Structure of spin groups associated with degenerate Clifford algebras

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Clifford algebras over finite-dimensional vector spaces endowed with degenerate quadratic form contain a nontrivial two-sided nilpotent ideal (the Jacobson radical) generated by the orthogonal complement of such spaces. Thus, they cannot be faithfully represented by matrix algebras. Following the theory of spin representations of classical Clifford algebras, the left regular (spin) representations of these degenerate algebras can be studied in suitably constructed left ideals. First, structure of the group of units of such algebras is examined for a quadratic form of arbitrary rank. It is shown to be a semidirect product of a group generated by the radical and the group of units of a maximal nondegenerate Clifford subalgebra. Next, in the special case of corank 1, Clifford, pin, and spin groups are defined an their structures are described. As an example, a Galilei–Clifford algebra over the Galilei space-time is considered. A covering theorem is then proved analogous to the one well known in the theory of spin and orthogonal groups.

I. INTRODUCTION

The theory of Clifford algebras over nondegenerate quadratic spaces and their spin representations are well known (Refs. 1–3). There have been few attempts, however, to expand this theory to algebras over degenerate spaces (i.e., endowed with a degenerate quadratic form) of any rank (Refs. 4 and 5). One has to keep in mind that whereas the former algebras are semisimple, hence representable faithfully by real, complex, or quaternion matrices, the latter are not since they contain a nontrivial two-sided nilpotent ideal called the Jacobson radical. The radical of a degenerate Clifford algebra is generated by the orthogonal complement of the associated quadratic space, i.e., by the set of null vectors orthogonal to the entire space. In fact, the radical contains every nilpotent right or left ideal in such algebras (Ref. 6).

In this paper $R_{d,p,k}$ denotes a real Clifford algebra over a real vector space $R^{d,p,k}$ of dimension $d+p+k$ and endowed with a quadratic form Q of rank $p+k$ and signature (d,p,k) (i.e., dim ker $Q=d$) whereas rad $R_{d,p,k}$ denotes its Jacobson radical. We examine structure of the group of units of a *degenerate* Clifford algebra of any rank ($d\neq 0$). Using general properties of the Jacobson radical of a ring with unity (Ref. 6) we show (Sec. II) that this group is a semidirect product of a group generated by the radical and the group of units of a maximal nondegenerate Clifford subalgebra $R_{p,k}$ contained in $R_{d,p,k}$ (here $R_{p,k}$ stands for $R_{0,p,k}$). We apply this result to a special case of degeneracy in one dimension ($d=1$). As an example we consider a Clifford algebra over the Galilei space-time of classical physics. Then we define Clifford, pin, and spin groups and analyze their structure by viewing them as subgroups of the group of units. We prove a covering theorem analogous to the one in the theory of spin and orthogonal groups associated with nondegenerate quadratic spaces (Sec. III).

II. GROUP OF UNITS OF A DEGENERATE CLIFFORD ALGEBRA AND ITS STRUCTURE

Throughout this section $R^{*}_{d,p,k}$ denotes the group of units of $R_{d,p,k}$. The following results can be immediately applied to complexified algebras $R^{c}_{d,p,k}$ and, in particular, to the Galilei–Clifford algebra $R^{c}_{1,3,0}$, which is our main interest. To simplify our notation we write $C(Q)$ [resp. $C^{*}(Q)$, $C(Q')$, $C^{*}(Q')$] for $R_{d,p,k}$ (resp. $R^{*}_{d,p,k}$, $R_{p,k}$, $R^{*}_{p,k}$), where Q' denotes the nondegenerate part of Q with signature (p,k) (the diagonalized form of Q' contains k plus ones and p minus ones).

Notice that for every m in $C(Q)$ there exist unique m' in $C(Q')$ (the latter is being considered as the semisimple subalgebra of the former) and r in rad $C(Q)$ such that $m=m'+r$. It is a direct consequence of writing m in terms of the standard basis of $C(Q)$, or from the direct sum decomposition $C(Q)=C(Q')\oplus \text{rad } C(Q)$ into $C(Q')$-modules. The next two lemmas follow from the above remark and from Nakayama's lemma for rings (Ref. 6).

Lemma 2.1: For every m in $C^{*}(Q)$ there exist unique m' in $C^{*}(Q')$ and r in rad $C(Q)$ such that $m=m'+r$.

Lemma 2.2: For every m in $C^{*}(Q)$ there exist unique x,y in rad $C(Q)$ and m' in $C^{*}(Q')$ such that $m=m'(1+x)=(1+y)m'$.

The following proposition describes the structure of the group of units of $C(Q)$. Here, $H\cdot G=\{hg|h\in H,\ g\in G\}$, $H\lhd G$ indicates that H is a normal subgroup of G, $H\circledS G$ denotes the semidirect product of H and G with G acting on H through a homomorphism $\chi: G\to \text{Aut } H$ such that $H\circledS G$ is the group $(H\times G,\cdot)$, with multiplication defined as $(h,g)(h',g')=(h\chi(g)(h'),\ gg')$ and $x\circ z=x+z+xz$ for any x, z in $C(Q)$.

Proposition 2.3:

(i) $C^{*}(Q)=C^{*}(Q')\cdot G=G\cdot C^{*}(Q')$,
where $G=\{1+x|x\in \text{rad } C(Q)\}\subset C^{*}(Q)$.

(ii) $G\lhd C^{*}(Q)$ and $G\cap C^{*}(Q')=\{1\}$.

(iii) $C^{*}(Q)=G\circledS C^{*}(Q')$ with the conjugate action of $C^{*}(Q')$ on G.

(iv) Let $z(G)=\{x\in C^{*}(Q)|xg=gx, g\in G\}$, G any subgroup of $C^{*}(Q)$, and $g=g'(1+x)\in z(G)$, $k=1+z\in G$, x, $z\in \text{rad } C(Q)$, $g'\in C^{*}(Q')$. Then $x\circ z=(g'^{-1}zg')\circ x$ and, similarly, if $g=g'(1+X)\in C^{*}(Q)$ and $x\circ z=(g'^{-1}zg')\circ x$, $z\in \text{rad } C(Q)$, then $g\in z(G)$.

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(v) If $g \in z(g)$ and $g = g'(1+x)$, $x \in \operatorname{rad} C(Q)$, then $g'x = xg'$.

(vi) $z(G) \cap C^*(Q')$
$= \{g' \in C^*(Q') | g'z = zg', z \in \operatorname{rad} C(Q)\}$.

Moreover, $z(G) \cap C^*(Q') = z(C(Q)) \cap C^*(Q') = R^*$, where R^* denotes the nonzero reals and $z(C(Q))$ denotes the center of $C(Q)$.

(vii) $C^*(Q)/R^* \simeq G \circledS (C^*(Q')/R^*)$.

Proof:

(i) See Lemma 2.2.

(ii) If $1+x \in G$, $m \in C^*(Q)$ then $m^{-1}(1+x)m = 1 + m^{-1}xm \in G$ since $\operatorname{rad} C(Q)$ is a two-sided ideal in $C(Q)$. For the second part notice that $\operatorname{rad} C(Q) \cap C(Q') = \emptyset$.

(iii) By part (i) we have $C^*(Q) = G \cdot C^*(Q')$. Let $m = gr$, $m' = g'r'$, $g, g' \in G$, and $r, r' \in C^*(Q')$. Then $mm' = g\chi(r)(g')rr'$ and $C^*(Q) = G \circledS C^*(Q')$, where $\chi: C^*(Q') \to \operatorname{Aut} G$ is the conjugation $g \to rgr^{-1}$.

(iv) Since $gk = kg$ we have $g'(1+x)(1+z)(1+x)^{-1}g'^{-1} = 1+z$, or $x \circ z = (g'^{-1}zg') \circ x$, $z \in \operatorname{rad} C(Q)$. On the other hand, $x \circ z = (g'^{-1}zg') \circ x$, $z \in C(Q)$, implies that $g(1+z) = (1+z)g$.

(v) Follows from part (iv): apply $x \circ z = (g'^{-1}zg') \circ x$ when $x = z$.

(vi) Let $g = g'(1+x) \in z(G) \cap C^*(Q')$. Thus $x = 0$ and for any $z \in \operatorname{rad} C(Q)$ we have by part (iv): $z = 0 \circ z = g'^{-1}zg' \circ 0 = g'^{-1}zg'$ or $g'z = zg'$. In the other direction, let $g' \in C^*(Q')$ be such that $g'z = zg'$, $z \in \operatorname{rad} C(Q)$. Then $g'(1+z) = (1+z)g'$ and $g' \in z(G) \cap C^*(Q')$.

We now set $K = z(G) \cap C^*(Q')$. Since $z(C(Q)) \subset z(G)$, we only need to show $K \subset z(C(Q)) \cap C^*(Q')$. If $g' \in K$ then $g'\tilde{e}_i = \tilde{e}_i g'$ for every generator $\tilde{e}_i$ of $R^{d,p,k}$ with vanishing square [i.e., $Q(\tilde{e}_i) = 0$]. If $(e_j)^2 = \pm 1$, then $g'e_j\tilde{e}_i = e_j\tilde{e}_i g'$ since $e_j\tilde{e}_i \in \operatorname{rad} C(Q)$. Also if $m = \Sigma_I m_I e_I$, $0 \leqslant |I| \leqslant p+k$, then by the linear independence of $\{e_I\tilde{e}_i\}$ in $C(Q)$, $m\tilde{e}_i = 0$ implies $m = 0$. Thus $(g'e_j - e_j g')\tilde{e}_i = 0$ for any generator e_j of $R^{d,p,k}$ implies $g' \in z(C(Q)) \cap C^*(Q')$.

Finally, since

$$z(R_{d,p,k}) = \begin{cases} R^{+}_{d,0,0}, & \text{if } d+p+k \text{ even}, \\ R^{+}_{d,0,0} + Re_1 \cdots e_{d+p+k}, & \text{if } d+p+k \text{ odd} \end{cases} \tag{2.1}$$

(Refs. 3–5) thus in either case $z(C(Q)) \cap C^*(Q') = R^*$.

(vii) See Refs. 7 and 8. □

We now recall that the complexification of any nondegenerate quadratic form is of maximum Witt index, i.e., the dimension of maximal totally isotropic subspaces of given complex quadratic space is maximum (Ref. 2). Following Ref. 9 one can then describe the generators of $C^c(Q)$ [resp. $C^c(Q')$], and, in particular, the generators of rad $C^c(Q)$ [considered as a $C^c(Q)$-submodule] using the limiting Witt decomposition. In the following, the superscript c denotes the complexification of the underlying algebraic structure, and we assume that $d+p+k = 2r$. There are two cases: (i) $d = 2t$,

$$\operatorname{rad} C^c(Q) = \Big\{ \sum a_{JK} \tilde{x}_J \tilde{y}_K,\ a_{KJ} \in C^c(Q'), \\ 0 \leqslant |J|, |K| \leqslant t,\ 1 \leqslant |J| + |K| \leqslant d \Big\}, \tag{2.2}$$

while the generator F of a spin space of $C^c(Q)$ can be expressed (modulo a scalar factor) as $F = \tilde{y}_1 \cdots \tilde{y}_t y_{t+1} \cdots y_r$; (ii) $d = 2t+1$,

$$\operatorname{rad} C^c(Q) = \Big\{ \sum a_{JKL} \tilde{e}_L \tilde{x}_J \tilde{y}_K,\ a_{JKL} \in C^c(Q'), \\ 0 \leqslant |L| \leqslant 1,\ 0 \leqslant |J|, |K| \leqslant t, \\ 1 \leqslant |J| + |K| + |L| \leqslant d \Big\}, \tag{2.3}$$

while $F = \tilde{y}_1 \cdots \tilde{y}_t \tilde{e}_{t+1} y_{t+2} \cdots y_r$.

Notice that in case (i)

$$\operatorname{rad} C^c(Q) \cap \operatorname{ann} F = \Big\{ \sum a_{JK} \tilde{x}_J \tilde{y}_K,\ |K| \geqslant 1 \Big\}, \tag{2.4}$$

while in case (ii)

$$\operatorname{rad} C^c(Q) \cap \operatorname{ann} F = \Big\{ \sum a_{JKL} \tilde{e}_L \tilde{x}_J \tilde{y}_K,\ |L| + |K| \geqslant 1 \Big\}, \tag{2.5}$$

where $\operatorname{ann} F = \{x \in C^c(Q) | xF = 0\}$.

Lemma 2.4: Let x, $y \in \operatorname{rad} C^c(Q) \cap \operatorname{ann} F$ and $G'' = \{1+x | x \in \operatorname{rad} C^c(Q) \cap \operatorname{ann} F\}$. (i) $x \circ y \in \operatorname{rad} C^c(Q) \cap \operatorname{ann} F$, (ii) G'' is a subgroup of G, and (iii) every generator $\tilde{x}_M F$ of the spin space $C^c(Q)F$, $0 < |M| < [d/2]$, is stabilized by G'', i.e., $g\tilde{x}_M F = \tilde{x}_M F$ for every g in G''.

Now we describe the structure of the group G, the normal subgroup of $C^{c*}(Q)$ (see Proposition 2.3). Let

$$G' = \{1+x | x = \sum a_J \tilde{x}_j \in \operatorname{rad} C^c(Q),\ a_j \in C^c(Q'), \\ 1 \leqslant |J| \leqslant [d/2]\},$$

if $d > 1$, and $G' = \{1\}$ if $d = 1$.

Lemma 2.5: Let G, G', and G'' be as above. Then (i) G' is a subgroup of G, (ii) $G = G' \cdot G'' = G'' \cdot G'$, (iii) $G' \cap G'' = \{1\}$, and (iv) G'' is a normal subgroup of G.

Proof:

(i) Let $1+x, 1+y \in G'$. Then $(1+x)(1+y) \in G'$ since $\operatorname{rad} C^c(Q)$ is a two-sided ideal of $C^c(Q)$ and $x \circ y \in \operatorname{rad} C^c(Q)$.

(ii) Let $1+x \in G$. Then there exist unique x', $x'' \in \operatorname{rad} C^c(Q)$ such that $x = x' + x''$ and $x'' \in \operatorname{ann} F$. Thus

$$1 + x = 1 + x' + x'' = (1+x')[1 + (1+x')^{-1}x''] \\ = [1 + x''(1+x')^{-1}](1+x')$$

since $1 + x' \in G'$. Moreover $x'^m = 0$ for some $m > 0$ and

$$(1+x')^{-1} = 1 + \sum_{i=1}^{m-1} (-x')^i.$$

Thus $1 + (1+x')^{-1}x'', 1 + x''(1+x')^{-1} \in G''$.

(iii) Immediate since $\{\tilde{x}_J \tilde{y}_K\}$ are linearly independent.

(iv) Let $1 + y'' \in G''$, $1 + x \in G$. We need to show that $(1+x)(1+y'')(1+x)^{-1} \in G''$. Let $(1+x)^{-1} = 1 + \tilde{x}$ for some $\tilde{x} \in \operatorname{rad} C^c(Q)$. Using the same argument as in (ii) we may write $x = x' + x''$ and $\tilde{x} = \tilde{x}' + \tilde{x}''$, x'', $\tilde{x}'' \in \operatorname{rad} C^c(Q) \cap \operatorname{ann} F$, x', $\tilde{x}' \in \operatorname{ann} F$, such that $1 + x'$, $1 + \tilde{x}' \in G'$ and $1 + x''$, $1 + \tilde{x}'' \in G''$. Then one can check that $(1+x)(1+y'')(1+x)^{-1}$ is in G''. □

Theorem 2.6: Let G, G', and G'' be as above. Then $G = G'' \circledS G'$ with the conjugate action of G' on G''.

Corollary 2.7: $C^{c^*}(Q) = G \circledS C^{c^*}(Q') = (G'' \circledS G') \circledS C^{c^*}(Q')$ where $C^{c^*}(Q')$ (resp. G') acts on G (resp. G'') by conjugation.

We consider now the following example of degeneracy in one dimension.

Example 2.8: In the Galilei–Clifford algebra $R^{\,c}_{1,3,0}$ we have $\operatorname{rad} R^{\,c}_{1,3,0} = \{m\tilde{e}_1 | m \in R^{\,c}_{3,0}\}$ and $F = \tilde{e}_1 y_2$, where $\tilde{e}_1$ spans the one-dimensional null subspace of the Galilei space (Ref. 9). Then the spin space $R^{\,c}_{1,3,0}F$ can be viewed as the limit spin ideal obtained by contracting a family of deformed twistor spaces. Thus $\operatorname{rad} R^{\,c}_{1,3,0} \subset \operatorname{ann} F$ and $G = G'' = \{1 + m\tilde{e}_1 | m \in R^{\,c}_{3,0}\}$, $G' = \{1\}$. In fact $1 + m\tilde{e}_1 = \exp(m\tilde{e}_1)$ and the Lie algebra of G (over $R^{\,c}_{3,0}$) is generated by one element $\tilde{e}_1$. Then

$$R^{\,c^*}_{1,3,0} = G \cdot R^{\,c^*}_{3,0} = G \circledS R^{\,c^*}_{3,0}$$

and G is normal in $R^{\,c^*}_{1,3,0}$.

III. SPIN AND PIN GROUPS OF A DEGENERATE CLIFFORD ALGEBRA

In this section we extend the definitions of Clifford, pin, and spin groups found in the theory of classical (nondegenerate) Clifford algebras (Refs. 2 and 10) to degenerate algebras $R_{d,p,k}$. In particular, we determine their structures when $d = 1$. The results presented below are similar to the ones in Ref. 4, where the groups above are defined with the main automorphism α of $R_{1,p,k}$.

Recall that when $d = 1$ then G' is the trivial group, $G = G'' = \{1 + m\tilde{e}_1 | m \in R^{\,c}_{p,k}\}$, and every invertible in $R^{\,c^*}_{1,p,k}$ can be uniquely written as $r(1 + m\tilde{e}_1)$, $r \in R^{\,c^*}_{p,k}$, and $1 + m\tilde{e}_1 \in G$. Then the inverse of the latter is $1 - m\tilde{e}_1$ since $(m\tilde{e}_1)^2 = m\alpha(m)\tilde{e}_1^2 = 0$, $m \in R^{\,c}_{p,k}$. In the following, the complexification of $R^{\,1,p,k}$ is denoted by X and we decompose X into the direct sum $(\tilde{e}_1) \oplus X'$, where X' denotes the nondegenerate part of X. Also, $C(Q)$ and $C(Q')$ will be used instead of $R_{1,p,k}$ and $R_{p,k}$, respectively, and $\langle m \rangle_r$ will be the r-vector part of m in $C(Q)$.

Definition 3.1: The *Clifford group* $\Gamma(1,p,k)$ of $C^c(Q)$ is the set $\{g \in C^{c^*}(Q) | gxg^{-1} \in X, x \in X\}$.

Lemma 3.2: Let X' be identified with the space of one-vectors in $C^c(Q')$ and $m \in C^c(Q')$. If $x'm + mx' = \langle x'm + mx' \rangle_0$, $x' \in X'$, then

$$m = \begin{cases} \langle m \rangle_1, & \text{if } p + k \text{ is odd,} \\ \langle m \rangle_1 + \langle m \rangle_{p+k}, & \text{if } p + k \text{ is even.} \end{cases} \tag{3.1}$$

Proof: Write $m = \langle m \rangle_0 + \langle m \rangle_1 + \Sigma_J m_J e_J + \langle m \rangle_{p+k}$, $2 \leqslant |J| \leqslant p + k - 1$. Let $p + k$ be even. Then $\langle m \rangle_{p+k} x' + x' \langle m \rangle_{p+k} = 0$ and for every e_i, $1 \leqslant i \leqslant p + k$,

$$e_i e_j = \begin{cases} (-1)^{|J|} e_J e_i, & \text{if } i \notin J, \\ (-1)^{|J|-1} e_J e_i, & \text{if } i \in J. \end{cases} \tag{3.2}$$

Thus $me_i + e_i m = 2\langle m \rangle_0 e_i + 2e_i \cdot \langle m \rangle_1 + \Sigma_{i \in J} m_J [1 + (-1)^{|J|}] e_J e_i + \Sigma_{i \in J} m_J [1 + (-1)^{|J|-1}] e_J e_i$ (summation over $2 \leqslant |J| \leqslant p + k - 1$), where $\cdot$ denotes the inner product in X' induced by the inner product in X. Separating the even and odd parts we get

$$\begin{aligned} (me_i + e_i m)^+ &= 2e_i \cdot \langle m \rangle_1 + \Sigma 2m_J e_J e_i, \\ &\quad i \in J, \ |J| \text{ odd}, \\ (me_i + e_i m)^- &= 2\langle m \rangle_0 e_i + \Sigma 2m_J e_J e_i, \\ &\quad i \in J, \ |J| \text{ even}. \end{aligned} \tag{3.3}$$

Due to the linear independence of the generators of $C^c(Q')$ we conclude that $\langle m \rangle_0 = m_J = 0$ if $|J|$ is odd and $i \in J$ or, if $|J|$ is even and $i \in J$. Thus $m_J = 0$, $2 \leqslant |J| \leqslant p + k - 1$ and $m = \langle m \rangle_1 + \langle m \rangle_{p+k}$.

Now let $p + k$ be odd. Then $\langle m \rangle_{p+k} x' = x' \langle m \rangle_{p+k}$ since $\langle m \rangle_{p+k} \in z(C^c(Q'))$ and

$$(me_i + e_i m)^+ = 2e_i \cdot \langle m \rangle_1 + 2\langle m \rangle_{p+k} e_i + \sum_{i \in J} 2m_J e_J, \tag{3.4}$$

for $|J|$ odd while the odd part is given in (3.3). Considering all vector parts and again using the linear independence argument we conclude that $m = \langle m \rangle_1$. □

Proposition 3.3: Let $\Gamma^{\pm}(p,k) = \{g \in \Gamma(p,k) | \alpha(g) = \pm g\}$, where α is the main automorphism in $C^c(Q)$ and let

$$\tilde{G} = \left\{ 1 + m\tilde{e}_1 | m = \begin{cases} \langle m \rangle_1, & p + k \text{ odd}, \\ \langle m \rangle_1 + \langle m \rangle_{p+k}, & p + k \text{ even} \end{cases} \right\}.$$

Then $\Gamma(1,p,k) = \tilde{G} \circledS \Gamma^{\pm}(p,k)$.

Proof: Let $g = r(1 + m\tilde{e}_1) \in C^{c^*}(Q)$, $r \in C^{c^*}(Q')$, $m \in C^c(Q')$, and $x = x' + x'' \in X = X' \oplus (\tilde{e}_1)$. Then

$$\begin{aligned} gxg^{-1} &= r(1 + m\tilde{e}_1)x(1 - m\tilde{e}_1)r^{-1} \\ &= \lambda' \tilde{e}_1 + rxr^{-1}, \end{aligned} \tag{3.5}$$

where $\lambda' = r[\lambda - (x'm + mx')]\alpha(r)^{-1}$ and $rx'r^{-1} \in X'$ since $gxg^{-1} \in X$, $r \in \Gamma(p,k)$, $\lambda, \lambda' \in \mathbb{C}$. In particular, if $x' = 0$ and $\lambda \neq 0$ then $r = \alpha(r)\mu$, $\mu = \lambda'/\lambda$ and $\alpha(r) = \mu r = \mu^2 \alpha(r)$, or $\mu = \pm 1$. Thus $r = r^{\pm} \in \Gamma^{\pm}(p,k) = \Gamma(p,k) \cap C^{c^{\pm}}(Q)$ and by Lemma 3.2 $m = \langle m \rangle_1$, $p + k$ odd, or $m = \langle m \rangle_{p+k} + \langle m \rangle_1$, $p + k$ even. Finally, $1 + m\tilde{e}_1 \in \tilde{G}$ and $\tilde{G} \cap C^{c^*}(Q') = \{1\}$.

Now let $r = r^{\pm} \in \Gamma^{\pm}(p,k)$. If $p + k$ is odd then

$$r^{\pm}(1 + \langle m \rangle_1 \tilde{e}_1)(r^{\pm})^{-1} = 1 \pm r^{\pm} \langle m \rangle_1 (r^{\pm})^{-1} \tilde{e}_1 \in \tilde{G}, \tag{3.6}$$

$1 + m\tilde{e}_1 \in \tilde{G}$, since $r^{\pm} \langle m \rangle_1 (r^{\pm})^{-1}$ is a one-vector for every $r^{\pm} \in \Gamma^{\pm}(p,k)$. Similarly, if $p + k$ is even then

$$\begin{aligned} &r^{\pm}(1 + \langle m \rangle_1 \tilde{e}_1 + \langle m \rangle_{p+k} \tilde{e}_1)(r^{\pm})^{-1} \\ &\quad = 1 \pm r^{\pm} \langle m \rangle_1 (r)^{-1} \tilde{e}_1 \pm r^{\pm} \langle m \rangle_{p+k} (r^{\pm})^{-1} \tilde{e}_1 \in \tilde{G}, \end{aligned} \tag{3.7}$$

since $r^{\pm} \langle m \rangle_{p+k} (r^{\pm})^{-1}$ is a $(p + k)$-vector in $C^c(Q')$. Thus $\Gamma^{\pm}(p,k)$ acts on G by conjugation. In fact one can show that $\tilde{G}$ is normal in $\Gamma(1,p,k)$. □

Following now the standard approach (Refs. 2 and 3) we define the homomorphism p: $\Gamma(1,p,k) \to \operatorname{End}_{\mathbb{C}}(X)$ as $p_g(x) = gxg^{-1}$ and the *spinor map* N: $\Gamma(1,p,k) \to C^{c^*}(Q)$ as $N(g) = \beta(g)g$, where β is the main antiautomorphism of $C^c(Q)$. Since gxg^{-1} above is a one-vector, $N(g) \in \ker p = z^*(C^c(Q))$, the set of invertibles in the center of $C^c(Q)$. Here $N(g)$ is called the *spinor norm* of g; notice that $N(g) \in \mathbb{C}^*$, $p + k$ odd, and $N(g) \in \mathbb{C}^* + \mathbb{C}e_N$, $p + k$ even, where e_N represents a $(1 + p + k)$-vector in $C^c(Q)$. Finally $N(gg') = N(g)N(g')$.

Using standard arguments one can show that for every $g \in \Gamma(1,p,k)$, p_g is an isometry defined on X and $p_a(x) = axa^{-1} + [2B(a,x)/Q(a)]a$ for every nonisotropic vector

$a \in X$, where B is the bilinear form associated with Q. Thus $-p_a$ is a reflection in the plane perpendicular to a. Following Ref. 3 we call the intersection $\Gamma(1,p,k) \cap C^{c+}(Q)$ [resp. $\Gamma(p,k) \cap C^{c+}(Q')$] the *special Clifford group* $\Gamma^+(1,p,k)$ [resp. $\Gamma^+(p,k)$]. Superscript + (resp. −) denotes the even (resp. odd) part of the given algebraic structure.

Corollary 3.4: $\Gamma^+(1,p,k) = \tilde{G}' \otimes \Gamma^+(p,k)$, where $\tilde{G}' = \{1 + \langle m \rangle_1 \tilde{e}_1 | m \in C^c(Q')\} \subset \tilde{G}$ for any $p+k$. Notice that if $g \in \Gamma^+(1,p,k)$ then $N(g) = N(r^+) \in \mathbb{C}^*$ for some $r^+ \in \Gamma^+(p,k)$. We define the *special reduced Clifford group* $\Gamma_0^+(1,p,k)$ [resp. $\Gamma_0^+(p,k)$] to be the intersection $\ker N \cap \Gamma(1,p,k)$ [resp. $\ker N \cap \Gamma^+(p,k)$].

Corollary 3.5: $\Gamma_0^+(1,p,k) = \tilde{G}' \otimes \Gamma_0^+(p,k)$.

Since we are primarily interested here in the case when $p+k=3$, we define the *reduced Clifford group* $\Gamma_0(1,p,k)$ ($p+k$ odd) to be the kernel of N in $\Gamma(1,p,k)$ and the *pin group* $\mathrm{Pin}(1,p,k) = \{g \in \Gamma(1,p,k) | N(g) = \pm 1\}$. Notice that $N(g) = N(r^\pm) \in z^*(C^c(Q))$, hence $N(g)$ is a scalar since $\beta(r^\pm) r^\pm$ is always even. Thus, a general element of $\mathrm{Pin}(1,p,k)$ is of the form $r^\pm(1 + \langle m \rangle_1 \tilde{e}_1, r^\pm \in \Gamma^\pm(p,k)$, and $[N(r^\pm)]^2 = 1$ (see Proposition 3.3).

If we let the *spin group* $\mathrm{Spin}(1,p,k)$ be the intersection $\mathrm{Pin}(1,p,k) \cap C^c(Q)$, then $r(1 + \langle m \rangle_1 \tilde{e}_1) \in \mathrm{Spin}(1,p,k)$ implies $r = r^+$. Recalling now that $\mathrm{Spin}(p,k) = \{r^+ \in \Gamma^+(p,k) | N(r^+) = \pm 1\}$ when $p+k$ is odd (Ref. 3) and denoting by $\Gamma_0^\pm(p,k) = \{r^\pm \in \Gamma^\pm(p,k) | [N(r^\pm)]^2 = 1\}$ we have the following proposition.

Proposition 3.6: Let $p+k$ be odd.

(i) $\mathrm{Pin}(1,p,k) = \tilde{G}' \otimes \Gamma_0^\pm(p,k)$.

(ii) $\mathrm{Spin}(1,p,k) = \tilde{G}' \otimes \mathrm{Spin}(p,k)$.

When $p+k$ is even we define the pin and spin groups in exactly the same way as above:

$$\begin{aligned} \mathrm{Pin}(1,p,k) &= \{g \in \Gamma(1,p,k) | N(g) = \pm 1\}, \\ \mathrm{Spin}(1,p,k) &= \{g \in \Gamma^+(1,p,k) | N(g) = \pm 1\}. \end{aligned} \tag{3.8}$$

Notice that $N(g)$ is not necessarily a scalar for all $g \in \Gamma(1,p,k)$ since the center of $C^c(Q)$ is nontrivial. However, we will view $N(g) = \pm 1$ in (3.8) as a condition on the elements of this group.

Thus let $g \in \Gamma(1,p,k)$, $p+k$ even. Proposition 3.3 shows that g can be factored into $r^\pm(1 + \langle m \rangle_1 \tilde{e}_1 + \langle m \rangle_{p+k} \tilde{e}_1)$, $r^\pm \in \Gamma^\pm(p,k)$ and

$$N(g) = N(r^\pm)(1 + [1 + (-1)^{(p+k)/2}] \langle m \rangle_{p+k} \tilde{e}_1). \tag{3.9}$$

The condition $N(g) = \pm 1$ together with (3.9) implies that $[N(r^\pm)]^2 = 1$ while

$$m = \begin{cases} \langle m \rangle_1 + \langle m \rangle_{p+k}, & (p+k) \equiv 2 \pmod 4, \\ \langle m \rangle_1, & \text{otherwise.} \end{cases} \tag{3.10}$$

Define a subgroup $\tilde{G}''$ of $\tilde{G}$ as the set $\{1 + m\tilde{e}_1 | m$ satisfies (3.10)$\}$. If $g \in \mathrm{Pin}(1,p,k) \cap C^{c+}(Q)$, then $g = r^+(1 + \langle m \rangle_1 \tilde{e}_1)$, where $1 + \langle m \rangle_1 \tilde{e}_1 \in \tilde{G}'$ and $r^+ \in \mathrm{Spin}(p,k)$.

Proposition 3.7: Let $p+k$ be even.

(i) $\mathrm{Pin}(1,p,k) = \tilde{G}'' \otimes \Gamma_0^\pm(p,k)$.

(ii) $\mathrm{Spin}(1,p,k) = \tilde{G}' \otimes \mathrm{Spin}(p,k)$.

Corollary 3.8: $\mathrm{Spin}(1,p,k) = \tilde{G}' \otimes \mathrm{Spin}(p,k)$ for any parity of $p+k$.

For the similar result when the action on X is defined using the principal automorphism α of $C^c(Q)$ see Ref. 4.

In physical applications we are mostly concerned with the orientation preserving component of the identity. For example, the proper Lorentz group L_6 is the identity component of SO(1,3) denoted usually by $\mathrm{SO}^+(1,3)$, the proper de Sitter group S_{10} is defined as $\mathrm{SO}^+(1,4)$, the homogeneous Galilei group $G_6 = R^3 \otimes \mathrm{SO}(3)$ is isomorphic to $\mathrm{SO}^+(1,0,3)$ and is doubly covered by $\mathrm{Spin}^+(1,0,3)$, the identity component of Spin(1,0,3). We define the component of the identity in pin, spin, and Clifford groups for any parity of $p+k$ as follows:

$$\begin{aligned} &\mathrm{Pin}_0(1,p,k) = \{g \in \Gamma(1,p,k) | N(g) = 1\}, \\ &\mathrm{Spin}_0(1,p,k) = \{g \in \Gamma^+(1,p,k) | N(g) = 1\}, \\ &{}^0\Gamma_0^\pm(p,k) = \{r \in \Gamma_0^\pm(p,k) | N(r) = 1\}. \end{aligned} \tag{3.11}$$

Proposition 3.8:

(i) $\mathrm{Pin}_0(1,p,k) = \tilde{G}'' \otimes {}^0\Gamma_0^\pm(p,k)$,

$\mathrm{Spin}_0(1,p,k) = \tilde{G}' \otimes \mathrm{Spin}_0(p,k)$, if $p+k$ is even.

(ii) $\mathrm{Pin}_0(1,p,k) = \tilde{G}' \otimes {}^0\Gamma_0^\pm(p,k)$,

$\mathrm{Spin}_0(1,p,k) = \tilde{G}' \otimes \mathrm{Spin}_0(p,k)$, if $p+k$ is odd,

where $\mathrm{Spin}_0(p,k)$ is the component of the identity of $\mathrm{Spin}(p,k)$.

Proof: If $g \in \mathrm{Pin}(1,p,k)$ then $g = r^\pm(1 + m\tilde{e}_1)$, where $1 + m\tilde{e}_1 \in \tilde{G}'$ (resp. $\tilde{G}''$), $p+k$ odd (resp. $p+k$ even). Then one can easily check that $N(g) = N(r^\pm) = 1$ implies $r^\pm \in {}^0\Gamma_0^\pm(p,k)$. □

As it was mentioned above, the conjugate action of the Clifford group $\Gamma(1,p,k)$ on X induces certain actions on the nondegenerate part X' and on the degenerate orthogonal complement $(\tilde{e}_1)$. We now proceed to find these actions explicitly.

Let $g = r^\pm(1 + m\tilde{e}_1) \in \Gamma(1,p,k)$, $r^\pm \in \Gamma^\pm(p,k)$, and $1 + m\tilde{e}_1 \in \tilde{G}$ (see Proposition 3.3) and let $x = \lambda\tilde{e}_1 + x' \in X$ (see Lemma 3.2). Then

$$\begin{aligned} p_g(x) &= gxg^{-1} \\ &= \pm(\lambda - \lambda'\tilde{e}_1 + r^\pm x'(r^\pm)^{-1} \\ &= p_g''(\lambda\tilde{e}_1) + p_g'(x'), \end{aligned} \tag{3.12}$$

where $\lambda' = mx' + x'm$ is a scalar (see Lemma 3.2) and the projection of $p_g(x)$ on X' [resp. on $(\tilde{e}_1)$] is denoted by $p_g'(x)$ [resp. $p_g''(x)$].

Lemma 3.9: Let p: $\Gamma(1,p,k) \to \mathrm{End}_C(X)$ be the homomorphism above.

(i) p_g is an isometry on X which reduces to $\pm\mathrm{Id}$ on $(\tilde{e}_1)$.

(ii) p induces orthogonal rotations on X'.

(iii) Let $a = a' + a''$ be isotropic in X. Then $-p_a$ is a reflection in the plane perpendicular to a and $-p_a'$ is a reflection in the plane perpendicular to a'.

Proof: (i) Clearly $(p_g(x))^2 = x^2$, $g \in \Gamma(1,p,k)$, $x \in X$. If $x = \lambda\tilde{e}_1$ then $p_g(x) = \pm\lambda\tilde{e}_1 = \pm x$ by (3.12).

(ii) Notice that $(p_g'(x'))^2 = '(r^\pm x'(r^\pm)^{-1})^2 = x'^2$ for $x' \in X'$.

(iii) Since $a^2 = a'^2 \neq 0$ in $C^c(Q)$ then

$$\begin{aligned} -p_a(x) = r_a(x) &= x - 2(a \cdot x/a \cdot a)a \\ &= [x'' - 2(a' \cdot x'/a' \cdot a')a''] \\ &\quad + [x' - 2(a' \cdot x'/a' \cdot a')a'] \\ &= -p_a''(x'') + r_a'(x'), \end{aligned} \tag{3.13}$$

where r_a' denotes the reflection in X' with respect to a plane perpendicular to a' induced by the reflection r_a and $\cdot$ is the inner product in X. □

Finally, we state and prove our last result which provides an extension of the Cartan–Dieudonné Theorem (Ref. 2) to real quadratic spaces endowed with a quadratic form of corank 1.

Proposition 3.10: Let ρ be the restriction of the homomorphism p: $\Gamma(1,p,k)\to\mathrm{End}_R(X)$, $X=R^{(1,p,k)}$, to $\tilde G'\subset\Gamma_0^{\pm}(p,k)$ and let T be the Abelian subgroup of the orthogonal group $O(1,p,k)$ generated by $\rho(\tilde G')$.

(i) The kernal of ρ is Z_2.

(ii) If $p+k$ is even then ρ: $\tilde G'\subset\Gamma_0^{\pm}(p,k)\to T\subset O(p,k)$ is a covering map. If $p+k$ is odd then ρ: $\tilde G'\subset\Gamma_0^{\pm}(p,k)\to T\subset SO(p,k)$ is a covering map.

Proof: (i) Recall that $\tilde G'<\tilde G<R^{*}_{1,p,k}$ (see Corollary 3.4). Let $g\in\ker\rho$. Then for every $x\in X=(\tilde e_1)\oplus X'$, $gx=xg$ or $g\in z^*(R_{1,p,k})\cap\mathrm{Pin}'(1,p,k)$, where $\mathrm{Pin}'(1,p,k)=\tilde G'\subset\Gamma_0^{\pm}(p,k)$ [notice that $\mathrm{Pin}'(1,p,k)=\mathrm{Pin}(1,p,k)$, $p+k$ odd, and $\mathrm{Pin}'(1,p,k)\neq\mathrm{Pin}(1,p,k)$, $p+k$ even]. Since

$$z^*(R_{1,p,k})=\begin{cases}R^*, & p+k \text{ odd},\\ R^*+R\tilde e_1e_2\cdots e_{p+k}, & p+k \text{ even}\end{cases}\tag{3.14}$$

(Ref. 4) and $N(g)=\pm1$, $\ker\rho=Z_2$ if $p+k$ is odd. If $p+k$ is even then an invertible element of the center of $R_{1,p,k}$ is of the form $\lambda_0+\lambda_1\tilde e_1e_2\cdots e_{p+k}$, $\lambda_0\neq0$, and it belongs to $\mathrm{Pin}'(1,p,k)$ if and only if $\lambda_1=0$. Again, $\ker\rho=Z_2$.

(ii) Notice that for every g in $\mathrm{Pin}'(1,p,k)$ we have $\rho_g(x)=\rho_r(\rho_m(x))$, where

$$\begin{aligned}\rho_m(x)&=(1+\langle m\rangle_1\tilde e_1)x(1-\langle m\rangle_1\tilde e_1)\\&=(\lambda_1-\lambda_2)\tilde e_1+x',\\ \rho_r(x)&=\alpha_r\lambda_1\tilde e_1+r^{\pm}x'(r^{\pm})^{-1},\end{aligned}\tag{3.15}$$

$\lambda_2=\langle m\rangle_1x'+x'\langle m\rangle_1$, $\alpha_r=1$ (resp. -1) if $r=r^+$ (resp. $r=r^-$) for every $x=\lambda_1\tilde e_1+x'\in X$. Thus the image set of ρ in $O(1,p,k)$ is generated by ρ_r, $r^{\pm}\in\Gamma_0^{\pm}(p,k)$, and ρ_m, $1+\langle m\rangle_1\tilde e_1\in\tilde G'$. We proceed now to find $\rho(\Gamma_0^{\pm}(p,k))$. Let p' be the projection of X', i.e., $p'(x)=x'$, $x\in X$. Then $(p'\circ\rho_r)(x)=r^{\pm}x'(r^{\pm})^{-1}$ and $p'\circ\rho_r$ is an isometry in X' for every $r^{\pm}\in\Gamma_0^{\pm}(p,k)$. Now let a be an anisotropic vector in X, i.e., $a^2=a'^2\neq0$ in $C(Q)$. Then $-p'\circ\rho_a$ is a reflection in the plane perpendicular to a' in X' (see Lemma 3.9). Thus if r_v is any reflection in X', $v^2\neq0$, let $a=b+v$ for some $b\in(\tilde e_1)$ and then $(-p'\circ\rho_a)(x')=r_v(x')$, $x'\in X'$. This implies that the negative of every reflection in X' is in the image of ρ.

If $n=p+k$ is even, then $-\mathrm{Id}=(-r_1)\cdots(-r_n)$ and if r is any reflection in X, then $r=(-\mathrm{Id})(-r)$, thus ρ covers $O(p,k)$ by the Cartan–Dieudonné theorem.

If $n=p+k$ is odd then the negative of a reflection has determinant $(-1)^n(-1)=1$, thus $-p'\circ\rho_a\in SO(p,k)$. But every element of $SO(p,k)$ must be a product of an even number of reflections or an even number of negative reflections each of which belongs to the image of ρ. Thus ρ covers $SO(p,k)$ by the theorem.

Finally, we establish the semidirect product structure of $\rho(\mathrm{Pin}'(1,p,k))$. It follows from (3.15) that $\rho(\mathrm{Pin}'(1,p,k))=T\cdot\rho(\Gamma_0^{\pm}(p,k))$. Thus we need only to show that $T\cap\rho(\Gamma_0^{\pm}(p,k))=\{1\}$, $z(T)\cap\rho(\Gamma_0^{\pm}(p,k))=\{1\}$, and $T\lhd\rho(\mathrm{Pin}'(1,p,k))$ since then we may refer to the classical result in the group theory (Ref. 7).

Suppose that $t\in T\cap\rho(\Gamma_0^{\pm}(p,k))$, i.e., $t=\rho_m=\rho_r$ for some $1+\langle m\rangle_1\tilde e_1\in\tilde G'$ and $r^{\pm}\in\Gamma_0^{\pm}(p,k)$. Since T is Abelian, for every $\langle m\rangle_1\in R^{1,p,k}$ we have $t\rho_m=\rho_mt$. But $\rho_r\rho_m(x)=\alpha_r(\lambda_1-\lambda_2)\tilde e_1+r^{\pm}x'(r^{\pm})^{-1}$, $x'\in X'$, and $\rho_m\rho_r(x)=(\alpha_r\lambda_1-\lambda_1')\tilde e_1+r^{\pm}x'(r^{\pm})^{-1}$, $\lambda_2=x'\langle m\rangle_1+\langle m\rangle_1x'$, $\lambda_2'=\langle m\rangle_1r^{\pm}x'(r^{\pm})^{-1}+r^{\pm}x'(r^{\pm})^{-1}\langle m\rangle_1$, $\alpha_r\lambda_2=\lambda_2'$. Since the bilinear form on X' is nondegenerate, we may conclude that $r^+\in z^*(R_{p,k})$ if $\alpha_r=1$. When $\alpha_r=-1$ then $r=r^-$, $-r^-\langle m\rangle_1=\langle m\rangle_1r^-$, and there are two cases to consider: if $p+k$ is even then multiplying both sides of the last equation by the volume element e_N of $R_{p,k}$ we see that $r^-e_N\langle m_1\rangle=\langle m\rangle_1r^-e_N$, $\langle m\rangle_1\in R^{1,p,k}$, or $r^-e_N\in z^*(R_{p,k})$. This is impossible since $r^-e_N\in R_{p,k}^-$ and $z^*(R_{p,k})=R^*$. If $p+k$ is odd then one can decompose r^- uniquely into s-vector parts $\langle r^-\rangle_s$, s odd and $1\leqslant s\leqslant p+k$. Moreover,

$$0=\langle m\rangle_1r^-+r^-\langle m\rangle_1=\sum_{s=1}^{p+k}(\langle m\rangle_1\langle r^-\rangle_s+\langle r^-\rangle_s\langle m\rangle_1).\tag{3.16}$$

It can be checked that each summand in (3.16) is a homogeneous element of order $s-1$, $1\leqslant s\leqslant p+k$ (Ref. 10), and, by the degree argument, is equal to 0. Therefore, every s-vector part of r^- vanishes and $r^-=0$. We may conclude that $\rho_r=t=1$, hence $T\cap\rho(\Gamma_0^{\pm}(p,k))=\{1\}$. This computation also shows that the intersection of the centralizer $z(T)$ of T in $\rho(\mathrm{Pin}'(1,p,k))$ with $\rho(\Gamma_0^{\pm}(p,k))$ contains only the identity element.

Now we show that T is normal in $\rho(\mathrm{Pin}'(1,p,k))$. Let ρ_m and ρ_r be as in (3.15). Then

$$\begin{aligned}\rho_r\rho_m\rho_{r'}(x)&=\rho_r\rho_m(r^{\pm\,-1}xr)\\&=\rho_r((1+\langle m\rangle_1\tilde e_1)r^{\pm\,-1}xr^{\pm})(1-\langle m\rangle_1\tilde e_1)\\&=(1+\langle m'\rangle_1\tilde e_1)x(1-\langle m'\rangle_1\tilde e_1)\\&=\rho_{m'}(x),\end{aligned}\tag{3.17}$$

where $r'=r^{-1}$, $\langle m'\rangle_1=\alpha_rr^{\pm}\langle m\rangle_1(r^{\pm})^{-1}$.

Finally, consider an Abelian subgroup T' of $O(1,p,k)$ whose action on $x\in X$ depends linearly on the x' part of $x=\lambda_1e_1+x'$

$$t(x)=x-\lambda_2(x')\tilde e_1,\tag{3.18}$$

for $t\in T'$, where λ_2 is a linear functional on X'. We want to show that for every $x'\neq0$ and λ_2 there exists $\langle m\rangle_1\in R^{1,p,k}$ such that $\rho_m(x)=t(x)$, i.e., $\lambda_2=\langle m\rangle_1x'+x'\langle m\rangle_1$.

Assume that x' is anisotropic and $\lambda_2\neq0$. Then take $\langle m\rangle_1=\lambda_2x'/2(x'\cdot x')$. For x' isotropic, i.e., $x'^2=0$, let $K=(x')$ be the one-dimensional totally isotropic subspace of $R^{p,k}$ spanned by x'. Hence $K\subseteq K^{\perp}$ and there exists a vector $v\in R^{p,k}$ such that $v\cdot x'\neq0$ due to the nondegeneracy of $X'=R^{p,k}$. Thus let $v\cdot x'/\lambda_2=1$ and $\langle m\rangle_1=v$. Therefore, $T'=T=\rho(G')$. □

IV. SUMMARY

The main result of this paper was to prove, using the theory of radicals for rings with unity, that the group of units of the degenerate Clifford algebra of any rank is the semidirect product of two groups: the group generated by the radical, and the group of units of the nondegenerate Clifford subalgebra. In the simpler example of degeneracy in one dimension this basic structure was carried over to nontwisted Clifford, pin, and spin groups which were defined here in analogy with the classical theory of Clifford algebras. Finally, we proved the covering theorem reminiscent of the well-known covering theorem in

the theory of spin and orthogonal groups (Ref. 11). Using the results presented in this paper and the ones formulated in Ref. 12 we will attempt to provide a classification of degenerate Clifford algebras of any rank according to the finite multiplicative groups which are uniquely associated with each algebra.

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Hamiltonian particle mechanics on curved space-times—A no-interaction theorem

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Hamiltonian particle mechanics is formulated on a space-time (M,g). The restrictions imposed by the isometry group G of g on the possible dynamics are analyzed; a no-interaction theorem is obtained on a large class of homogeneous space-times. The results are in particular applied to the de Sitter space-time: here it is proven that a G-invariant dynamics can describe geodesic particle motion only.

I. INTRODUCTION

The last two decades have witnessed a growing interest in the study of relativistic direct particle interactions. This has lead to extensive investigations[1] of systems consisting of two or more particles in Minkowski space-time M [3.1]. A major obstacle encountered in these studies is the Currie–Jordan–Sudarshan no-interaction theorem[2,3]: it says, loosely stated, that Hamiltonian particle mechanics on phase space, when coupled with Poincaré invariance, can only describe free particles. In other words, the dynamics is completely determined by the kinematic framework, in particular by the symmetry group, and it is trivial.

The role played by the phase space formulation of Poincaré-invariant particle mechanics in obtaining the no-interaction result has extensively been investigated.[1] However, the question of whether this result is an idiosyncrasy of Minkowski space and its large isometry group has been left open. In this paper, we therefore examine the phase space formulation of particle mechanics on a general space-time (M,g) with Lorentz metric g and isometry group G; we determine in particular conditions on G for a no-interaction result to hold.

In order to formulate Hamiltonian particle mechanics on a space-time (M,g), we first need to generalize to the new context the kinematic framework of nonrelativistic Hamiltonian particle mechanics: i.e., the notions of observer, phase space, and symmetry. This is done in Sec. II, where we also give a precise definition of a Hamiltonian n-particle system. It is then proven that the G-invariance of the particle systems considered induces a (local) action of G on the phase space. Actions arising in this fashion satisfy a number of conditions that are a generalization to the new framework of the worldline conditions, well known for the case where M is Minkowski space-time. They express the compatibility of the action of G on phase space with its action on M and are essential for the worldline interpretation of the theory. In Sec. III we introduce a local and observer-dependent notion of time and the concept of dynamics, associated with it. We consider the case where the observer's worldline is the flowline of a one-parameter subgroup of isometries. It is then shown that complete information about the dynamics of the n-particle system can be obtained from knowledge of the action of G on phase space. It is in particular possible to give a precise definition of the notion of a free n-particle system in terms of the action of G on phase space. This framework allows us to formulate and prove, in Sec. IV, a no-interaction theorem for Hamiltonian particle mechanics on a space-time (M,g), provided its isometry group is large enough, in a sense to be made precise. The theorem states assumptions under which a Hamiltonian n-particle system is necessarily free in the sense of Sec. III. The assumptions can be summarized as follows. First, we require that the action of G on phase space is realized by canonical transformations [Theorem 4.1, assumption (i)]. Second, we consider the case (as in Sec. III) where the observer's worldline is a flowline of a one-parameter subgroup of isometries [Theorem 4.1, assumption (ii)]. Third, we express the fact that initial positions and velocities determine the motion uniquely [Theorem 4.1, assumption (iii)]. Finally, we impose a crucial condition on G: we require that the local notion of simultaneity, introduced in Sec. III, is not preserved under the action of G on M. In Sec. V, we first show how the original no-interaction theorem can be obtained as a special case of the theorem proved in Sec. IV. We then give other examples and, in particular, study in detail the case where (M,g) is the de Sitter space-time.

II. HAMILTONIAN PARTICLE MECHANICS ON (M,g): KINEMATICS

Let (M,g) be a space-time with Lorentz metric g and isometry group G. Denote by

$$\Phi:\ G\times M\to M\,, \tag{2.1}$$

the action of G on M. In the following, G will always be a Lie group. First, we define the notions of particle and particle system. A particle is a one-dimensional, timelike, and connected submanifold $\gamma^{(k)}$ of M; in other words, a particle is a worldline. An n-particle system is a G-stable collection Γ of n-tuples $\gamma=(\gamma^{(1)},\gamma^{(2)},\ldots,\gamma^{(n)})$ of particles. It is the goal of relativistic particle mechanics to explicitly construct, in a mathematically convenient way, physically meaningful n-particle systems.

We illustrate the above definition with an example of its nonrelativistic analog. Consider two masses m_1 and m_2 connected by a spring with spring constant κ. This system can be identified with all couples of trajectories in $\mathbb{R}^3\times\mathbb{R}$ that describe the possible motions the system can execute. Another choice of interaction between the two masses would have

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yielded other trajectories. Moreover, the Galilei invariance of the system manifests itself in the invariance of the collection of pairs of trajectories under the action of the Galilei group on $\mathbf{R}^3\times\mathbf{R}$. In other words, "the transform of a possible motion is a possible motion."

Returning to the definition of an n-particle system on $(M,\mathscr{g})$, we see that a choice of Γ is interpreted as a choice of interaction between the particles. The G-stability of Γ expresses the invariance of the dynamics under the isometry group of $(M,\mathscr{g})$. We will refer to elements of Γ as possible motions.

The purpose of this paper can now be rephrased as follows: we investigate which n-particle systems Γ can be described by a Hamiltonian particle mechanics on phase space.

We now introduce the notion of an instantaneous observer. An instantaneous observer w at $m\in M$ is an orthonormal basis $\{e_1,e_2,e_3,e_4\}$ of the tangent space T_mM of M at m, with e_4 a timelike, future-pointing unit vector.[4] Two instantaneous observers w and w' are equivalent if there exists an element $g\in G$ such that $T_m\Phi_g\cdot e_i=e_i'$, for $i=1,2,3,4$. We write $w'=g[w]$.

We now show how to use the notion of an instantaneous observer w at $m\in M$ to describe the properties of certain n-particle systems Γ in a neighborhood of $m\in M$. First remark that the geodesics generated by span $\{e_1,e_2,e_3\}$ form locally a three-dimensional spacelike hypersurface H_w of M. Given an open subset Σ_w of H_w containing m, we define the n-particle phase space S_w associated to w as the cotangent bundle $S_w=T^*(\Sigma_w\times\cdots\times\Sigma_w)$ (n copies). We denote by τ_α^{w*}: $S_w\to\Sigma_w$ the natural projection of S_w onto the αth copy of Σ_w ($\alpha=1,2,\ldots,n$). On Minkowski space, to the choice of w corresponds a unique geodesic coordinate system (x,y,z,t) with $m\equiv(0,0,0,0)$ and $e_1=\partial/\partial x$, $e_2=\partial/\partial y$, $e_3=\partial/\partial z$, $e_4=\partial/\partial t$. Then H_w is given by the hypersurface $t=0$. Taking $\Sigma_w=H_w$, S_w can indeed be identified with $T^*\mathbf{R}^{3n}$, the usual phase space for an n-particle system. On other spacetimes $(M,\mathscr{g})$, Σ_w can usually not sensibly be taken equal to H_w, as will be seen later. Next, recalling the nonrelativistic example of the harmonic oscillator, we remark that in this case the possible motions are labeled in a one-to-one fashion by points in phase space. This would no longer be true if the two masses had additional degrees of freedom, such as spin, for example. In that case, one would have to use a larger space to label the possible motions of the system. In other words, it is a restriction on the system to say that its possible motions can be labeled by points in phase space. Applying the preceding considerations to the general case, we arrive at the following definition.

Definition 2.1: An n-particle system Γ is a Hamiltonian n-particle system with respect to an instantaneous observer w if there exists an open subset $\Sigma_w\subset H_w$ and a map

$$b_w:\quad s\in S_w\to b_w(s)\in\Gamma\,, \tag{2.2}$$

such that (1) b_w is injective; (2) if for every $\gamma^{(\alpha)}$ in $\gamma=(\gamma^{(1)},\ldots,\gamma^{(n)})\in\Gamma$, the intersection $\gamma^{(\alpha)}\cap\Sigma_a$ is a singleton, then $\gamma\in\operatorname{Im} b_w$; and (3) if $s=b_w^{-1}((\gamma^{(1)},\ldots,\gamma^{(n)}))$, then $\gamma^{(\alpha)}\cap\Sigma_w=\{\tau_\alpha^{w*}(s)\}$, for $\alpha=1,2,\ldots,n$. If $b_w(s)=\gamma$, we refer to s as the state of the possible motion γ for w. Condition (3) guarantees the interpretation of $\tau_\alpha^{w*}(s)$ as the "position" of the αth particle in the possible motion $b_w(s)=\gamma$. Given $\sigma=(\sigma_1,\ldots,\sigma_n)\in\Sigma_w\times\cdots\times\Sigma_w$, we consider

$$\Gamma_\sigma=\{\gamma=(\gamma^{(1)},\gamma^{(2)},\ldots,\gamma^{(n)})\in\Gamma\,|\,\gamma^{(\alpha)}\cap\Sigma_w=\{\sigma_\alpha\}\,,\ \alpha=1,2,\ldots,n\}\,. \tag{2.3}$$

Conditions (1)–(3) assure that b_w maps the fiber $T^*_\sigma(\Sigma_w\times\cdots\times\Sigma_w)$ bijectively onto Γ_σ. In other words: initial positions and momenta determine uniquely a possible motion.

In order to exploit the G stability of Γ, we make the following smoothness assumption: for $\gamma\in\operatorname{Im} b_w$, there exists a neighborhood $\mathscr{N}(\gamma)$ of $e\in G$, such that $\Phi_g(\gamma)\in\operatorname{Im} b_w$ for all $g\in\mathscr{N}(\gamma)$. We can then define a local group action[5] ψ^w of G on S_w as follows:

$$\psi^w:\quad (g,s)\in\mathscr{D}_w\subset G\times S_w\to\psi_g^w(s)\in S_w\,, \tag{2.4}$$

with

$$\mathscr{D}_w=\{(g,s)\in G\times S_w\,|\,g\in\mathscr{N}(b_w(s))\} \tag{2.5}$$

and

$$\psi_g^w(s)=b_w^{-1}\circ\Phi_g\circ b_w(s)\,. \tag{2.6}$$

The interpretation of ψ^w is as follows: if s is the state of γ for w, then $\psi_g^w(s)$ is the state of $\Phi_g(\gamma)$ for w.

In the following, we investigate the properties of n-particle systems Γ which are Hamiltonian with respect to an instantaneous observer w by analyzing the corresponding local group action ψ^w on S_w.

As a first remark, we notice that ψ^w satisfies what is known as the worldline conditions. This is an immediate consequence of condition (3) in Definition 2.1. A convenient form of the worldline conditions is given in the following lemma. (Notice that the lemma holds for every value of $\alpha\in\{1,2,\ldots,n\}$ separately.)

Lemma 2.1: If Γ is a Hamiltonian n-particle system with respect to an instantaneous observer w then the corresponding local group action ψ^w of G on S_w satisfies

$$(\Phi_g\circ\tau_\alpha^{w*})(\psi_{g^{-1}}^w(s))=\tau_\alpha^{w*}(s)\,, \tag{2.7}$$

for all $(g^{-1},s)\in\mathscr{D}_w$ such that $\Phi_{g^{-1}}(\tau_\alpha^{w*}(s))\in\Sigma_w$.

Proof: Take $(g^{-1},s)\in\mathscr{D}_w$ such that $\Phi_{g^{-1}}(\tau_\alpha^{w*}(s))\in\Sigma_w$. Write $b_w(s)=\gamma=(\gamma^{(1)},\gamma^{(2)},\ldots,\gamma^{(n)})$. Then

$$\Phi_{g^{-1}}(\gamma^{(\alpha)})\cap\Sigma_w\supset\{\Phi_{g^{-1}}(\tau_\alpha^{w*}(s))\}\,. \tag{2.8}$$

But $(g^{-1},s)\in\mathscr{D}_w$, so that $\Phi_{g^{-1}}(\gamma)\in\operatorname{Im} b_w$. Hence, by (3) of Definition 2.1, $\Phi_{g^{-1}}(\gamma^{(\alpha)})\cap\Sigma_w$ is a singleton. Consequently,

$$\Phi_{g^{-1}}(\gamma^{(\alpha)})\cap\Sigma_w=\{\Phi_{g^{-1}}(\tau_\alpha^{w*}(s))\}\,. \tag{2.9}$$

Moreover, from (2.6) and (3) of Definition 2.1

$$\Phi_{g^{-1}}(\gamma^{(\alpha)})\cap\Sigma_w=\{\tau_\alpha^{w*}(\psi_{g^{-1}}^w(s))\}\,. \tag{2.10}$$

From (2.9) and (2.10), (2.7) follows immediately. □

The worldline conditions will be of crucial importance in proving the no-interaction theorem of Sec. IV.

In order to make further contact with Hamiltonian mechanics, we assume from now on that the local action ψ^w of G on the phase space S_w is strongly symplectic, i.e., all the generators of ψ^w are Hamiltonian vector fields. In other words, if $\mathscr{L}(G)$ is the Lie algebra of G, if ω is the natural

symplectic form on $S_w = T^*(\Sigma_w \times \cdots \times \Sigma_w)$, and if we denote by $(\xi)_{S_w}$ the generator of the action ψ^w corresponding to $\xi \in \mathscr{L}(G)$, we have

$$(\xi)_{S_w} \lrcorner \omega = dK(\xi), \tag{2.11}$$

for some $K(\xi) \in \mathscr{F}(S_w)$, the smooth functions on S_w. We write $\{\cdot,\cdot\}$ for the Poisson bracket on S_w.

III. HAMILTONIAN PARTICLE MECHANICS ON $(M,\mathscr{G})$: DYNAMICS

We first introduce in this section a local and observer-dependent notion of time as follows. Let $w = \{e_1,e_2,e_3,e_4\}$ be an instantaneous observer at a point m of the space-time $(M,\mathscr{G})$. Assume the existence of an element in $\mathscr{L}(G)$ that we shall denote by ξ_4 such that its corresponding infinitesimal generator $(\xi_4)_M$ on M satisfies $(\xi_4)_M(m) = e_4$. We then construct a one-parameter family of instantaneous observers $w(t) \equiv \exp t\xi_4[w]$, $t \in \mathbb{R}$. A straightforward application of the "straightening out theorem[6]" assures the existence of an open neighborhood $\mathscr{N} \subset H_w$ of $m \in M$ and a positive real number $a \in \mathbb{R}^+$ such that the map

$$\tau: \quad (t,\sigma) \in (-a,a) \times \mathscr{N} \to \Phi(\exp t\xi_4,\sigma) \in M \tag{3.1}$$

is injective and onto a neighborhood U of $m \in M$. Consequently, given $m' \in U$, $\exists!(t,\sigma) \in (-a,a) \times \mathscr{N}$ such that

$$\Phi(\exp t\xi_4,\sigma) = m'. \tag{3.2}$$

The value of t is interpreted as the value of the time at m'; it depends on the choice of w and of ξ_4. On Minkowski space ξ_4 is usually taken to be the generator of translations in the e_4 direction and t is then the usual notion of observer time.

Now let Γ be a Hamiltonian n-particle system with respect to w. We can take, without loss of generality, $\Sigma_w = \mathscr{N}$. We prove that Γ is locally fully determined by the knowledge of the action ψ^w of G on the phase space S_w. Consider a state $s \in S_w$, the phase space associated to w, and denote the corresponding possible motion $b_w(s)$ by γ:

$$b_w(s) = \gamma = (\gamma^{(1)},\gamma^{(2)},\ldots,\gamma^{(n)}). \tag{3.3}$$

From (2.5), it follows that $\exists b \in \mathbb{R}^+$ such that $\forall t \in (-b,b)$, $(\exp -t\xi_4,s) \in \mathscr{D}_w$. Without loss of generality, we can take $a = b$. For fixed α in $\{1,2,\ldots,n\}$, choose $m' \in \gamma^{(\alpha)} \cap U$. Then, by (3.2), $\exists!(t,\sigma_\alpha) \in (-a,a) \times \Sigma_w$ such that

$$\Phi(\exp -t\xi_4,m') = \sigma_\alpha. \tag{3.4}$$

Clearly, by (3) of Definition 2.1, and the definition (2.4)–(2.6) of ψ^w,

$$\{\sigma_\alpha\} = \Sigma_w \cap \Phi_{\exp -t\xi_4}(\gamma^{(\alpha)}) \tag{3.5}$$

and

$$\sigma_\alpha = \tau_\alpha^{w*}(\psi^w_{\exp -t\xi_4}(s)). \tag{3.6}$$

From (3.4) and (3.6), we conclude

$$m' = \Phi(\exp t\xi_4,\tau_\alpha^{w*}(\psi^w_{\exp -t\xi_4}(s))). \tag{3.7}$$

Since we can repeat the argument for every $m' \in \gamma^{(\alpha)} \cap U$, we conclude that

$$\operatorname{Im} \hat{\gamma}^{(\alpha)} = \gamma^{(\alpha)} \cap U, \tag{3.8}$$

where

$$\hat{\gamma}^{(\alpha)}: \quad t \in (-b,b) \subset \mathbb{R} \to \Phi(\exp t\xi_4,\tau_\alpha^{w*}(\psi^w_{\exp -t\xi_4}(s))). \tag{3.9}$$

This proves indeed that, given a state $s \in S_w$ and the local action ψ^w of G on S_w, we can reconstruct locally the possible motion $b_w(s) = \gamma$ corresponding to the state s by considering (3.9).

We are now justified in calling $(\xi_4)_{S_w}$ the dynamic vector field on S_w and $K(\xi_4)$ [see (2.11)] the corresponding Hamiltonian: indeed, considering the special case where M is Minkowski space-time and ξ_4 the generator of time translations in the e_4 direction, (3.9) expresses that the "time evolution" is given by the Hamiltonian flow corresponding to $K(\xi_4) \equiv K_4$.

In the sequel we will only consider the case where the Legendre transformation (fiber derivative[4])

$$\mathbf{FK}_4: \quad S_w = T^*(\Sigma_w \times \cdots \times \Sigma_w) \to T(\Sigma_w \times \cdots \times \Sigma_w) \tag{3.10}$$

is a diffeomorphism onto its image. This expresses the fact that, instead of "initial positions and momenta," we can use "initial positions and velocities" to label the possible motions.

Given ψ^w and $\mathbf{FK}_4$, we construct a local group action $\hat{\psi}^w$ of G on $TQ_w \equiv T(\Sigma_w \times \cdots \times \Sigma_w)$ as follows:

$$\hat{\psi}^w: \quad (g,v) \in \hat{D}_w \subset G \times TQ_w \to \hat{\psi}^w_g(v) \in TQ_w, \tag{3.11}$$

where

$$\hat{\psi}^w_g(v) = (\mathbf{FK}_4 \circ \psi^w_g \circ \mathbf{FK}_4^{-1})(v) \tag{3.12}$$

and

$$\hat{D}_w = \{(g,v) \in G \times TQ_w \mid (g,(\mathbf{FK}_4)^{-1}(v)) \in \mathscr{D}_w\}. \tag{3.13}$$

One can make TQ_w into a symplectic manifold by constructing the Lagrange two-form,[4] using $\mathbf{FK}_4$ in the usual way. The action $\hat{\psi}^w$ is then symplectic with respect to this symplectic structure. In particular, the infinitesimal generator $(\xi_4)_{TQ_w}$ of the action $\hat{\psi}^w$ corresponding to ξ_4 (i.e., the dynamic vector field on TQ_w) is a second-order Lagrangian vector field on TQ_w. In local coordinates on TQ_w,

$$(\xi_4)_{TQ_w}(v) = \dot{q}_i^{(\alpha)} \frac{\partial}{\partial q_i^{(\alpha)}}\bigg|_v + A_i^{(\alpha)}(v) \frac{\partial}{\partial v_i^{(\alpha)}}\bigg|_v, \tag{3.14}$$

where the summation of $\alpha \in \{1,2,\ldots,n\}$ and $i \in \{1,2,3\}$ is understood and

$$v \equiv (q_i^{(1)},q_i^{(2)},\ldots,q_i^{(n)},\dot{q}_i^{(1)},\ldots,\dot{q}_i^{(n)}) \equiv (q^{(\alpha)},\dot{q}^{(\alpha)}). \tag{3.15}$$

We now say that an n-particle system Γ is free if the "acceleration" $A_i^{(\alpha)}$, $i = 1,2,3$, of the αth particle only depends on the position and velocity of the αth particle itself. This idea is expressed in the following definition.

Definition 3.1: Let (i) Γ be a Hamiltonian n-particle system with respect to an instantaneous observer $w = \{e_1,\ldots,e_4\}$; (ii) the corresponding local group action ψ^w of G on S_w be strongly symplectic; and (iii) $\xi_4 \in \mathscr{L}(G)$ be such that $((\xi_4)_M(m) = e_4$ and such that $\mathbf{FK}_4$ is a diffeomorphism onto its image. Then we say that Γ is a free n-particle system with respect to w and ξ_4 if there exist local group actions $\chi^{(\alpha)}$ of G on $T\Sigma_w$ such that $\forall (g,v) \in \mathscr{D}_w$, with $v \equiv (v^{(1)},v^{(2)},\ldots,v^{(n)})$,

$$\hat{\psi}^w_g(v) = (\chi^{(1)}_g(v^{(1)}),\chi^{(2)}_g(v^{(2)}),\ldots,\chi^{(n)}_g(v^{(n)})). \tag{3.16}$$

In other words, the local action $\hat{\psi}^w$ "factorizes" into the n-fold product of the local actions $\chi^{(\alpha)}$.

IV. A NO-INTERACTION THEOREM

We are now ready to state and prove the main result of this paper.

Theorem 4.1: Let $w=\{e_1,...,e_4\}$ be an instantaneous observer at a point m of a space-time (M,φ) with isometry group G. Let Γ be a Hamiltonian n-particle system with respect to w. If (i) the corresponding local action ψ^w of G on the phase space S_w is strongly symplectic; (ii) there exists an element $\xi_4\in\mathscr{L}(G)$, the Lie algebra of G, such that $(\xi_4)_M(m)=e_4$; (iii) the Legendre transformation $\mathbf{F}K_4$ is a diffeomorphism onto its image; and (iv) for every $\sigma\in\Sigma_w$, the isotropy group of σ does not leave the normal to Σ_w at σ invariant; then Γ is a free n-particle system with respect to (w,ξ_4).

In physical terms, condition (iv) requires that the local notions of time and simultaneity, associated with the pair (w,ξ_4) by (3.1) and (3.2) are not preserved under the invariance group G. We break the proof of the theorem up into several lemmas. The flow of the argument is a generalization of a proof of the original no-interaction theorem, given for the first time in that form in Ref. 3.

As a first step, we exploit in Lemma 4.1 the worldline conditions (2.7) to determine the infinitesimal generators $(\xi)_{TQ_w}(\xi\in\mathscr{L}(G))$ of the local action $\hat{\psi}^w$: the result shows that, independently of assumption (iv) of Theorem 4.1, all the generators are determined uniquely by $(\xi_4)_{TQ_w}$.

We assume for simplicity that there exists a global coordinate system on Σ_w:

$$\phi:\ \sigma\in\Sigma_w\to\phi(\sigma)\in\mathbf{R}^3, \tag{4.1}$$

with $\phi(\sigma)=(\phi_1(\sigma),\phi_2(\sigma),\phi_3(\sigma))\equiv(q_1,q_2,q_3)$. Correspondingly, we have coordinates $(q_i^{(\alpha)},\dot{q}_i^{(\alpha)})$ on TQ_w and $(q_i^{(\alpha)},p_i^{(\alpha)})$ on $T^*Q_w=S_w$ (i = 1,2,3; $\alpha=1,2,...n$). Moreover, defining

$$v_i^{(\alpha)}(s)=\{q_i^{(\alpha)},K_4\}(s), \tag{4.2}$$

we have

$$\mathbf{F}K_4:\quad s=(q_i^{(\alpha)},p_i^{(\alpha)})\in S_w\to(q_i^{(\alpha)},v_i^{(\alpha)}(s))\in TQ_w. \tag{4.3}$$

We can now write, using the definition (3.11)–(3.13) of $\hat{\Psi}^w$ and summing over $\alpha\in\{1,2,...,n\}$ and $i\in\{1,2,3\}$,

$$(\xi)_{TQ_w}(\mathbf{F}K_4(s))=\{q_i^{(\alpha)},K(\xi)\}(s)\frac{\partial}{\partial q_i^{(\alpha)}}\bigg|_{\mathbf{F}K_4(s)}+\{v_i^{(\alpha)},K(\xi)\}(s)\frac{\partial}{\partial\dot{q}_i^{(\alpha)}}\bigg|_{\mathbf{F}K_4(s)}, \tag{4.4}$$

with $\xi\in\mathscr{L}(G)$ and $s\in T^*Q_w$. In particular, for $\xi=\xi_4$, and in obvious shorthand notation

$$(\xi_4)_{TQ_w}=\dot{q}_i^{(\alpha)}\frac{\partial}{\partial q_i^{(\alpha)}}+\{v_i^{(\alpha)},K_4\}\frac{\partial}{\partial\dot{q}_i^{(\alpha)}}. \tag{4.5}$$

Comparing with (3.14), we have

$$A_i^{(\alpha)}=\{v_i^{(\alpha)},K_4\}. \tag{4.6}$$

(We will use the same notation $A_i^{(\alpha)}$, whether considered as a function on S_w or TQ_w.)

In Lemma 4.1 we compute the functions $\{K(\xi),q_i^{(\alpha)}\}$ and $\{K(\xi),v_i^{(\alpha)}\}$ in terms of $v_i^{(\alpha)}$ and $A_i^{(\alpha)}$. For that purpose, we need the following function:

$$T:\ (\sigma,\xi)\in\Sigma_w\times\mathscr{L}(G)\to T(\sigma,\xi)\in(-a,a)\subset\mathbf{R}, \tag{4.7}$$

which is defined, using (3.1) and (3.2), by

$$\Phi(\exp -T(\sigma,\xi)\xi_4,\Phi(\exp\xi,\sigma))\in\Sigma_w. \tag{4.8}$$

Here T is well defined on an open subset of $\Sigma_w\times\mathscr{L}(G)$ that contains $\Sigma_w\times\{0\}$: indeed, if ξ is small enough, then $\Phi(\exp\xi,\sigma)\in U\subset M$ [see (3.1) and (3.2)]; hence $T(\sigma,\xi)$ in (4.8) is unique by (3.2). Now $T(\sigma,\xi)$ is the time value associated to the point $\Phi(\exp\xi,\sigma)$ by w. Notice that $T(\sigma,0)=0$, $\forall\sigma\in\Sigma_w$.

Let $\{\xi_1,...,\xi_k\}$ be a basis of $\mathscr{L}(G)$. We write $K_m\equiv K(\xi_m)$ (see 2.11). For the partial derivative of T (4.7) with respect to the mth component of $\xi\in\mathscr{L}(G)$, we use the notation $T_{,m}(\sigma,\xi)$. Notice also that we can construct a coordinate system (q_1,q_2,q_3,t) on U, using (3.1) and (3.2), and (4.1). As a consequence, we will consider the function ϕ in (4.1) alternatively as defined on U or on Σ_w, without using different notations. In the sequel $\alpha,\ \beta\in\{1,2,...,n\}$, $i,j\in\{1,2,3\}$, $l,m\in\{1,2,...,k\}$.

Lemma 4.1: Under conditions (i)–(iii) of Theorem 4.1, summing over m and j, $\forall\ s\in S_w$,

$$\{q_i^{(\alpha)},K_l\}(s)=(G_l^i\circ\tau_\alpha^{w^*})(s)+T_{,l}(\tau_\alpha^{w^*}(s),0)v_i^{(\alpha)}(s), \tag{4.9}$$

$$\begin{aligned}&\{v_i^{(\alpha)},K_l\}(s)\\&=c_{4l}^m\{q_i^{(\alpha)},K_m\}(s)+(G_l^i)_{,j}(\tau_\alpha^{w^*}(s)v_j^{(\alpha)}(s)\\&\quad+(T_{,l})_{,j}(\tau_\alpha^{w^*}(s),0)v_i^{(\alpha)}(s)v_j^{(\alpha)}(s)\\&\quad+T_{,j}(\tau_\alpha^{w^*}(s),0)A_i^{(\alpha)}(s),\end{aligned} \tag{4.10}$$

with

$$G_l^i:\sigma\in\Sigma_w\to(\xi_l)_M(\phi_i)(\sigma)\in\mathbf{R}, \tag{4.11}$$

$$[\xi_4,\xi_l]=c_{4l}^m\xi_m, \tag{4.12}$$

and

$$(T_{,l})_{,j}=\frac{\partial T_{,l}}{\partial q_j},\quad (G_l^i)_{,j}=\frac{\partial G_l^i}{\partial q_j}.$$

Proof: Take $s\in S_w$. Choose $\mu\in\mathbf{R}$ small enough such that (i) $T(\tau_\alpha^{w^*}(s),\mu\xi_l)$ exists, and (ii) $(g^{-1},s)\in D_w$, with

$$g=\exp -\mu\xi_l\ \exp T(\tau_\alpha^{w^*}(s),\mu\xi_l)\xi_4\in G. \tag{4.13}$$

It follows from (4.8) that

$$\Phi(g^{-1},\tau_\alpha^{w^*}(s))\in\Sigma_w. \tag{4.14}$$

Hence, Lemma 2.1 applies: for $f\in\mathscr{F}(M)$, Eq. (2.7) yields

$$(f\circ\tau_\alpha^{w^*})(\psi_{g^{-1}}^w(s))=(f\circ\Phi_{g^{-1}})(\tau_\alpha^{w^*}(s)). \tag{4.15}$$

Choosing $f=\phi_i$, taking the derivative for $\mu=0$ in both sides of (4.15) and remembering that $T(\tau_\alpha^{w^*}(s),0)=0$, one obtains (4.9) upon using $(\xi_4)_M(\phi_i)(\sigma)=0$.

In order to derive (4.10), one first writes, using the Jacobi identity,

$$\begin{aligned}\{v_i^{(\alpha)},K_l\}(s)&=\{\{q_i^{(\alpha)},K_4\},K_l\}(s)\\&=\{\{K_4,K_l\},q_i^{(\alpha)}\}-\{\{K_l,q_i^{(\alpha)}\},K_4\}.\end{aligned} \tag{4.16}$$

Inserting (4.12) and (4.9) into (4.16), (4.10) follows. □

The next lemma uses assumption (iv) of Theorem 4.1 in a crucial way.

Lemma 4.2: Under the conditions of Theorem 4.1, for all $s\in S_w$ and for $\alpha\neq\beta$,

$$\{q_i^{(\alpha)},v_j^{(\beta)}\}(s)=0, \tag{4.17}$$

$$\{v_i^{(\alpha)},v_j^{(\beta)}\}(s)=0, \tag{4.18}$$

$$\{q_i^{(\alpha)},A_j^{(\beta)}\}(s)=0, \tag{4.19}$$

$$\{v_i^{(\alpha)},A_j^{(\beta)}\}(s)=0. \tag{4.20}$$

Proof: Upon using, in that order, the Jacobi identity, $\{q_i^{(\alpha)},q_j^{(\beta)}\}=0$, and Eq. (4.9), one calculates, $\forall s\in S_w$,

$$\{\{K_l,q_i^{(\alpha)}\},q_j^{(\beta)}\}(s) = -T_{,l}(\tau_\beta^{w^*}(s),0)\{v_j^{(\beta)},q_i^{(\alpha)}\}(s). \tag{4.21}$$

Alternatively, using (4.9) directly, one has

$$\{\{K_l,q_i^{(\alpha)}\},q_j^{(\beta)}\}(s) = -T_{,l}(\tau_\alpha^{w^*}(s),0)\{v_i^{(\alpha)},q_j^{(\beta)}\}(s). \tag{4.22}$$

But, with (4.2) and the Jacobi identity,

$$\begin{aligned}\{v_j^{(\beta)},q_i^{(\alpha)}\} &= \{\{q_j^{(\beta)},K_4\},q_i^{(\alpha)}\}\\ &= -\{\{K_4,q_i^{(\alpha)}\},q_j^{(\beta)}\} - \{\{q_i^{(\alpha)},q_j^{(\beta)}\},K_4\}\\ &= \{v_i^{(\alpha)},q_j^{(\beta)}\}.\end{aligned} \tag{4.23}$$

Hence, from (4.21)–(4.23), $\forall s\in S_w$,

$$(T_{,l}(\tau_\beta^{w^*}(s),0) - T_{,l}(\tau_\alpha^{w^*}(s)0))\{q_i^{(\alpha)},v_j^{(\beta)}\}(s) = 0. \tag{4.24}$$

Consequently we have, $\forall s\in S_w$ and $\forall\xi\in\mathscr{L}(G)$,

$$\frac{d}{d\lambda}(T(\tau_\beta^{w^*}(s),\lambda\xi) - T(\tau_\alpha^{w^*}(s),\lambda\xi))\Big|_{\lambda=0}\{q_i^{(\alpha)},v_j^{(\beta)}\}(s) = 0. \tag{4.25}$$

It follows from (4.25) that $\{q_i^{(\alpha)},v_j^{(\beta)}\}(s) = 0$ whenever $\exists\xi\in\mathscr{L}(G)$ such that

$$\frac{d}{d\lambda}(T(\tau_\beta^{w^*}(s),\lambda\xi) - T(\tau_\alpha^{w^*}(s),\lambda\xi))\Big|_{\lambda=0} \neq 0. \tag{4.26}$$

In order to prove (4.17), we need to prove that, even if, for some $s\in S_w$,

$$\frac{d}{d\lambda}(T(\tau_\beta^{w^*}(s),\lambda\xi) - T(\tau_\alpha^{w^*}(s),\lambda\xi))\Big|_{\lambda=0} = 0,$$
$$\forall\xi\in\mathscr{L}(G), \tag{4.27}$$

$\{q_i^{(\alpha)},v_j^{(\beta)}\}(s)$ is nevertheless equal to zero.

Suppose therefore that for some $s\in S_w$, (4.27) is satisfied. Choose ξ_0 in the Lie algebra of the isotropy group of $\tau_\alpha^{w^*}(s)$ such that the flow $\Phi_{\exp\lambda\xi_0}$ of the corresponding one-parameter group $\exp\lambda\xi_0(\lambda\in\mathbb{R})$ does not leave the normal to Σ_w at $\tau_\alpha^{w^*}(s)$ invariant. Alternatively,

$$(\Phi_{\exp\lambda\xi_0})_*(T_{\tau_\alpha^{w^*}(s)}\Sigma_w) \neq T_{\tau_\alpha^{w^*}(s)}\Sigma_w. \tag{4.28}$$

Such a ξ_0 exists by assumption (iv) of Theorem 4.1. Since $\exp\lambda\xi_0(\lambda\in\mathbb{R})$ is in the isotropy group of $\tau_\alpha^{w^*}(s)$, it follows from (4.7) and (4.8) that

$$T(\tau_\alpha^{w^*}(s),\lambda\xi_0) = 0,\ \lambda\in\mathbb{R}. \tag{4.29}$$

Hence, from (4.27), with $\xi = \xi_0$,

$$\frac{d}{d\lambda}T(\tau_\beta^{w^*}(s),\lambda\xi_0)\Big|_{\lambda=0} = 0. \tag{4.30}$$

We now prove by contradiction that

$$\forall N\subset\Sigma_w,\ \text{neighborhood of } \tau_\alpha^{w^*}(s),$$
$$\exists\sigma\in N \text{ such that } \frac{d}{d\lambda}T(\sigma,\lambda\xi_0)|_{\lambda=0}\neq 0. \tag{4.31}$$

Indeed, suppose there exists a neighborhood $N\subset\Sigma_w$ of $\tau_\alpha^{w^*}(s)$ such that $\forall\sigma\in N$, $(d/d\lambda)\,T(\sigma,\lambda\xi_0)|_{\lambda=0} = 0$; recall that, in the coordinate system (q_1,q_2,q_3,t) introduced before Lemma 4.1, we can write

$$\Phi(\exp\lambda\xi_0,\sigma) = (q_1(\lambda),q_2(\lambda),q_3(\lambda),T(\sigma,\lambda\xi_0)), \tag{4.32}$$

with $\sigma = (q_1(0),q_2(0),q_3(0),0)$. Consequently,

$$(d/d\lambda)T(\sigma,\lambda\xi_0)|_{\lambda=0} = 0$$

implies $(\xi_0)_M(\sigma)\in T_\sigma\Sigma_w$. If this is true for all $\sigma\in N$, $(\xi_0)_M$, when restricted to N, is a vector field on N. Hence, Eq. (4.28) cannot be satisfied. This proves (4.31) by contradiction.

Consider therefore a sequence of points $\sigma_k\in\Sigma_w$, $k\in\mathbb{N}$, such that σ_k approaches $\tau_\alpha^{w^*}(s)$ as $k\to\infty$ and satisfying $(d/d\lambda)T(\sigma_k,\lambda\xi_0)|_{\lambda=0}\neq 0$. Writing $\sigma_k\equiv(q_{k1},q_{k2},q_{k3})$, construct a sequence of points $s_k\in S_w$ as follows: if

$$s\equiv(q_i^{(1)},q_i^{(2)},\ldots,q_i^{(\alpha)},\ldots,q_i^{(\beta)},\ldots,q_i^{(n)},p_i^{(1)},\ldots,p_i^{(n)}), \tag{4.33}$$

then

$$s_k\equiv(q_i^{(1)},q_i^{(2)},\ldots,q_{ki},\ldots,q_i^{(\beta)},\ldots,q_i^{(n)},p_i^{(1)},\ldots,p_i^{(n)}). \tag{4.34}$$

Here $\alpha\neq\beta$; clearly s_k approaches s as k goes to infinity. Upon using (4.30), (4.33), and (4.34), Eq. (4.25) reads, $\forall k\in\mathbb{N}$,

$$\frac{d}{d\lambda}T(\tau_\alpha^{w^*}(s_k),\lambda\xi_0)\Big|_{\lambda=0}\{q_i^{(\alpha)},v_j^{(\beta)}\}(s_k) = 0. \tag{4.35}$$

Hence $\{q_i^{(\alpha)},v_j^{(\beta)}\}(s_k) = 0$, $\forall k\in\mathbb{N}$. It follows by continuity that $\{q_i^{(\alpha)},v_j^{(\beta)}\}(s) = 0$. This proves (4.17).

Equations (4.18)–(4.20) are proved in a similar way. First, using the Jacobi identity, Eqs. (4.9) and (4.17), one finds, $\forall s\in S_w$,

$$\{\{K_l,v_i^{(\beta)}\},q_j^{(\alpha)}\}(s) = -T_{,l}(\tau_\alpha^{w^*}(s),0)\{v_j^{(\alpha)},v_i^{(\beta)}\}(s). \tag{4.36}$$

Alternatively, from (4.10) and (4.17) and $\forall s\in S_w$,

$$\{\{K_l,v_i^{(\beta)},q_j^{(\alpha)}\}(s) = -T_{,l}(\tau_\beta^{w^*}(s),0)\{A_i^{(\beta)},q_j^{(\alpha)}\}(s). \tag{4.37}$$

Furthermore, from the Jacobi identity and (4.17) one obtains, $\forall s\in S_w$,

$$\{A_i^{(\beta)},q_j^{(\alpha)}\} = \{v_j^{(\alpha)},v_i^{(\beta)}\}. \tag{4.38}$$

Inserting (4.38) into (4.37) and comparing to (4.36), one has $\forall s\in S_w$ and $\forall\xi\in\mathscr{L}(G)$,

$$\frac{d}{d\lambda}(T(\tau_\beta^{w^*}(s),\lambda\xi) - T(\tau_\alpha^{w^*}(s),\lambda\xi))\Big|_{\lambda=0}\{v_j^{(\alpha)},v_i^{(\beta)}(s) = 0. \tag{4.39}$$

Comparing (4.39) to (4.25), we see that (4.18) follows if we repeat the arguments in (4.26)–(4.34).

Equation (4.20) is proven in a similar way. To prove (4.19), note that

$$\begin{aligned}\{A_j^{(\beta)},q_i^{(\alpha)}\} &= \{\{v_j^{(\beta)},K_4\},q_i^{(\alpha)}\}\\ &= \{\{K_4,q_i^{(\alpha)}\},v_j^{(\beta)}\} - \{\{q_i^{(\alpha)},v_j^{(\beta)}\},K_4\}\\ &= 0,\end{aligned} \tag{4.19'}$$

where we used (4.6), (4.2), (4.17), (4.18) and the Jacobi identity. □

Having obtained Lemma 4.2, the proof of the theorem now follows along precisely the same lines as in the flat case. We briefly recall the argument.

Proof of Theorem 4.1: From (4.17)–(4.20) and the definition of the Poisson bracket on S_w, we obtain, for $\alpha\neq\beta$,

$$\begin{aligned}\{q_i^{(\alpha)},A_j^{(\beta)}\} &= 0 = \{q_i^{(\alpha)},v_k^{(\alpha)}\}\frac{\partial A_j^{(\beta)}}{\partial v_k^{(\alpha)}},\\ \{v_i^{(\alpha)},A_j^{(\beta)}\} &= 0 = \{v_i^{(\alpha)},v_k^{(\alpha)}\}\frac{\partial A_j^{(\beta)}}{\partial v_k^{(\alpha)}} + \{v_i^{(\alpha)},q_k^{(\alpha)}\}\frac{\partial A_j^{(\beta)}}{\partial v_k^{(\alpha)}},\end{aligned} \tag{4.40}$$

where k is summed over from 1 to 3. From (4.17) and condition (iii) of Theorem 4.1, we also have

$$\det\{q_i^{(\alpha)},v_j^{(\alpha)}\}\neq 0,\quad \forall\alpha\in\{1,2,\ldots,n\}. \tag{4.41}$$

Consequently, the only solutions to (4.40) are

$$\frac{\partial A_j^{(\beta)}}{\partial v_i^{(\alpha)}} = 0 = \frac{\partial A_j^{(\beta)}}{\partial q_i^{(\alpha)}}, \quad \forall i,j \in \{1,2,3\}, \ \forall \alpha \neq \beta \in \{\alpha,\ldots,n\}. \tag{4.42}$$

In other words, the acceleration $A_j^{(\beta)}$ does not depend on the position or the velocity of the αth particle, provided $\alpha \neq \beta$. Inserting (4.42), (4.9), and (4.10), into (4.4), we see that we can write

$$(\xi)_{TQ_w} = \sum_{\alpha=1}^{n} (\xi)_{T\Sigma_w}^{(\alpha)},$$

where $(\xi)_{T\Sigma_w}^{(\alpha)}$ is a vector field on the αth copy of $T\Sigma_w$ in $TQ_w = T\Sigma_w \times T\Sigma_w \times \cdots \times T\Sigma_w$. We construct local group actions $\chi^{(\alpha)}$ of G on $T\Sigma_w$ by exponentiation of the infinitesimal generators $(\xi)_{T\Sigma_w}^{(\alpha)}$. Hence, (3.16) is satisfied and Γ is free with respect to w and ξ_4. □

V. EXAMPLES

As an immediate example, we recover the original no-interaction theorem. In this case $(M,\mathscr{P})$ is Minkowski space-time $M^{3,1}$ with the Poincaré group as isometry group. All instantaneous observers are equivalent. Choosing $w \equiv (e_1,\ldots,e_4)$, at $m \in M$, we can set up the unique geodesic coordinate system (x,y,z,t) determined by $m \equiv (0,0,0,0)$ and $e_1 = \partial/\partial x, e_2 = \partial/\partial y, e_3 = \partial/\partial z, e_4 = \partial/\partial t$. Here H_w is the hyperplane $t = 0$. For ξ_4 we choose the generator for translations in the t direction and condition (iv) of Theorem 4.1 is now satisfied everywhere on H_w. Choosing $\Sigma_w = H_w$, we can apply Theorem 4.1. A little extra algebra proves moreover that the particles move in geodesics, i.e., the accelerations are identically equal to zero.[3] Notice that in this case the curve

$$\lambda \in \mathbb{R} \to \Phi(\exp \lambda \xi_4, m) \in M^{3,1} \tag{5.1}$$

is a geodesic: hence it makes sense to refer to the family of instantaneous observers $w(\lambda) = \exp \lambda \xi_4[w]$ as a "freely falling observer." The no-interaction theorem stated in Sec. IV also applies to the so-called "uniformly accelerated observers[7]" on Minkowski space-time. Choose a geodesic coordinate system (x,y,z,t) on $M^{3,1}$ and consider $w \equiv (\partial/\partial x, \partial/\partial y, \partial/\partial z, \partial/\partial t)$ at $m \equiv (x,y,z,t) = (1,0,0,0)$. Let ξ_4 be the generator of the Lorentz boosts in the x direction; these leave the origin (0,0,0,0) fixed. Moreover, with this choice of w and ξ_4, the curve (5.1) now represents a uniformly accelerated motion, asymptotically approaching the speed of light. Again, H_w is the surface $t = 0$, but Σ_w is given by $\{(x,y,z,t) | t = 0, x > 0\}$. Theorem 4.1 applies here also: Hamiltonian particle mechanics with respect to w and ξ_4 only describes free particles.

We now give examples where $(M,\mathscr{P})$ is not Minkowski space-time. First note that conditions (ii) and (iv) of Theorem 4.1 put restrictions on the space-times to which the theorem can be applied. A large class of examples is found among the homogeneous space-times; condition (ii) can then be satisfied for any choice of w. If the isometry group is at least five-dimensional, then (iv) can also be satisfied for some choice of w. Indeed, the isotropy group of any point is now at least one-dimensional and therefore cannot leave every timelike direction invariant. Hence, we can choose w such that e_4 is not invariant and so (iv) is satisfied.

More specifically, we are interested in the homogeneous solutions of the Einstein equations. Those have been studied extensively.[8] We already mentioned Minkowski space-time as a first example.

We now apply Theorem 4.1 to the de Sitter space-time, $M_+^{3,1}$. $M_+^{3,1}$ has the topology of $\mathbb{R}^1 \times S^3$ and can be identified with the hyperboloid

$$u^2 + x^2 + y^2 + z^2 - t^2 = R^2 \tag{5.2}$$

in the five-dimensional Minkowski space-time $M^{4,1}$. Its isometry group is the ten-dimensional Lorentz group in $M^{4,1}$; the isotropy group of any point is isomorphic to the six-dimensional Lorentz group in $M^{3,1}$. $M_+^{3,1}$ is a homogeneous space-time of constant positive curvature. Let $m \equiv (R,0,0,0,0)$ and $w \equiv (e_1,e_2,e_3,e_4) = (\partial/\partial x, \partial/\partial y, \partial/\partial z, \partial/\partial t)$; then H_w is given by the hypersurface $t = 0$ in $M_+^{3,1}$.

Let ξ_4 be the generator of the Lorentz boosts in the (u,t) plane. Notice that the curve

$$\lambda \in \mathbb{R} \to \Phi(\exp \lambda \xi_4, m) \in M_+^{3,1} \tag{5.3}$$

is a geodesic so that we are again dealing with a "freely falling observer." The theorem immediately applies: the particles move independently of one another. We now prove that the particle motion is actually geodesic.

We first remark that it is sufficient to show that a particle at rest at the origin (i.e., at $m = (R,0,0,0,0) \in M_+^{3,1}$) feels no acceleration. Indeed, in this case it will remain at rest and consequently move on the curve (5.3), which is geodesic. Moreover, every other initial position and velocity can be obtained from the first one using an element of the isometry group. As the isometry group maps geodesics into geodesics and since initial positions and velocities determine the motion uniquely, every particle motion has to be geodesic. We now prove

$$A_l(q,\dot{q}) = 0 \tag{5.4}$$

for

$$(q,\dot{q}) = (q_1,q_2,q_3,\dot{q}_1,\dot{q}_2,\dot{q}_3) = (0,0)$$

[cf. (3.14) and (3.15), where we dropped the superscript α].

First, returning to (4.7)–(4.12), note that we have, in the coordinate system (q_1,q_2,q_3,t) on a neighborhood U of m,

$$(\xi_l)_M(\sigma) = G_l^i(\sigma)\frac{\partial}{\partial q^i} + T_{,l}(\sigma,0)\frac{\partial}{\partial t}, \quad \forall \sigma \in \Sigma_w, \tag{5.5}$$

for $l = \{1,2,\ldots,k\}$. (On $M_+^{3,1}$, we have $k = 10$.)

The isotropy group of $m = (R,0,0,0,0)$ contains as a subgroup the group SO(3) of rotations around the u axis, leaving the hypersurface H_w invariant. We write $\{\xi_1,\xi_2,\xi_3\}$ for the corresponding generators and notice that

$$[\xi_l,\xi_4] = 0, \quad \text{for } l = 1,2,3, \tag{5.6}$$

and

$$T_{,l}(\sigma,0) = 0, \quad \text{for } l = 1,2,3, \forall \sigma \in \Sigma_w. \tag{5.7}$$

Using (4.3), (4.4), (4.9), (4.10), (5.6), and (5.7) we have

$$(\xi_l)_{T\Sigma_w} = G_l^i\frac{\partial}{\partial q_i} + (G_l^i)_{,j}\dot{q}_j\frac{\partial}{\partial \dot{q}_i}, \quad \text{for } l = 1,2,3. \tag{5.8}$$

For the $\dot{q}_l$ component of $[(\xi_l)_{T\Sigma_w}, (\xi_4)_{T\Sigma_w}](q,\dot{q}) = 0$ at $(q,\dot{q}) = (0,0)$, we have, summing over $j \in \{1,2,3\}$,

$$-(G_l^i),_j(0)A_j(0,0)=0, \quad i=1,2,3, \tag{5.9}$$

where we used $(G_l^i)(0)=0$ since the ξ_l are generators of the isotropy group of m. Finally, as the three matrices $(G_1^i),_j(0), (G_2^i),_j(0), (G_3^i),_j(0)$ form an irreducible representation of the SO(3) Lie algebra on $T_m\Sigma_w$, (5.4) immediately follows from (5.9).

This concludes the proof of our assertion that, on de Sitter space-time $M_+^{3,1}$, particle motion is necessarily geodesic.

Notice that, upon taking the limit for R to ifinity in (5.2), the isometry group of $M_+^{3,1}$ contracts to the Poincaré group. In this sense we can recover the original no-interaction theorem on Minkowski space-time as a limiting case. Notice, however, that the Poincaré group similarly contracts to the Galilei group, but that the no-interaction theorem no longer holds in the limit! This illustrates the crucial role played by condition (iv) in obtaining the conclusion of Theorem 4.1.

We finally consider the Einstein static universe. This is a homogeneous space-time with a seven-dimensional isometry group. The isotropy group is three dimensional and leaves a preferred ("cosmic") time direction invariant. For an observer traveling with the substratum, the theorem therefore does not apply; other observers can be chosen, however, such that it does! This brings about the peculiar situation that, depending on the choice of observer, interaction can or cannot be described by the Hamiltonian formalism outlined in this paper. This situation is reminiscent of the situation in quantum field theory on curved space-times, where the choice of observer also can be of crucial importance.[9]

Finally, we remark that the proof of the theorem given here makes implicit use of the Lagrange two-form on TQ_w. For the flat case, this has been exploited further recently by several authors[10]: their results also carry over to the general case considered in this paper.

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Simple subgroups of simple Lie groups and nonlinear differential equations with superposition principles

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Nonlinear ordinary differential equations admitting a superposition principle based on the action of the group SL(*n*,C) on the homogeneous spaces SL(*n*,C)/O(*n*,C) and SL(*n*,C)/Sp(*n*,C) are derived. The superposition formulas are presented explicitly. In the O(*n*,C) case the general solution is expressed in terms of three particular solutions (for any *n*). For the Sp(*n*,C) case three solutions are needed for $n = 2k \geq 8$, four solutions for $n = 6$, and five solutions for $n = 4$.

I. INTRODUCTION

Almost exactly one hundred years ago Lie showed that certain systems of n ordinary differential equations, not necessarily linear ones, admit a "nonlinear superposition principle." That is to say, their general solution can be expressed in terms of a finite number m of particular solutions and n constants.[1,2] For $n = 1$ [one ordinary differential equation (ODE)] only one nontrivial, i.e., nonlinear, equation of this type exists, namely the Riccati equation

$$\dot{y} = a(t) + b(t)y + c(t)y^2 . \tag{1.1}$$

It is well known that the general solution of this equation can be expressed algebraically (but not linearly) in terms of three particular solutions. The Riccati equation is quite important in many branches of physics. In particular it figures in Bäcklund transformations for such important integrable partial differential equations as the Korteweg–de Vries equation, the sine–Gordon equation, the nonlinear Schrödinger equation, and many others.[3,4]

For systems of $n \geq 2$ nonlinear ordinary differential equations the situation is much richer. Indeed, a system of ODE's with a superposition formula can be associated with every group–subgroup pair $G \supset G_0$. The system of equations will be nonlinear if the action of the group G on the homogeneous space $M \sim G/G_0$ is nonlinear. The number of equations is

$$n = \dim G - \dim G_0 , \tag{1.2}$$

where G_0 is the isotropy group of the origin in M. The equations can be obtained by introducing local coordinates $(x^1,..., x^n)$ in the neighborhood of the origin on M and expressing the elements of the Lie algebra L of G as vector fields

$$\hat{\xi}_i = f_i^{\mu}(x^1,..., x^n)\frac{\partial}{\partial x^{\mu}}, \quad i = 1,..., r , \tag{1.3}$$

where r is the dimension of the Lie algebra. The corresponding ODE's are

$$\dot{x}^{\mu} = \sum_{i=1}^{r} Z_i(t) f_i^{\mu}(x^1,..., x^n) , \tag{1.4}$$

where $Z_i(t)$ are arbitrary functions of t. Conversely, a system of ODE's

$$\dot{x}^{\mu} = f^{\mu}(x^1,..., x^n, t) , \tag{1.5}$$

will allow a superposition formula, precisely if (1.5) has the form (1.4) and the vector fields (1.3) generate a finite dimensional Lie algebra with respect to the usual commutator bracket.[2] The superposition formula itself can be written as the mapping

$$\mathbf{x}(t) = \mathbf{S}(\mathbf{x}_1(t),..., \mathbf{x}_m(t), \mathbf{a}) , \tag{1.6}$$

where $\mathbf{x}_1(t),..., \mathbf{x}_m(t)$ are particular solutions of (1.4) and $\mathbf{a}$ is a constant vector related to the initial conditions. The vector function $\mathbf{S}$ can be explicitly calculated for each equation of the considered type.

The problem that arises is twofold: (1) to classify all systems of ODE's with superposition formulas, and (2) to obtain the superposition formula (1.6) in each case.

A series of recent publications has been devoted to the above problem.[5–11] In particular, it has been shown[11] that an additional requirement, namely that the system of ODE's (1.4) be "indecomposable," implies that the action of the group G on the space $M \sim G/G_0$ should not only be transitive, but also primitive.[12–15] Indecomposability in this case means that it is not possible to introduce coordinates on M in such a manner that a subset of the equations (1.4) splits off and has a superposition law of its own. This would occur if the space M allowed an invariant foliation. For details see Ref. 11, where the classification of indecomposable systems of equations with superposition laws is reduced to a classification of transitive primitive Lie algebras[11–15] (L, L_0).

Much of the previous work concentrated on the case where L [the Lie algebra of the vector fields (1.3)] is simple, and L_0 (the subalgebra of vector fields vanishing at the origin) is a maximal parabolic algebra.

The purpose of this article is to start a systematic treatment of the most complicated case, when L is again simple, but L_0 is a maximal reductive subalgebra (i.e., L_0 is the direct sum of one or more simple Lie algebras and possibly of an Abelian Lie algebra). More specifically, we analyze the ODE's related to two series of homogeneous spaces, namely SL(*n*,C)/SO(*n*,C) and SL(2*n*,C)/Sp(2*n*,C).

In Sec. II we discuss the construction of these homogeneous spaces and the action of G on G/G_0 (in several different manners). In Sec. III we present the corresponding ODE's

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explicitly. The superposition formula for both cases is obtained in Sec. IV. Section V is devoted to low-dimensional examples where special features occur. The conclusions and perspectives for future work are outlined in the final section, Sec. VI.

II. REALIZATIONS OF HOMOGENEOUS SPACES

In order to construct the systems of ODE's (1.4) associated with a homogeneous space $M \sim G/G_0$, we need a specific and explicit realization of this space. This can be achieved by a direct construction of the left cosets gG_0.[16] The action of G on G/G_0 is given in terms of a section of the homogeneous space. The vector fields $\hat{\xi}_i$ of (1.3) are invariant with respect to the choice of a section s of G/G_0 on G. Hence Eqs. (1.4), which can be written as

$$\frac{dx^\mu}{dt} = \sum_{i=1}^{r} Z_i(t)\hat{\xi}_i \cdot x^\mu , \tag{2.1}$$

are also invariant under changes of section.

The explicit construction of G/G_0 and of the action of G may involve considerable algebraic complications. The remainder of this section is devoted precisely to this problem, concentrating on the case when the group G is $SL(n,F)$ (with $F = \mathbb{R}$ or $\mathbb{C}$) and the subgroup G_0 leaves a nondegenerate symmetric or skew-symmetric bilinear form K invariant.

A. The direct construction of G/G_0

Let G be a simple Lie group and G_0 a maximal reductive subgroup of G (i.e., G_0 can be a simple Lie group, the direct product of several simple Lie groups, or the direct product of one or more simple Lie groups with an Abelian group). We consider the homogeneous space G/G_0, i.e., the set of left cosets gG_0, $g \in G$. The action of G on G/G_0 is, by assumption, primitive, i.e., there does not exist an invariant foliation of G/G_0. This is assured by the maximality of G_0 in G (see Ref. 15).

If we take a continuous local section

$$s: G/G_0 \to G , \tag{2.2}$$

we obtain a decomposition of the elements of G

$$g = s(gG_0)\gamma(g) , \tag{2.3}$$

where γ is a local map from G into G_0. The transitive left action of G on G/G_0 is defined by

$$G \times G/G_0 \to G/G_0, \quad (g,x) \to gx .$$

In terms of the section s we can write

$$s(gx) = gs(x)[\gamma(gs(x))]^{-1} , \tag{2.4}$$

having made use of (2.2) to decompose $gs(x)$ as

$$gs(x) = s(gx)\gamma(gs(x)) .$$

We must now choose a local section s and determine $s(gx)$, i.e., specify $\gamma(gs(x))$. This is often quite difficult, but once $s(gx)$ is known it is quite straightforward to calculate the vector fields $\hat{\xi}_i(x)$ and hence Eq. (2.1). The variables x^μ are then coordinates in some appropriate chart on G/G_0.

Two different local sections of G/G_0, say s and s', are related by

$$s'(x) = s(x)\delta(x) , \tag{2.5}$$

where $\delta: G/G_0 \to G_0$ is a continuous local map. The vector fields are invariant under (2.5). We shall work with normalized sections, i.e., put

$$s(eG_0) \equiv s(x_0) = e .$$

Let us now restrict ourselves to the case of interest for this article, namely let G act linearly on F^n (with $F = \mathbb{R}$, or $F = \mathbb{C}$) and let G_0 be the subgroup of G leaving a nondegenerate symmetric or skewsymmetric bilinear form invariant

$$G_0 = \{ g \in G \mid gKg^T = K \}, \quad \det K \neq 0,$$
$$K = \rho K^T, \quad \rho = \pm 1 . \tag{2.6}$$

Here, K is the matrix of the bilinear form in some chosen basis.

Since $\gamma(gs(x)) \in G_0$, we have

$$\gamma(gs(x))K[\gamma(gs(x))]^T = K .$$

Using (2.4) we can write

$$[s(gx)]^{-1}gs(x)K[[s(gx)]^{-1}gs(x)]^T = K .$$

From here we obtain

$$s(gx)K[s(gx)]^T = gs(x)K[gs(x)]^T .$$

Defining

$$W \equiv s(x)K[s(x)]^T , \tag{2.7}$$

we obtain

$$W' = gWg^T , \tag{2.8}$$

where we have

$$W' \equiv s(gx)K[s(gx)]^T .$$

Notice that if K is symmetric (skew symmetric) then the same holds for W:

$$W = \rho W^T .$$

Note also that W is not a section.

Relation (2.8) realizes the action of G on G/G_0, i.e., W provides a coordinate patch for this space. This will prove to be very useful below, where G_0 will be chosen to be $SO(n,\mathbb{C})$ or $Sp(2n,\mathbb{C})$.

The differential equations (2.1) associated with the action (2.8) are given by

$$\dot{W} = AW + WA^T , \tag{2.9}$$

where $A(t)$ is an element of the Lie algebra of the group G. The equations are thus linear, however, in general W will be subject to nonlinear constraints.

B. Homogeneous spaces via Lie algebra

There are many ways of choosing the section s and, as a consequence, W. Let us discuss now a special section associated with the decomposition of the Lie algebra of G.

Let L and L_0 be the Lie algebras of G and G_0 respectively, and consider the direct sum decomposition of L as a vector space[14]:

$$L = L_0 \dot{+} L_1 \tag{2.10}$$

where L_1 is a subspace of L. In the cases we will treat below, this is always possible, in view of (2.6). The definitions of L_0 and L_1 are

$$L_0 = \{ A \in L \mid AK + KA^T = 0 \} , \tag{2.11}$$

$$L_1 = \{A \in L \mid AK - KA^T = 0\}\,. \tag{2.12}$$

It is easy to show that the sum is a direct one and that the following properties are true:

$$[L_0, L_0] \subseteq L_0, \quad [L_0, L_1] \subseteq L_1, \quad [L_1, L_1] \subseteq L_0\,.$$

The subspaces L_0 and L_1 are orthogonal with respect to the Killing form of L. The decomposition (2.10) is related to the existence of an involutive automorphism θ of L,

$$\theta(A) = -KA^T K^{-1}\,,$$

L_0 and L_1 are identified with the eigenspaces of eigenvalues $+1$ and -1, respectively, and L is a Z_2-graded Lie algebra.

It is also interesting to remark that this decomposition corresponds to a splitting of L into two parts, symmetric and skew symmetric with respect to the metric given by K, that is,

$$A_a = (A - KA^T K^{-1})/2, \quad A_s = (A + KA^T K^{-1})/2\,,$$

and $A_s K = (A_s K)^T$, $A_a K = -(A_a K)^T$. Then $L_0 = \{A_a\}$ and $L_1 = \{A_s\}$. Using known properties of Lie groups and Lie algebras, we can construct a continuous local section s given by the exponential of L_1. Its existence is due to the isomorphism between L_1 and the tangent space at the point $x_0 \equiv eG_0$ of G/G_0 [We have a local chart at x_0, (V_{x_0}, ψ) such that, $\psi: V_{x_0} \to U \subset \mathbb{R}^n$ and $\mathbb{R}^n$ is isomorphic to $T_{x_0}(G/G_0)$]; that is, for every $X \in L_1$, $\exp(X)$ belongs to G and evidently, to a coset of G/G_0, so that we choose $\exp(X)$ as the representative of this coset. [It is easily shown that if X and Y belong to L_1 and $\exp(X)$, and $\exp(Y)$ are in the same coset, then $X = Y$.]

The matrix W of (2.7) is now

$$W = \exp(X) K \exp(X)^T = \exp(2X)\,, \tag{2.13}$$

because $X \in L_1$ and $XK = KX^T$ (2.12). If we define $Y \equiv 2X$, the action of G on G/G_0 is given by (2.8):

$$\exp(Y') = g \exp(Y) g^T\,. \tag{2.14}$$

It is not always easy to calculate $\exp(Y)$.

C. Homogeneous spaces via maximal parabolic subgroups and Grassmannians

If the isotropy subgroup is a maximal parabolic one (defined, for $F = \mathbb{C}$, as a maximal subgroup of G containing the maximal solvable subgroup), then the corresponding homogeneous space is easily realized as a Grassmannian of k-dimensional planes in some higher-dimensional linear space. In some cases, when G is simple and G_0 reductive, use can be made of certain diffeomorphisms, given by Kobayashi and Nagano,[14] to reduce the construction of G/G_0 to that of a Grassmannian.

This is possible if there exists a group $\tilde{G}$, such that G is a subgroup of $\tilde{G}$ and G_0 is the intersection of G with some maximal parabolic subgroup $P \subset \tilde{G}$. We then have

$$G/G_0 \approx \tilde{G}/P, \quad G_0 = G \cap P\,. \tag{2.15}$$

The following diffeomorphisms were established for $F = \mathbb{R}$:

$$\mathrm{Sp}(2n,\mathbb{R})/P \approx \mathrm{U}(n)/\mathrm{O}(n)\,, \tag{2.16}$$

$$\mathrm{SO}^*(4n)/P \approx \mathrm{U}(2n)/\mathrm{Sp}(2n)\,, \tag{2.17}$$

where P is the corresponding parabolic subgroup in each case. Note that the pairs appearing in the Kobayashi–Nagano list are given up to a local group isomorphism. If we complexify the relations (2.16) and (2.17) we get

$$\mathrm{Sp}(2n,\mathbb{C})/P \approx \mathrm{GL}(n,\mathbb{C})/\mathrm{O}(n,\mathbb{C})\,,$$

$$\mathrm{SO}(4n,\mathbb{C})/P \approx \mathrm{GL}(2n,\mathbb{C})/\mathrm{Sp}(2n,\mathbb{C})\,,$$

where P is again the appropriate complexified parabolic subgroup.

Let us consider the first case; the second has been recently studied in some detail.[11]

The group $\mathrm{Sp}(2n,\mathbb{C})$ can be defined by

$$\mathrm{Sp}(2n,\mathbb{C}) = \{g \in \mathrm{SL}(2n,\mathbb{C}):\ gKg^T = K\} \tag{2.18}$$

where K is given by

$$K = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \tag{2.19}$$

(I is the $n \times n$ identity matrix).

We want to give a particular realization of $\mathrm{GL}(n,\mathbb{C})$, $\widetilde{\mathrm{GL}}(n,\mathbb{C})$, as a subgroup of $\mathrm{Sp}(2n,\mathbb{C})$ with the property

$$\tilde{\mathrm{O}}(n,\mathbb{C}) = \widetilde{\mathrm{GL}}(n,\mathbb{C}) \cap P\,, \tag{2.20}$$

where $\tilde{\mathrm{O}}(n,\mathbb{C})$ is a particular imbedding of $\mathrm{O}(n,\mathbb{C})$ into $\mathrm{Sp}(2n,\mathbb{C})$ and P is a maximal parabolic subgroup of $\mathrm{Sp}(2n,\mathbb{C})$.

To give an explicit form to the subgroup P, we make use of the $\mathrm{Sp}(2n,\mathbb{C})$ action over a submanifold of $G_n(\mathbb{C}^{2n})$, the Grassmannian of n-planes in $\mathbb{C}^{2n}$. While $\mathrm{Sp}(2n,\mathbb{C})$ does not act transitively on $G_n(\mathbb{C}^{2n})$, it does so on the isotropic n-plane manifold $G_n^0(\mathbb{C}^{2n})$:

$$G_n^0(\mathbb{C}^{2n}) = \left\{ \begin{pmatrix} X \\ Y \end{pmatrix}:\ X, Y \in \mathbb{C}^{n\times n},\ X^T Y - Y^T X = 0 \right\}, \tag{2.21}$$

$\binom{X}{Y}$ are homogeneous coordinates in $G_n(\mathbb{C}^{2n})$.

The isotropy group of the point $x_0 = \binom{0}{I}$ in $G_n^0(\mathbb{C}^{2n})$ is a maximal parabolic subgroup[17] of $\mathrm{Sp}(2n,\mathbb{C})$ and is given by

$$P = \left\{ \begin{bmatrix} g_{11} & 0 \\ g_{21} & g_{22} \end{bmatrix} \in \mathrm{Sp}(2n,\mathbb{C}) \right\},$$

where $g_{ij} \in \mathbb{C}^{n\times n}$.

The most obvious way of realizing $\mathrm{GL}(n,\mathbb{C})$ as a subgroup of $\mathrm{Sp}(2n,\mathbb{C})$ is

$$g \in \mathrm{GL}(n,\mathbb{C}) \to \begin{bmatrix} g & 0 \\ 0 & (g^T)^{-1} \end{bmatrix} \in \widetilde{\mathrm{GL}}(n,\mathbb{C}) \subset \mathrm{Sp}(2n,\mathbb{C})\,. \tag{2.22}$$

This is, however, not the correct realization, since we have $\widetilde{\mathrm{GL}}(n,\mathbb{C}) \subset P$ and hence (2.20) is not satisfied. If we conjugate (2.22) by a matrix

$$g_0 = \begin{bmatrix} I & I \\ 0 & I \end{bmatrix}, \tag{2.23}$$

preserving the chosen form of K (2.19), but shifting the origin to $\binom{I}{I} = g_0 \binom{0}{I}$, we obtain a different realization of $\mathrm{GL}(n,\mathbb{C})$, namely

$$\widetilde{\mathrm{GL}}(n,\mathbb{C}) = g_0^{-1}\, \widetilde{\mathrm{GL}}(n,\mathbb{C}) g_0$$

$$= \left\{ \begin{bmatrix} g & g - (g^T)^{-1} \\ 0 & (g^T)^{-1} \end{bmatrix},\ g \in \mathrm{GL}(n,\mathbb{C}) \right\}. \tag{2.24}$$

With this realization of $\mathrm{GL}(n,\mathbb{C})$ we find that (2.20) is satisfied, i.e., $\tilde{\mathrm{O}}(n,\mathbb{C})$ is obtained as the intersection of $\widetilde{\mathrm{GL}}(n,\mathbb{C})$

and P. Here, $\tilde{O}(n,\mathbb{C})$ is a particular choice of $O(n,\mathbb{C})$ as a subgroup of $Sp(2n,\mathbb{C})$. In fact,

$$\tilde{O}(n,\mathbb{C}) = \left\{ \begin{bmatrix} g & 0 \\ 0 & (g^T)^{-1} \end{bmatrix} : g \in O(n,\mathbb{C}) \right\} . \tag{2.25}$$

The action of $\tilde{GL}(n,\mathbb{C})$ on $G_n^0(\mathbb{C}^{2n})$ is

$$\tilde{g}\begin{pmatrix} X \\ I \end{pmatrix} = \begin{bmatrix} gX + g - (g^T)^{-1} \\ ((g^T)^{-1} \end{bmatrix} \sim \begin{bmatrix} gXg^T + g\,g^T - I \\ I \end{bmatrix}, \tag{2.26}$$

in a neighborhood of the point x_0; we have $X = X^T$ (2.21).

The action of $\tilde{GL}(n,\mathbb{C})$ is transitive and in particular, acting on the origin, we have (locally)

$$\begin{pmatrix} X \\ I \end{pmatrix} = \tilde{g}\begin{pmatrix} 0 \\ I \end{pmatrix} = \begin{bmatrix} g\,g^T - I \\ I \end{bmatrix}, \tag{2.27}$$

so that $X = X^T$.

The isotropy group of x_0 [when one considers the $\tilde{GL}(n,\mathbb{C})$ action] is evidently $\tilde{O}(n,\mathbb{C})$.

We want to find the $SL(n,\mathbb{C})$ action so that we must impose the constraint $\det g = 1$. The isotropy group of x_0 is $SO(n,\mathbb{C})$ [a realization of $SO(n,\mathbb{C})$ as given in (2.25)], and the orbit of x_0 is (2.27), with the condition $g \in SL(n,\mathbb{C})$. As a consequence,

$$\det (X + I) = 1. \tag{2.28}$$

The differential equations corresponding to the action of $SL(n,\mathbb{C})$ are obtained from the concrete realization (2.24) and its Lie algebra

$$\begin{bmatrix} \dot{X} \\ \dot{Y} \end{bmatrix} = \begin{bmatrix} A & A + A^T \\ 0 & -A^T \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix}, \tag{2.29}$$

where $A \in sl(n,\mathbb{C})$, that is $\operatorname{tr} A = 0$.

If we use affine coordinates $\hat{W} = XY^{-1}$ (in a neighborhood of the point x_0) we get

$$\dot{\hat{W}} = A\hat{W} + \hat{W}A^T + A + A^T,$$

or, calling $W = \hat{W} + I$,

$$\dot{W} = AW + WA^T, \tag{2.30}$$

with constraints coming from (2.21) and (2.28):

$$W = W^T, \tag{2.31}$$

$$\det W = 1 . \tag{2.32}$$

The case $SL(2n,\mathbb{C})/Sp(2n,\mathbb{C})$ was treated earlier[11] in a similar way and lead to the same equation with different constraints, given (after some trivial changes) by

$$\dot{W} = AW + WA^T, \tag{2.33}$$

$$W^T = -W, \tag{2.34}$$

$$\det W = 1 . \tag{2.35}$$

The same equation was obtained above [see formula (2.9)] by a different method. There we have $W = s(x)K[s(x)]^T$ [see (2.7)] so that if $G = SL(n,\mathbb{C})$ and $G_0 = SO(n,\mathbb{C})$, K is a symmetric matrix and $W = W^T$ (and $\det W = 1$). If $G = SL(2n,\mathbb{C})$ and $G_0 = Sp(2n,\mathbb{C})$, K is skew symmetric and $W = -W^T$ (and $\det W = 1$).

III. EXPLICIT FORM OF THE DIFFERENTIAL EQUATIONS

In Sec. II we found the general form (2.9) of the differential equations, independently of the local section or the parametrization of the group. We will now give an explicit form of these equations, related to concrete choices for the section and the parametrization.

A. $SL(n,\mathbb{C})/SO(n,\mathbb{C})$

In this case the equations are

$$\dot{W} = AW + WA^T, \quad \operatorname{Tr} A = 0, \quad W = W^T, \quad \det W = 1 . \tag{3.1}$$

The constraint $\det W = 1$ can be eliminated if we solve for one of the matrix elements of W, for instance w_{nn},

$$w_{nn} = \frac{1 - \sum_{j=1}^{n-1} w_{nj}\hat{W}_{nj}}{\hat{W}_{nn}}, \tag{3.2}$$

where $\hat{W}_{ij}$ is the determinant (with the appropriate sign) of the matrix adjoint to the element w_{ij}. In this way (3.1) yields

$$\dot{w}_{ij} = \sum_{k=1}^{n} (a_{ik}w_{kj} + a_{jk}w_{ik}), \quad \text{if } 1 \leqslant j \leqslant i \leqslant n-1, \tag{3.3a}$$

$$\dot{w}_{nj} = \sum_{k=1}^{n} a_{nk}w_{kj} + \sum_{k=1}^{n-1} a_{jk}w_{nk} + a_{jn}\frac{1 - \sum_{j=1}^{n-1} w_{nj}\hat{W}_{nj}}{\hat{W}_{nn}}, \tag{3.3b}$$

$$\text{if } j = 1,\ldots, n-1.$$

The nonlinear term in (3.3a) can be further simplified by using a specific section. In particular if we use the section

$$s:\ \mathrm{SL(n,\mathbb{C})}/SO(n,\mathbb{C}) \to SL(n,\mathbb{C}),$$
$$x \to s(x),$$

where $s(x)$ is a lower triangular matrix with determinant equal to one, that is

$$s(x)_{ij} = x_{ij}, \quad \text{if } i \geqslant j, \quad s(x)_{ij} = 0, \quad \text{if } i < j,$$
$$x_{11}\cdots x_{nn} = 1 . \tag{3.4}$$

(It can be easily shown that this is a continuous local section.) The system of differential equations is given in a recurrent way by

$$\dot{x}_{ij} = \frac{1}{x_{jj}}\left\{ h_{ij} - (1 - \delta_{ij}) \sum_{k=1}^{j} x_{ik}\dot{x}_{jk} - \sum_{k=1}^{j-1} x_{jk}\dot{x}_{ik} \right\},$$
$$j \leqslant i, \quad 1 \leqslant j \leqslant n-1, \quad 1 \leqslant i \leqslant n, \tag{3.5}$$

where

$$h_{ij} = \sum_{l=1}^{j} x_{jl} \sum_{k=l}^{n} a_{ik}x_{kl} + (1 - \delta_{ij}) \sum_{l=1}^{i} x_{il} \sum_{\kappa=l}^{n} a_{jk}x_{kl}, \quad i \geqslant j . \tag{3.6}$$

B. $SL(2n,\mathbb{C})/Sp(2n,\mathbb{C})$

As in the previous case we can express one of the functions appearing in W as a function of the other w_{ij}, using the constraint $\det W = 1$. However, in this case W is a skew-symmetric matrix, and we choose to solve for $w_{n,n-1}$ (which is equal to $-w_{n-1,n}$).

The determinant of a skew-symmetric matrix of even dimension can be written as the square of an expression in the matrix elements,

$$\det W = \left[\sum_{j=1}^{n-1} w_{nj}\tilde{W}_{nj}\right]^2 = 1\,. \tag{3.7}$$

We can obtain equations with rational nonlinearities by taking, for instance, the positive root:

$$w_{nn-1} = \frac{1 - \Sigma_{j=1}^{n-2} w_{nj}\tilde{W}_{nj}}{\tilde{W}_{n,n-1}}\,. \tag{3.8}$$

The expressions $\tilde{W}_{nj}$ are determinants of the matrices (as in the previous case, with a sign $+$ or $-$, depending on the position of w_{nj}) obtained by removing from the matrix W two rows and two columns, containing the elements w_{nj} and $w_{jn}(=-w_{nj})$. The equations can then be written in the same way (see Eq. 3.3), as in the orthogonal case (now $i>j$, because W is skew symmetric), with the appropriate interpretation of $\tilde{W}_{nj}$.

We can always use a particular section to write the equations. For instance,

$$\text{s: } \mathrm{SL}(2n,\mathbb{C})/\mathrm{Sp}(2n,\mathbb{C}) \to \mathrm{SL}(2n,\mathbb{C})\,,$$

$$x \to s(x)\,,$$

where $s(x)$ is a lower triangular 2×2 block matrix and the blocks on the diagonal are multiples of the 2×2 identity matrix:

$$s_{ij}(x) = X_{ij} \in \mathbb{C}^{2\times 2}\,, \quad i>j\,,$$

$$s_{ij}(x) = 0, \qquad i<j,$$

$$s_{ii}(x) = x_{ii}I, \qquad i = 1,\ldots, n.$$

Equations (2.9) are now constructed in the following way:

$$W = s(x)Ks(x)^T\,,$$

with

$$K = \begin{bmatrix} J & & \\ & \ddots & \\ & & J \end{bmatrix}, \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

We consider W as consisting of 2×2 matrices W_{ij}. Then

$$W_{ij} = \sum_{k=1}^{j} X_{ik}\,JX_{jk}^T\,, \quad i\geqslant j\,, \tag{3.9}$$

and the system is given in a recurrent form by

$$\dot{X}_{ij} = \frac{1}{(1+\delta_{ij})x_{ii}}\left\{\sum_{k=1}^{j-1}\dot{X}_{ik}\,JX_{jk}^T + \sum_{k=1}^{j-1} X_{ik}\,J\dot{X}_{jk}^T + (1-\delta_{ij})X_{ij}\,J\dot{X}_{jj}^T - H_{ij}\right\}J, \quad i\geqslant j\,, \tag{3.10}$$

where

$$H_{ij} = \sum_{l=1}^{j}\sum_{k=l}^{n} A_{ik}X_{kl}\,JX_{jl}^T + \sum_{l=1}^{i}\sum_{k=l}^{n} X_{il}\,JX_{kl}^T A_{jk}^T\,. \tag{3.11}$$

Note that the particular sections taken in these paragraphs correspond to a neighborhood of the point $x_{ij}=0$, $i>1$, $x_{ii}=1$, $i=1,\ldots,n-1$. If we want to work with the origin, $x_{ij}=0$, we should make a translation in the x_{ii} coordinates, $x_{ii}\to x_{ii}-1$.

IV. THE SUPERPOSITION FORMULAS

The general solution of the system of equations (2.1) is given by[6]

$$\mathbf{x}(t) = g(t)\mathbf{x}(t_0)\,, \tag{4.1}$$

where $g(t)$ is a curve in the group G, the solution of the equation

$$\frac{dg(t)}{dt}g^{-1}(t) = \sum_{i=1}^{n} Z_i(t)\hat{\xi}_i\,,$$

with some initial condition $g(t_0)=g_0$.

Our aim is to construct $g(t)$ from a finite number m of particular solutions of Eqs. (2.1), $\mathbf{x}_k(t)$, $k=1,\ldots,m$, with initial conditions $\mathbf{x}_k(t_0)$. The number m is determined as the smallest number of initial conditions for which the joint isotropy group is the identity group only. Such a minimal set of solutions, satisfying certain independence conditions is called a fundamental set of solutions.

Solving the equations

$$\mathbf{x}_k(t) = g(t)\mathbf{x}_k(t_0), \quad k=1,\ldots,m\,, \tag{4.2}$$

for $g(t)$, we obtain the expression for g as a function of $\mathbf{x}_k(t)$ and substituting into (4.1), the general solution for our system (2.1). For more details see Refs. 6 and 7.

We shall obtain the superposition formulas for the two cases we have studied above.

A. SL(n,C)/SO(n,C)

The equations in this case are given by (2.9)

$$\dot{W}(t) = A(t)W(t) + W(t)A^T(t)\,, \tag{4.3a}$$

with the constraints

$$W(t) = W(t)^T, \quad \det W(t) = 1, \quad \mathrm{Tr}\,A(t) = 0. \tag{4.3b}$$

The general solution can hence be written in the form (2.8)

$$W(t) = g(t)W(t_0)[g(t)]^T\,, \tag{4.4}$$

with

$$\det g(t) = 1, \quad W(t_0) = [W(t_0)]^T, \quad \det W(t_0) = 1,$$

where $g(t)\in\mathrm{SL}(n,\mathbb{C})$ is a curve in the group manifold to be determined in terms of a fundamental set of particular solutions.

Let us first show that a fundamental set of solutions in this case consists of three generically chosen particular solutions.

Theorem 1: A fundamental set of solutions of Eqs. (4.3) consists of three particular solutions $W_i(t)$ $(i=1,2,3)$ with initial conditions satisfying the following.

(i) $W_i(t_0) = W_i^T(t_0)$, $\det W_i(t_0) = 1$.

(ii) The matrix $W_1(t_0)$ has all eigenvalues distinct.

(iii) The matrix $Q_2(t_0) = W_2(t_0)W_1^{-1}(t_0)$ has all eigenvalues distinct.

(iv) The matrices $Q_2(t_0)$ and $Q_3(t_0) = W_3(t_0)W_1^{-1}(t_0)$ have no common nontrivial invariant eigenspaces.

Proof: We must show that the joint isotropy group of $W_i(t_0)$ in $\mathrm{SL}(n,\mathbb{C})$ is $G_I = I$. Notice, first of all, that two elements $\pm g(t)$ must be identified, since they produce the same $W(t)$ in (4.4). For n odd this is imposed by the requirement $\det g(t) = 1$, for n even we impose a consistent choice of sign

by continuity. In view of the group condition in (4.4) we can replace the initial conditions $W_i(t_0)$, with no loss of generality, by

$$W_i(t_0) = h\, W_i(t_0) h^T, \tag{4.5}$$

where $h \in SL(n,\mathbb{C})$ is a constant matrix. Put $h = R_1 D R_2$, where $R_2 \in O(n,\mathbb{C})$ diagonalizes $W_1(t_0)$, $D = \mathrm{diag}(1/\sqrt{\lambda_1}, \ldots, 1/\sqrt{\lambda_n})$, where λ_i are the eigenvalues of $W_1(t_0)$, and $R_1 \in O(n,\mathbb{C})$ is an arbitrary orthogonal matrix. We then have

$$\begin{aligned} &\tilde{W}_1(t_0) = I \\ &\tilde{W}_a(t_0) = R_1 D R_2 W_a(t_0) R_2^T D R_1^T \\ &\qquad = R_1 D R_2 W_a(t_0) [W_1(t_0)]^{-1} R_2^{-1} D^{-1} R_1^{-1}, \\ &\qquad a = 2, 3 . \end{aligned} \tag{4.6}$$

Conditions (i) and (ii) allowed us to transform $W_1(t_0)$ into I; conditions (iii) and (iv) make it possible to choose R_1 such that

$$\tilde{W}_2(t_0) = \Lambda, \quad \tilde{W}_3(t_0) = \Omega, \tag{4.7}$$

where Λ is a diagonal matrix with all eigenvalues distinct, and $\tilde{W}_3(t_0)$ is a matrix corresponding to a connected graph. (That is, if we draw a graph with n vertices, labeled 1,..., n, and connect two points, i and k, whenever $\Omega_{ik} = \Omega_{ki} \neq 0$, then we obtain a connected graph.) Let us now determine the isotropy group of the triplet $\{I,\Lambda,\Omega\}$. The condition $gIg^T = I$ implies $g \in O(n,\mathbb{C})$; $g\Lambda g^T = \Lambda$ implies further that g is a diagonal matrix, hence $g_{ik} = \pm \delta_{ik}$. Finally, the condition $g\Omega g^T = \Omega$ implies $g = \pm I$. Q. E. D.

Let us now obtain the superposition formula explicitly, i.e., express $g(t)$ in terms of three solutions $W_i(t)$, satisfying the conditions of Theorem 1. With no loss of generality we can choose these solutions to satisfy

$$W_1(t_0) = I, \quad W_2(t_0) = \Lambda, \quad W_3(t_0) = \Omega, \tag{4.8}$$

with Λ and Ω as in (4.7), in particular $\Lambda = \mathrm{diag}(\lambda_1,\ldots,\lambda_n)$, $\lambda_i \neq \lambda_k$ for $i \neq k$.

Let us represent $g(t) \in SL(n,\mathbb{C})$ as the product of four matrices

$$g(t) = R_1(t) D(t) R_2(t) E(t), \tag{4.9}$$

where R_1 and R_2 are orthogonal, D and E are diagonal, and the eigenvalues of E are all equal to ± 1. In view of (4.4) we have

$$W_1(t) = R_1(t) D^2(t) R_1(t)^T, \tag{4.10}$$

so that

$$D = \mathrm{diag}(\sqrt{\lambda_1(t)},\ldots,\sqrt{\lambda_n(t)}), \tag{4.11}$$

where $\lambda_i(t)$ are the eigenvalues of $W_1(t)$, and $R_1(t) \in SO(n,\mathbb{C})$ is a matrix diagonalizing $W_1(t)$. The matrix D is made unique by choosing an ordering, say $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$; $R_1(t)$ is made unique say by choosing the first nonzero element in each column to be positive for all t. Further, we have

$$\tilde{W}_2(t) \equiv D^{-1} R_1^T W_2(t) R_1 D^{-1} = R_2(t) \Lambda R_2(t)^T, \tag{4.12}$$

i.e., $R_2(t) \in SO(n,\mathbb{C})$ diagonalizes $\tilde{W}_2(t)$ and is made unique by an appropriate choice of signs in each column. Finally we have

$$\tilde{W}_3(t) = R_2^T D^{-1} R_1^T W_3(t) R_1 D^{-1} R_2 = E\, \Omega\, E^T. \tag{4.13}$$

We have $E = \mathrm{diag}(\epsilon_1,\ldots,\epsilon_n)$, $\epsilon_i = \pm 1$ and (4.13) is equivalent to a set of linear algebraic equations for ϵ_i,

$$\tilde{W}_3 E = E\, \Omega, \tag{4.14}$$

determining ϵ_i uniquely up to an irrevelant overall sign.

B. SL(2n,C)/Sp(2n,C), n⩾2

The equations in this case are again given by (4.3a) but the constraints are

$$W(t) = -W^T(t), \quad \det W(t) = 1, \quad \mathrm{Tr}\, A(t) = 0 . \tag{4.15}$$

The general solution is again given by (4.4) with

$$\det g(t) = 1, \quad W(t_0) = -W^T(t_0), \quad \det W(t_0) = 1 . \tag{4.16}$$

Let us first establish the number of solutions needed to determine $g(t)$.

Theorem 2: A fundamental set of solutions of equations (4.3a) with the constraints (4.15) consists of three solutions for $n \geqslant 4$, four solutions for $n = 3$, and five solutions for $n = 2$. A sufficient set of conditions on the initial conditions for these solutions is the following.

(i) $W_i(t_0) = -W_i^T(t_0)$, $\det W_i(t_0) = 1$.

(ii) The matrix $W_1(t_0)$ has $2n$ distinct eigenvalues.

(iii) The matrix $W_2(t_0) W_1^{-1}(t_0)$ is diagonalizable and has n distinct eigenvalues, each of multiplicity 2.

These conditions assure the existence of a matrix g_0 that transforms $W_1(t_0)$ and $W_2(t_0)$ into[18]

$$K = g_0 W_1(t_0) g_0^T, \quad \Lambda_J = g_0 W_2(t_0) g_0^T,$$

$$K = \begin{bmatrix} J & & & \\ & J & & \\ & & \ddots & \\ & & & J \end{bmatrix}, \quad \Lambda_J = \begin{bmatrix} \lambda_1 J & & & \\ & \lambda_2 J & & \\ & & \ddots & \\ & & & \lambda_n J \end{bmatrix}, \tag{4.17}$$

$$J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \lambda_i \neq \lambda_j, \quad \text{for } i \neq j .$$

(iv) In the basis (4.17) further initial conditions are

$$\Omega_a = g_0 W_a(t_0) g_0^T = \{X^a_{ik}\}, \quad \det \Omega_a = 1, \tag{4.18}$$

$$X^a_{ii} = \begin{bmatrix} 0 & a_i \\ -a_i & 0 \end{bmatrix}, \quad X^{aT}_{ki} = -X^a_{ik} = -\begin{bmatrix} x^a_{ik} & y^a_{ik} \\ z^a_{ik} & t^a_{ik} \end{bmatrix},$$

$$1 \leqslant i < k \leqslant n ,$$

where $n+1$ nonsingular entries X^a_{ik} $(i<k)$ are needed, at least three of them linearly independent. For $n \geqslant 4$, and $a = 1$, these $n+1$ entries can be taken to be X^1_{1k} $(2 \leqslant k \leqslant n)$, X^1_{23}, and X^1_{24}. For $n = 3$ we need two matrices Ω_1 and Ω_2; the entries can be chosen to be X^1_{12}, X^1_{13}, X^1_{23}, and X^2_{12}. For $n = 2$ we need three matrices Ω_1, Ω_2, and Ω_3; the entries are X^a_{12} $(a = 1, 2, 3)$.

Proof: The condition $gKg^T = K$ implies $g \in Sp(2n,\mathbb{C})$. The condition $g\Lambda_J g^T = \Lambda_J$ then implies

$$g = \begin{bmatrix} g_1 & & & \\ & g_2 & & \\ & & \ddots & \\ & & & g_n \end{bmatrix}, \tag{4.19}$$

with $g_i \in Sp(2,\mathbb{C})$, i.e., $g_i J g_i^T = J$.

Requiring $g\,\Omega_a g^T = \Omega_a$ we obtain

$$g_i\, X^a_{ik}\, J = X^a_{ik}\, J g_k\,, \tag{4.20}$$

and $n-1$ of these relations will express $g_2,\ldots,g_n$ in terms of g_1. Two more relations will then fix $g_1 = \pm I_2$ and hence $g = \pm I$. Q. E. D.

In order to reconstruct $g(t)$ in (4.4) explicitly we make a convenient choice of particular solutions. First let us take $W_1(t)$ and $W_2(t)$ satisfying

$$W_1(t_0) = K, \quad W_2(t_0) = \Lambda_J\,, \tag{4.21}$$

as in (4.17). Let us represent $g(t) \in \mathrm{SL}(2n,\mathbb{C})$ as

$$g(t) = S_1 D S_2 S_3\,, \tag{4.22}$$

where $S_i\, K S_i^T = K$, i.e., $S_i \in \mathrm{Sp}(2n,\mathbb{C})$. We have

$$W_1(t) = S_1 D S_2 S_3\, K S_3^T S_2^T D S_1^T\,,$$
$$W_1 K = S_1 (DK)^2 S_1^{-1}\,. \tag{4.23}$$

Thus, S_1 is a symplectic matrix that diagonalizes W_1K; this is always possible since $X \equiv W_1K$ satisfies $XK = KX^T$, i.e., X is symmetric under the symplectic involution.[18] The matrix D is

$$D = \begin{bmatrix} \sqrt{-\lambda_1}\, I_2 & & & \\ & \sqrt{-\lambda_2}\, I_2 & & \\ & & \ddots & \\ & & & \epsilon\sqrt{-\lambda_n}\, I_2 \end{bmatrix}, \tag{4.24}$$

with $\Pi_{i=1}^n \lambda_i^2 = 1$ and $\det D = 1$, where λ_i are eigenvalues of (W_1K) and $\epsilon = \pm 1$ is chosen so that $\det D = 1$. Using the second solution $W_2(t)$ we find

$$\tilde{W}_2 = D^{-1} S^{-1} W_2 (S_1^T)^{-1} D^{-1} = S_2 S_3 \Lambda_J\, S_3^T S_2^T\,, \tag{4.25}$$

where

$$S_3 \Lambda_J\, S_3^T = \Lambda_J, \quad \text{i.e.,}\ S_3 \in [\mathrm{Sp}(2,\mathbb{C})]^n\,, \tag{4.26}$$

and S_2 is a matrix that diagonalizes $\tilde{W}_2 K$. Any remaining ambiguities in S_1 and S_2 can be removed, e.g., by postulating that the first nonzero entry in each column be real and positive. So far, we know S_1, D, and S_2 and have limited S_3 to

$$S_3 = \begin{bmatrix} g_{11} & & & \\ & g_{22} & & \\ & & \ddots & \\ & & & g_{nn} \end{bmatrix}, \tag{4.27}$$

with $g_{ii} \in \mathrm{Sp}(2,\mathbb{C})$, i.e., $g_{ii}\, J g_{ii}^T = J$.

Let us first consider the case $n \geqslant 4$. We have

$$\tilde{W}_3(t) \equiv S_2^{-1} D^{-1} S_1^{-1} W_3(t) (S_1^T)^{-1} D^{-1} (S_2^T)^{-1}$$
$$= S_3 W_3(t_0) S_3^T\,, \tag{4.28}$$

with $\tilde{W}_3(t_0) = W_3(t_0)$ since we can choose $S_i(t_0) = D(t_0) = I$.

For $n = 4$ we put

$$W_3(t_0) = \Omega = \begin{bmatrix} 0 & J & J & J \\ J & 0 & I & \sigma \\ J & -I & 0 & \sigma \\ J & -\sigma & -\sigma & 0 \end{bmatrix}, \quad \sigma = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{4.29}$$

For $n = 2k \geqslant 6$, we put

$$W_3(t_0) = \Omega = \begin{bmatrix} 0 & J & J & \cdots & & & \cdots & J & J & J & J \\ J & 0 & 0 & \cdots & & & \cdots & 0 & \sigma & I & 0 \\ J & 0 & 0 & \cdots & & & \cdots & 0 & I & 0 & 0 \\ \vdots & & & & & & \cdots & I & 0 & 0 & 0 \\ & & & & & & \iddots & & & & \\ & & & & 0 & I & & & & & \\ & & & & -I & 0 & & & & & \\ & & & \iddots & & & & & & & \\ J & 0 & 0 & -I & & & & & & & \\ J & -\sigma & -I & 0 & & & & & & & \\ J & -I & 0 & 0 & & & & & & & \\ J & 0 & 0 & 0 & & & & & & & \end{bmatrix} \tag{4.30}$$

For $n = 2k+1 \geqslant 5$, we put

$$W_3(t_0) = \Omega = \begin{bmatrix} 0 & J & J & \cdots & & & \cdots & J & J & J & J \\ J & 0 & 0 & \cdots & & & \cdots & 0 & \sigma & I & 0 \\ J & 0 & 0 & \cdots & & & \cdots & 0 & I & 0 & 0 \\ \vdots & & & & & & & I & 0 & 0 & 0 \\ & & & & & & \iddots & & & & \\ & & & & 0 & 0 & I & & & & \\ & & & & 0 & J & 0 & & & & \\ & & & & -I & 0 & 0 & & & & \\ & & & \iddots & & & & & & & \\ J & 0 & 0 & -I & & & & & & & \\ J & -\sigma & -I & 0 & & & & & & & \\ J & -I & 0 & 0 & & & & & & & \\ J & 0 & 0 & 0 & & & & & & & \end{bmatrix} \tag{4.31}$$

(we always have $\Omega = -\Omega^T$, $\det \Omega = 1$).

Equation (4.28) rewritten in terms of 2×2 blocks implies

$$[\tilde{W}_3(t)]_{ik} J = g_{ii}\Omega_{ik} J g_{kk}^{-1} \tag{4.32}$$

(no summation). Choosing $k = 1$ we obtain

$$g_{ii} = -[\tilde{W}_3(t)]_{i1} J g_{11}, \quad i = 2,\ldots, n, \tag{4.33}$$

i.e., express all g_{ii} in terms of g_{11}. Two more relations are needed to determine g_{11}. One is obtained by taking $i = 2$, $k = n-1$ in (4.32)

$$J[\tilde{W}_3(t)]_{21}^{-1}[\tilde{W}_3(t)]_{2,n-1} J[\tilde{W}_3(t)]_{n-1,1} J g_{11} + g_{11} J = 0; \tag{4.34}$$

the existence of $[\tilde{W}_3(t)]_{21}^{-1}$ is guaranteed, at least locally, for small t by the fact that $\tilde{W}_3(t_0)_{21} = J$ is nonsingular. Finally take $i = 2$ and $k = a$, where $a = 4$ for $n = 4$, and $a = n-2$ for $n \geqslant 5$. We obtain

$$J(\tilde{W}_3)_{21}^{-1}(\tilde{W}_3)_{2a} J(\tilde{W}_3)_{a1} J g_{11} + g_{11}\sigma J = 0. \tag{4.35}$$

The linear algebraic equations (4.34) and (4.35) determine g_{11} (up to an irrelevant sign); (4.33) then determines $S_3(t)$, and ultimately (4.22) determines $g(t)$ in terms of known quantities, and the superposition formula (4.4) is complete.

For $n = 2$ and 3 the procedure up to formula (4.28) is the same as above. For $n = 3$ we use a fourth solution $W_4(t)$, construct $\tilde{W}_4(t)$ similarly as $\tilde{W}_3(t)$, and put

$$\begin{aligned}\tilde{W}_4(t) &= S_2^{-1} D^{-1} S_1^{-1} W_4(t)(S_1^T)^{-1} D^{-1}(S_2^T)^{-1} \\ &= S_3 W_4(t_0) S_3^T.\end{aligned} \tag{4.36}$$

A convenient choice is

$$\begin{aligned} W_3(t_0) = \Omega_3 &= \begin{bmatrix} 0 & J & J \\ J & J & I \\ J & -I & 0 \end{bmatrix}, \\ W_4(t_0) = \Omega_4 &= \begin{bmatrix} 0 & \sigma & 0 \\ -\sigma & 0 & 0 \\ 0 & 0 & J \end{bmatrix}. \end{aligned} \tag{4.37}$$

We now have two formulas of the type (4.32). They yield formula (4.33) expressing g_{22} and g_{33} in terms of g_{11}. For g_{11} we obtain

$$J[\tilde{W}_3(t)]_{21}^{-1}[\tilde{W}_3(t)]_{23} J[\tilde{W}_3(t)]_{31} J g_{11} + g_{11} J = 0, \tag{4.38}$$

and

$$(\tilde{W}_4(t))_{12} J(\tilde{W}_3(t))_{21} J g_{11} + g_{11}\sigma J = 0. \tag{4.39}$$

Equations (4.38) and (4.39) determine g_{11} and hence also g_{22}, g_{33}, S_3, and finally, $g(t)$ completely.

Finally, for $n = 2$ we choose

$$\begin{aligned} W_3(t_0) = \Omega_3 &= \begin{bmatrix} 0 & J \\ J & 0 \end{bmatrix}, \quad W_4(t_0) = \Omega_4 = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \\ W_5(t_0) &= \begin{bmatrix} 0 & \sigma \\ -\sigma & 0 \end{bmatrix}. \end{aligned} \tag{4.40}$$

Using $W_3(t)$ we find

$$g_{22} = -[\tilde{W}_3(t)]_{21} J g_{11}, \tag{4.41}$$

and $W_4(t)$ and $W_5(t)$ yield

$$\begin{aligned} &(\tilde{W}_4(t))_{12} J(\tilde{W}_3(t))_{21} J g_{11} + g_{11} J = 0, \\ &(\tilde{W}_5(t))_{12} J(\tilde{W}_3(t))_{21} J g_{11} + g_{11}\sigma J = 0. \end{aligned} \tag{4.42}$$

V. LOW DIMENSIONAL EXAMPLES

The number of equations associated with a transitive primitive Lie algebra $\{L, L_0\}$ is equal to the dimension of the homogeneous space G/G_0:

$$N = \dim G - \dim G_0.$$

In the cases considered in this article we have

$$N_1 = \dim \mathrm{SL}(n,\mathbb{C}) - \dim \mathrm{SO}(n,\mathbb{C}) = n(n+1)/2 - 1, \tag{5.1}$$

$$N_2 = \dim \mathrm{SL}(2n,\mathbb{C}) - \dim \mathrm{Sp}(2n,\mathbb{C}) = n(2n-1) - 1, \tag{5.2}$$

where N_1 and N_2 are complex dimensions.

The differential equations corresponding to the two series $\mathrm{SL}(n,\mathbb{C})/\mathrm{SO}(n,\mathbb{C})$ and $\mathrm{SL}(2n,\mathbb{C})/\mathrm{Sp}(2n,\mathbb{C})$ can be written compactly as linear equations (2.9) with a nonlinear constraint $\det W = 1$ (and $W = W^T$ or $W = -W^T$, as the case may be). On the other hand, the constraint can be solved to yield precisely N unconstrained nonlinear ODE's. This was done in general terms in Sec. III. Since low-dimensional cases are of particular interest in applications, we shall give the nonlinear equations explicitly for $N \leqslant 9$.

A. SL(n,C)/SO(n,C)

The case $n = 2$ is of no interest in this context since $\mathrm{SO}(2,\mathbb{C})$ is not a maximal subgroup of $\mathrm{SL}(2,\mathbb{C})$. This is, hence, a decomposable case and indeed, we would obtain two uncoupled complex Riccati equations.

For $n = 3$ the homogeneous space $\mathrm{SL}(3,\mathbb{C})/\mathrm{SO}(3,\mathbb{C})$ has complex dimension $N = 5$. We can obtain the equations from (2.9) using Eq. (3.4), i.e.,

$$s(x) = \begin{bmatrix} x_{11} & 0 & 0 \\ x_{21} & x_{22} & 0 \\ x_{31} & x_{32} & (x_{11}x_{22})^{-1} \end{bmatrix}, \tag{5.3}$$

and putting

$$W(x) = s(x)s^T(x), \tag{5.4}$$

as in (2.7). The five nonlinear ODE's are

$$\begin{aligned} \dot{x}_{11} &= a_{11}x_{11} + a_{12}x_{21} + a_{13}x_{31}, \\ \dot{x}_{21} &= a_{21}x_{11} + a_{22}x_{21} + a_{23}x_{31} \\ &\quad + (x_{22}/x_{11})(a_{12}x_{22} + a_{13}x_{32}), \\ \dot{x}_{31} &= a_{31}x_{11} + a_{32}x_{21} + (-a_{11} - a_{22})x_{31} \\ &\quad + (x_{32}/x_{11})(a_{12}x_{22} + a_{13}x_{32}) + a_{13}/x_{11}^3 x_{22}^2, \\ \dot{x}_{22} &= a_{22}x_{22} + a_{23}x_{32} - (x_{21}/x_{11})(a_{12}x_{22} + a_{13}x_{32}), \\ \dot{x}_{32} &= a_{32}x_{22} + (-a_{11} - a_{22})x_{32} \\ &\quad - (x_{31}/x_{11})(a_{12}x_{22} + a_{13}x_{32}) \\ &\quad + (1/x_{11}^3 x_{22}^3)(a_{23}x_{11} - a_{13}x_{21}). \end{aligned} \tag{5.5}$$

We see that the removal of the constraint $\det W = 1$, i.e., $\det s = 1$ has introduced rational nonpolynomial nonlinearities and also singularities in the hyperplanes $x_{11} = 0$ and $x_{22} = 0$. An equivalent, but different, system of five nonlinear equations can be obtained directly from (3.1), using (3.2).

For $n = 4$ the homogeneous space has dimension $N = 9$. Taking the section $s(x)$ of SL(4,C)/SO(4,C) as

$$x \to s(x) = \begin{bmatrix} x_{11} & 0 & 0 & 0 \\ x_{21} & x_{22} & 0 & 0 \\ x_{31} & x_{32} & x_{33} & 0 \\ x_{41} & x_{42} & x_{43} & x_{44} \end{bmatrix},$$

$$x_{44} = (x_{11}x_{22}x_{33})^{-1} \tag{5.6}$$

we obtain the following system of nine equations:

$$\begin{aligned}
\dot{x}_{11} &= \sum_{i=1}^{4} a_{1i}x_{i1}, \\
\dot{x}_{21} &= \sum_{i=1}^{4} a_{2i}x_{i1} + \frac{x_{22}}{x_{11}} \sum_{i=2}^{4} a_{1i}x_{i2}, \\
\dot{x}_{31} &= \sum_{i=1}^{4} a_{3i}x_{i1} + \frac{x_{32}}{x_{11}} \sum_{i=2}^{4} a_{1i}x_{i2} + \frac{x_{33}}{x_{11}} \sum_{i=3}^{4} a_{1i}x_{i3}, \\
\dot{x}_{41} &= \sum_{i=1}^{4} a_{4i}x_{i1} + \frac{x_{42}}{x_{11}} \sum_{i=2}^{4} a_{1i}x_{i2} + \frac{x_{43}}{x_{11}} \sum_{i=3}^{4} a_{1i}x_{i3} \\
&\quad + \frac{a_{14}}{x_{11}^3 x_{22}^2 x_{33}^2}, \\
\dot{x}_{22} &= \sum_{i=2}^{4} a_{2i}x_{i2} - \frac{x_{21}}{x_{11}} \sum_{i=2}^{4} a_{1i}x_{i2}, \\
\dot{x}_{32} &= \sum_{i=2}^{4} a_{3i}x_{i3} + \frac{x_{33}}{x_{22}} \sum_{i=3}^{4} a_{2i}x_{i3} - \frac{x_{31}}{x_{11}} \sum_{i=2}^{4} a_{1i}x_{i2} \\
&\quad - \frac{x_{21}x_{33}}{x_{11}x_{22}} \sum_{i=3}^{4} a_{1i}x_{i3}, \\
\dot{x}_{42} &= \sum_{i=2}^{4} a_{4i}x_{i4} + \frac{x_{43}}{x_{22}} \sum_{i=3}^{4} a_{2i}x_{i3} + \frac{a_{24}}{x_{11}^2 x_{22}^3 x_{33}^2} \\
&\quad - \frac{x_{41}}{x_{11}} \sum_{i=2}^{4} a_{1i}x_{i2} - \frac{x_{21}x_{43}}{x_{11}x_{22}} \sum_{i=3}^{4} a_{1i}x_{i3} \\
&\quad - \frac{a_{14}x_{21}}{x_{11}^3 x_{22}^3 x_{33}^2}, \\
\dot{x}_{33} &= \sum_{i=3}^{4} a_{3i}x_{i3} - \frac{x_{31}}{x_{11}} \sum_{i=3}^{4} a_{1i}x_{i3} - \frac{x_{32}}{x_{22}} \sum_{i=3}^{4} a_{2i}x_{i3} \\
&\quad + \frac{x_{21}x_{32}}{x_{11}x_{22}} \sum_{i=3}^{4} a_{1i}x_{i3}, \\
\dot{x}_{43} &= \sum_{i=3}^{4} a_{4i}x_{i3} - \frac{x_{41}}{x_{11}} \sum_{i=3}^{4} a_{1i}x_{i3} - \frac{x_{42}}{x_{22}} \sum_{i=3}^{4} a_{2i}x_{i3} \\
&\quad + \frac{x_{21}x_{42}}{x_{11}x_{22}} \sum_{i=3}^{4} a_{1i}x_{i3} + \frac{a_{34}}{x_{11}^2 x_{22}^2 x_{33}^3} - \frac{a_{14}x_{31}}{x_{11}^3 x_{22}^2 x_{33}^3} \\
&\quad - \frac{a_{24}x_{32}}{x_{11}^2 x_{22}^3 x_{33}^3} + \frac{a_{14}x_{21}x_{32}}{x_{11}^3 x_{22}^3 x_{33}^3},
\end{aligned} \tag{5.7}$$

where $A = \{a_{ij}\}$ is an element of the Lie algebra sl(4,C).

Again, the nonlinearities are rational, rather than polynomial, and singularities occur for $x_{11} = 0$, $x_{22} = 0$, and $x_{33} = 0$.

B. SL(2n,C)/Sp(2n,C)

Here we restrict ourselves to the case $n = 2$, i.e., the case SL(4,C)/Sp(4,C) leading to five equations. We use the occasion to give an example of the construction described in Sec. II B. We take the symplectic metric in the form

$$K = \begin{bmatrix} J & 0 \\ 0 & J \end{bmatrix}. \tag{5.8}$$

The subspace $L_1 \subset \mathrm{sl}(4,\mathbb{C})$ of (2.12) in this case is

$$L_1 = \left\{ B = \begin{bmatrix} hI & R \\ -JR^{T}J & -hI \end{bmatrix},\ h \in \mathbb{C},\ R \in \mathbb{C}^{2\times 2} \right\}. \tag{5.9}$$

Exponentiating B we have

$$\exp B = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \cosh\lambda + B\frac{\sinh\lambda}{\lambda}, \tag{5.10}$$

where

$$\lambda^2 = h^2 + \det R. \tag{5.11}$$

The ODE's could be written directly in terms of the variable h and $R = \{r_{ik}\}$; they take a simpler (polynomial) form in the variables

$$Z_1 = \begin{bmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{bmatrix} = \frac{\tanh\lambda}{\lambda} R, \quad z_2 = \frac{\tanh\lambda}{\lambda} h. \tag{5.12}$$

The SL(4,C)/Sp(4,C) equations in these variables are

$$\begin{aligned}
\dot{z}_{11} &= (A_1 - A_4)z_{11} - A_6 z_{12} + A_2 z_{21} - 2A_7 z_2 \\
&\quad + z_{11}(-2A_{11}z_2 - A_{15}z_{11} + A_{14}z_{12} + A_{13}z_{21}) \\
&\quad + A_{12}(1 + z_2^2 - z_{12}z_{21}), \\
\dot{z}_{12} &= -A_5 z_{11} + (A_1 + A_4)z_{12} + A_2 z_{22} - 2A_8 z_2 \\
&\quad + z_{12}(-2A_{11}z_2 - A_{15}z_{11} + A_{14}z_{12} - A_{12}z_{22}) \\
&\quad + A_{13}(1 + z_2^2 + z_{11}z_{12}), \\
\dot{z}_{21} &= A_3 z_{11} + (-A_1 - A_4)z_{21} - A_6 z_{22} - 2A_9 z_2 \\
&\quad + z_{21}(-2A_{11}z_2 - A_{15}z_{11} + A_{13}z_{21} - A_{12}z_{22}) \\
&\quad + A_{14}(1 + z_2^2 + z_{11}z_{22}), \\
\dot{z}_{22} &= A_3 z_{12} - A_5 z_{21} + (-A_1 + A_4)z_{22} - 2A_{10} z_2 \\
&\quad + z_{22}(-2A_{11}z_2 + A_{14}z_{12} + A_{13}z_{21} - A_{12}z_{22}) \\
&\quad + A_{15}(1 + z_2^2 - z_{12}z_{21}), \\
\dot{z}_2 &= A_{10} z_{11} - A_9 z_{12} - A_8 z_{21} + A_7 z_{22} \\
&\quad + z_2(-A_{15}z_{11} + A_{14}z_{12} + A_{13}z_{21} - A_{12}z_{22}) \\
&\quad + A_{11}(1 - z_2^2 + z_{11}z_{22} - z_{12}z_{21}).
\end{aligned} \tag{5.13}$$

The $A_i(t)$ $(i = 1,\ldots, 15)$ are arbitrary functions of t, each of them corresponding to a specifically chosen one parameter subalgebra of sl(4,C). Similar equations in different coordinates were presented in Ref. 11.

Equations (5.13) can be transformed into a more concise form, making use of the local isomorphisms SL(4,C)~SO(6,C) and Sp(4,C)~SO(5,C). Indeed, denoting

$$z = (z_{11}, z_{12}, z_{21}, z_{22}, z_2)^{T}, \tag{5.14}$$

$$A=\begin{bmatrix} A_1-A_4 & -A_6 & A_2 & 0 & -2A_7 \\ -A_5 & A_1+A_4 & 0 & A_2 & -2A_8 \\ A_3 & 0 & -A_1-A_4 & -A_6 & -2A_9 \\ 0 & A_3 & -A_5 & -A_1+A_4 & -2A_{10} \\ A_{10} & -A_9 & -A_8 & A_7 & 0 \end{bmatrix}, \tag{5.15}$$

we have $A\in so(5,\mathbb{C})$, i.e., $A\hat{K}+\hat{K}A^{T}=0$ with

$$\hat{K}=\begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \tag{5.16}$$

and $E=(A_{12},A_{13},A_{14},A_{15},A_{11})^{T}$, we rewrite (15.13) as

$$\dot{z}=Az+(z^{T}\hat{K}zI_5-2zz^{T}\hat{K})E+E. \tag{5.17}$$

If we let $y=P^{-1}z$, where $P^{T}\hat{K}P=I$, we find that (5.16) is equivalent to

$$\dot{y}=By+\{y^{T}yI_5-2yy^{T}\}D+D, \tag{5.18}$$

where B is a skew-symmetric 5×5 matrix and D is a five-dimensional vector.

Equation (5.17), or (5.18), is actually a special case of "conformal Riccati equations," based on the conformal action of the group $O(n+2,\mathbb{C})$ on an n-dimensional complex Euclidean plane.[6,11] The isomorphism $SL(4,\mathbb{C})/Sp(4,\mathbb{C})\sim SO(6,\mathbb{C})/SO(5,\mathbb{C})$ does not generalize to other dimensions; the $SL(2n,\mathbb{C})/Sp(2n,\mathbb{C})$ equations for $n\geqslant3$ can hence not be cast into the form (5.18).

VI. CONCLUSIONS

This paper is to be viewed as the first step in the systematic study of systems of nonlinear ODE's with superposition principles, based on the action of a Lie group G on a homogeneous space G/G_0, where G is a simple Lie group and G_0 a maximal reductive subgroup. In this paper G is taken to be $SL(n,\mathbb{C})$, G_0 was either $SO(n,\mathbb{C})$ or $Sp(n,\mathbb{C})$ (for n even). In both cases the ODE's can either be written as linear matrix equations with a nonlinear constraint, or as unconstrained nonlinear equations.The nonlinearities are rational, but in general not polynomial. Indeed, Riccati type equations, i.e., equations with quadratic nonlinearities, are obtained only in the case $SL(4,\mathbb{C})/Sp(4,\mathbb{C})$.

We obtained the superposition formulas explicitly. For $G_0=O(n,\mathbb{C})$ the general solution is expressed in terms of three particular solutions for any $n\geqslant3$. For $G_0=Sp(2n,\mathbb{C})$ five solutions are needed for $n=2$, four solutions for $n=3$, and only three solutions for $n\geqslant4$.

Work is in progress on other group–subgroup pairs. The emphasis in this article, as well as previous "classification" articles, has been on the classical complex Lie algebras. The case of real Lie algebras is richer and more complicated and will be approached in the near future.

Finally we mention applications of the constructed systems of nonlinear ODE's with superposition formulas. All of these equations are, in some sense, integrable. They have the "Painlevé property,"[19,20] i.e., their solutions do not have moving singularities other than poles. Such systems of ODE's figure prominently in studies of integrability. For instance, ODE's with superposition formulas occur as Bäcklund transformations for integrable partial differential equations such as those of the σ model.[4,21,22] Furthermore, these equations serve as a useful tool in a study of such phenomena as nonintegrability and onset of chaos.[23]

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A class of unitary representations of the Lie group Sp(3, ℝ), its coherent states, and its map to a symplectic realization on sp*(3, ℝ)

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Unitary representations from the positive discrete series of Sp(3, R) with lowest weight $w = \{w_0 w_0 w_0\}$ are considered. By use of new relations on the enveloping algebra, the generators are constructed as differential operators acting on functions of six real variables. Coherent states for these representations are constructed with the help of the Iwasawa decomposition and used to map the representation space to a symplectic realization on the dual sp*(3, R).

I. INTRODUCTION

The group Sp(3, ℝ) and its subgroups $GL_+(3, \mathbb{R})$ and SL(3, ℝ) have found a great deal of attention in the study of collective motion in nuclei.[1–5]

In Refs. 6–8 the present authors started a geometric study of this group both for the quantum and classical collective dynamics. In Refs. 6 and 7 we studied in particular the representations of Sp(3, R) on the coset U(3)\Sp(3, R). This coset was parametrized by a 3×3 symmetric complex matrix B restricted to the classical symmetric bounded domain Ω_3^{II}: $I - BB^+ > 0$. General results on the harmonic analysis in the classical symmetric domains are given in Ref. 9, and the quantization in these domains is discussed in Ref. 10. Analytic parametrizations and representations for semisimple compact groups are studied in Ref. 11 and references given therein.

The coset U(3)\Sp(3, ℝ) arises in the representations of the positive discrete series of the group Sp(3, R) for the lowest weight $w = \{w_0 w_0 w_0\}$. In Sec. III we prove new relations on the enveloping algebra for these representations. In Secs. IV and V we use these relations to construct the representations on a Hilbert space of square-integrable functions of six real variables. The aim of the present paper is to introduce real parameters for the coset U(3)\Sp(3, ℝ). In Sec. II we determine these parameters from the Iwasawa decomposition; we use them in Sec. VI in order to define coherent states. By use of these coherent states we associate to the operators in the representation space functions on an orbit on the dual sp*(3, R) with a generalized Poisson bracket.

The results of the present paper apply to collective motion of nuclei with a closed-shell ground state. The collective dynamics in terms of these real parameters is studied in Refs. 12 and 13 on the classical and quantum level.

II. THE IWASAWA DECOMPOSITION OF THE SYMPLECTIC GROUP Sp(3, R) AND THE COSET U(3)\Sp(3, R)

The Lie group Sp(3, ℝ) is connected, noncompact, and semisimple and therefore possesses a unique Iwasawa decomposition (Refs. 14, p. 41, and Ref. 15, p. 104). The first factor in this decomposition is the maximal compact subgroup U(3), and therefore the Iwasawa decomposition yields in particular a parametrization of the cosets U(3)\Sp(3, ℝ). By a modification of the Iwasawa decomposition of Sp(3, ℝ), we derive a new parametrization of these cosets.

Definition 2.1: The real Lie algebra sp(3, ℝ): We choose the basis $B(\mathrm{sp}(3,\mathbb{R})) = \{A_{ij}, Q_{ij}, P_{ij} | Q_{ij} = Q_{ji}, P_{ij} = P_{ji}, i,j = 1,2,3\}$ with the structure constants given by[8]

$$
\begin{aligned}
&[A_{ij}, Q_{rs}] = i(-\delta_{jr}Q_{is} - \delta_{js}Q_{ir}),\\
&[A_{ij}, P_{rs}] = i(\delta_{ir}P_{js} + \delta_{is}P_{jr}),\\
&[A_{ij}, A_{rs}] = i(\delta_{is}A_{rj} - \delta_{rj}A_{is}),\\
&[Q_{ij}, Q_{rs}] = 0,\\
&[Q_{ij}, P_{rs}] = i(\delta_{ir}A_{js} + \delta_{is}A_{jr} + \delta_{jr}A_{is} + \delta_{js}A_{ir}),\\
&[P_{ij}, P_{rs}] = 0.
\end{aligned}
$$

Proposition 2.2: Iwasawa decomposition of $\mathbb{L} = \mathrm{sp}(3, \mathbb{R})$: (a) The maximal compact subalgebra $\mathbb{K}$ of $\mathbb{L}$ has the basis $B(\mathbb{K}) = \{C_{ij} | C_{ij} = \frac{1}{2}(Q_{ij} + P_{ij}) + (i/2)(A_{ij} - {}^tA_{ij}), i,j = 1,2,3\}$.

(b) The Cartan decomposition $\mathbb{L} = \mathbb{K} + \mathbb{P}$ yields for $\mathbb{P}$ the basis

$$B(\mathbb{P}) = \{K_{ij,\pm} | K_{ij,\pm} = \tfrac{1}{4}(Q_{ij} - P_{ij}) \mp (i/4)(A_{ij} + {}^tA_{ij}), \quad i,j = 1,2,3\}.$$

(c) The maximal Abelian subalgebra $\mathbb{A}$ of $\mathbb{P}$ has the basis

$$B(\mathbb{A}) = \{A_{ii} | i = 1,2,3\}.$$

(d) The Lie algebra $\mathbb{N}_-$ with the basis

$$B(\mathbb{N}_-) = \{A_{ij}, i>j, i,j = 1,2,3; Q_{rs}, r,s = 1,2,3\}$$

is nilpotent.

(e) The algebra $\mathbb{A} + \mathbb{N}_-$ is solvable.

(f) The Iwasawa decomposition of sp(3, ℝ) is

$$\mathbb{L} = \mathbb{K} + \mathbb{A} + \mathbb{N}_-.$$

Proof: We follow the prescription given by Hermann (Ref. 15, Chap. 7).

Proposition 2.3: Global Iwasawa decomposition[14,15] of Sp(3, ℝ): The global Iwasawa decomposition of Sp(3, ℝ) is given by

$$\mathrm{Sp}(3, \mathbb{R}) = \mathrm{U}(3)AN_-,$$

where the three subgroups U(3), A, and N_- are generated by the Lie algebras $\mathbb{K}$, $\mathbb{A}$, and $\mathbb{N}_-$, respectively.

Definition 2.4: The collective motion group is the semidirect product group[16,17]

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$$\mathrm{GL}_+(3,\mathbb{R})N^2,$$

where $\mathrm{GL}_+(3,\mathbb{R})$ is the subgroup of $\mathrm{GL}(3,\mathbb{R})$ with positive determinant and where the invariant subgroup N^2 is generated by

$$B(\mathbf{N}^2)=\{Q_{ij}, i,j=1,2,3\}.$$

Proposition 2.5: The group $\mathrm{Sp}(3,\mathbb{R})$ admits the factorization

$$\mathrm{Sp}(3,\mathbb{R})=\mathrm{U}(3)\,C,$$

where C is a set of coset representatives from the coset $\mathrm{SO}(3,\mathbb{R})\backslash(\mathrm{GL}_+(3,\mathbb{R})N^2)$.

Proof: The group $\mathrm{SL}(3,\mathbb{R})$ has the global Iwasawa decomposition (Ref. 15, p. 42)[18]

$$\mathrm{SL}(3,\mathbb{R})=\mathrm{SO}(3,\mathbb{R})\,A^1N^1_-,$$

where the subgroups are generated by the bases

$$B(\mathrm{so}(3,\mathbb{R}))=\{A_{ij}-A_{ji}\,|\,i<j,\ i,j=1,2,3\},$$

$$B(\mathbf{A}^1)=\{A_{11}-A_{22},\ A_{33}-\tfrac{1}{2}(A_{11}+A_{22})\},$$

$$B(\mathbf{N}^1_-)=\{A_{ij}\,|\,i>j,\ i,j=1,2,3\}.$$

This decomposition may be extended to the nonsemisimple group $\mathrm{GL}_+(3,\mathbb{R})$ since

$$\mathrm{GL}_+(3,\mathbb{R})=A^0\,\mathrm{SL}(3,\mathbb{R}),$$

with the subgroup A^0 generated by

$$B(\mathbf{A}^0)=\{A_{11}+A_{22}+A_{33}\}.$$

Using this factorization for $\mathrm{GL}_+(3,\mathbb{R})N^2$ given in Definition 2.4, one finds

$$\begin{aligned}\mathrm{GL}_+(3,\mathbb{R})N^2&=\mathrm{SO}(3,\mathbb{R})\,A^0A^1N^1_-\,N^2\\&=\mathrm{SO}(3,\mathbb{R})\,AN_-.\end{aligned}$$

Hence the group AN_- runs over the different cosets of the form $\mathrm{SO}(3,\mathbb{R})\backslash(\mathrm{GL}_+(3,\mathbb{R})N^2)$. Let $C=\{c\}$ be an arbitrary but fixed set of representatives of this coset. Then there must exist a one-to-one mapping between AN_- and C such that

$$an=hc,\quad a\in A,\quad n\in N_-,\quad h\in\mathrm{SO}(3,\mathbb{R}),\quad c\in C.$$

Since $\mathrm{U}(3)h=\mathrm{U}(3)$, the Iwasawa decomposition of $\mathrm{Sp}(3,\mathbb{R})$ can be modified as

$$\mathrm{Sp}(3,\mathbb{R})=\mathrm{U}(3)AN_-=\mathrm{U}(3)C.\qquad\square$$

III. THE REPRESENTATIONS OF WEIGHT $\{w_0w_0w_0\}$ OF Sp(3, ℝ)

The unitary irreducible representations of the positive discrete series of $\mathrm{Sp}(3,\mathbb{R})$ are characterized by a lowest weight. We consider representations with degenerate weight, and derive relations between operators from the enveloping algebra.

Definition 3.1: The complex form of $\mathrm{Sp}(3,\mathbb{R})$ is given by

$$\mathrm{Sp}(3,\mathbb{C})\cap\mathrm{U}(3,3)=R\,\mathrm{Sp}(3,\mathbb{R})R^{-1},$$

$$R=\frac{1}{\sqrt{2}}\begin{bmatrix}I & iI\\ I & -iI\end{bmatrix}.$$

We denote by g the complex elements related to the real ones g' by $g=Rg'R^{-1}$.

Definition 3.2: The 6×6 operator-valued matrices $\hat{T}'$ and $\hat{T}$ (Refs. 6 and 8) are defined as

$$\hat{T}'=\begin{bmatrix}\hat{A} & \hat{Q}\\ -\hat{P} & -{}^t\hat{A}\end{bmatrix},\quad \hat{T}=\begin{bmatrix}\hat{C} & -2\hat{K}_+\\ 2\hat{K}_- & -{}^t\hat{C}\end{bmatrix}.$$

Under the adjoint action these matrices transform as

$$g'\in\mathrm{Sp}(3,\mathbb{R}),\quad g=Rg'R^{-1},$$

$$\hat{T}'\to(g')^{-1}\hat{T}'g',\quad \hat{T}\to g^{-1}\hat{T}g.$$

Definition 3.3: The unitary representations of the positive discrete series of $\mathrm{Sp}(3,\mathbb{R})$ are characterized by an extremal state $|\{w_1w_2w_3\}\rangle$ such that

$$\hat{K}_{ij,-}\,|\{w_1w_2w_3\}\rangle=0,\quad i,j=1,2,3,$$

$$\hat{C}_{ij}|\{w_1w_2w_3\}\rangle=0,\quad i<j,\quad i,j=1,2,3,$$

$$\hat{C}_{ll}|\{w_1w_2w_3\}\rangle=|\{w_1w_2w_3\}\rangle w_l,\quad l=1,2,3,$$

and by the Hermitian properties

$$(\hat{K}_{ij,-})^+=\hat{K}_{ij,+},\quad (\hat{C}_{ij})^+=\hat{C}_{ji}.$$

By L^{w_0} we denote the special representation space with $w_1=w_2=w_3=w_0$. Note that in L^{w_0} the lowest weight state is stable under the subgroup $\mathrm{U}(3)$ or $\mathrm{Sp}(3,\mathbb{R})$.

Proposition 3.4: The operator-valued matrices $\hat{T}'$ and $\hat{T}$ when restricted to the representation space L^{w_0} obey the matrix relations

$$\hat{T}'\hat{T}'=-4i\hat{T}'-w_0(w_0-4)\hat{I},\quad \hat{T}\hat{T}=4\hat{T}+w_0(w_0-4)\hat{I},$$

where $\hat{I}$ is the 6×6 operator-valued matrix with the identity operator on diagonal entries and with the zero operator elsewhere.

Proof: It was shown[7] that a special form of L^{w_0} is given in terms of a complex symmetric 3×3 matrix $b=\{b_{ij}\}$ by

$$\hat{K}_{ij,-}=\nabla_{ij},\quad \hat{K}_{ij,+}=\sum_{p,q=1}^{3}b_{qi}b_{pj}\nabla_{pq}+w_0b_{ij},$$

$$\hat{C}_{ij}=2\sum_{q=1}^{3}b_{iq}\nabla_{qj}+w_0\delta_{ij},$$

where

$$\nabla_{ij}=\frac{1}{2}\left(\frac{\partial}{\partial b_{ij}}+\frac{\partial}{\partial b_{ji}}\right).$$

The symmetrized derivative is used to simplify the application of these operators to functions of b. An explicit computation with this special representation yields the result. $\square$

IV. THE SUBGROUPS $\mathrm{GL}_+(3,\mathbb{R})$ AND $\mathrm{GL}_+(3,\mathbb{R})N^2$ OF Sp(3, ℝ)

In Sec. II we found the correspondence of the cosets $\mathrm{U}(3)\backslash\mathrm{Sp}(3,\mathbb{R})$ and $\mathrm{SO}(3,\mathbb{R})\backslash\mathrm{GL}_+(3,\mathbb{R})N^2$. In Sec. III we considered the irreducible representation L^{w_0} of $\mathrm{Sp}(3,\mathbb{R})$ and noted that its lowest weight state is stable under $\mathrm{U}(3)$. These two observations suggest that the representation L^{w_0} of $\mathrm{Sp}(3,\mathbb{R})$ could be constructed with the help of the coset $\mathrm{SO}(3,\mathbb{R})\backslash\mathrm{GL}_+(3,\mathbb{R})N^2$. The group $\mathrm{Sp}(3,\mathbb{R})$ acts as a transformation group on its coset $\mathrm{U}(3)\backslash\mathrm{Sp}(3,\mathbb{R})$. This action will be considered in Sec. VI, where this coset will be considered as a symplectic manifold with a generalized Poisson bracket. It will be shown that the six parameters of the coset $\mathrm{So}(3,\mathbb{R})\backslash\mathrm{GL}_+(3,\mathbb{R})$ serve as generalized coordinates of this symplectic manifold. In this and the following section we construct the representation L^{w_0} on a Hilbert space of square-integrable functions of this coset.

Definition 4.1: The matrix form of the groups $Sp(3,\mathbb{R})$, N^2, and $GL_+(3,\mathbb{R})$: The 6×6 matrix forms of the groups are given by

$$Sp(3,\mathbb{R}) = \left\{ g' \,|\, g' K\, {}^t g' = K, \quad K = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \right\}$$

$$N^2 = \left\{ g_1' \,|\, g_1' = g_1'(Z) = \begin{bmatrix} I & 0 \\ Z & I \end{bmatrix}, \quad {}^t Z = Z \right\},$$

$$Gl_+(3,\mathbb{R}) = \left\{ g_2' \,|\, g_2' = g_2'(k) = \begin{bmatrix} k & 0 \\ 0 & {}^t k^{-1} \end{bmatrix} \sim k \in GL_+(3,\mathbb{R}) \right\}.$$

The group $GL_+(3,\mathbb{R})$ has the invariant measure (Ref. 14, p. 74)

$$x' \in GL_+(3,\mathbb{R}), \quad d\mu(x') = (\det x')^{-3} \prod_{i,j=1}^{3} dx'_{ij}.$$

Proposition 4.2: On $\mathcal{L}^2(GL_+(3,\mathbb{R}),\mu)$, the group $GL_+(3,\mathbb{R})N^2$ has the unitary representation L:

$$(\hat{U}_{g_1'(Z)}\chi)(x') = \exp\left(-\frac{1}{2} i \sum_{i,j=1}^{3} Z_{ij}\hat{Q}_{ij} \right)\chi(x'),$$

$$(\hat{Q}_{ij}\chi)(x') = \left(\sum_{q=1}^{3} x'_{iq}x'_{jq} \right)\chi(x'),$$

$$(\hat{U}_{g_2(k)}\chi)(x') = \chi(k^{-1}x') = \exp\left(-i \sum_{i,j=1}^{3} \kappa_{ij}\, \hat{A}_{ij} \right)\chi(x'),$$

$$(\hat{A}_{ij}\chi)(x') = \left(-i \sum_{q=1}^{3} x'_{iq} \frac{\partial}{\partial x'_{jq}} \right)\chi(x'),$$

$$k = \exp \kappa.$$

This representation was constructed by Rosensteel and Rowe[17] in relation with the mass quadrupole collective model, except for the fact that they constructed it only on the coset $SO(3,\mathbb{R})\backslash GL_+(3,\mathbb{R})$. It arises[17] from the representation of the same group in the many-body Hilbert space.

V. CONSTRUCTION OF THE REPRESENTATION L^{w_0} OF $Sp(3,\mathbb{R})$ ON THE COSET $GL_+(3,\mathbb{R})/SO(3,\mathbb{R})$

As mentioned before, the representation of the subgroup $GL_+(3,\mathbb{R})N^2$ given in Sec. IV was already constructed by Rosensteel and Rowe.[17] We now show that this representation can be extended to the representation L^{w_0} of $Sp(3,\mathbb{R})$. The proof will be based essentially on the results of Sec. III, Proposition 3.4.

Written out in detail, Proposition 3.4 yields the two independent matrix conditions

$$\sum_{j=1}^{3} \hat{A}_{ij}\hat{Q}_{jl} - \sum_{j=1}^{3} \hat{Q}_{ij}\hat{A}_{lj} = -4i\hat{Q}_{il}, \quad i,l = 1,2,3, \tag{5.1}$$

$$\sum_{j=1}^{3} \hat{A}_{ij}\hat{A}_{jl} - \sum_{j=1}^{3} \hat{Q}_{ij}\hat{P}_{jl} = -4i\hat{A}_{il} - w_0(w_0-4)\delta_{il}, \quad i,l = 1,2,3. \tag{5.2}$$

The part of Proposition 3.4 given by Eq. (5.1) will be shown to imply a condition on the representations of $Gl_+(3,\mathbb{R})N^2$; Equation (5.2) will determine the generators $\hat{P}_{jl}$ of $Sp(3,\mathbb{R})$ which do not belong to $GL_+(3,\mathbb{R})N^2$.

Proposition 5.1: Extension of the representation L of $GL_+(3,\mathbb{R})N^2$ to L^{w_0} of $Sp(3,\mathbb{R})$ requires that the functions $\chi(x')$ be stable under the right action of $SO(3,\mathbb{R})$, $(T_h\chi)(x') = \chi(x'h) = \chi(x')$.

Proof: Using the commutators of $\hat{A}$ and $\hat{Q}$, Eq. (5.1) may be rewritten as

$$\sum_{j=1}^{3} \hat{Q}_{lj}\hat{A}_{ij} - \sum_{j=1}^{3} \hat{Q}_{ij}\hat{A}_{lj} = 0. \tag{5.3}$$

The action of $GL_+(3,\mathbb{R})$ on $GL_+(3,\mathbb{R})$ is generated by the differential operators

$$\hat{A}^{R}_{\alpha\beta} = -i \sum_{q=1}^{3} x'_{q\alpha} \frac{\partial}{\partial x'_{q\beta}},$$

which are related to the left action generators by

$$\hat{A}_{ij} = \sum_{\alpha,\beta=1}^{3} x'_{i\beta}(x'^{-1})_{\alpha j}\hat{A}^{R}_{\alpha\beta}.$$

The left-hand side of Eq. (5.3) becomes

$$\sum_{j=1}^{3} \hat{Q}_{lj}\hat{A}_{ij} - \sum_{j=1}^{3} \hat{Q}_{ij}\hat{A}_{lj} = \sum_{\alpha,\beta=1}^{3} x'_{l\alpha}x'_{i\beta}\mathcal{L}^{R}_{\alpha\beta},$$

where

$$\hat{\mathcal{L}}^{R}_{\alpha\beta} = \hat{A}^{R}_{\alpha\beta} - \hat{A}^{R}_{\beta\alpha}$$

are the three generators of the right action of $SO(3,\mathbb{R})$ on $GL_+(3,\mathbb{R})$. Equation (5.1) now implies the vanishing of these operators when acting in L^{w_0}. □

Corollary 5.1': Under the conditions of Proposition 5.1 the vortex spin[1] vanishes.[19]

Proof: The vortex spin is linearly related to the generators $\mathcal{L}^{R}_{\alpha\beta}$. □

The conditions implied by Proposition 3.4 restrict the representations of $GL_+(3,\mathbb{R})N^2$ to those induced by the identity representation of $SO(3,\mathbb{R})$. The functions χ and the measure $d\mu$ should therefore be restricted to the coset $GL_+(3,\mathbb{R})/SO(3,\mathbb{R})$. This coset can be parametrized by the matrix $Q = (Q_{il})$. In terms of this matrix we get the following.

Proposition 5.2: The generators of $GL_+(3,\mathbb{R})N^2$ on the coset $GL_+(3,\mathbb{R})/SO(3,\mathbb{R})$: The generators in terms of Q become

$$(\hat{A}_{il}\chi)(Q) = \left(\sum_{j=1}^{3} \hat{Q}_{ij}\hat{X}_{jl} \right)\chi(Q), \quad i,l = 1,2,3,$$

$$(\hat{Q}_{il}\chi)(Q) = Q_{il}\chi(Q), \quad i,l = 1,2,3,$$

where $\hat{X}$ are the differential operators

$$(\hat{X}_{jl}\chi)(Q) = -i\left(\frac{\partial}{\partial Q_{jl}} + \frac{\partial}{\partial Q_{lj}} \right)\chi(Q), \quad j,l = 1,2,3.$$

We turn now to the equation (5.2) related to Proposition 3.4.

Proposition 5.3: Extension to the representation of $Sp(3,\mathbb{R})$: On the coset $GL_+(3,\mathbb{R})/SO(3,\mathbb{R})$, the representation of $GL_+(3,\mathbb{R})N^2$ of Proposition 5.2 can be extended to the representation L^{w_0} of $Sp(3,\mathbb{R})$ by including the generators

$$\hat{P}_{il} = \sum_{k,q=1}^{3} (\hat{Q})_{kq}\hat{X}_{ik}\hat{X}_{lq} + w_0(w_0-4)(\hat{Q}^{-1})_{il}.$$

Proof: Assuming $\hat{Q}$ to be invertible we can isolate $\hat{P}$ in Eq. (5.2), insert the form of $\hat{A}$ in terms of $\hat{Q}$ and $\hat{X}$ by use of

Proposition 5.2, and move the differential operators to the right to get the result. □

Proposition 5.4: The lowest weight state of L^{w_0}: Define on $GL_+(3,\mathbb{R})/SO(3,\mathbb{R})$ the state

$$\chi^{w_0}(Q) = c_0(\det Q)^{w_0/2}\exp\left[-\frac{1}{2}\sum_i^3 Q_{ii}\right].$$

This state is of lowest weight in L^{w_0}.

VI. ORBITS ON THE DUAL sp*(3, R), COHERENT STATES, AND THE DEQUANTIZATION MAP OF THE REPRESENTATION L^{w_0}

The symplectic group acts on its Lie algebra sp(3, R) through the adjoint representation and on the dual sp*(3, R) through the coadjoint representation. As shown by Kostant,[20] the orbits under the coadjoint action yield symplectic manifolds. We shall consider a special class of these orbits and construct a set of coherent states in L^{w_0} and a map from operators on L^{w_0} to functions on these orbits.

The semisimple group Sp(3, R) has a nondegenerate Killing metric on its Lie algebra sp(3, R). As a consequence, the adjoint and coadjoint representations are equivalent. Hence we can introduce on sp*(3, R) covariant coordinates, i.e., coordinates which transform according to the adjoint rather than to the coadjoint representation. Since we are dealing with a matrix group, it is convenient to describe these parameters of sp*(3, R) by matrices.

Definition 6.1: For the group Sp(3, R) given in the real and complex form of Definition 3.1, introduce as covariant parameters of sp*(3, R) the 6×6 matrices

$$\mathcal{T}' = \begin{bmatrix} \mathcal{A} & \mathcal{Q} \\ -\mathcal{P} & -{}^t\mathcal{A} \end{bmatrix},$$

$$\mathcal{Q} = {}^t\mathcal{Q},\quad {}^t\mathcal{P} = \mathcal{P},\quad \mathcal{A},\ \mathcal{Q},\ \mathcal{P} \text{ real},$$

$$\mathcal{T} = \begin{bmatrix} \mathcal{C} & -2\mathcal{K}_+ \\ 2\mathcal{K}_- & -{}^t\mathcal{C} \end{bmatrix},$$

$$\mathcal{C}^+ = {}^t\mathcal{C},\quad (\mathcal{K}_+)^+ = \mathcal{K}_-,$$

with the adjoint action of Sp(3, R) given by

$$g' \in \mathrm{Sp}(3,\mathbb{R}),\quad g = Rg'R^{-1},$$

$$\mathcal{T}' \to (g')^{-1}\mathcal{T}'g',\quad \mathcal{T} \to g^{-1}\mathcal{T}g.$$

The matrices $\mathcal{T}$ and $\mathcal{T}'$ were introduced in Refs. 6 and 8.

With the definitions for 6×6 matrices

$$q^* =: -K\,{}^tqK,\quad q^{\S} =: Mq^+M,\quad M = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix},$$

the conditions given in Definition 6.1 are equivalent to

$$(\mathcal{T}')^* = -\mathcal{T}',\quad \overline{\mathcal{T}'} = \mathcal{T}',\quad \mathcal{T}^* = -\mathcal{T},\quad \mathcal{T}^{\S} = \mathcal{T}.$$

Note the similarity of the matrices $\mathcal{T}'$, $\mathcal{T}$ to the operator-valued matrices of Definition 3.2. By use of the adjoint action as given in Definition 6.1, the determination of orbits on sp*(3, R) becomes equivalent to the search for standard forms of the matrices $\mathcal{T}'$ and $\mathcal{T}$. It was shown[6] that only the part with $\mathcal{T}$: $M\mathcal{T} \geqslant 0$ can arise in a moment map[21] from many-body phase space to sp*(3, R). For $M\mathcal{T} > 0$ the standard forms of $\mathcal{T}'$ and $\mathcal{T}$ were given as

$$\mathring{\mathcal{T}} = \begin{bmatrix} \sigma & 0 \\ 0 & -\sigma \end{bmatrix},\quad \mathring{\mathcal{T}}' = \begin{bmatrix} 0 & \sigma \\ -\sigma & 0 \end{bmatrix},$$

$$\sigma = (\sigma_i\delta_{ij}),\quad \sigma > 0.$$

We consider in detail the degenerate case $\sigma = \sigma_0 I$ and denote the corresponding orbits by ℓ^{σ_0}.

Proposition 6.2: The orbits ℓ^{σ_0} on sp*(3, R) characterized by the standard forms

$$\mathring{\mathcal{T}}' = \sigma_0\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},\quad \mathring{\mathcal{T}} = \sigma_0\begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}$$

have the properties (a) $\mathring{\mathcal{T}}'$ and $\mathring{\mathcal{T}}$ have the stability group U(3); and (b) the matrices $\mathcal{T}'$, $\mathcal{T}$ belonging to ℓ^{σ_0} have the property

$$\mathcal{T}'\mathcal{T}' = -\sigma_0^2 I,\quad \mathcal{T}\mathcal{T} = \sigma_0^2 I.$$

Proof: The stability group of $\mathring{\mathcal{T}}$ is easily determined from the adjoint action. The second property follows by writing, for example, for $\mathcal{T}$

$$\mathcal{T} = g^{-1}\mathring{\mathcal{T}}g,\quad \mathcal{T}\cdot\mathcal{T} = g^{-1}\mathring{\mathcal{T}}\mathring{\mathcal{T}}g = \sigma_0^2 I.$$ □

In Ref. 6, the orbits ℓ^{σ_0} were characterized by a complex parametrization of the coset $U(3)\backslash Sp(3,\mathbb{R})$. Here we use Proposition 2.5, replace the coset $U(3)\backslash Sp(3,\mathbb{R})$ by the coset $SO(3,\mathbb{R})\backslash GL_+(3,\mathbb{R})N^2$, and introduce for this coset the representation

$$c(s,Z) = g_2'(s^{-1})g_1'(Z),\quad s = {}^ts > 0,\quad Z = {}^tZ$$

in the notation of Definition 4.1. The first factor arises by factorizing the elements of $Gl_+(3,\mathbb{R})$ into products of an orthogonal and a positive definite symmetric matrix s^{-1}.

Proposition 6.3: The parameters s and Z provide coordinates for the orbit ℓ^{σ_0} of sp*(3, R). The matrix $\mathcal{T}'$ on these orbits has the blocks

$$\mathcal{Q} = \sigma_0 s^2,\quad \mathcal{A} = \sigma_0 s^2 Z,\quad \mathcal{P} = \sigma_0(Zs^2Z + s^{-2}),$$

The nondegenerate Poisson bracket on ℓ^{σ_0} for functions $\mathcal{F}$, $\mathcal{G}$ is given by

$$\{\mathcal{F},\mathcal{G}\}(s^2,Z) = \frac{1}{2\sigma_0}\sum_{l,k=1}^{3}\left[\left(\frac{\partial}{\partial s_{lk}^2}+\frac{\partial}{\partial s_{kl}^2}\right)\mathcal{F}\left(\frac{\partial}{\partial Z_{lk}}+\frac{\partial}{\partial Z_{kl}}\right)\mathcal{G} - \left(\frac{\partial}{\partial Z_{lk}}+\frac{\partial}{\partial Z_{kl}}\right)\mathcal{F}\left(\frac{\partial}{\partial s_{lk}^2}+\frac{\partial}{\partial s_{kl}^2}\right)\mathcal{G}\right].$$

Here we use derivatives with respect to s^2 which for $s > 0$ is in one-to-one correspondence to s. With this Poisson bracket, the functions $\mathcal{Q}$, $\mathcal{A}$, $\mathcal{P}$ generate the Poisson action of Sp(3, R) and yield a realization of the Lie algebra with structure constants given as in Definition 2.1.

Proof: The block form of $\mathcal{T}'$ follows from the computation of

$$\mathcal{T}' = (c(s,Z))^{-1}\mathring{\mathcal{T}}'c(s,Z).$$

The Poisson bracket can in principle be obtained by restricting a degenerate bracket to the orbit ℓ^{σ_0}. In practice it has been derived from the dequantization procedure described below in Proposition 6.5. □

The first-order differential operators given by $\{\mathcal{Q},\}$, $\{\mathcal{A},\}$, $\{\mathcal{P},\}$ generate the action of Sp(3, R) on the orbit ℓ^{σ_0}. These operators are completely different from the operators constructed in Sec. V, Propositions 5.2 and 5.3.

We shall now link the representation space L^{w_0} and the orbits ℓ^{σ_0}. To this purpose we define coherent states according to the general prescription of Perelomov[22] by acting with the unitary operators corresponding to the coset of the stability group U(3) on the lowest weight state in L^{w_0}.

Definition 6.4: The coherent states $|s,Z\rangle$ for the representation space L^{w_0} of Sp(3, R) are defined as

$$|s,Z\rangle = \exp\left[-i\frac{1}{2}\sum_{k,l=1}^{3} Z_{kl}\hat{Q}_{lk}\right] \times \exp\left[-i\frac{1}{2}\sum_{k,l=1}^{3}\theta_{lk}(\hat{A}_{kl}+\hat{A}_{lk})\right]|\{w_0 w_0 w_0\}\rangle$$

$$s = \exp\theta, \quad {}^t\theta = \theta.$$

Each coherent state is normalized and the scalar product is given by

$$\langle s',Z'|s,Z\rangle = (\det\lambda)^{-w_0},$$

$$\lambda = \tfrac{1}{2}[(s')^{-1}s + s's^{-1} + is'(Z'-Z)s].$$

Given a set of coherent states for a representation space of a Lie group, one can map the operators from the enveloping algebra to functions on the coset associated with the coherent states by taking these functions as expectation values of the operators. This map was studied[23] and associated with a Poisson bracket such that, for the elements of the Lie algebra, the image of the commutator becomes the Poisson bracket of the images of these operators. The construction of the Poisson bracket was given in Ref. 23 in terms of derivatives of the overlap of coherent states with respect to the parameters of the coset. This technique can be applied in the present case.

Proposition 6.5: Define a map from operators in the enveloping algebra of sp(3, R) on the representation space L^{w_0} to functions of (s,Z) by the prescription

$$\hat{Y} \to \mathscr{Y} = \langle s,Z|\hat{Y}|s,Z\rangle = \mathscr{Y}(s,Z).$$

This map determines functions on ℓ^{σ_0} for $\sigma_0 = w_0$, yields for elements $\hat{X}_\alpha, \hat{X}_\beta \in$ sp(3, R) the relations

$$\{\mathscr{X}_\alpha, \mathscr{X}_\beta\} = -i\langle s,Z|[\hat{X}_\alpha, \hat{X}_\beta]|s,Z\rangle,$$

and determines the basis of sp(3, R) in the form given in Proposition 6.3 for $\sigma_0 = w_0$.

Proof: The expectation values are best obtained by first evaluating expectation values of finite transformations and using them as generating functions. □

Note that in the map from operators to functions one selects the discrete set of orbits ℓ^{σ_0} such that $\sigma_0 = w_0$. We call this map a dequantization map since it associates to a quantum system with the dynamical group Sp(3, R) a classical system on a generalized phase space with a Poisson bracket. The time-dependent variational principle shows how the classical equations of motion are obtained from the quantum equations.[23]

The fundamental Poisson brackets in terms of the functions $\mathscr{Q}$ and Z become

$$\{\mathscr{Q}_{ij}, \mathscr{Q}_{rs}\} = 0, \quad \{Z_{ij}, Z_{rs}\} = 0,$$

$$\{\mathscr{Q}_{ij}, Z_{rs}\} = \delta_{ir}\delta_{js} + \delta_{is}\delta_{jr},$$

in complete analogy to the quantum commutators of the operators $\hat{Q}$ and $\hat{X}$ constructed in Sec. V, Proposition 5.2. The coset $SO(3,R)\backslash GL_+(3,R)$ parametrized by $\mathscr{Q}$ yields the generalized coordinates whereas the matrix Z provides the generalized momenta.

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The metaplectic group within the Heisenberg–Weyl ring

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The Heisenberg–Weyl ring contains the metaplectic group of canonical transforms acting unitarily on $\mathscr{L}^2(\mathscr{R})$. These ring elements are characterized through (i) the integral transform kernels, (ii) coset distributions, and (iii) classical functions under any quantization scheme. The isomorphism under group composition leads to several new relations involving twisted products and quantization of Gaussian classical functions. The Wigner inversion operator is a special central group element. It is shown that the only quantization scheme invariant under metaplectic transformations is the Weyl scheme. The structure studied here appears to be relevant to the study of wave optics with aberration.

I. INTRODUCTION

A *group ring* is the structure composed out of formal linear combinations of the group elements. The group multiplication law induces an operation of multiplication for ring elements; the group unit serves as a ring unit but, since no inverse under multiplication is assured, the structure is not a group, but a *ring*. The Heisenberg–Weyl algebra w and group W were introduced as foundations for quantum mechanics by Heisenberg[1] and Weyl,[2] respectively. The former lead to the representation of canonically conjugate observables (having the real line for its spectrum) by Schrödinger. (The requirement on the spectra of the algebra elements is partially circumvented in Weyl's approach.) The Stone-von Neumann theorem[3] assures us of the existence and uniqueness of the Schrödinger operators representing position and momentum.

The Heisenberg–Weyl group W in N dimensions has $2N+1$ generators, is nilpotent, is an extension of the group of translations of the phase space, and is a non-Abelian group with a nontrivial center. Its early association with quantum mechanics should not hide the fact that it has been most useful recently as a frame to describe wave systems—optical and radar—where a meaningful phase space and geometric (i.e., classical) limit exist.

One of the peculiar features of the Heisenberg–Weyl algebra w, is that its isomorphism group is larger than the group W of Heisenberg and Weyl. The endomorphism of the enveloping algebra $\overline{w}$ (factorized by $(\mathbb{H}\text{-}\mathbf{1})$, where $\mathbb{H}$ is the central generator) of the Heisenberg–Weyl algebra have been studied by Dixmier.[4] The Heisenberg–Weyl algebra can undergo *symplectic* real linear transformations in the position and momentum generators[5]; these are the linear canonical transformations in quantum mechanics studied by Moshinsky and Quesne,[6] who also inquired into the representation of these on the $\mathscr{L}^2(\mathscr{R}^N)$ Hilbert space of wave functions. On this space, the group has a two-valued representation that is faithful for the twofold cover of the symplectic group [$\mathrm{Sp}(2N,\mathscr{R})$ is infinitely connected], i.e., the *metaplectic* group $\mathrm{Mp}(2N,\mathscr{R})$ (see Ref. 7). The latter is a subgroup of the universal covering group $\overline{\mathrm{Sp}(2N,\mathscr{R})}$; $\mathrm{Sp}(2N,\mathscr{R}) \simeq \overline{\mathrm{Sp}(2N,\mathscr{R})}/\mathscr{Z}$.

For continuous groups the elements of the group ring may be characterized by a function over the group, which takes the place of generalized linear combination coefficients for the group elements. If, besides functions within some subspace of $\mathscr{L}^2(W)$ over the group manifold, we allow distributions—Dirac δ's and their derivatives up to arbitrarily high order, then the group ring $\mathscr{W}$ comes to contain the group W itself, its Lie algebra w, and its enveloping algebra $\overline{w}$. In this context one of us examined[8] some time ago the question of quantization in physics, using the fact that the Heisenberg–Weyl ring $\mathscr{W}$ contained all operators $\mathbf{A}$ one would wish to quantize, and that these could be described either through their group function $A(g)$, $g \in W$, or through their *integral-kernel* representative $A^{\times}(q,q')$, or through a *classical function* $a_{\phi}(q,p)$ in some quantization scheme ϕ. The integral kernels were derivatives of δ's and Hermiticity of the operators in $\mathscr{L}^2(\mathscr{R})$ was required.

Here we wish to use the rich structure of the Heisenberg–Weyl ring $\mathscr{W}$ to study another object, namely the metaplectic group $\mathrm{Mp}(2,\mathscr{R})$ of linear canonical transformations,[9] which lies within the ring. The set of these ring elements is characterized by a set of proper functions over the group, by integral transform kernels, and by classical functions. These compose under multiplication of ring elements as a group. The last two realizations, in particular, are interesting even as mathematical relations. For this reason, we work in $N=1$ dimension. The purpose in physics of these will be, in following papers, to treat wave optics with aberration. The Gaussian limit[10] of lens optics is served by the

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results obtained here, which come to describe the results of Nazarathy and Shamir,[11] who used canonical integral transforms. The group-theoretical treatment of wave optics with *aberration*[12] will need further structures within the Heisenberg–Weyl ring, which are under development.

In Sec. II we formally introduce the characteristics freely used above, and Sec. III describes the ring elements in terms of the three functions we have mentioned, particularly under multiplication. The metaplectic group is treated in Sec. IV and shown to contain among its elements the Fourier transform, the free-space propagation, the Gaussian lens transformation, and the Wigner operator (one of the two central elements of the ring). Section V ends showing that the only quantization scheme that is invariant under metaplectic transformations is the Weyl–McCoy rule.[13,14] This fact is probably crucial in the process of quantization (or waveization) of geometrical optics with aberration.

II. CAST OF CHARACTERS AND ROLES

We shall be dealing with the following mathematical objects, all named after Heisenberg and Weyl (HW): The HW algebra w, the HW universal enveloping algebra $\overline{w}$, the HW group W, and the HW ring $\mathscr{W}$. Succinct definitions follow.

The HW algebra w: This is a three-dimensional vector space generated by $\mathbb{Q}$, $\mathbb{P}$, and $\mathbb{H}$, with the commutator Lie bracket

$$[\mathbb{Q},\mathbb{P}] = i\mathbb{H}, \quad [\mathbb{Q},\mathbb{H}] = 0, \quad [\mathbb{P},\mathbb{H}] = 0 . \tag{2.1}$$

It is two-step nilpotent and $\mathbb{H}$ is the central generator. Due to the Stone–von Neumann theorem,[3] the generic Hermitian representation of w is the usual Schrödinger representation on a space of smooth functions:

$$(\mathbb{Q}f)(q) = qf(q), \quad (\mathbb{P}f)(q) = -i\hbar\frac{df(q)}{dq},$$
$$(\mathbb{H}f)(q) = \hbar f(q), \tag{2.2}$$

where $\hbar \in \mathscr{R}$ labels the representation. We write $\hbar = \lambda/2\pi$ in optics and $\hbar = \hbar$ in quantum mechanics.

The HW enveloping algebra $\overline{w}$: The generators of w are multiplied (noncommutatively) to form monomials $\mathbb{Q}^m\mathbb{P}^n\mathbb{H}^k$, on which the commutator Lie bracket acts distributively through the Leibnitz identity. These monomials generate an infinite-dimensional algebra $\overline{w}$ under the commutator. Of course, $w \subset \overline{w}$.

Within $\overline{w}$ we also have a *symplectic* $\mathrm{sp}(2,\mathscr{R})$ subalgebra, generated by

$$\mathbb{X}^1_{+1} := \mathbb{P}^2, \quad \mathbb{X}^1_0 := \tfrac{1}{2}(\mathbb{P}\mathbb{Q} + \mathbb{Q}\mathbb{P}), \quad \mathbb{X}^1_{-1} := \mathbb{Q}^2 , \tag{2.3a}$$

with the well-known commutation relations

$$[\mathbb{X}^1_0,\mathbb{X}^1_{\pm 1}] = \pm 2i\hbar\mathbb{X}^1_{\pm 1}, \quad [\mathbb{X}^1_{+1},\mathbb{X}^1_{-1}] = -4i\hbar\mathbb{X}^1_0 . \tag{2.3b}$$

When writing down the "basic monomials," we may do it (i) in *standard* order, i.e., all $\mathbb{Q}$'s to the left of all $\mathbb{P}$'s as $\mathbb{Q}^m\mathbb{P}^n$; (ii) in *antistandard* order, i.e., all $\mathbb{Q}$'s to the right of all $\mathbb{P}$'s as $\mathbb{P}^n\mathbb{Q}^m$; (iii) in *symmetrized* order;[13] i.e., one-half of (i) plus (ii); (iv) in Weyl order, i.e., the sum of all permutations of the $\mathbb{Q}$'s and $\mathbb{P}$'s considered as individual objects, divided by their total factorial (the explicit expressions furnished by McCoy[14] will be given in the next section); and (v) any of an infinity of orderings, defined by Cohen's[15] ordering function ϕ, which will be given below.

The HW group W: The Lie group W generated by w has elements ω, which may be parametrized[8] through

$$\omega(x,y,z) := \exp i(x\mathbb{Q} + y\mathbb{P} + z\mathbb{H})$$
$$= \exp(ix\mathbb{Q})\exp(iy\mathbb{P})\exp(i[z + \tfrac{1}{2}xy]\mathbb{H})$$
$$= \exp(iy\mathbb{P})\exp(ix\mathbb{Q})\exp(i[z - \tfrac{1}{2}xy]\mathbb{H}) , \tag{2.4a}$$

and have the composition rule

$$\omega(x_1,y_1,z_1)\omega(x_2,y_2,z_2)$$
$$= \omega(x_1 + x_2, y_1 + y_2, z_1 + z_2 + \tfrac{1}{2}[y_1x_2 - x_1y_2]) . \tag{2.4b}$$

The group unit is $e = \omega(0,0,0)$ and the inverse $\omega(x,y,z)^{-1} = \omega(-x,-y,-z)$; the Haar measure is $d\omega = dx\,dy\,dz$. The space of self-adjoint irreducible representations of $w,\hat{w}$ is parametrized by $\hbar \in \mathscr{R}$, with Plancherel measure $d\hat{\omega}(\hbar) = |\hbar|\,d\hbar/4\pi^2$.

In the Schrödinger realization, where the algebra generators are (2.2), the unitary group action on functions $f \in \mathscr{L}^2(\mathscr{R})$ is given by

$$[\omega(x,y,z):f](q) = \exp i(qx + \hbar[z + \tfrac{1}{2}xy])f(q + \hbar y) . \tag{2.5}$$

The inner product in $\mathscr{L}^2(\mathscr{R})$ of a function f_1 and $\omega:f_2$ yields the bilinear functional on W given by

$$H(f_1,f_2;x,y,z) := (f_1,\omega(x,y,z):f_2)$$
$$= \int dq\, f_1(q)^*[\omega(x,y,z):f_2](q)$$
$$= e^{i\hbar z}\int dq\, f_1(q - \tfrac{1}{2}\hbar y)^* e^{iqx} f_2(q + \tfrac{1}{2}\hbar y) . \tag{2.6}$$

This is the *cross correlation* of f_1 and f_2; $\hbar y$ is the spatial correlation parameter between the two functions and x the *frequency* correlation parameter. When f_1 and f_2 are allowed to run over the elements $\{f_\mu\}$ of a *basis* of $\mathscr{L}^2(\mathscr{R})$ (denumerable or generalized), then $D^\hbar_{\mu\nu}(\omega) := H(f_\mu,f_\nu;\omega)$ constitute the (matrix or integral kernel) *representations* of W. For the generalized eigenfunctions $\delta(q - q_0)$ of $\mathbb{Q}$, this yields the representation *kernel*

$$D^\hbar_{qq'}(\omega(x,y,z))$$
$$= \delta(\hbar y - [q' - q])\exp i(\hbar z + \tfrac{1}{2}x[q + q']) , \tag{2.7}$$

which basically one obtains from (2.5). It is unitary and irreducible. The generalized eigenfunctions of $\mathbb{P}$, $(2\pi)^{-1/2}e^{ipq/\hbar}$, $p \in \mathscr{R}$, may be used to yield [Ref. 8, Eq. (2.24)] $D^\hbar_{pp'}(\omega)$. For the harmonic oscillator eigenfunctions of $\frac{1}{2}(\mathbb{P}^2 + \mathbb{Q}^2)$ one obtains [Ref. 8, Eq. (2.43) with the exponent sign correction remarked by Dahl, Ref. 16, Eq. (35)] a half-infinite matrix.

The HW ring $\mathscr{W}$: The elements of W are taken as the formal basis for a linear vector space $\mathscr{W}$, which thus inherits the multiplication law, and whose elements are in the (Haar, formal) integrals

$$\mathbb{A} = \int_W d\omega\, A(\omega)\omega$$
$$= \int dx\,dy\,dz\, A(x,y,z)\exp i(x\mathbb{Q} + y\mathbb{P} + z\mathbb{H}) , \tag{2.8}$$

with $A(\omega)$ a distribution over W called[8] the *group representative* of $\mathrm{A}\in\mathscr{W}$. The elements of $\mathscr{W}$ may be linearly combined and multiplied but, since no inverse A^{-1} is assured for every A, the structure of $\mathscr{W}$ is that of a *ring*.

III. DESCRIPTION OF THE HW RING ELEMENTS

When the elements of $\mathscr{W}$ act on functions in $\mathscr{L}^2(\mathscr{R})$ carrying a definite representation $\hbar$ of W, the third generator H is simply replaced by the real number $\hbar$. The integration over z in (2.8) may be thus performed defining the *coset distribution* over the space W/Z, Z being the one-parameter central subgroup generated by H, as

$$\hat{A}^{\hbar}(x,y) := \int_{\mathscr{R}} dz\, A(\omega(x,y,z)e^{i\hbar z}. \tag{3.1}$$

We shall henceforth drop $\hbar$ as an index in the quantities which bear it. We take $\hbar>0$. The ring element (2.8) appears as

$$\begin{aligned}\mathrm{A} &= \int_{\mathscr{R}^2} dx\,dy\,\hat{A}(x,y)\exp i(x\mathbb{Q}+y\mathbb{P})\\ &= \int_{\mathscr{R}^2} dx\,dy\,\hat{A}_{\mathrm{s}}(x,y)\exp(ix\mathbb{Q})\exp(iy\mathbb{P})\\ &= \int_{\mathscr{R}^2} dx\,dy\,\hat{A}_{a}(x,y)\exp(iy\mathbb{P})\exp(ix\mathbb{Q}).\end{aligned} \tag{3.2a}$$

We have also defined the *standard* and *antistandard* coset distributions, $\hat{A}_{\mathrm{s}}, \hat{A}_{\mathrm{a}}$, over the space W/Z using (2.4a), that is

$$\hat{A}_{\mathrm{s}}(x,y) := \hat{A}(x,y)e^{i\hbar xy/2},\quad \hat{A}_{\mathrm{a}}(x,y) := \hat{A}(x,y)e^{-i\hbar xy/2}. \tag{3.2b}$$

We shall associate the coset distribution $\hat{A}(x,y)$ with the name of Weyl and write it as $\hat{A}_{\mathrm{w}}(x,y)$ when convenient.

The names of "standard," "antistandard," and "Weyl" should bring to mind the quantization-scheme and operator-ordering problems. In this paper we *start* from a ring element $\mathrm{A}\in\mathscr{W}$ whose action on $\mathscr{L}^2(\mathscr{R})$ is that of an integral transform

$$\begin{aligned}(\mathrm{A}:f)(q) &= \int_{\mathscr{R}^2} dx\,dy\,\hat{A}(x,y)\int_{\mathscr{R}} dq'\,D_{qq'}(\omega(x,y,0))f(q')\\ &=: \int_{\mathscr{R}} dq'\,A(q,q')f(q'),\end{aligned} \tag{3.3}$$

with an *integral kernel* $A(q,q')$, which will be well defined, and in terms of which we shall find the coset distributions in the following way:

$$\begin{aligned}A(q,q') &:= \int_{\mathscr{R}^2} dx\,dy\,\hat{A}(x,y)D_{qq'}(\omega(x,y,0))\\ &= \frac{1}{|\hbar|}\int_{\mathscr{R}} dx\,\hat{A}(x,[q-q']/\hbar)\exp i(\tfrac{1}{2}[q+q']),\end{aligned} \tag{3.4a}$$

$$\hat{A}(x,y) = \frac{|\hbar|}{2\pi}\int_{\mathscr{R}} dq\,A(q-\tfrac{1}{2}\hbar y, q+\tfrac{1}{2}\hbar y)e^{-ixq}. \tag{3.4b}$$

We may now speak of (at least) three *classical functions* $a_c(q,p)$, the Weyl, standard, and antistandard classical functions, denoted by the subindices c = W, s, or a, just as their corresponding coset distributions. The former are defined as the Fourier transforms of the latter:

$$\hat{A}_c(x,y) = \frac{1}{4\pi^2}\int_{\mathscr{R}^2} dq\,dp\,a_c(q,p)\exp(-i[xq+yp]), \tag{3.5}$$

with its well-known inverse (which simply changes the sign of the exponent and removes the $1/4\pi^2$ factor). Since we choose to regard the integral kernel as that which primarily defines the ring element, we write the composition of (3.2b), (3,4), and (3.5) to find the three classical functions as

$$a_{\mathrm{w}}(q,p) = \int_{\mathscr{R}} dr\,A(q+\tfrac{1}{2}r, q-\tfrac{1}{2}r)e^{-ipr/\hbar}, \tag{3.6a}$$

$$a_{\mathrm{s}}(q,p) = e^{-iqp/\hbar}\int dq'\,A(q,q')e^{iq'p/\hbar}, \tag{3.6b}$$

$$a_{\mathrm{a}}(q,p) = e^{iqb/\hbar}\int dq'\,A(q',q)e^{-iq'p/\hbar}. \tag{3.6c}$$

We should remind the reader that to quantize in the standard (antistandard) scheme means to propose functions a_{s} (resp. a_{a}) of phase space (q,p) and to replace the monomials (in the Taylor expansion, if need be) by the same functions of the Schrödinger operators $\mathbb{Q}$ and $\mathbb{P}$, all $\mathbb{Q}$'s being left (resp. right) of all $\mathbb{P}$'s. Rather trivially, thus we have a linear mapping $\mathbf{\Omega}_{\mathrm{s}}$ (resp. $\mathbf{\Omega}_{\mathrm{a}}$) between functions $a(q,p)$ of phase space and elements $\mathrm{A}\in\mathscr{W}$ (which also lie in $\bar{w}$), which effect

$$\mathbf{\Omega}_{\mathrm{s}}(q^m p^n) = \mathbb{Q}^m\mathbb{P}^n, \tag{3.7a}$$

$$\mathbf{\Omega}_{\mathrm{a}}(q^m p^n) = \mathbb{P}^n\mathbb{Q}^m. \tag{3.7b}$$

The Weyl quantization scheme $\mathbf{\Omega}_{\mathrm{w}}$ is not so trivial, but the correspondence

$$\begin{aligned}\mathbf{\Omega}_{\mathrm{w}}(q^m p^n) &= \frac{1}{2^m}\sum_{k=0}^{m}\binom{m}{k}\mathbb{Q}^{m-k}\mathbb{P}^n\mathbb{Q}^k\\ &= \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\mathbb{P}^{n-k}\mathbb{Q}^m\mathbb{P}^k\end{aligned} \tag{3.7c}$$

has been given by McCoy,[14] as well as the next displayed equation. Basically, the Weyl–McCoy scheme permutes all operators and divides by the factorial of their number.

In what appears to be a characterization of all such schemes $\mathbf{\Omega}_{\phi}$, Cohen[15] introduced an *ordering* function $\phi(u)$, defining $\hat{A}_{\phi}(x,y) = \hat{A}_{\mathrm{w}}(x,y)\phi(\frac{1}{2}\hbar xy)$ and, through (3.5), a corresponding coset distribution to be entered in (3.2) to yield the ring element. Written in standard order, this is

$$\begin{aligned}\mathbf{\Omega}_{\phi}(q^m p^n) = &\sum_{k=0}^{\min(m,n)}\binom{m}{k}\binom{n}{k}k!\\ &\times\phi_k(-\tfrac{1}{2}i\hbar)^k\mathbb{Q}^{m-k}\mathbb{P}^{n-k},\end{aligned} \tag{3.7d}$$

$$\phi_k := \sum_{l=0}^{k}\binom{k}{l}(-2i)^l\frac{\partial^l\phi(u)}{\partial u^l}\bigg|_{u=0}. \tag{3.7d'}$$

In terms of Cohen functions, the Weyl quantization scheme (3.7d) corresponds to $\phi_{\mathrm{w}}(u)=1$, while the standard and antistandard schemes come from $\phi_{\mathrm{s}}(u)=e^{iu}$ and $\phi_{\mathrm{a}}(u)=e^{-iu}$. The often-used Born–Jordan[17] and symmetrization[13] schemes correspond to $\phi(u)=u^{-1}\sin u$ and $\cos u$, respectively.

There are restrictions on the Cohen function $\phi(u)$, though. If one requires the usual quantization for q^m to $\mathbb{Q}^m$ and p^n to $\mathbb{P}^n$, as demanded by Dirac[18] and von Neumann,[18,19] then $\phi(0)=1$ (so $\phi_0=1$). If one wants qp to have its correspondence with $\frac{1}{2}(\mathbb{QP}+\mathbb{PQ})$, as in (2.3), then $\phi'(0)=0$ (so

$\phi_1 = 1$ also). This last requirement is, of course, violated by the s and a schemes, but it is not a great fault; we shall use it below.

The classical monomials $q^m p^n$, under Fourier transformation inverse to (3.6), yield[8] derivatives of Dirac δ's and/or powers in $q+q'$ and $q-q'$ for the integral transform kernels (so they become differential operators). In this article, we are mostly interested in a *group* of ring elements whose kernels are proper functions of q and q'.

The inner product in $\mathscr{L}^2(\mathscr{R})$ allows us to introduce the *adjoint* of a ring element A, as that $\mathbb{B} = :\mathbb{A}^\dagger$, which satisfies $(\mathbb{B}f,g) = (f,\mathbb{A}g)$ for all f and g in a dense subspace of $\mathscr{L}^2(\mathscr{R})$. The integral kernel of $\mathbb{B}$ is, from (3.3), $B(q,q') = A(q',q)^*$. The coset distributions of these elements relate, from (3.4b), as $\hat{B}(x,y) = \hat{A}(-x,-y)^*$, while, for any Cohen function ϕ, $\hat{B}_\phi(x,y) = \hat{A}_\phi(-x,-y)^*(\phi/\phi^*)$. From (3.6a), thus, $b_\phi(q,p) = a_\phi(q,p)^*$ for all classical functions with a *real* Cohen function $\phi(\frac{1}{2}\hbar xy)$. When the quantization-scheme function is not real, one remains, in general, with a convolution integral relation between $b_\phi(q,p)$ and $a_\phi(q,p)$. Between the standard and antistandard quantization schemes, for which ϕ_s, ϕ_a are not real but $e^{i\hbar xy/2}$, $e^{-i\hbar xy/2}$, one has $b_s(q,p) = a_a(q,p)^*$. Hence, *if* a real classical function is to quantize to a self-adjoint operator, it is *necessary* that the Cohen function ϕ be real.

Quantum mechanics is mostly preoccupied with Heisenberg–Weyl ring elements which are self-adjoint. In this work we shall regard *unitary* ring elements, i.e., those which when multiplied by their adjoint—in either order—yield back the identity operator. To detail multiplication we turn now to find explicit forms for the three views we have on ring elements through their integral kernel, coset distribution, and classical function.

Let $\mathbb{C} = \mathbb{A}\mathbb{B}$ be the ring element that is the product of A and B. From (3.3) it follows that the representing integral kernels compose simply as

$$C(q,q') = \int_{\mathscr{R}} dq''\, A(q,q'')B(q'',q')\,. \tag{3.8}$$

The corresponding functions over the group follow a convolution product[8] and the coset distributions (3.1) then compose, from (3.4), as

$$\hat{C}(x,y) = \int_{\mathscr{R}^2} dx'\,dy'\,\hat{A}(x',\tfrac{1}{2}y+y')\hat{B}(x-x',\tfrac{1}{2}y-y') \times\exp\left[i\tfrac{1}{2}\hbar(xy'-x'y+\tfrac{1}{2}xy)\right]. \tag{3.9}$$

Similarly, from (3.6) and its inversion follows, for the classical function (in the Weyl scheme),

$$\begin{aligned} c_W(q,b) &= \frac{1}{\pi^1|\hbar|^2}\int_{\mathscr{R}^4} dq'\,dq''\,dp'\,dp''\,a_W(q',p')b_W(q'',p'') \\ &\quad\times\exp[2i\{q(p'-p'')+q'(p''-p)+q''(p-p')\}/\hbar] \\ &= \sum_{m=0}^{\infty}\frac{(\hbar/2)^m}{m!}\left(\frac{\partial}{\partial q'}\frac{\partial}{\partial p''}-\frac{\partial}{\partial q''}\frac{\partial}{\partial p'}\right)^m \\ &\quad\times a_W(q',p')b_W(q'',p'')\big|_{\substack{q'=q''=q\\ p'=p''=p}}. \end{aligned} \tag{3.10a}$$

For the classical functions which quantize in the standard scheme, one has

$$\begin{aligned} c_s(q,p) &= \frac{1}{2\pi|\hbar|}\int_{\mathscr{R}^2} dq'\,dp'\,a_s(q,p')b_s(q',p) \\ &\quad\times\exp[-i(q-q')(p-p')/\hbar] \\ &= \sum_{m=0}^{\infty}\frac{(-i\hbar)^m}{m!}\left(\frac{\partial}{\partial q'}\frac{\partial}{\partial p'}\right)^m a_s(q,p')b_s(q',p)\big|_{\substack{q'=q\\ p'=p}}, \end{aligned} \tag{3.10b}$$

and for the classical functions in the antistandard scheme,

$$\begin{aligned} c_a(q,p) &= \frac{1}{2\pi|\hbar|}\int_{\mathscr{R}^2} dq'\,dp'\,a_a(q,p')b_a(q',p) \\ &\quad\times\exp[i(q-q')(p-p')/\hbar] \\ &= \sum_{m=0}^{\infty}\frac{(i\hbar)^m}{m!}\left(\frac{\partial}{\partial q'}\frac{\partial}{\partial p'}\right)^m a_a(q',p)b_a(q,p')\big|_{\substack{q'=q\\ p'=p}}. \end{aligned} \tag{3.10c}$$

These equations between the classical functions define so-called twisted products. Twisted products are known from the theory of operator symbols[20] (pseudodifferential operators[21]) in mathematical literature and phase-space methods in physical literature.[22,23] The second members in the last three equations are simplest to apply to polynomials (and special rational) functions, the case in which the sum is finite. Twisted products have been also applied for calculations in noncommutative algebra by use of computer-algebra systems.[24,25] The integral form we offer seems to be most appropriate for the cases where the factor functions are exponentials or Gaussians.

The unit element $\mathbb{E}$ in the ring $\mathscr{W}$ is described by an integral kernel $E(q,q') = \delta(q-q')$ [see (3.3)], a coset distribution $\hat{E}(x,y) = \delta(x)\delta(y)$ [see (3.4)], and a classical function $a_\phi(q,p) = 1$ in all quantization schemes ϕ. This may be used to verify the coefficients in (3.10).

Unitary ring elements are described by unitary integral kernels in the usual $\mathscr{L}^2(\mathscr{R})$ sense.

The HW group W is contained in the ring $\mathscr{W}$; the describing distribution over the group [see (2.8)] of a group element $G_0 = \omega(x_0,y_0,z_0)$ is $G_0(\omega) = \delta_W(\omega_0\omega^{-1}) := \delta(x-x_0)\delta(y-y_0)\delta(z-z_0)$; from (3.1), the coset distribution is $\hat{G}_0(x,y) = \delta(x-x_0)\ \delta(y-y_0)e^{i\hbar z_0}$, from (3.4a) the integral kernel is $G_0(q,q') = D_{qq'}(\omega(x_0,y_0,z_0))$. The Weyl classical function of G_0 is $g_{0W}(g,p) = \exp i(x_0q + y_0p + \hbar z_0)$, while any other scheme function ϕ yields a well-defined classical function $g_{0\phi}(q,p) = g_{0W}(q,p)\phi(\frac{1}{2}\hbar x_0y_0)$ for this subset of ring elements. Multiplication in W may be followed in the classical functions for the s, a, and W cases through the integral or twisted product composition expressions (3.10).

In the next section we shall introduce the set of ring elements that constitute a metaplectic group. It should be noted that here we have generally a *fixed* ring element (defined through its integral kernel or coset distribution) and a whole ϕ range of "classical" functions, the Weyl among them. This is different from the usual stance in quantum mechanics, where one has a classical function to start with, and a ϕ range of elements of the ring, among which we try to choose.

IV. CANONICAL TRANSFORMS AS RING ELEMENTS

We may be sure the HW ring $\mathscr{W}$ contains other subsets which are groups, besides W itself. The enveloping algebra $\overline{w}$, we noted in Sec. II, contains the symplectic algebra $\mathrm{sp}(2,\mathscr{R})$, explicitly given by (2.3). The embeddings of $\mathrm{sp}(2,\mathscr{R})$ in $\overline{w}$ [and of $\mathrm{sp}(2N,\mathscr{R})$ in the generalization of $\overline{w}$ to N canonical pairs $(\mathbb{Q}_1,\ldots,\mathbb{Q}_N,\mathbb{P}_1,\ldots,\mathbb{P}_N)$ and in its quotient division ring] have been systematically studied.[26] Moreover, embeddings (canonical realizations) have been constructed filling the gap between minimal and maximal (with respect to the number N of canonical pairs) canonical (Schurean, anti-Hermitian, nonequivalent) realizations.[26]

Now, integral transform representations[27] of the [universal cover $\overline{\mathrm{Sp}(2,\mathscr{R})}$ of the] symplectic group $\mathrm{Sp}(2,\mathscr{R})$ on $\mathscr{L}^2(\mathscr{R})$ are known for some time under the name of canonical transforms.[6,9] They are special in that they are generated by second-order differential operators. If the generators are (2.3a) and the space is $\mathscr{L}^2(\mathscr{R})$, the representation is called the *oscillator* (or metaplectic) representation. It is not irreducible, but consists of a direct sum of the lower-bound discrete series $D^+_{1/4}$ and $D^+_{3/4}$ irreducible representations in the notation of Bargmann.[27,28] The integral transform operators $\mathbb{C}_M$, which act adjointly on w as the linear transformation

$$\mathbb{C}_{\mathbf{M}}\begin{pmatrix}\mathbb{Q}\\ \mathbb{P}\end{pmatrix}\mathbb{C}_{\mathbf{M}}^{-1}=\mathbf{M}^{-1}\begin{pmatrix}\mathbb{Q}\\ \mathbb{P}\end{pmatrix} \tag{4.1a}$$

(using an obvious vector notation and not changing the central element), are specified through their integral kernel,[6,9] which depends on the matrix parameters of

$$\mathbf{M}=\begin{pmatrix}a & b\\ c & d\end{pmatrix},\quad ad-bc=1\,. \tag{4.1b}$$

The integral kernels are given by

$$C_{\mathbf{M}}(q,q')=\begin{cases}\dfrac{e^{-i\pi/4}}{\sqrt{2\pi b\hbar}}\exp\left[\dfrac{i(dq^2-2qq'+aq'^2)}{2b\hbar}\right], & b\neq 0\,,\\ (1/\sqrt{a})e^{icq^2/2a\hbar}\delta(q-q'/a)\,, & b=0\,.\end{cases} \tag{4.1c}$$

For lower-triangular matrices ($b=0$), the integral kernels become one of the sequences leading to a Dirac δ, and the integral transform becomes a Lie transformation (with multiplier factor). This subgroup is generated by the first-order differential operators in (2.3a), $\mathbb{X}^1_0$ generating the scale transformations and $\mathbb{X}^1_{-1}$ generating the multiplier.

Through the integral kernel composition (3.8), it follows that the ring elements (4.1) have the composition property

$$\mathbb{C}_{\mathbf{M}_1}\mathbb{C}_{\mathbf{M}_2}=\sigma(\mathbf{M}_1,\mathbf{M}_2)\mathbb{C}_{\mathbf{M}}\,,\quad \mathbf{M}=\mathbf{M}_1\mathbf{M}_2\,, \tag{4.2a}$$

where σ is a *sign* given by

$$\sigma(\mathbf{M}_1,\mathbf{M}_2)=\exp\left[\frac{i\pi}{4}\left(\operatorname{sgn} b-\operatorname{sgn} b_1-\operatorname{sgn} b_2+\operatorname{sgn}\frac{b}{b_1b_2}\right)\right]. \tag{4.2b}$$

This sign is quite fundamental and it may be observable. It may be a wave-mechanics counterpart of spin, for here it is the symplectic group $\mathrm{Sp}(2,\mathscr{R})$, which is doubly covered. To uncover its significance, consider the ($\hbar=1$) harmonic oscillator Hamiltonian $\mathbb{H}=\frac{1}{2}(\mathbb{P}^2+\mathbb{Q}^2)+\frac{1}{2}(\mathbb{X}^1_{+1}+\mathbb{X}^1_{-1})$, which lies in $\overline{w}$ and exponentiate it. This yields a line of integral transforms

$$e^{i\alpha\mathbb{H}}=\mathbb{C}\begin{pmatrix}\cos\alpha & -\sin\alpha\\ \sin\alpha & \cos\alpha\end{pmatrix},$$

where for $\alpha=\pi/2$ we have the inverse Fourier transform *times* $e^{+i\pi/4}$. For $\alpha=\pi$ we have the square of this, which is $e^{i\pi/2}$ times the inversion operator; $\alpha=3\pi/2$ corresponds to $e^{3i\pi/4}$ times the Fourier transform, and for $\alpha=2\pi$ we have the operator $-\mathbf{1}$, which is the unit ($\mathbf{1}=\mathbb{C}_{\mathbf{1}}$) operator times -1. When $\mathbb{C}_{\mathbf{M}}$ acts *adjointly* on w, this yields the transformation $(-\mathbf{1})\mathbb{X}(-\mathbf{1})^{-1}=\mathbb{X}$, which is an identity transformation of the algebra, but not for functions in $\mathscr{L}^2(\mathscr{R})$, where $-\mathbf{1}$ acts. It is only when we let $\alpha=4\pi$ that we obtain back the unit operator in $\mathscr{L}^2(\mathscr{R})$. On $\mathscr{L}^2(\mathscr{R})$ we thus have a group of operators that is the double cover of the circle matrices

$$\begin{pmatrix}\cos\alpha & -\sin\alpha\\ \sin\alpha & \cos\alpha\end{pmatrix}.$$

When Bargmann[27] described the connectivity properties of the Lorentz group (in three dimensions) SO(2,1), he also introduced a proper parametrization of the metaplectic group, which for fourth-integer k, D^+_k representations are faithful. For our purposes here we shall not need the composition formula (4.2a), and it suffices to consider group elements near the identity of the metaplectic group, corresponding to elements near the symplectic group identity element. In this regard it is helpful to note that $\mathbb{C}_{\mathbf{M}}$ is a Hilbert–Schmidt operator when its integral kernel has parameters a, b, c, d with small imaginary parts such that the integral kernel is a decreasing (rather than increasing) Gaussian, i.e., for $\mathrm{Im}\,(a/b)>0$. For real $a>0$ we can ascribe to b a small negative imaginary part, so that the limit of real parameters a, b, c, d can be approached from b's in the *lower-half complex plane*. In that case, the argument of positive b is zero and that of negative b is $-\pi$. When b vanishes from negative values (as when we followed the Fourier circle above), then a can be thought to be constrained to the lower-half plane (so $a<0$ means $\arg a=-\pi$); when b vanishes from positive values, a is contrained to the upper-half plane (so $a<0$ means $\arg a=+\pi$).

In order to investigate the properties of the coset distributions and classical functions of the ring elements $\mathbb{C}_{\mathbf{M}}$ we use integral kernels we have defined above. The following integrals (regularized for real values of the parameters) are useful:

$$I(R,S):=\int_{\mathscr{R}}dx\,\exp i(Rx^2+Sx)=e^{i\pi/4}\sqrt{\frac{\pi}{R}}\exp(-iS^2/4R)\,,\quad \mathrm{Im}\,R\geqslant 0\,, \tag{4.3a}$$

$$I(A,B,C,D,E) := \int_{\mathscr{R}^2} dx\,dy \exp i(Ax^2 + Bxy + Cy^2 + Dx + Ey) = \frac{2\pi i}{\sqrt{4AC - B^2}} \exp\left(- i\frac{D^2C + E^2A - EBD}{4AC - B^2}\right),$$

$$\operatorname{Im} A \geqslant 0, \quad \operatorname{Im}(C - B^2/4A) \geqslant 0, \quad \operatorname{Im} C \geqslant 0, \quad \operatorname{Im}(A - B^2/4C) \geqslant 0. \tag{4.3b}$$

From (3.4b) we find the coset distribution of $\mathbb{C}_{\mathrm{M}}$:

$$\hat{C}_{\mathrm{M}}(x,y) = \begin{cases} \dfrac{1}{2\pi\hbar\sqrt{a+d-2}} \\ \quad \times \exp\left(i\dfrac{-bx^2 + (a-d)xy + cy^2}{\hbar\, 2(a+d-2)}\right), \\ \quad b \neq 0, \\ \dfrac{1}{2\pi\hbar}\dfrac{\sqrt{a}}{a-1} \\ \quad \times \exp\left(i\hbar\left[\dfrac{cay^2}{2(a-1)^2} + \dfrac{1}{2}\dfrac{a+1}{a-1}xy\right]\right), \\ \quad b = 0. \end{cases} \tag{4.4}$$

The Weyl, standard, and antistandard classical functions are obtained as

$$C_{\mathrm{M,w}}(q,p) = \frac{2}{\sqrt{a+d+2}} \times \exp\left(\frac{2i}{\hbar(a+d+2)}[-bp^2 + (d-a)pq + cq^2]\right), \tag{4.5a}$$

$$C_{\mathrm{M,s}}(q,p) = \frac{1}{\sqrt{a}} \exp\left(\frac{i}{2a\hbar}[-bp^2 + 2(1-a)pq + cq^2]\right), \tag{4.5b}$$

$$C_{\mathrm{M,a}}(q,p) = \frac{1}{\sqrt{d}} \exp\left(\frac{i}{2d\hbar}[-bp^2 + 2(d-1)pq + cq^2]\right). \tag{4.5c}$$

The Weyl classical function as presented above reproduces correctly the results of Combe *et al.*[29] and Burdet and Perrin[30] contained in the metaplectic group. The product composition is (3.10a), (3.10b), and (3.10c), respectively.

The Lie algebra corresponding to the integral kernel action of $\mathbb{C}_{\mathrm{M}}$ on $\mathscr{L}^2(\mathscr{R})$ yields up-to-second-order differential operators, and $\mathbb{C}_{\mathrm{M}}$ may be written directly as the exponential of second-order operators in various alternative forms using the product (4.2); similarly, as an integral over exponentials of first-order operators we may use (3.2)–(4.4). We thus obtain

$$\begin{aligned} &\mathbb{C}\begin{pmatrix} a & b \\ c & d \end{pmatrix} \\ &= \exp\left(-\frac{ib}{2d\hbar}\mathbb{P}^2\right)\exp\left(i\ln d\cdot\frac{1}{2\hbar}[\mathbb{PQ} + \mathbb{QP}]\right) \\ &\quad \times \exp\left(\frac{ic}{2d\hbar}\mathbb{Q}^2\right) \\ &= \exp\left(\frac{ic}{2a\hbar}\mathbb{Q}^2\right)\exp\left(-i\ln a\cdot\frac{1}{2\hbar}[\mathbb{PQ} + \mathbb{QP}]\right) \\ &\quad \times \exp\left(\frac{-ib}{2d\hbar}\mathbb{P}^2\right) \\ &= \exp\left(i\frac{\operatorname{arccosh}\frac{1}{2}(a+d)}{\hbar\sqrt{(a+d)^2-4}}\right. \\ &\quad \left.\times\left[b\mathbb{P}^2 + \frac{1}{2}(a-d)(\mathbb{PQ} + \mathbb{QP}) - c\mathbb{Q}^2\right]\right) \\ &= \frac{\hbar}{2\pi\sqrt{a+d-2}}\int_{\mathscr{R}^2} dx\,dy \\ &\quad \times\exp\left(i\frac{-bx^2 + [a-d]xy + cy^2}{\hbar\, 2(a+d-2)}\right) \\ &\quad \times\exp i(x\mathbb{Q} + y\mathbb{P}), \end{aligned} \tag{4.6}$$

as the Weyl, standard, and antistandard quantization of (4.5a), (4.5b), and (4.5c), respectively.

Particularizing, we may obtain several interesting relations. The exponential function of qp in different quantization schemes, expressed in terms of the anticommutator $\frac{1}{2}(\mathbb{PQ} + \mathbb{QP})$, is

$$\begin{aligned} &\mathbf{\Omega}_{\mathrm{w}}(e^{ixqp/\hbar}) \\ &\quad = \frac{1}{\sqrt{1-(x/2)^2}} \exp\left[2i\arctan\frac{x}{2}\cdot\frac{1}{2}(\mathbb{PQ} + \mathbb{QP})\right], \\ &\mathbf{\Omega}_{\mathrm{s}}(e^{1xqb/\hbar}) \\ &\quad = \frac{1}{\sqrt{1+x}} \exp\left[i\ln(1+x)\cdot\frac{1}{2}(\mathbb{PQ} + \mathbb{QP})\right], \\ &\mathbf{\Omega}_{\mathrm{a}}(e^{ixqp/\hbar}) \\ &\quad = \frac{1}{\sqrt{1-x}} \exp\left[-i\ln(1-x)\cdot\frac{1}{2}(\mathbb{PQ} + \mathbb{QP})\right]. \end{aligned} \tag{4.7}$$

The (normalized) Fourier transform operator may be written as the ring element

$$\mathbb{C}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}_{\hbar=1}$$

applied to a smooth function (multiplied by $e^{-i\pi/4}$):

$$\tilde{f}(q)=\left[\mathbb{C}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}f\right](q)$$
$$=\frac{e^{-i\pi/4}}{\sqrt{2\pi}}\int_{\mathscr{R}}dq'\,e^{-iqq'}f(q')$$
$$=\frac{-i}{2\pi\sqrt{2}}\int_{\mathscr{R}^2}dx\,dy\,\exp\left[\frac{i(x+y)^2}{4}\right]e^{ixq}f(q+y)\,. \tag{4.8}$$

The correctness of the last result may be verified reducing the twofold integral to a single one by means of (4.3a).

Corresponding to the matrix $-\mathbf{1}$ one has one of the central elements in the group,

$$\mathbb{C}\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}.$$

This is the Wigner inversion operator studied by Grossmann,[31] Huguenin,[32] Royer,[33] and Dahl.[16] Indeed, following the one-parameter "harmonic oscillator" subgroup

$$\begin{pmatrix}\cos\alpha & -\sin\alpha\\ \sin\alpha & \cos\alpha\end{pmatrix},$$

we arrive, for $\alpha\to\pi^-$, at the ring element given through (4.7) by

$$\mathbb{C}_{-1}=\frac{i\hbar}{4\pi}\int_{\mathscr{R}^2}dx\,dy\,\exp(i[x\mathbb{Q}+y\mathbb{P}])\,. \tag{4.9}$$

This corresponds to a coset distribution constant over the manifold, an integral kernel $\delta(q+q')$, and the Weyl quantization of a classical Dirac δ at the origin of phase space.

In Gaussian geometrical optics,[5] the Hamiltonian formulation introduces a momentum canonically conjugate to the position q of a ray at a plane perpendicular to the optical axis z. This momentum is $p=n\sin\theta$, where n is the refraction index of the medium and θ is the angle between the optical axis and the light ray.

For lens systems,[11] the subsets of $\mathrm{Mp}(2,\mathscr{R})$ that are of interest are the parabolic subgroup of upper-triangular matrices

$$\mathbb{F}_z:=\mathbb{C}\begin{pmatrix}1 & -z/n\\ 0 & 1\end{pmatrix}=\exp\left(-i\frac{z}{n}\mathbb{P}^2\right),\quad z\geqslant 0\,, \tag{4.10a}$$

corresponding to free propagation through a length z in a medium with refraction index n, and the group elements

$$\mathbb{S}_P:=\mathbb{C}\begin{pmatrix}1 & 0\\ P & 1\end{pmatrix},\quad P=2\beta(n'-n)\,, \tag{4.10b}$$

which corresponds to the action on optical phase space of a refracting surface $z=\zeta(q)=\beta q^2$, where light passes from a medium n to a medium n'. If standing for a lens, P is the Gaussian power.

From these optical elements we may build as a limit any $\mathrm{Mp}(2,R)$ transformation of optical phase space.[34] The corresponding canonical transform is the Huygens–Fresnel integral cut to the quadratic exponential term. This acts on the object phase function to yield the image.

One further development, which is immediate but not of central import to this paper, is the consideration of the semidirect product between the Heisenberg–Weyl group W and the metaplectic group explored above, $W\,\mathrm{Mp}(2,\mathscr{R})=W\wedge\mathrm{Mp}(2,\mathscr{R})$, with W a normal ideal. In terms of the results of Combe *et al.*,[29] Burdet and Perrin,[30] this allows the inclusion of the linear potential (free-fall) Hamiltonian. The group of translations and inversions of Dahl[16] is simply (4.9) in semidirect product with W.

V. SYMPLECTIC IDEALS AND WEYL QUANTIZATION

As we stated in the Introduction, our eventual aim is to apply the structure of the Heisenberg–Weyl ring $\mathscr{W}$ to the description of wave optics in aberration. The metaplectic group within $\mathscr{W}$ describes Gaussian optics, its elements acting on the object phase function to yield the image phase function.

The study of geometrical optics of aligned systems with third aberration order has been done using the "classical" Poisson-bracket Lie algebra of observables quadratic and quartic in the phase-space variables[12,35] *modulo* higher-order terms. Preliminary results suggest that the relevant algebraic structure is $\nu\wedge\mathrm{sp}(2,\mathscr{R})$, where ν is a nilpotent ideal under the Gaussian algebra $\mathrm{sp}(2,\mathscr{R})$. This ideal *decomposes* into Nth-order aberration ideals[36] under $\mathrm{sp}(2,\mathscr{R})$. Concretely (in one dimension), if we denote

$$\chi^j_m:=p^{j+m}q^{j-m}\,,$$
$$m=j,j-1,\ldots,-j,\ 2j=0,1,2,\ldots, \tag{5.1}$$

then the Poisson bracket $\{\cdot,\cdot\}$ between these elements is given by

$$\{\chi^j_m,\chi^{j'}_{m'}\}=2(jm'-j'm)\chi^{j+j'-1}_{m+m'}\,. \tag{5.2}$$

Now, it is a well-known fact that the quantities (5.1) with Lie bracket given by the Poisson bracket form an infinite-dimensional Lie algebra with a grading. If we now consider χ^j_m as classical functions to be quantized according to some scheme, it is also a well-known fact that the algebra whose Lie bracket is the commutator will *not* be isomorphic to the previous one. Classical Poisson brackets and quantum commutators do *not* follow each other, except[8] for (i) up-to-quadratic expressions in the basic Heisenberg–Weyl constituents, (ii) classical functions of the form $pf(q)+g(q)$ and their corresponding quantum operators, and (iii) classical functions $qf(p)+g(p)$ and their quantized operators. [We have not included some finite-dimensional Lie subalgebras of $\overline{w}$ $\{(1,\mathbb{Q}\mathbb{P},\mathbb{Q}^k\mathbb{P}^l,)k,\ l$ fixed, $k\neq l$, $k,l\leqslant 2\}$ and Abelian infinite-dimensional Lie subalgebras (polynomials in one element, e.g., $\mathbb{Q}^k\mathbb{P}^k$, $k=0,1,2,\ldots$), which are also isomorphic to the corresponding Lie algebras of their classical functions under Poisson bracket.] The algebraic span of any two of the above classes is outside the span of each class by itself.

In Gaussian optics (with prisms) the geometrical and wave treatments follow each other since the generating operators all belong to class (i). Optics with aberration lacks this isomorphism due to the fact that it uses quantities (5.1) with $j>1$.

In following papers we intend to show that a quantization analog of wave optics out of geometrical optics—in an approximation still to be explored—*is* achieved if we retain only the requirement

$$\{\chi^1_m,\chi^j_{m'}\}=2(m'-jm)\chi^j_{m+m'}\,, \tag{5.3a}$$

so that the quantized version of this relation,

$$[\mathbb{X}^1_m,\mathbb{X}^j_{m'}]=2i\hbar(m'-jm)\mathbb{X}^j_{m+m'}\,, \tag{5.3b}$$

holds. We show here that this is possible *if and only if* $\mathbb{X}^j_m$ is the Heisenberg–Weyl ring element corresponding to the classical function χ^j_m *in the Weyl quantization scheme*. What

we are asking for is that $\{X^j_m\}^j_{m=-j}$ transform under the symplectic group in the same way as the classical quantities $\{\chi^j_m\}^j_{m=-j}$ do. We shall detail elsewhere the association between the *multiplet* χ^j and *Sp(2,R)-classified* aberrations of order $A = 2j - 1$. In the following we prove that (5.3b) follows from (5.3a) in (and only in) Weyl quantization.

We refer to (3.7) for the general-scheme quantization of the basic monomial $q^m p^n$, and calculate its commutator with $X^1_{-1} = Q^2$, the sp(2,R) lowering operator in (2.3):

$$
\begin{aligned}
[Q^2, \Omega_\phi(q^m p^n)] &= \sum_k \binom{m}{n}\binom{n}{k} k!\,\phi_k \\
&\quad \times \left(-\frac{1}{2} i\hbar\right)^k Q^{m-k}\,[Q^2, P^{n-k}] \\
&= 2i\hbar n \sum_k \binom{m+1}{k}\binom{n-1}{k} k! \\
&\quad \times \left\{\phi_k - \frac{k}{m+1}(\phi_k - \phi_{k-1})\right\} \\
&\quad \times \left(-\frac{1}{2} i\hbar\right)^k Q^{m+1-k} P^{n-1-k}. \qquad (5.4)
\end{aligned}
$$

If the last member is to be an operator quantized from a classical monomial function in the same scheme, the quantity in curly brackets must be again ϕ_k and independent of m. This is possible if and only if $\phi_k = \text{const}$. This is the trademark of the Weyl scheme. The same derivation applies for the commutator between $X^1_1 = P^2$ and $\Omega_\phi(q^m p^n)$ and thus for any sp(2,R) element and its exponential to the group. The Weyl rule is thus invariant under metaplectic transformations. The proof given here is algebraic; a geometric proof would be of interest.

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Generating relations for reducing matrices. I. Ordinary representations

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Auxiliary groups are constructed that make it possible to reduce the multiplicity problem and to derive consistent generating relations for the elements of reducing matrices. Three examples are worked out to illustrate the general scheme.

I. INTRODUCTION

One of the standard problems in representation theory is to find a matrix which transforms a given reducible matrix representation into a direct sum of its irreducible constituents. In the last years there have been several attempts to systematize the calculation of these *reducing matrices*, especially for those reducible representations that are the tensor product of two irreducible ones (Kronecker products, Clebsch–Gordan matrices). The various approaches all had a common feature: They started from operations (e.g., complex conjugation or multiplication with one-dimensional representations) that establish relations between matrix representations of the same dimension irrespective of whether they have been constructed explicitly or not. These relations between representations were then used to derive relations between the elements of the reducing matrix. Finally these relations were exploited to generate the elements of the reducing matrix from a certain subset that has to be calculated by standard methods.[1–6] To make the generating relations simpler and hence more useful the irreducible representations (irreps) are usually chosen or implicitly restricted to be of a form especially adapted to the operations one started with.

Several kinds of operations have been considered in the literature: multiplication with one-dimensional representations[7–13] (hereafter denoted as "association"), complex conjugation,[2,5,14–20] permutations,[2,7,14–16,21] automorphisms,[12,17,20] and transposition of subgroup–irrep labels[22–24] (when the subgroup in a group–subgroup chain has a direct product structure). Each of these operations gives some useful results, but usually their separate and independent application does not completely solve the ambiguities of the reducing matrices, while their correlated application may considerably help to solve the considered problem.

For the present paper only three operations, namely association, automorphisms, and complex conjugation, are of relevance. The reasons why we limit our considerations to these operations comes from the fact that we want to make our approach applicable to the most general situation. The general situation is to decompose a reducible representation into its irreducible constituents where neither the reducible representation nor the occurring irreps are constrained. So we neither want to consider now irreps that are adapted to group chains nor is the reducible representation assumed to have a peculiar structure (e.g., to be a Kronecker product of irreps or to be chain adapted).

In this paper it is shown that the three approaches may be combined into one single scheme. The crucial point of the present procedure is that the operations belonging to associations, automorphisms, and complex conjugation can be closed to form a group. The structure of this auxiliary group, hereafter denoted as Q^{REP}, turns out to be

$$Q^{\mathrm{REP}} = \mathrm{ASS} \leftthreetimes (\mathrm{AUT} \times \mathrm{CON}), \tag{1.1}$$

where $\leftthreetimes$ characterizes a semidirect product and $\times$ a direct one. The central outcome of this paper is (i) to define operator groups that are associated with Q^{REP} or subgroups thereof that allow us to reduce (resolve) the multiplicity problem on group theoretical grounds only and (ii) to define consistent generating relations for subsets of the reducing matrices.

Reducing matrices S are defined by

$$R(g)S = S \sum_k \oplus\, m_k D^k(g), \tag{1.2}$$

where $R(g)$ is the reducible representation of G that will be decomposed into a direct sum of its irreducible constituents. The irreps of G are denoted by D^k and the multiplicity of D^k in R is termed by m_k. For our purpose it is useful to split the square reducing matrix S, where $\dim S = \dim R = n_R$, into rectangular submatrices consisting of n_k $(= \dim D^k)$ columns and n_R rows. Accordingly the defining equations (1.2) can be rewritten as

$$R(g)S^{k;m} = S^{k;m} D^k(g), \tag{1.3}$$

where the multiplicity index m ranges from 1 to m_k. It is worth noting that for given irreps D^k, Eqs. (1.3) fix $S^{k;m}$ up to arbitrary m_k-dimensional unitary transformations. Irrespective of which solution for the multiplicity problem has been chosen, Eqs. (1.3) are necessary and sufficient to fulfill Eqs. (1.2) assuming that the $S^{k;m}$ are orthonormalized with respect to the index m.

For a given representation R our approach starts with finding a subgroup Q of Q^{REP} that leaves R invariant up to similarity transformations. Analogously, we can find a subgroup Q^k of Q leaving D^k [occurring in (1.2)] invariant up to unitary equivalence. Due to our procedure we define operator groups $\tilde{Q}^k$ that are associated with Q^k and act on the multiplicity index m of $S^{k;m}$ only, i.e.,

$$T(q)S^{k;m} = \sum_{m'} \Delta_{m'm}(q) S^{k;m'}, \tag{1.4}$$

where q denotes elements of Q^k. Accordingly the auxiliary

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operator group $\tilde{Q}^k$ defines a m_k-dimensional representation which, in general, turns out to be a matrix corepresentation Δ owing to the structure of Q^{REP}. If Δ decomposes into inequivalent coirreps only the multiplicity problem is, by definition, resolved. That is the orthogonality of the blocks $S^{k;m}$ with respect to m may then be explained in terms of the orthogonality relations of the coirreps of Q^k. If Δ contains a coirrep at least twice the multiplicity problem is resolved only in part and further conventions are necessary to fix the multiplicity index.

Apart from this "partner blocks" $S^{q'k;m}$ are obtained from $S^{k;m}$ by means of generating relations of the form

$$S^{q'k;m} = U(q')S^{k;m}, \tag{1.5}$$

where the q' are coset representatives of Q with respect to Q^k, $q'k$ is the correspondingly transformed G-irrep label, and $U(q')$ a similarity transformation of R.

Comparing our method with other approaches we may infer that our scheme is more systematic as the various operations are closed to form a group. This allows to obtain by group theoretical considerations only both a reduction (resolution) of the multiplicity problem and a systematic derivation of consistent generating relations for subsets of the reducing matrix. However, it must be admitted that one drawback of the present approach is that many different auxiliary groups have to be constructed. So it might happen that for an example at hand a direct method is more efficient and quicker (e.g., solution of the multiplicity problem by applying Schmidt's procedure or other methods) than our scheme. Nevertheless if one is interested in a group theoretical explanation of the multiplicity problem the present method is a useful tool to tackle this task. Clearly the more generating relations that can be established between the various elements of the reducing matrix S the more this method simplifies tabulations of such coefficients. This is the main reason for investigating the problem along these lines.

It is intended to modify the present method for corepresentations and to extend it by including further operations such as permutations if Kronecker products are considered.

The rest of the paper is organized as follows: In Sec. II we introduce all necessary concepts and develop our scheme. In its last subsection the method is summarized suitable to its practical application. Section III contains three examples that illustrate the general considerations and show the feasibility of our approach.

II. THE GENERAL SCHEME

A. Preliminaries

In the following we consider a fixed finite or compact continuous group G with elements g. We denote by REP the set of all unitary matrix representations of G. This set decomposes into equivalence classes if the equivalence of two representations is defined in the usual way: $D_1 \sim D_2$ if, and only if, there exists a unitary matrix U such that $D_1(g) = U^+ D_2(g) U$ for all $g \in G$. Furthermore, $D_1 \in \mathrm{REP}$ is said to be contained in $D \in \mathrm{REP}$, if $D \sim D_1 \oplus D_2$ (direct sum) for some $D_2 \in \mathrm{REP}$. Irreducible unitary matrix representations (irreps) are denoted by D^k, $k = 1,2,\ldots$. Note that the symbol D^k represents always one definite irrep, not the whole equivalence class. Conventions that can be used to interrelate inequivalent standard irreps will be discussed in the next two subsections.

B. The group Q^{REP}

Now we introduce an auxiliary group Q consisting of bijective mappings of REP. Three kinds of mappings are considered: associations, automorphisms, and complex conjugation. The first of these mappings are in one-to-one correspondence with the one-dimensional representations of G:

$$(a_j D)(g) = D^j(g) D(g), \quad \dim D^j = 1. \tag{2.1}$$

These mappings, called associations, obviously form an Abelian group. We denote this group by ASS and use the letter a for its elements.

The next class of mappings is related to automorphisms of G. An automorphism is a bijective mapping β: $G \to G$ such that $\beta(g_1)\beta(g_2) = \beta(g_3)$ if $g_1 g_2 = g_3$. The inner automorphisms $g \to g_1 g g_1^{-1}$ are not interesting for the applications we have in mind. They are only introduced if they are needed to close a set of outer automorphisms into a group. Outer automorphisms are mappings $g \to \beta(g)$ that are not of the form $\beta(g) = g_1 g g_1^{-1}$. To each automorphism β_k of G we assign a mapping b_k of REP by setting

$$(b_k D)(g) = D(\beta_k^{-1}(g)), \quad \beta_k = \text{automorphism of } G. \tag{2.2}$$

Like the set of all automorphisms of G the set of the associated mappings of REP forms also a group. This group is denoted by AUT.

The last kind of mappings is the complex conjugation.

$$(c_l D)(g) = D(g)^{c_l} = \begin{cases} D(g), & c_l = c_0, \\ D(g)^*, & c_l = c_1 = c. \end{cases} \tag{2.3}$$

Therefore c^2 is the identical mapping and the group $\{c_0, c\}$ is denoted by CON.

A general element of Q^{REP} is

$$q = a_j b_k c_l \tag{2.4}$$

and its action onto a representation $D \in \mathrm{REP}$ is defined by

$$(qD)(g) = (a_j(b_k(c_l D))) = D^j(g) D(\beta^{-1}(g))^{c_l}. \tag{2.5}$$

It follows from these definitions that Q^{REP} has the structure

$$Q^{\mathrm{REP}} = \mathrm{ASS} \,\textcircled{\times}\, (\mathrm{AUT} \times \mathrm{CON}), \tag{2.6}$$

where $\textcircled{\times}$ denotes a semidirect product and $\times$ a direct one. The group Q^{REP} retains this structure if ASS and/or AUT are restricted to subgroups. For a finite group G the subgroups ASS and AUT are finite and the auxiliary group Q^{REP} is therefore a finite group.

The definition of Q^{REP} entails that each q maps equivalence classes onto equivalence classes. This transformation is most easily followed by looking at how the characters change under a transformation q. The mappings $\chi = \mathrm{trace}\, D \to q\chi = \mathrm{trace}\, qD$ clearly show which irreps can be related by the operations of the auxiliary group Q^{REP}. We write

$$qk = l \quad \text{if } qD^k \sim D^l. \tag{2.7}$$

If G and hence Q^{REP} is finite it is illustrative to construct a

table exhibiting how the generating elements of Q^{REP} act onto the various irreps k (qk-table).

Q^{REP} induces an equivalence relation, called Q^{REP} equivalence, for equivalence classes of irreps: $k \sim l$ if $l = qk$ from some $q \in Q^{\mathrm{REP}}$. The equivalence classes of irreps can therefore be partitioned into disjoint sets and standard irreps can be defined in the following manner: First we choose one member of each Q^{REP} class, say D^k, as standard irrep; then remaining inequivalent standard irreps D^l belonging to the same Q^{REP} class as D^k are generated from this irrep by applying suitable transformations of Q^{REP}, i.e., $D^l = qD^k$ for some $q \in Q^{\mathrm{REP}}$. Since $q_1 D^k = q_2 D^k$ implies $q_1 k = q_2 k$, but not vice versa, the generator q has to be fixed for each irrep D^k by a convention to arrive at a unique and consistent definition of standard irreps.

For the following discussion it is advantageous to introduce the subgroup

$$Q_0^{\mathrm{REP}} = \mathrm{ASS} \circledS \mathrm{AUT}, \tag{2.8}$$

with elements $q = a_j\, b_k$ and the corresponding coset decomposition of Q^{REP}:

$$Q^{\mathrm{REP}} = Q_0^{\mathrm{REP}} \cup Q_1^{\mathrm{REP}}, \quad Q_0^{\mathrm{REP}} \cap Q_1^{\mathrm{REP}} = \varnothing. \tag{2.9}$$

C. The groups Q and Q^k

Now we focus onto one single reducible representation $R \in \mathrm{REP}$ and the irreps contained in R:

$$R \sim \sum_k \oplus\, m_k D^k. \tag{2.10}$$

The multiplicities m_k can be calculated by means of the characters $\chi = \mathrm{trace}\, R$ and $\chi^k = \mathrm{trace}\, D^k$. Both χ and the m_k's depend on the specific representation R, and so do the definitions of the various quantities (groups, matrices, etc.) introduced later on. We do not indicate this dependence explicitly (e.g., by writing $m_{R;k}, \chi_R, \ldots$ instead of $m_k, \chi, \ldots$) since this would make the notation too clumsy and the formulas less transparent. In fact this dependence has to be kept in mind only in case one wants to reduce a few representations or a whole class of them.

The problem we want to solve is to find a unitary matrix S that relates the two representations occurring in (2.10). This is achieved by a number of steps the first of which consists of restricting Q^{REP} to the subgroup Q defined by

$$Q = \{ q \in Q^{\mathrm{REP}} | qR \sim R \}. \tag{2.11}$$

If Q^{REP} is finite and the transformations $k \to qk$ are known (e.g., from the table mentioned in Sec. II B), Q is easily deduced from (2.10). While $qR \sim R$ by definition, if $q \in Q$, an irrep D^k contained in R may transform into an inequivalent irrep qD^k. If the equivalence classes k of the irreps contained in R are combined into Q-classes,

$$[k] = \{ qk \,|\, q \in Q \}, \tag{2.12}$$

the multiplicity m_k is obviously the same for all members of such a class:

$$m_l = m_k \quad \text{if} \quad l \in [k]. \tag{2.13}$$

In the following we also need some subgroups of Q, namely one for each Q-class $[k]$. Let k be the representative of $[k]$ then Q^k is defined by

$$Q^k = \{ q \in Q \,|\, qk = k \} \tag{2.14}$$

and

$$[k] = \{ q_1^{(k)} k, q_2^{(k)} k, \ldots \}, \tag{2.15}$$

where the $q_l^{(k)}$'s are suitable coset representatives of Q^k in Q:

$$Q = q_1^{(k)} Q^k \cup q_2^{(k)} Q^k \cup \cdots. \tag{2.16}$$

For the moment we assume that we are allowed to choose the set of standard irreps at our convenience. We exploit this freedom to set

$$D^l = q_l^{(k)} D^k, \quad q_k^{(k)} = q_0 = \text{identical transformation}. \tag{2.17}$$

If a different set of standard irreps is wanted the scheme developed in the following has to be supplemented according to item (9) of Sec. II G.

The subsets $Q_i \subset Q$ and $Q_i^k \subset Q^k$ to which we refer in the sequel are defined analogous to the subsets $Q_i^{\mathrm{REP}} \subset Q^{\mathrm{REP}}$, Eqs. (2.8) and (2.9):

$$Q_i = Q \cap Q_i^{\mathrm{REP}}, \quad Q_i^k = Q^k \cap Q_i^{\mathrm{REP}}, \quad i = 0,1. \tag{2.18}$$

D. The groups $\bar{Q}$ and $\bar{Q}^k$

If $q \in Q$ there exists a unitary matrix $U(q)$ such that

$$(qR)(g) = U^+(q) R(g) U(q). \tag{2.19}$$

Repeated application of transformations q_i onto R show that the matrix

$$\begin{aligned} &U(q_1) * U(q_2) * \cdots * U(q_n) \\ &\quad = U(q_1)(q_1 U)(q_2) \cdots (q_1 q_2 \cdots q_{n-1} U)(q_n) \end{aligned} \tag{2.20}$$

transforms R into $q_1 q_2 \cdots q_n R$ if the matrices $U(q_i)$ satisfy (2.19) for $q = q_i$. In Eqs. (2.20) we used the notation

$$qM = \begin{cases} M, & \text{for } q \in Q_0^{\mathrm{REP}}, \\ M^*, & \text{for } q \in Q_1^{\mathrm{REP}}, \end{cases} \tag{2.21}$$

for the matrices $M = U(q)$. In the literature qM is usually written as M^q but we prefer (2.21) since later on we have to label the q's with double indices [see, e.g., (2.41)]. We shall use notation (2.21) in the following also for other matrices, except for matrix representations of G where the meaning of qD has already been defined in Eqs. (2.1)–(2.5). The product (2.20) is well known in the theory of corepresentations[25–27] whence we refer to this composition law as comultiplication. The inverse of $U(q)$ with respect to comultiplication is

$$U^{\#}(q) = (qU)^+(q) = (qU^+)(q) \tag{2.22}$$

and this matrix can be used to transform R into $q^{-1}R$:

$$U(q^{-1}) = U^{\#}(q). \tag{2.23}$$

Now let

$$\{ q_x, q_y, \ldots \} = \text{set of generators of } Q, \tag{2.24}$$

$U(q_x), U(q_y), \ldots$ be a set of matrices satisfying (2.19) for the transformations $q_x, q_y, \ldots$, and the matrices $U(q_x^{-1})$, $U(q_y^{-1}), \ldots$ be related to the matrices $U(q_x), U(q_y), \ldots$ through Eqs. (2.22) and (2.23). It is then possible to define a matrix cogroup by forming all coproducts of the matrices $U(q)$, $q \in \{ q_x, q_y, \ldots, q_x^{-1}, q_y^{-1}, \ldots \}$. The matrix cogroup constructed

this way will be denoted by $\overline{Q}$. Each element of $\overline{Q}$ is uniquely fixed by a unitary matrix U and a label indicating whether $U*U_1$ is equal to UU_1 or to UU_1^* (U "unitary" or "antiunitary"). Both the matrix and this label may be characterized by a word $q = q_1 q_2 \cdots q_n$ that is composed of letters $q_i \in \{q_x,\ldots,q_x^{-1},\ldots\}$, but different words need not necessarily denote different elements of $\overline{Q}$.

It should be noted that there is a great freedom in the definition of $\overline{Q}$, especially if some of the multiplicities m_k in (2.10) are greater than 1. The great variety of possible definitions of $\overline{Q}$ results from the fact that the matrix $U(q)$ in (2.19) is not uniquely determined by R and q. In fact if $U(q)$ is a matrix satisfying (2.19) and if C_1, C_2 are unitary elements of the commuting algebras of R and of qR, respectively, i.e., $C_1 R = R C_1$ and $C_2(qR) = (qR)C_2$ for all $g \in G$, $C_i^+ = C_i^{-1}$, then the matrix $C_1 U(q) C_2^+$ satisfies also (2.19) and is therefore equally well-suited to describe the action of q onto R. While the factors C_i may be added to $U(q)$ without changing the relation between R and qR, they enter essentially into the result of a comultiplication if $U(q)$ is one of the factors of the product. The structure of the group $\overline{Q}$ therefore depends strongly on the selection of the generating matrices $U(q_x)$, $U(q_y)$, etc. Though a judicious choice of generating matrices can make the group $\overline{Q}$ isomorphic to Q in some cases, $U(q_1)*U(q_2)$ will, in general, differ from $U(q_3)$ by factors C of the kind mentioned above even if $q_1 q_2 = q_3$. There is some general relation between $\overline{Q}$ and Q but its discussion is postponed to Sec. II F since the knowledge of this relation does not help much in calculating the reducing matrix S. To this end it suffices to see how the group $\overline{Q}$ can be obtained in a constructive manner and the examples provided in Sec. III should convince the reader that the matrix cogroups obtained in this way need not be monstrous groups.

All these remarks apply also for the matrix cogroups $\overline{Q}^k$ that are generated from the matrices $U^k(q)$ in quite the same way as $\overline{Q}$ is generated from the matrices $U(q)$. Here $q \in \{q_r,\ldots,q_r^{-1},\ldots\}$, where

$$\{q_r, q_s, \ldots\} = \text{set of generators of } Q^k, \tag{2.25}$$

the matrices $U^k(q)$ satisfy

$$(qD^k)(g) = U^{k+}(q) D^k(g) U^k(q), \tag{2.26}$$

and

$$U^k(q^{-1}) = U^{k*}(q) \tag{2.27}$$

for the generating elements $q = q_r, q_s, \ldots$. In the following one such group is needed for each Q-class $[k]$.

The partition of these matrix cogroups into unitary and antiunitary elements,

$$\begin{aligned} &\overline{Q} = \overline{Q}_0 \cup \overline{Q}_1, \quad \overline{Q}_0 \cap \overline{Q}_1 = \varnothing, \\ &\overline{Q}^k = \overline{Q}_0^k \cup \overline{Q}_1^k, \quad \overline{Q}_0^k \cap \overline{Q}_1^k = \varnothing, \end{aligned} \tag{2.28}$$

follows from their construction and the corresponding partition of the groups Q and Q^k:

$$\begin{aligned} &U(q) \in \overline{Q}_i, \quad \text{iff } q \in Q_i, \\ &U^k(q) \in \overline{Q}_i^k, \quad \text{iff } q \in Q_i^k. \end{aligned} \tag{2.29}$$

In (2.29) the U's are matrices of the form (2.20) and are labeled by a word $q_1 q_2 \cdots q_n$ while the q's are those transformations that are obtained by reducing this word by means of the multiplication law of Q.

E. The groups $\tilde{Q}^k$ and the transformation properties of the reducing matrix S

Equation (2.10) means that there exists a unitary matrix S such that

$$R(g)S = S \sum_k \oplus\, m_k D^k(g). \tag{2.30}$$

If we split the square matrix S into rectangular submatrices ("blocks") S^k with n_R rows and n_k columns,

$$n_R = \dim R, \quad n_k = \dim D^k, \tag{2.31}$$

we may rewrite (2.30) as a set of equations of the form

$$R(g)S^k = S^k D^k(g). \tag{2.32}$$

From the existence of S we infer that there exist exactly m_k nonvanishing linearly independent blocks S^k for each irreducible representation D^k. If the scalar product of two rectangular matrices M_i of equal size is defined by

$$\langle M_1, M_2 \rangle = \text{trace } M_1^+ M_2, \tag{2.33}$$

they are even orthogonal because S is unitary. Hence if we succeed in finding m_k blocks S^{km} satisfying (2.32) and

$$\langle S^{km}, S^{km'} \rangle = n_k \delta_{mm'}, \tag{2.34}$$

we obtain a solution for all columns of the unknown matrix S that belong to one of the m_k irreps D^k contained in R. A straightforward solution of this problem is offered by the so-called projection method,[3,7,28–30] which consists of two steps: In the first one Eq. (2.32) is transcribed in such a way that S_1^k, the first column of S^k, is seen to be an eigenvector of a projection matrix of dimension n_R. By applying this projection matrix onto an arbitrary column vector one obtains m_k linearly independent column vectors that have to be orthonormalized by a Schmidt process. This yields the first column of the m_k blocks S^{km}. In the second step the remaining columns are determined from the first ones by multiplying them with square matrices ("shift" matrices) that are also special linear combinations of the matrices $R(g)$, $g \in G$.

According to the philosophy outlined in the Introduction we approach the same goal in a way that relies upon the transformation properties of the involved representations. To transfer this information from the matrix representations to the rectangular blocks S^k we assume first that $q \in Q^k$ and again consider the three kinds of transformations separately. If $a = a_j \in Q^k$ we multiply both sides of (2.32) with $D^j(g)$ and employ (2.19) and (2.26). Multiplying the resulting equation with $U(a)$ from the left and $U^{k+}(a)$ from the right we obtain

$$R(g)[U(a)S^k U^{k+}(a)] = [U(a)S^k U^{k+}(a)] D^k(g). \tag{2.35}$$

If $b \in Q^k$ we substitute $\beta^{-1}(g)$ for g on both sides of (2.32) and use again (2.19) and (2.26). The result analogous to (2.35) reads

$$R(g)[U(b)S^k U^{k+}(b)] = [U(b)S^k U^{k+}(b)] D^k(g). \tag{2.36}$$

Similarly if $c \in Q^k$ we consider the complex conjugate equation of (2.32) and obtain

$$R(g)[U(c)S^{k*}U^{k+}(c)] = [U(c)S^{k*}U^{k+}(c)]D^k(g). \tag{2.37}$$

Using the convention (2.21) for $M = S^k$, Eqs. (2.35)–(2.37) can be combined into one single equation

$$R(g)[T(q)S^k] = [T(q)S^k]D^k(g), \quad \text{for } q \in Q^k, \tag{2.38}$$

where

$$T(q)S^k = U(q)(qS^k)U^{k+}(q) \tag{2.39}$$

and the right-hand side of this equation defines the transformation of S^k for a general element $q \in Q^k$. Comparison of Eqs. (2.39) with (2.32) shows that the blocks $T(q)S^k$, $q \in Q^k$, are equally well suited as constituents of the reducing matrix S as the block S^k. We already concluded from the existence of S that there exist m_k linearly independent blocks S^{km} that all satisfy Eq. (2.32). Since this relation is linear in S^k any complex linear combination of the S^{km}'s is also a solution of (2.32). Endowed with the scalar product (2.33) the set of solutions of (2.32) therefore forms a unitary space of dimension m_k. In this space the transformation $S^k \to T(q)S^k$ defines a norm-preserving operator that is linear for $q \in Q_0^k$ and antilinear for $q \in Q_1^k$.

It should be noted that each operator $T(q)$ is defined by a pair of matrices, $U(q) \in \overline{Q}$ and $U^k(q) \in \overline{Q}^k$, where in both cases q has to be identified with a word composed of letters $q_x, q_y, \ldots$ and $q_r, q_s, \ldots$, respectively. To define $T(q)$ explicitly one can start with expressing the generators $q_r, q_s, \ldots$ of Q^k as words composed of the generators $q_x, q_y, \ldots$ of Q and compute the corresponding matrices $U(q_r), U(q_s), \ldots \in \overline{Q}$. These matrices, combined with the generators $U^k(q_r)$, $U^k(q_s), \ldots$ of $\overline{Q}^k$, then define the operators $T(q_r), T(q_s), \ldots$ for all generators q_r, $q_s, \ldots$ of Q^k. This set of operators can be closed into a group, if the product $T(q_2)T(q_1)$ is defined as that transformation of the blocks S^k that is obtained by applying first $T(q_1)$ and then $T(q_2)$. Because of (2.39) and (2.20) the product $T(q_2)T(q_1)$ can be equally well-defined by means of the coproducts of the matrices $U(q_i)$ and $U^k(q_i)$, respectively. We denote the resulting group of unitary/antiunitary operators by $\tilde{Q}^k$. There exists no simple general relation between this group and the matrix cogroups $\overline{Q}$ and $\overline{Q}^k$ as the form of the generating matrices $U(q_r), U(q_s), \ldots$ depends on those products of q_x, $q_y, \ldots$ that one chooses to represent the transformations q_r, $q_s, \ldots$. Moreover since $U(q)$ is always combined with $U^k(q)$ in the definition of $T(q)$ it is, in general, impossible to recognize the multiplication law of $\overline{Q}^k$ or the corresponding subgroups of $\overline{Q}$ from that of $\tilde{Q}^k$. However, similar to the matrix cogroups $\overline{Q}$ and $\overline{Q}^k$, it is sufficient to assume that starting from well-defined generating elements $T(q_r), T(q_s), \ldots$ the group $\tilde{Q}^k$ may always be obtained in a constructive way as shown in the examples of Sec. III. Similar to Q^k and $\overline{Q}^k$ the group $\tilde{Q}^k$ contains a subgroup $\tilde{Q}_0^k$ of index 2; it consists of all operators $T(q)$ that are unitary (i.e., norm preserving and linear):

$$T(q) \in \tilde{Q}_i^k \quad \text{iff } q \in Q_i^k, \quad i = 0,1. \tag{2.40}$$

The space spanned by the blocks S^k is invariant under the operations of $\tilde{Q}^k$ but in general not irreducible. A decomposition of this space into irreducible subspaces reduces the multiplicity problem since blocks transforming according to inequivalent irreducible corepresentations of $\tilde{Q}^k$ are orthogonal. The orthogonality relations of irreducible corepresentations[31–33] also tell us that blocks transforming according to different rows of the same representation have to be orthogonal. Therefore if the corepresentation of $\tilde{Q}^k$ carried by the m_k-dimensional vector space contains each irreducible corepresentation at most once the multiplicity problem is resolved by finding blocks S^k that transform according to these representations. This situation is, however, not the rule because, in general, one or more coirreps will occur more than once, especially if the multiplicity problem is only reduced, but not completely solved, and pairwise orthogonal blocks transforming according to the same row of the coirrep have to be found by Schmidt's procedure (see, e.g., example B of Sec. III).

Up to now we considered only one irrep D^k, which tacitly has been assumed to be the representative of the Q-class $[k]$. If the corresponding blocks S^k are known the remaining blocks S^l belonging to this class are easily generated from the blocks S^k. To this end we only have to apply the transformations $q_l^{(k)}$ to Eq. (2.32) in exactly the same way as the transformations $q \in Q^k$ were applied previously, and to consider convention (2.17) that relates D^l to D^k. This yields

$$R(g)[U(q_l^{(k)})(q_l^{(k)}S^k)] = [U(q_l^{(k)})(q_l^{(k)}S^k)]D^l(g), \tag{2.41}$$

which allows us to set

$$S^l = U(q_l^{(k)})(q_l^{(k)}S^k). \tag{2.42}$$

This is a convention the explicit form of which depends on the coproduct of the matrices $U(q_x), U(q_y), \ldots$ that is chosen to represent $U(q_l^{(k)})$.

The pattern along which the reducing matrix S can be constructed should now be obvious. However, before it is summarized as a list of practical rules, it seems appropriate to reflect the mathematical background of the procedure to realize the extent of freedom one is left in obeying these rules.

F. Interrelations of the various groups

This subsection contains some material for the mathematically interested reader and may be dropped by those who only want to see how the method proposed here works in practice.

In discussing the relations between the various groups introduced in the preceding subsections we start with the groups Q and $\overline{Q}$. Since Q is a subgroup of Q^{REP} each $q \in Q$ is defined on all $D \in \text{REP}$. On the other hand, if $U(q) \in \overline{Q}$, then the transformation $R \to U^+(q)RU(q)$ transforms only R into qR. Repeated application of transformations of this kind allow us to extend the domain of $\overline{Q}$ to the set

$$\text{orbit of } R = \{D \in Q^{\text{REP}} | D = qR, \quad q \in Q\}. \tag{2.43}$$

It is clear that we can compare Q with $\overline{Q}$ only if the transformations of the former group are restricted to the orbit of R. Technically this can be done in the following way: Let $N \subset Q$ be defined by

$$N = \{q' \in Q | q'qR = qR, \quad \text{for all } q \in Q\}. \tag{2.44}$$

This subgroup is a normal subgroup of Q and the factor group Q/N may be identified with a set of transformations $q' \in Q$ which act onto the orbit in a nontrivial way, i.e., interchange at least two members of it. There exists a similar normal subgroup of $\overline{Q}$, namely,

$$\overline{N} = \{ U(q') \in \overline{Q} \mid U^+(q')(qR)U(q') = (qR), \quad \text{for all } q \in Q \}, \tag{2.45}$$

and

$$Q/N \cong \overline{Q}/\overline{N}. \tag{2.46}$$

The isomorphism can be proved by considering q and q' in (2.44) and (2.45) as words composed of letters $q_x, q_y, \ldots$. It is evident from (2.46) that Q and $\overline{Q}$ will have a different structure if N is not isomorphic to $\overline{N}$. But there exists no general relation between these two groups for several reasons: First, the multiplication law of N not only depends on R or its orbit but also on all other representations $D \in \mathrm{REP}$ because $N \subset Q \subset Q^{\mathrm{REP}}$. Second, as already pointed out in Sec. II D, there is some arbitrariness in the definition of $\overline{Q}$ and hence $\overline{N}$, since the generating matrices $U(q_x), U(q_y), \ldots$ are not uniquely determined by the generators $q_x, q_y, \ldots$ of Q. The structure of $\overline{N}$, the sole unknown part of $\overline{Q}$ assuming that Q and N are already known, is only restricted by the fact that the matrices $U(q') \in \overline{N}$ have to commute with all elements of the orbit of R. To what extent this property fixes the multiplication law of $\overline{N}$ depends on the irreducible constituents of R. If R is irreducible the matrices $U(q') \in \overline{N}$ have to be scalar matrices. The group $\overline{N}_0 = \overline{N} \cap \overline{Q}_0$ is then Abelian and is either equal to $\overline{N}$ or a normal subgroup of $\overline{N}$ of index 2. This holds also for a representation R that is a direct sum of inequivalent irreps (or equivalent to such a direct sum) because the commuting algebras of two equivalent representations are isomorphic and the index of $\overline{N}_0$ in $\overline{N}$ is always either 1 or 2. However if R contains an irrep more than once its commuting algebra is no longer commutative. Consequently $\overline{N}_0$ need not be Abelian so that, after having constructed $\overline{Q}$ from its generating elements, one may be faced with a normal subgroup $\overline{N}_0$ of very complicated structure. Of course one would like to exploit the freedom one has in choosing the generating matrices $U(q_x), U(q_y), \ldots$ to make $\overline{N}_0$ as small and as simple as possible. But the only constructive method we know that restricts $\overline{Q}$ to a small subset of the commuting algebra and guarantees that $\overline{N}_0$ is Abelian also in the general case presupposes the knowledge of a special reducing matrix S. Let us assume that R has already been reduced to a blockform D where the irreps D^l are combined according to the Q-classes $[k]$. Since the transformations $q \in Q$ do not intertwine the submatrices $D^{[k]} = \Sigma \oplus D^l$, $l \in [k]$, the generating matrices $U^D(q_x)$, $U^D(q_y), \ldots$ may be chosen in a corresponding blockform (one block for each Q-class, repetitions are allowed). With this choice $\overline{N}_0^D$ will be an Abelian group as follows from the previous considerations. Now since $R(g) = SD(g)S^+$ and

$$q(SDS^+)(g) = (qS)(qD)(g)(qS)^+, \tag{2.47}$$

we may define $\overline{Q}^R$ in such a way that it is isomorphic to $\overline{Q}^D$:

$$\begin{aligned} U^R(q) &= SU^D(q)S^+, \quad \text{for } q \in Q_0, \\ U^R(q) &= SU^D(q)S^T, \quad \text{for } q \in Q_1. \end{aligned} \tag{2.48}$$

This isomorphism maps $\overline{N}_0^D$ onto the matrix group $\overline{N}_0^R$, which is therefore also Abelian. This shows that it is always possible to find generating matrices $U(q_x), U(q_y), \ldots$ such that $\overline{N}$ is Abelian. But to find them before knowing the matrix S, the object one is primarily interested in, is more an art than a science.

Isomorphisms similar to (2.46) exist for all groups Q^k and $\overline{Q}^k$ if the normal subgroups N^k and $\overline{N}^k$ are defined analogously to Eqs. (2.44) and (2.45). The structure of the groups $\overline{Q}^k$ is in general simpler than that of $\overline{Q}$ because all the normal subgroups $\overline{N}_0^k$ have to be Abelian.

The relation of the operator group $\tilde{Q}^k$ to the matrix cogroups $\overline{Q}$ and $\overline{Q}^k$ depends even more on the details of its definition, i.e., on the choice of its generating elements. Each generating operator $T(q_r)$ is characterized by a pair of matrices, $U(q_r) \in \overline{Q}$, $U^k(q_r) \in \overline{Q}^k$, and a label indicating whether $T(q_r)$ is unitary ($q_r \in Q_0^k$) or antiunitary ($q_r \in Q_1^k$). Since $U(q_r)$ and $U^k(q_r)$ appear in (2.39) on different sides of the blocks S^k the product of two operators $T(q)$ is determined by the coproduct of the corresponding matrices $U(q) \otimes U^k(q)$, where $M \otimes N$ denotes the tensor product of the matrices M and N:

$$(M \otimes N)_{iI,jJ} = M_{ij} N_{IJ}. \tag{2.49}$$

Since the multiplication of the matrices $U(q)$ does not affect that of the matrices $U^k(q)$ and vice versa, the matrices $U(q_r) \otimes U^k(q_r)$ obviously generate a subgroup of $\overline{Q} \times \overline{Q}^k$. The elements in $\overline{N} \times \overline{N}^k$ form a normal subgroup and the corresponding factor group is isomorphic to a subgroup of $Q/N \times Q^k/N^k$. In general this is all that can be said about the matrix cogroups in advance.

It should be noted that $\tilde{Q}^k$ cannot be simply identified with this matrix cogroup because an operator $T(q)$ related by (2.29) to a matrix $U(q) \otimes U^k(q)$ defines a transformation in the space of all blocks of the same size as the blocks S^k. In this linear space of dimension $n_R n_k$ the blocks satisfying Eq. (2.32) form only a subspace of dimension m_k so that in general $\tilde{Q}^k$ will only be a homomorphic image of the matrix cogroup considered above.

G. Summary of the scheme

We conclude the general discussion by summarizing our approach in a set of rules. This should enable the reader to construct a reducing matrix in which he is interested, in the form proposed here.

(1) Determine the multiplication law of G and the classes of conjugate elements. Use this information to find outer automorphisms of G and close them into a group (definition of the subgroup AUT).

(2) Determine the simple characters of G, i.e., the character table if G is finite. This provides you with all one-dimensional representations of G (definition of ASS). Use ASS, AUT, and the complex conjugation (definition of CON) to define Q^{REP}, Eqs. (2.1)–(2.5). Determine the action of the transformations $q \in Q^{\mathrm{REP}}$ onto the equivalence classes of the G-irreps. If G is finite it is convenient to construct a table showing the labels qk, Eq. (2.7), for all irreps k and a set $\{a_1, a_2, \ldots; b_1, b_2, \ldots; c\}$ of generating elements of Q^{REP}.

(3) Consider the reducible representation R; use its character and the simple characters found previously to calculate the multiplicities $m_k \neq 0$. Use this information and the transformation properties of the irreps D^k [the qk-table of item (2)] to find Q, the subgroup of Q^{REP} that leaves $\chi = \text{trace } R$ invariant [cf. Eq. (2.11)]. Then find a set of generators q_x, q_y,... of Q, preferable a small one, and construct for each of the generators q_z a unitary matrix $U(q_z)$ that satisfies $U(q_z)(q_z R)(g) = R(g)U(q_z)$ [cf. Eq. (2.19)].

(4) Combine the irreps contained in R into Q-classes $[k]$ according to (2.12). Choose a representative k for each class and determine the corresponding group Q^k, Eq. (2.19), using the facts of item (2). For each group Q^k find a set of coset representatives with respect to Q, Eq. (2.16).

(5) Consider the first Q-class, say $[k]$, and fix the standard irrep D^k of its representative k. Then determine a rectangular matrix S^k that satisfies (2.32). This matrix must contain m_k free complex parameters (e.g., matrix elements). If $m_k = 1$ continue with item (7).

(6) If $m_k > 1$ find generators q_r, q_s,... of Q^k (again small sets are preferred). For each q_w construct a unitary matrix $U^k(q_w)$ that satisfies $U^k(q_w)(q_w D^k)(g) = D^k(g)U^k(q_w)$ [cf. Eq. (2.26)]. Then express each generator q_w as a product of the generators q_x, q_y,... of Q and calculate the matrices $U(q_w)$ by forming the corresponding coproducts of the matrices $U(q_x), U(q_y)$,... [Eq. (2.20)]. Next use the matrices $U(q_w)$ and $U^k(q_w)$ to define the operators $T(q_w)$ according to Eq. (2.39). Close these operators into the group $\tilde{Q}^k$ and decompose the space spanned by the blocks S^k into irreducible subspaces. In each of these subspaces construct a basis which is orthonormalized due to (2.34). This provides you with m_k blocks S^{km} which (i) intertwine $R(g)$ with $D^k(g)$, (ii) are orthogonal and properly normalized, and (iii) transform according to coirreps of the operator group $\tilde{Q}^k$.

(7) Express the coset representatives $q_l^{(k)}$ as products of the generators q_x, q_y,... of Q and calculate the matrices $U(q_l^{(k)})$ by forming the corresponding coproducts. Use these matrices to generate the blocks S^{lm} from the blocks S^{km}, Eq. (2.42).

(8) Repeat steps (5)–(7) until all Q-classes $[k]$ are exhausted and combine the blocks into the matrix S.

(9) If you prefer standard irreps $\bar{D}^l \neq D^l = q_l^{(k)} D^k$ you have at first to find unitary matrices W^l that relate these equivalent irreps:

$$W^l \bar{D}^l(g) = D^l(g) W^l. \tag{2.50}$$

The blocks S^{lm} have then to be multiplied with W^l,

$$\bar{S}^{lm} = S^{lm} W^l, \tag{2.51}$$

to obtain a matrix $\bar{S}$ which decomposes R into a direct sum of irreps $\bar{D}^l$.

III. EXAMPLES

A. The regular representation of the double point group T^*

If R is the regular representation of a compact group G, Q coincides with Q^{REP} because $\chi(g) = 0$ for $g \neq e$ (unit element). Moreover, if G is finite and a complete set of standard irreps D^k is known one may set[1,34]

$$S_{g,kmj} = (S^{km})_{g,j} = (n_k/|G|)^{1/2} D^k_{jm}(g)^*, \tag{3.1}$$

for the elements of the reducing matrix S or its block constituents S^{km}, respectively. That this matrix decomposes the permutation matrices of the regular representation into a direct sum of irreps D^k follows from the form of the matrix $R(g)$ representing $g \in G$,

$$R_{g_1, g_2}(g) = \delta_{g_1, gg_2}, \tag{3.2}$$

the multiplication law of the irreps, $D^k(g_1 g_2) = D^k(g_1) D^k(g_2)$, and their unitarity, $D^k_{jm}(g)^* = D^k_{mj}(g^{-1})$.

Here we consider the double point group T^* as defined by Bradley and Cracknell.[27] Since a complete set of irreps of T^* is known[35] the reducing matrix is immediately obtained from (3.1). Therefore the present example serves only to reveal relations between the columns of S that are not evident from (3.1). For the elements of T^* we adopt the shorthand notation $x, +1, -1, \bar{x}, +\bar{1}, -\bar{1}$, etc. instead of the symbols $C_{2x}, C_{31}^+, C_{31}^-, \bar{C}_{2x}, \bar{C}_{31}^+, \bar{C}_{31}^-$, etc. used in Ref. 27. The multiplication law of T^* can be extracted from that of the double point group O^* that contains T^* as a normal subgroup.[36] Denoting the unit element by E the group T^* may also be defined by the generating relations

$$\begin{aligned} &x^2 = y^2 = (-1)^3 = \bar{E}, \\ &\bar{E}x = x\bar{E}, \quad \bar{E}y = y\bar{E}, \quad (-1)\bar{E} = \bar{E}(-1), \\ &\bar{E}^2 = E, \\ &(-1)x = \bar{E}xy(-1), \quad (-1)y = \bar{E}x(-1), \end{aligned} \tag{3.3}$$

T^* has the elements

$$\begin{aligned} &E, x, y, z = xy, \\ &-1, -2 = x(-1), \quad -3 = \bar{E}y(-1), \\ &-4 = \bar{E}z(-1), \\ &+1 = (-1)^{-1}, \quad +2 = (-2)^{-1}, \\ &+3 = (-1)^{-1}, \quad +4 = (-4)^{-1}, \end{aligned} \tag{3.4}$$

and twelve more elements $\bar{g}$ related to the elements (3.4) by

$$\bar{g} = \bar{E}g. \tag{3.5}$$

These 24 elements decompose into seven classes. Conjugation with the element $C_{2b} \in O^* \setminus T^*$ defines an outer automorphism of T^* of order 2:

$$\beta(x) = y, \quad \beta(y) = x, \quad \beta(-1) = (-1)^{-1}. \tag{3.6}$$

The character table of T^* (see Ref. 37) shows that this group has three one-dimensional irreps that are labeled by $k = 1,2,3$. For associations it is sufficient to consider D^2 where

$$D^2(x) = D^2(y) = 1, \quad D^2(-1) = \omega^2, \quad \omega = e^{2\pi i/3}. \tag{3.7}$$

If we assign the generating association a to D^2 and the (only nontrivial) automorphism b to β the group $Q = Q^{\text{REP}}$ is easily seen to have the structure

$$Q \cong C_3 \otimes (C_2 \times C_2), \quad Q_0 \cong C_3 \otimes C_2. \tag{3.8}$$

The rows and columns of the matrices $R(g)$ and $U(q)$ are labeled in the sequence (3.4), followed by (3.5). The nonvan-

ishing matrix elements (g_1, g_2) of the unitary matrices $U(a)$ and $U(b)$ are the following ones:

$$\begin{aligned} U(a):\ & (E,E)=(x,x)=(y,y)=(z,z)=1, \\ & (-1,-1)=(-2,-2)=(-3,-3) \\ & \qquad =(-4,-4)=\omega, \\ & (+1,+1)=(+2,+2)=(+3,+3) \\ & \qquad =(+4,+4)=\omega^2, \\ & (\bar{g},\bar{g})=(g,g); \end{aligned} \tag{3.9}$$

$$\begin{aligned} U(b):\ & (E,E)=(x,y)=(y,x)=(z,\bar{z}) \\ & \qquad =(-1,+1)=(-2,+2) \\ & \qquad =(-3,+4)=(-4,+3) \\ & \qquad =(+1,-1)=(+2,-2) \\ & \qquad =(+3,-4)=(+4,-3)=1, \\ & (\bar{g}_1,\bar{g}_2)=(g_1,g_2). \end{aligned} \tag{3.10}$$

Since R is a real representation, $U(c)$ may be chosen to be the antiunitary unit matrix. With this choice

$$\bar{Q}\cong Q. \tag{3.11}$$

The action of the generating elements a, b, and c onto the equivalence classes of irreps shows the following table:

qk	1	2	3	4	5	6	7
a	2	3	1	4	7	5	6
b	1	3	2	4	5	7	6
c	1	3	2	4	5	7	6.

(3.12)

The Q-classes are therefore

$$[1]=\{1,2,3\},\quad [4]=\{4\},\quad [5]=\{5,6,7\}. \tag{3.13}$$

The corresponding subgroups Q^k that transform the irreps D^1, D^4, and D^5 into equivalent ones and the coset representatives $q_l^{(k)}$ are listed below (q_0 = identical transformation):

$$\begin{aligned} & Q^1=\{q_0,b,c,bc\}, \\ & q_1^{(1)}=q_0,\quad q_2^{(1)}=a,\quad q_3^{(1)}=a^2, \end{aligned} \tag{3.14}$$

$$Q^4=Q, \tag{3.15}$$

$$\begin{aligned} & Q^5=\{q_0,b,c,bc\} \\ & q_5^{(5)}=q_0,\quad q_1^{(5)}=a^2,\quad q_2^{(5)}=a. \end{aligned} \tag{3.16}$$

The standard irreps D^k for $k=1,4,5$ are defined by

$$D^1(g)=1, \tag{3.17}$$

$$\begin{aligned} & D^4(x)=\mathrm{diag}(1,-1,-1), \\ & D^4(y)=\mathrm{diag}(-1,1,-1), \\ & D^4(-1)=\begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix}, \end{aligned} \tag{3.18}$$

$$\begin{aligned} & D^5(x)=\begin{bmatrix}0&-i\\-i&0\end{bmatrix}, \\ & D^5(y)=\begin{bmatrix}0&-1\\1&0\end{bmatrix}, \\ & D^5(-1)=\frac{1}{2}\begin{bmatrix}1-i&-1+i\\1+i&1+i\end{bmatrix}, \end{aligned} \tag{3.19}$$

and the coset representatives (3.14) and (3.16) have been chosen in such a way that the irreps D^k coincide with those given by Bradley and Cracknell.[35]

The block S^1 multiplied by the normalization factor $\sqrt{24}$ is the column matrix with elements

$$\sqrt{24}\,S^1_{g,1}=1 \tag{3.20}$$

[cf. (3.1) and (3.17)]. Because of (3.20) and (3.10), $U(b)S^1=S^{1*}=S^1$. If we choose $U^1(q)=1$ for all $q\in Q^1$ the group $\tilde{Q}^1$ consists of the identical transformation only. Furthermore,

$$S^2=U(a)S^1,\quad S^3=(U(a))^2S^1, \tag{3.21}$$

in accordance with the general theory [cf. Eq. (2.14)].

The block S^{41} has 72 matrix elements. Fourty-eight of them vanish; the remaining are listed below, where (g,j) stands for $\sqrt{8}(S^{41})_{g,j}$, $g\in T^*$, and $j=1,2,3$:

$$\begin{aligned} \sqrt{8}\,S^{41}:\ & (E,1)=(x,1)=(-1,3)=(-4,3) \\ & \qquad =(+1,2)=(+2,2)=1, \\ & (y,1)=(z,1)=(-2,3)=(-3,3) \\ & \qquad =(+3,2)=(+4,3)=-1, \\ & (\bar{g},j)=(g,j). \end{aligned} \tag{3.22}$$

As generators of $\bar{Q}^4$ we choose the unitary matrices

$$\begin{aligned} & U^4(a)=\mathrm{diag}(\omega^2,\omega,1), \\ & U^4(b)=\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}, \end{aligned} \tag{3.23}$$

and the antiunitary matrix

$$U^4(c)=\mathrm{diag}(1,1,1). \tag{3.24}$$

This makes

$$\bar{Q}^4\cong Q. \tag{3.25}$$

The generating operators $T(q)$, $q=a,b,c$, are defined as

$$\begin{aligned} & T(a)S^4=U(a)S^4U^{4+}(a), \\ & T(b)S^4=U(b)S^4U^{4+}(b), \\ & T(c)S^4=S^{4*}. \end{aligned} \tag{3.26}$$

If the blocks S^{42} and S^{43} are calculated from the irrep D^4 due to Eqs. (3.1), (3.4), (3.5), and (3.18), one finds

$$\begin{aligned} & T(a)S^{4m}=\omega^m S^{4m}, \\ & T(b)S^{41}=S^{42}, \\ & T(b)S^{42}=S^{41}, \\ & T(b)S^{43}=S^{43}, \\ & T(c)S^{4m}=S^{4m}. \end{aligned} \tag{3.27}$$

That is, S^{41} and S^{42} carry the two-dimensional coirrep

$$\Delta(a) = \mathrm{diag}(\omega,\omega^2),$$
$$\Delta(c) = \mathrm{diag}(1,1), \tag{3.28}$$
$$\Delta(b) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

while S^{43} carries the one-dimensional coirrep

$$\Delta(q) = 1, \quad \text{for } q = a,b,c. \tag{3.29}$$

This shows that in this case the multiplicity problem may be completely solved by finding irreducible matrix corepresentations of the auxiliary group $\tilde{Q}^4$, where

$$\tilde{Q}^4 \cong Q. \tag{3.30}$$

The blocks S^{km}, $k = 5,6,7$, $m = 1,2$, can be calculated by means of (3.1) once the representations D^5, $D^6 = a^2 D^5$, and $D^7 = aD^5$ are obtained from (3.19), (3.7), and (3.4), and (3.5). The irrep D^5 yields the following matrix elements (g,j) of the block $\sqrt{24}\,S^{51}$:

$$\begin{aligned}
\sqrt{24}\,S^{51}:\ & (E,1) = \sqrt{2}, \quad (x,1) = (y,1) = 0, \quad (z,1) = i\sqrt{2}, \\
& (-1,1) = (-2,1) = (+3,1) = (+4,1) = \gamma, \\
& (-3,1) = (-4,1) = (+1,1) = (+2,1) = \gamma^*, \\
& (E,2) = (z,2) = 0, \quad (x,2) = i\sqrt{2}, \quad (y,2) = \sqrt{2}, \\
& (-1,2) = (+2,2) = \gamma^*, \\
& (-2,2) = (+1,2) = -\gamma^*, \\
& (-3,2) = (+4,2) = -\gamma, \\
& (-4,2) = (+3,2) = \gamma, \\
& (\bar{g},j) = -(g,j), \quad \gamma = e^{i\pi/4}.
\end{aligned} \tag{3.31}$$

The block S^{52} is related to S^{51} by operators $T(q) \in \tilde{Q}^5$, but in order to define this operator group one has to define first the generating elements of the matrix cogroup $\overline{Q}^5$:

$$U^5(b) = \begin{bmatrix} 0 & \gamma^* \\ \gamma & 0 \end{bmatrix},$$
$$U^5(c) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{3.32}$$

$$T(b)S^5 = U(b)S^5U^5(b),$$
$$T(c)S^5 = -S^5{}^*U^5(c). \tag{3.33}$$

The block S^{52} can be generated from the block S^{51} in several ways because

$$T(b)S^{51} = \gamma^* S^{52}, \quad T(b)S^{52} = \gamma S^{51},$$
$$T(c)S^{51} = -S^{52}, \quad T(c)S^{52} = S^{51}. \tag{3.34}$$

Equations (3.34) show that the blocks S^{51} and S^{52} transform according to the corepresentation (3.32), which is irreducible though not in standard form. That $m_5 = 2$ may therefore be deduced from the existence of the operator group

$$\tilde{Q}^5 \cong C_2 \circledS C_4, \quad \tilde{Q}_0^5 \cong C_2 \times C_2. \tag{3.35}$$

The remaining blocks can be generated from the blocks S^{5m}, $m = 1,2$, by multiplication with the matrix (3.9):

$$S^{6m} = (U(a))^2 S^{5m}, \quad S^{7m} = U(a)S^{5m}. \tag{3.36}$$

These relations explain why the multiplicities m_k coincide for $k = 5,6,7$.

B. A 12-dimensional representation of the double point group D_3^*

The group D_3^* can be generated by two elements -1 and $2b$ (again shorthand notations for $C_{3\bar{1}}$ and C_{2b}) satisfying the relations

$$\begin{aligned}
&(-1)^3 = (2b)^2 = \bar{E}, \\
&\bar{E}^2 = E, \\
&(2b)(-1) = \bar{E}(-1)^2(2b).
\end{aligned} \tag{3.37}$$

The twelve elements of the form $(-1)^n(2b)^m$ decompose into six classes of conjugate elements

n	1	2	3	4	5	6
$(-1)^n$	-1	$+\bar{1}$	$\bar{E}$	$-\bar{1}$	$+1$	E
$(-1)^n(2b)$	$2f$	$2\bar{e}$	$2\bar{b}$	$2\bar{f}$	$2e$	$2b$,

(3.38)

Classes: E

$\bar{E}$

$-1, +1$

$-\bar{1}, +\bar{1}$

$2b, 2\bar{e}, 2\bar{f}$

$2\bar{b}, 2e, 2f.$ (3.39)

The automorphism β of order 2,

$$\beta(-1) = -1, \quad \beta(2b) = 2\bar{b}, \tag{3.40}$$

leaves the first four classes invariant and interchanges the last two of them.

The character table of D_3^* has the following form:

	E	$\bar{E}$	-1	$-\bar{1}$	$2b$	$2\bar{b}$
1	1	1	1	1	1	1
2	1	1	1	1	-1	-1
3	1	-1	-1	1	i	$-i$
4	1	-1	-1	-1	$-i$	i
5	2	2	-1	-1	0	0
6	2	-2	1	-1	0	0.

(3.41)

We take the irrep D^3 to define the generating association

$$(a_3 D)(g) = D^3(g)D(g). \tag{3.42}$$

It follows from (3.40)–(3.42) that

$$Q^{\mathrm{REP}} \cong C_4 \circledS (C_2 \times C_2). \tag{3.43}$$

How the transformations of this group relate the irreps D^k is

seen from the table below:

qk	1	2	3	4	5	6
a_3	3	4	2	1	6	5
b	1	2	4	3	5	6
c	1	2	4	3	5	6.

(3.44)

The reducible representation R we consider is the tensor product of two representations,

$$R(g) = D^{\pi}(g) \otimes D^{6}(g) \tag{3.45}$$

[for a definition of $D^{\pi} \otimes D^{6}$ see (2.49)], where D^{π} is a six-dimensional permutation representation defined by

$$D^{\pi}(-1) = \begin{bmatrix} d(-1) & 0 \\ 0 & d(-1) \end{bmatrix},$$

$$D^{\pi}(2b) = \begin{bmatrix} 0 & d(2b) \\ d(2b) & 0 \end{bmatrix},$$

$$d(-1) = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad d(2b) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \tag{3.46}$$

and D^{6} is one of the standard irreps,

$$D^{6}(-1) = \begin{bmatrix} \xi & 0 \\ 0 & \xi^{5} \end{bmatrix}, \quad D^{6}(2b) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{3.47}$$

$$\xi = e^{i\pi/3}, \quad \xi + \xi^{5} = \xi^{6} = 1. \tag{3.48}$$

If the character $\chi(g) = \chi^{\pi}(g)\chi^{6}(g)$ is calculated from (3.46)–(3.48) and (3.38) it is easily seen from the character table (3.41) that

$$R \sim 2D^{3} \oplus 2D^{4} \oplus 4D^{6}. \tag{3.49}$$

It follows from this and the transformation properties of the irreps D^{k}, table (3.44), that Q is a proper subgroup of Q^{REP}:

$$\mathrm{ASS} \cap Q = \{q_0, a\}, \quad a = a_2 = a_3^2, \tag{3.50}$$

$$Q \cong C_2 \times C_2 \times C_2. \tag{3.51}$$

The matrices $U(a), U(b), U(c)$, which transform R into aR, bR, cR, may be chosen as direct sums of six two-dimensional matrices:

$$U(a) = U(b) = 3E^{6} \oplus 3(-E^{6}), \quad U(c) = 6U^{6}(c), \tag{3.52}$$

$$E^{6} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad U^{6}(c) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{3.53}$$

Accordingly

$$\overline{Q} \cong C_2 \times C_4, \quad \overline{Q}_0 \cong C_2 \times C_2. \tag{3.54}$$

The irreps contained in R belong to two Q-classes, namely

$$[3] = \{3,4\}, \quad [6] = \{6\}, \tag{3.55}$$

$$Q^{3} = \{q_0, ab, ac, bc\}, \quad q_3^{(3)} = q_0, \quad q_4^{(3)} = a, \tag{3.56}$$

$$Q^{6} = Q. \tag{3.57}$$

The blocks S^{3m} are column matrices for which

$$R(g)S^{3} = S^{3}D^{3}(g) \tag{3.58}$$

holds true. If this equation is considered for $g = -1$ and $g = 2b$ and if the correpsonding matrices, given in Eqs. (3.46)–(3.48) and (3.41), are inserted one finds that S^{3} is uniquely determined by a column matrix α with two elements:

$$S^{3} = \begin{bmatrix} \alpha \\ (-\bar{1})\alpha \\ (+\bar{1})\alpha \\ -i(2b)\alpha \\ -i(2\bar{f})\alpha \\ -i(2\bar{e})\alpha \end{bmatrix},$$

$$\alpha = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}, \quad g\alpha \mathrel{\hat{=}} D^{6}(g)\alpha. \tag{3.59}$$

Since $\dim D^{3} = 1$ we may set $U^{3}(q) = 1$ for all $q \in Q^{3}$. To define the operators $T(q) \in \tilde{Q}^{3}$ we also need the matrices $U(q)$ for the generators of Q^{3}, i.e., $q = ab$ and $q = ac$. We choose

$$\begin{aligned} U(ab) &= U(a)U(b) = 6E^{6} \quad \text{(unit matrix)}, \\ U(ac) &= U(a)U(c) = 3U^{6}(c) \oplus 3U^{6T}(c), \end{aligned} \tag{3.60}$$

which fixes the action of $T(ab)$ and $T(ac)$:

$$\begin{aligned} &T(ab)S^{3} = U(ab)S^{3} = S^{3}, \\ &T(ac)S^{3} = U(ac)S^{3*}, \\ &(T(ac))^{2}S^{3} = (U(ac))^{2}S^{3} = -S^{3}, \end{aligned} \tag{3.61}$$

$$\tilde{Q}^{3} \cong C_4, \quad \tilde{Q}_0^{3} \cong C_2. \tag{3.62}$$

There exist no eigenvectors of $T(ac)$ since this operator is antilinear and the eigenvalues would have to be $\pm i$ because of (3.61). Therefore the space of blocks S^{3} satisfying (3.58) has to be of even dimension whence the multiplicities $m_3 = m_4 = 2$ may be explained by the operator group $\tilde{Q}^{3}$. If we choose the basis

$$\begin{aligned} &S^{31}: \quad \alpha_1 = 1, \quad \alpha_2 = 0, \\ &S^{32}: \quad \alpha_1 = 0, \quad \alpha_2 = 1, \end{aligned} \tag{3.63}$$

then

$$S^{32} = T(ac)S^{31} = U(ac)S^{31*} \tag{3.64}$$

and $T(ac)$ is represented by the antiunitary matrix $U^{6T}(c)$, the transpose of the matrix $U^{6}(c)$ as given in (3.53). From the columns S^{3m} the columns S^{4m} are obtained according to

$$S^{4m} = U(a)S^{3m}. \tag{3.65}$$

The general form of the blocks S^{6} may be derived from the defining relations

$$R(g)S^{6} = S^{6}D^{6}(g), \tag{3.66}$$

in quite the same way as the general form of S^{3} has been obtained from (3.58):

$$S^{6} = \begin{bmatrix} \alpha \\ (-1)\alpha(+\bar{1}) \\ (+1)\alpha(-\bar{1}) \\ (2b)\alpha(2\bar{b}) \\ (2f)\alpha(2\bar{f}) \\ (2\bar{e})\alpha(2e) \end{bmatrix},$$

$$\alpha = \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix}, \quad g\alpha g' \mathrel{\hat{=}} D^{6}(g)\alpha D^{6}(g'). \tag{3.67}$$

The number of free parameters α_{ij} coincides with the multiplicity $m_6 = 4$. The generating matrices of $\bar{Q}^6$ are

$$U^6(a) = \mathrm{diag}(-i, i), \tag{3.68}$$

$$U^6(b) = \mathrm{diag}(1, -1), \tag{3.69}$$

and the matrix $U^6(c)$. Combined with the matrices (3.52) these matrices determine the operators $T(a)$, $T(b)$, and $T(c)$, which generate $\tilde{Q}^6$. One finds

$$\left.\begin{aligned} T(a)S^6 &= iS^6 \\ T(b)S^6 &= S^6 \end{aligned}\right\} \text{ iff } \alpha_{12} = \alpha_{22} = 0, \tag{3.70}$$

$$\left.\begin{aligned} T(a)S^6 &= -iS^6 \\ T(b)S^6 &= -S^6 \end{aligned}\right\} \text{ iff } \alpha_{11} = \alpha_{21} = 0. \tag{3.71}$$

The choice of the generating matrices $U(q)$ and $U^6(q)$, Eqs. (3.52)–(3.53), and (3.67), entails

$$\tilde{Q}^6 \cong (C_4 \times C_2) \circledS C_2, \quad Q_0^6 = C_4 \times C_2. \tag{3.72}$$

Accordingly the antiunitary operator $T(c)$ transforms blocks of the form (3.70) into blocks of the form (3.71). But there are still two undetermined parameters, e.g., α_{11} and α_{12}, that cannot be fixed by the auxiliary group $\tilde{Q}^6$. In other words, this group reduces the multiplicity problem but does not solve it completely. Two orthogonal blocks both of which are eigenvectors of $T(a)$ and $T(b)$ with eigenvalues i and 1, respectively, have to be found by a Schmidt process. A rather obvious choice is

$$\begin{aligned} &S^{61}\colon \quad \alpha_{11} = 1/\sqrt{3}, \quad \alpha_{12} = \alpha_{21} = \alpha_{22} = 0, \\ &S^{63}\colon \quad \alpha_{21} = 1/\sqrt{3}, \quad \alpha_{11} = \alpha_{12} = \alpha_{22} = 0. \end{aligned} \tag{3.73}$$

From these two blocks the remaining ones can be generated by $T(c)$:

$$\begin{aligned} &S^{62} = T(c)S^{61}\colon \quad \alpha_{22} = 1/\sqrt{3}, \quad \alpha_{11} = \alpha_{12} = \alpha_{21} = 0, \\ &S^{64} = T(c)S^{63}\colon \quad \alpha_{12} = -1/\sqrt{3}, \quad \alpha_{11} = \alpha_{21} = \alpha_{22} = 0. \end{aligned} \tag{3.74}$$

The pairs S^{61}, S^{62} and S^{63}, S^{64} each carry the corepresentation

$$\begin{aligned} \Delta(a) &= \mathrm{diag}(i, -i), \\ \Delta(b) &= \mathrm{diag}(1, -1), \\ \Delta(c) &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \end{aligned} \tag{3.75}$$

which is faithful, irreducible, and in standard form.

C. An 18-dimensional representation of the double space group $(C_3 \times C_3) \circledS C_2^*$

In this example we consider a finite homomorphic image of the two-dimensional space group $p211$ (see Ref. 38) by imposing Born–von Karman boundary conditions. We assume the corresponding Bravais lattice to be square and choose the boundary integer $N = 3$. The notation we adopt for the group elements $g \in G^*$ (= double space group) and the G^*-irrep labels is closely related to space groups and their representation theory, i.e., differs from the notion we introduced in Sec. II. As the finite space group G^* is symmorphic[27,38] it can be defined as a semidirect product group:

$$G^* = T \circledS P^*. \tag{3.76}$$

The symbol T denotes a translation group of order 9 and P^* a double point group of order 4:

$$T = \left\{ \mathbf{t} \in \mathbb{R}^2 \middle| \mathbf{t} = \sum_i n_i \mathbf{i}, \quad n_i = 0, \pm 1 \right\}, \tag{3.77}$$

$$P^* = \{E, z, \bar{E}, \bar{z}\}. \tag{3.78}$$

The basis translations $\mathbf{i}$ ($i = 1,2$) are assumed to form the basis of a square Bravais lattice where the lattice constant is chosen as unit length:

$$\mathbf{i} \cdot \mathbf{i}' = \delta_{i,i'}. \tag{3.79}$$

The dot occurring on the left-hand side of (3.79) denotes the scalar product of $\mathbf{i}$ with $\mathbf{i}'$. We retain this notation henceforward. Because of (3.77) and (3.78) we infer that

$$G^* = (C_3 \times C_3) \circledS C_2^*. \tag{3.80}$$

Usually the group elements of G^* are denoted by

$$(p|\mathbf{t}) \in G^*, \quad \text{where } p \in P^* \text{ and } \mathbf{t} \in T. \tag{3.81}$$

The multiplication law of G^* is established by

$$(p|\mathbf{t})(p'|\mathbf{t}') = (pp'|\mathbf{t} + (p)\mathbf{t}'), \tag{3.82}$$

where $pp' \in P^*$ and $\mathbf{t} + (p)\mathbf{t}' \in T$. It is worth noting that $\mathbf{t} + (p)\mathbf{t}'$, where (p) is a linear operator acting on $\mathbb{R}^2$, has to be understood modulo T, i.e., whenever $\mathbf{t} + (p)\mathbf{t}'$ lies "outside" of the T there exists a vector $\mathbf{t}'' \in T$ that is uniquely determined by $\mathbf{t} + (p)\mathbf{t}'$. For instance, $\mathbf{1} + \mathbf{1}$ has to be identified with $-\mathbf{1}$. We choose, as generating elements of G^*,

$$(E|\mathbf{1}), \quad (E|\mathbf{2}); \quad (z|\mathbf{0}), \tag{3.83}$$

and the generating relations in the form

$$(z|\mathbf{0})(z|\mathbf{0}) = (\bar{E}|\mathbf{0}), \tag{3.84}$$

$$(z)\mathbf{i} = (\bar{z})\mathbf{i} = -\mathbf{i} \quad (i = 1,2). \tag{3.85}$$

A straightforward inspection of (3.82) yields that the 36 elements of G^* subdivide into 12 classes of conjugate group elements.

Classes of G^*:

$$\begin{aligned} &\{(E|\mathbf{0})\} && = K_1 \\ &\{(E|\mathbf{1}), (E|-\mathbf{1})\} && = K_2 \\ &\{(E|\mathbf{2}), (E|-\mathbf{2})\} && = K_3 \\ &\{(E|\mathbf{1}+\mathbf{2}), (E|-\mathbf{1}-\mathbf{2})\} && = K_4 \\ &\{(E|\mathbf{1}-\mathbf{2}), (E|-\mathbf{1}+\mathbf{2})\} && = K_5 \\ &\{(\bar{E}|\mathbf{0})\} && = K_6 \\ &\{(\bar{E}|\mathbf{1}), (\bar{E}|-\mathbf{1})\} && = K_7 \\ &\{(\bar{E}|\mathbf{2}), (\bar{E}|-\mathbf{2})\} && = K_8 \\ &\{(\bar{E}|\mathbf{1}+\mathbf{2}), (\bar{E}|-\mathbf{1}-\mathbf{2})\} && = K_9 \\ &\{(\bar{E}|\mathbf{1}-\mathbf{2}), (\bar{E}|-\mathbf{1}+\mathbf{2})\} && = K_{10} \\ &\{(z|\mathbf{t}), \mathbf{t} \in T\} && = K_{11} \\ &\{(\bar{z}|\mathbf{t}), \mathbf{t} \in T\} && = K_{12}. \end{aligned} \tag{3.86}$$

As regards the derivation of an automorphism group of G^*, we do not want to go into any details and therefore leave this discussion to the reader. The automorphism group turns out to be

$$\mathrm{AUT} = C_{4v}, \quad C_{4v} = C_4 \circledS C_2. \tag{3.87}$$

The generating elements of AUT are chosen as

$$\beta \leftrightarrow +z \leftrightarrow C_{4z}^{+}$$
$$\beta'' \leftrightarrow db \leftrightarrow \sigma_{db}, \tag{3.88}$$

which are in one-to-one correspondence with the point group elements C_{4z}^{+} and σ_{db}, respectively. Again we prefer to employ a concise notation instead of the extended one used in Bradley and Cracknell.[27] A general element of AUT reads

$$\beta^{m}\beta''^{n} \in \mathrm{AUT}, \quad m = 1,2,3,4 \quad \text{and} \quad n = 1,2. \tag{3.89}$$

Moreover it holds that

$$\beta^{4} = \beta''^{2} = \epsilon \ \text{(unit element)},$$
$$\beta''\beta\beta''^{-1} = \beta^{3} \leftrightarrow C_{4z}^{-}. \tag{3.90}$$

Taking into account the transformations

$$(+z)\mathbf{1} = \mathbf{2}, \quad (+z)\mathbf{2} = -\mathbf{1}, \tag{3.91}$$
$$(db)\mathbf{1} = \mathbf{2}, \quad (db)\mathbf{2} = \mathbf{1}, \tag{3.92}$$

it is readily verified that the generating elements β,β'' of AUT define the following mappings of G^*:

$$\beta((E\,|\mathbf{1})) = (E\,|\mathbf{2}),$$
$$\beta((E\,|\mathbf{2})) = (E\,|-\mathbf{1}), \tag{3.93}$$
$$\beta((z|\mathbf{0})) = (z|\mathbf{0});$$
$$\beta''((E\,|\mathbf{1})) = (E\,|\mathbf{2}),$$
$$\beta''((E\,|\mathbf{2})) = (E\,|\mathbf{1}), \tag{3.94}$$
$$\beta''((z|\mathbf{0})) = (\bar{z}|\mathbf{0}).$$

It is worth noting that the automorphism β^2 can be identified with $(z|\mathbf{0}) \in G^*$, i.e., it turns out to be an inner automorphism. Accordingly this is an example where we have to close the set of outer automorphism to form a group by taking into account inner automorphisms.

Proceeding as proposed in our general scheme we have to construct the character table of G^*. Such a calculation is usually done without knowing explicitly irreps of G^*. But since the G^*-irreps are readily determined by means of induction,[27] we construct at first a complete set of G^*-irreps to extract from them the character table.

To construct G^*-irreps by means of induction one has to start from the one-dimensional irreps of T. They are given by

$$D^{\mathbf{v}}(\mathbf{t}) = e^{i\mathbf{v}\cdot\mathbf{t}}, \quad \mathbf{t} \in T, \tag{3.95}$$

where

$$\mathbf{v} = \sum_i n_i \mathbf{v}_i, \quad \mathbf{v}_i = \frac{2\pi}{3}\mathbf{i} \quad \text{and} \quad n_i = 0, \pm 1. \tag{3.96}$$

Hence the Brillouin zone (BZ) of G^* consists of nine vectors. The next step is to determine for each $\mathbf{v} \in \mathrm{BZ}$ the corresponding little cogroup $P^*(\mathbf{v})$:

$$P^*(\mathbf{v}) = \{\, p \in P^* \,|\, (p)\mathbf{v} = \mathbf{v}\}. \tag{3.97}$$

One immediately finds

$$P^*(\mathbf{0}) = P^*, \tag{3.98}$$
$$P^*(\mathbf{v}) = \{E,\bar{E}\}, \quad \text{for all } \mathbf{v} \neq \mathbf{0}. \tag{3.99}$$

Then one has to calculate sets of irreps for each $P^*(\mathbf{v})$. But to avoid redundancies we have to partition BZ into disjoint subsets ("star" of v-vector) and have to take from each star one element which requires some conventions. These peculiar elements define the so-called "representation domain" ΔBZ of BZ. In our case ΔBZ consists of the following five vectors:

$$\Delta\mathrm{BZ} = \{\mathbf{G},\mathbf{M},\mathbf{N},\mathbf{X},\mathbf{Y}\},$$
$$\mathbf{G} = \mathbf{0},$$
$$\mathbf{M} = \mathbf{v}_1, \quad \mathbf{N} = \mathbf{v}_2, \tag{3.100}$$
$$\mathbf{X} = \mathbf{v}_1 + \mathbf{v}_2, \quad \mathbf{Y} = \mathbf{v}_1 - \mathbf{v}_2,$$

where the notation G,M,N,X,Y for the various points has no deeper meaning.

Since $P^*(\mathbf{0})$ and $P^*(\mathbf{v})$, $\mathbf{v} \in \Delta\mathrm{BZ}$ with $\mathbf{v} \neq \mathbf{0}$, are Abelian, it is sufficient to give the character tables for these two groups:

$P^*(\mathbf{0})$	E	z	$\bar{E}$	$\bar{z}$
1	1	1	1	1
2	1	−1	1	−1
3	1	i	−1	$-i$
4	1	$-i$	−1	i,

(3.101)

$P^*(\mathbf{v})$	E	$\bar{E}$
1	1	1
2	1	−1.

(3.102)

The last step of the induction procedure consists of inducing from the irreps of little groups $G^*(\mathbf{v}) = T \otimes P^*(\mathbf{v})$, $\mathbf{v} \in \Delta\mathrm{BZ}$ to the full G^*-irreps, where $G^*(\mathbf{v})$-irreps are defined by

$$d^{\mathbf{v}k}(p|\mathbf{t}) = D^{k}(p)D^{\mathbf{v}}(\mathbf{t}), \quad p \in P^*(\mathbf{v}) \quad \text{and} \quad \mathbf{t} \in T. \tag{3.103}$$

For that purpose it is necessary to establish coset representatives of $P^*(\mathbf{v})$ in P^*. The case (3.98) is trivial and for (3.99) we choose E and z as coset representatives. Finally we obtain the following G^*-irreps:

$$\mathbf{0}\text{-point:} \quad D^{\mathbf{0}k}(p|\mathbf{t}) = D^{k}(p), \quad k = 1,2,3,4; \tag{3.104}$$
$$\mathbf{v}\text{-point:} \quad \mathbf{v} \in \Delta\mathrm{BZ} \quad \text{and} \quad \mathbf{v} \neq \mathbf{0},$$
$$D^{\mathbf{v}k}(E\,|\mathbf{t}) = \begin{bmatrix} e^{i\mathbf{v}\cdot\mathbf{t}} & 0 \\ 0 & e^{-i\mathbf{v}\cdot\mathbf{t}} \end{bmatrix},$$
$$D^{\mathbf{v}k}(z|\mathbf{0}) = \begin{bmatrix} 0 & D^{k}(\bar{E}) \\ D^{k}(E) & 0 \end{bmatrix}, \quad k = 1,2. \tag{3.105}$$

The row and column indices of the two-dimensional irreps (3.105) are indexed by E and z in consecutive order due to the choice of the coset representatives. It is worth repeating that (3.105) is valid for each $\mathbf{v} \in \{\mathbf{M},\mathbf{N},\mathbf{X},\mathbf{Y}\}$. Taking into account (3.101), (3.102), (3.104), and (3.105) the character table of G^* takes the following form:

	K_1	K_2	K_3	K_4	K_5	K_6	K_7	K_8	K_9	K_{10}	K_{11}	K_{12}
G1	1	1	1	1	1	1	1	1	1	1	1	1
G2	1	1	1	1	1	1	1	1	1	1	−1	−1
G3	1	1	1	1	1	−1	−1	−1	−1	−1	i	$-i$
G4	1	1	1	1	1	−1	−1	−1	−1	−1	$-i$	i
M1	2	−1	2	−1	−1	2	−1	2	−1	−1	0	0
M2	2	−1	2	−1	−1	−2	1	−2	1	1	0	0
N1	2	2	−1	−1	−1	2	2	−1	−1	−1	0	0
N2	2	2	−1	−1	−1	−2	−2	1	1	1	0	0
X1	2	−1	−1	−1	2	2	−1	−1	−1	2	0	0
X2	2	−1	−1	−1	2	−2	1	1	1	−2	0	0
Y1	2	−1	−1	2	−1	2	−1	−1	2	−1	0	0
Y2	2	−1	−1	2	−1	−2	1	1	−2	1	0	0

(3.106)

Now we may easily infer from this character table that ASS is a cyclic group of order 4. We take G3 to define the generating association, i.e., $a_3 \leftrightarrow$ G3:

$$(a_3 D)(p|\mathbf{t}) = D^{\mathrm{G3}}(p|\mathbf{t}) D(p|\mathbf{t}). \tag{3.107}$$

Combining the three different transformations [cf. (3.87), (3.93), (3.94), (3.107), and the complex conjugation] we have

$$Q^{\mathrm{REP}} \cong C_4 \wr (C_{4v} \times C_2), \tag{3.108}$$

which is a group of order 64. Due to our approach we summarize by means of the table below how the various transformations (generating elements only) are acting on the G^*-irreps. Thereby we assign b to β and b'' to β''. We have

qk	G1	G2	G3	G4	M1	M2	N1	N2	X1	X2	Y1	Y2
a_3	G3	G4	G2	G1	M2	M1	N2	N1	X2	X1	Y2	Y1
b	G1	G2	G3	G4	N1	N2	M1	M2	Y1	Y2	X1	X2
b''	G1	G2	G4	G3	N1	N2	M1	M2	X1	X2	Y1	Y2
c	G1	G2	G4	G3	M1	M2	N1	N2	X1	X2	Y1	Y2

(3.109)

The reducible representation R we want to decompose, and for which we want to resolve the multiplicity problem by means of the auxiliary operator groups $\tilde{Q}^{\nu k}$, is defined by the tensor product of two representations

$$R(p|\mathbf{t}) = D^{\pi}(p|\mathbf{t}) \otimes D^{\mathrm{M2}}(p|\mathbf{t}). \tag{3.110}$$

For the definition of the tensor product (3.110) once more consult (2.49). The permutational representation D^{π} occurring as first constituent on the right-hand side of (3.110) is defined by

$$D^{\pi}_{\mathbf{m},\mathbf{n}}(p|\mathbf{t}) = \delta_{\mathbf{m},\mathbf{t}+(p)\mathbf{n}}, \quad \mathbf{m},\mathbf{n} \in T. \tag{3.111}$$

The representation (3.111) is nine dimensional, so R is 18 dimensional. The character of R,

$$\chi(p|\mathbf{t}) = \chi^{\pi}(p|\mathbf{t})\chi^{\mathrm{M2}}(p|\mathbf{t}), \tag{3.112}$$

follows immediately from (3.106) and

$$\begin{aligned} &\chi^{\pi}(E|\mathbf{0}) = \chi^{\pi}(\bar{E}|\mathbf{0}) = 9, \\ &\chi^{\pi}(E|\mathbf{t}) = \chi^{\pi}(\bar{E}|\mathbf{t}) = 0, \quad \text{for } \mathbf{t} \neq \mathbf{0}, \\ &\chi^{\pi}(z|\mathbf{t}) = \chi^{\pi}(\bar{E}|\mathbf{t}) = 1. \end{aligned} \tag{3.113}$$

This determines the irreducible constituents of R,

$$R \sim D^{\mathrm{G3}} \oplus D^{\mathrm{G4}} \oplus 2D^{\mathrm{M2}} \oplus 2D^{\mathrm{N2}} \oplus 2D^{\mathrm{X2}} \oplus 2D^{\mathrm{Y2}}. \tag{3.114}$$

A simple inspection of (3.114) and (3.109) shows that Q is a proper subgroup of Q^{REP}:

$$\mathrm{ASS} \cap Q = \{q_0, a\}, \quad a = a_3^2, \tag{3.115}$$

$$Q \cong C_2 \times C_{4v} \times C_2, \quad Q_0 \cong C_2 \times C_{4v}. \tag{3.116}$$

It is worth noting that $a = a_3^2$ corresponds to G2. The set of generating elements of Q can be chosen as $\{a;b,b'';c\}$. To construct $\bar{Q}$ we have to determine the matrices $U(q)$ for $q = a,b,b'',c$ that satisfy (2.19).

To simplify the following calculations (concerning R) we employ, in part, matrix notation. We write

$$(U(q))_{\mathbf{m},\mathbf{n}} = U_{\mathbf{m},\mathbf{n}}(q) = u(q;\mathbf{m},\mathbf{n}), \quad \mathbf{m},\mathbf{n} \in T, \tag{3.117}$$

where the $u(q;\mathbf{m},\mathbf{n})$'s are two-dimensional square matrices which, apart from q, in general depend on $\mathbf{m}$ and $\mathbf{n}$. Straightforward calculations yield

$$U_{\mathbf{m},\mathbf{n}}(a) = \delta_{\mathbf{m},\mathbf{n}} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{3.118}$$

$$U_{\mathbf{m},\mathbf{n}}(b) = \delta_{\mathbf{m},(+z)\mathbf{n}} \begin{bmatrix} e^{i\mathbf{Y}\cdot\mathbf{m}} & 0 \\ 0 & e^{-i\mathbf{Y}\cdot\mathbf{m}} \end{bmatrix}, \tag{3.119}$$

$$U_{\mathbf{m},\mathbf{n}}(b'') = \delta_{\mathbf{m},(db)\mathbf{n}} \begin{bmatrix} e^{-i\mathbf{Y}\cdot\mathbf{n}} & 0 \\ 0 & -e^{i\mathbf{Y}\cdot\mathbf{n}} \end{bmatrix}, \tag{3.120}$$

$$U_{\mathbf{m},\mathbf{n}}(c) = \delta_{\mathbf{m},\mathbf{n}} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{3.121}$$

Therefrom it follows that

$$\bar{Q} \cong C_2 \times (C_{4v} \wr C_4), \quad \bar{Q}_0 \cong C_2 \times C_{4v} \times C_2. \tag{3.122}$$

Step (4) of our general scheme requires us to subdivide the G^*-irreps occurring in R into Q-classes. This is readily achieved by employing table (3.109):

$$[\mathbf{G3}] = \{\mathbf{G3},\mathbf{G4}\}, \quad [\mathbf{M2}] = \{\mathbf{M2},\mathbf{N2}\},$$
$$[\mathbf{X2}] = \{\mathbf{X2},\mathbf{Y2}\}. \tag{3.123}$$

Using once more table (3.109) the corresponding groups $Q^{\nu k}$ turn out to be the following groups:

$$Q^{\mathbf{G3}} = Q_0^{\mathbf{G3}} \circledS \{q_0, b'' c\},$$
$$Q_0^{\mathbf{G3}} = \{q_0, b, b^2, b^3\} \circledS \{q_0, ab''\}, \tag{3.124}$$
$$q_{\mathbf{G3}}^{(\mathbf{G3})} = q_0, \quad q_{\mathbf{G4}}^{(\mathbf{G3})} = c;$$
$$Q^{\mathbf{M2}} = Q_0^{\mathbf{M2}} \times \{q_0, c\},$$
$$Q_0^{\mathbf{M2}} = \{q_0, a\} \times \{q_0, b^2, b'' b^3\}, \tag{3.125}$$
$$q_{\mathbf{M2}}^{(\mathbf{M2})} = q_0, \quad q_{\mathbf{N2}}^{(\mathbf{M2})} = b'';$$
$$Q^{\mathbf{X2}} = Q_0^{\mathbf{X2}} \times \{q_0, c\},$$
$$Q_0^{\mathbf{X2}} = \{q_0, a\} \times \{q_0, b^2\} \times \{q_0, b''\}, \tag{3.126}$$
$$q_{\mathbf{X2}}^{(\mathbf{X2})} = q_0, \quad q_{\mathbf{Y2}}^{(\mathbf{X2})} = b.$$

Due to our general approach now we have to determine for the various representatives $\nu k \in \{\mathbf{G3},\mathbf{M2},\mathbf{X2}\}$ the general solution of the defining equations:

$$R(p|\mathbf{t}) S^{\nu k} = S^{\nu k} D^{\nu k}(p|\mathbf{t}). \tag{3.127}$$

After having done this we try to resolve the multiplicity problem by means of the coirreps of the auxiliary groups $Q^{\nu k}$. Finally we have to find the "partner" blocks belonging to the orbits $[\nu k]$ by means of the generating relations (2.42).

At first we discuss the case $\nu k = \mathbf{G3}$. Since $D^{\mathbf{G3}}$ is a one-dimensional irrep we make for $S^{\mathbf{G3}}$ the ansatz

$$S_{\mathbf{m}}^{\mathbf{G3}} = \begin{bmatrix} \alpha_1(\mathbf{m}) \\ \alpha_2(\mathbf{m}) \end{bmatrix}, \quad \mathbf{m} \in T, \tag{3.128}$$

where again we employed in part matrix notation for the components of the column vector $S^{\mathbf{G3}}$. To sketch how we proceed to construct $S^{\mathbf{G3}}$ we specify (3.127) to this case by using matrix notation. In detail, (3.127) reads

$$D^{\mathbf{M2}}(p|\mathbf{t}) S^{\mathbf{G3}}_{(p^{-1})(\mathbf{m}-\mathbf{t})} = S_{\mathbf{m}}^{\mathbf{G3}} D^{\mathbf{G3}}(p|\mathbf{t}). \tag{3.129}$$

If we specify $(p|\mathbf{t})$ to $(E|\mathbf{t})$ and $(z|\mathbf{0})$, respectively, we obtain the following set of equations:

$$\alpha_1(\mathbf{m}+\mathbf{t}) = e^{i\mathbf{M}\cdot\mathbf{t}} \alpha_1(\mathbf{m}), \quad \alpha_2(\mathbf{m}+\mathbf{t}) = e^{-i\mathbf{M}\cdot\mathbf{t}} \alpha_2(\mathbf{m}), \tag{3.130}$$

$$\alpha_1(-\mathbf{m}) = i\alpha_2(\mathbf{m}). \tag{3.131}$$

As (3.130) is independent of $\mathbf{m}$ we set $\mathbf{m} = 0$ and replace in (3.131) $\mathbf{m}$ by $\mathbf{t}$. From this follows that $\alpha_1(\mathbf{0})$ is the sole free parameter. Therefore

$$\alpha_1(\mathbf{t}) = e^{i\mathbf{M}\cdot\mathbf{t}} \alpha_1(\mathbf{0}), \quad \alpha_2(\mathbf{t}) = -ie^{i\mathbf{M}\cdot\mathbf{t}} \alpha_1(\mathbf{0}). \tag{3.132}$$

Finally choosing $\alpha_1(\mathbf{0}) = 1$ and normalizing suitably the column $S^{\mathbf{G3}}$ we arrive at the result

$$\sqrt{18}\, S_{\mathbf{m}}^{\mathbf{G3}} = \begin{bmatrix} e^{i\mathbf{M}\cdot\mathbf{m}} \\ -ie^{i\mathbf{M}\cdot\mathbf{m}} \end{bmatrix}, \quad \mathbf{m} \in T. \tag{3.133}$$

Clearly because of $m_{\mathbf{G3}} = 1$ there is no need of investigating in detail the operator group $\tilde{Q}^{\mathbf{G3}}$. For obvious reasons we choose $U^{\mathbf{G3}}(q) = 1$ for $q = a, b, b''$. Since it is easily verified that

$$T(q) S^{\mathbf{G3}} = S^{\mathbf{G3}}, \quad \text{for } q = a, b, b'' \tag{3.134}$$

holds, we infer

$$\tilde{Q}^{\mathbf{G3}} \cong C_1 \quad \text{(trivial group)}. \tag{3.135}$$

To conclude this part of our example we have to determine $S^{\mathbf{G4}}$ by means of the generating relations (2.42). Due to (3.124) we have

$$S^{\mathbf{G4}} = U(c) S^{\mathbf{G3}*}. \tag{3.136}$$

Inserting (3.121) and (3.133) into (3.136) we obtain

$$\sqrt{18}\, S_{\mathbf{m}}^{\mathbf{G4}} = \begin{bmatrix} -ie^{-i\mathbf{M}\cdot\mathbf{m}} \\ e^{-i\mathbf{M}\cdot\mathbf{m}} \end{bmatrix}, \quad \mathbf{m} \in T. \tag{3.137}$$

The next representative we consider is M2. Since $D^{\mathbf{M2}}$ is two dimensional we have to modify the ansatz (3.128) correspondingly:

$$S_{\mathbf{m}}^{\mathbf{M2}} = \begin{bmatrix} \alpha_{11}(\mathbf{m}) & \alpha_{12}(\mathbf{m}) \\ \alpha_{21}(\mathbf{m}) & \alpha_{22}(\mathbf{m}) \end{bmatrix}, \quad \mathbf{m} \in T. \tag{3.138}$$

The defining equations (3.127) read

$$D^{\mathbf{M2}}(p|\mathbf{t}) S^{\mathbf{M2}}_{(p^{-1})(\mathbf{m}-\mathbf{t})} = S_{\mathbf{m}}^{\mathbf{M2}} D^{\mathbf{M2}}(p|\mathbf{t}). \tag{3.139}$$

Setting the group elements $(p|\mathbf{t})$ equal to $(E|\mathbf{t})$ and $(z|\mathbf{0})$, respectively, we derive the following set of equations for the unknown matrix elements of (3.138):

$$\alpha_{11}(\mathbf{m}+\mathbf{t}) = \alpha_{11}(\mathbf{m}), \quad \alpha_{12}(\mathbf{m}+\mathbf{t}) = e^{-i\mathbf{M}\cdot\mathbf{t}} \alpha_{12}(\mathbf{m}), \tag{3.140}$$

$$\alpha_{21}(\mathbf{m}+\mathbf{t}) = e^{i\mathbf{M}\cdot\mathbf{t}} \alpha_{21}(\mathbf{m}), \quad \alpha_{22}(\mathbf{m}+\mathbf{t}) = \alpha_{22}(\mathbf{m}),$$
$$\alpha_{11}(-\mathbf{m}) = \alpha_{22}(\mathbf{m}), \quad \alpha_{12}(-\mathbf{m}) = -\alpha_{21}(\mathbf{m}), \tag{3.141}$$
$$\alpha_{21}(-\mathbf{m}) = -\alpha_{12}(\mathbf{m}), \quad \alpha_{22}(-\mathbf{m}) = \alpha_{11}(\mathbf{m}).$$

Since Eqs. (3.140) are independent of $\mathbf{m}$ we arrive at a two-parameter solution

$$\alpha_{11}(\mathbf{m}) = \alpha_{11}(\mathbf{0}), \quad \alpha_{12}(\mathbf{m}) = e^{-i\mathbf{M}\cdot\mathbf{m}} \alpha_{12}(\mathbf{0}),$$
$$\alpha_{21}(\mathbf{m}) = -e^{i\mathbf{M}\cdot\mathbf{m}} \alpha_{12}(\mathbf{0}), \quad \alpha_{22}(\mathbf{m}) = \alpha_{11}(\mathbf{0}), \tag{3.142}$$

where $\alpha_{11}(\mathbf{0})$ and $\alpha_{12}(\mathbf{0})$ are the free parameters. This is in accordance with $m_{\mathbf{M2}} = 2$. Consequently our general solution must be of the form

$$S_{\mathbf{m}}^{\mathbf{M2}} = \alpha_{11}(\mathbf{0}) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \alpha_{12}(\mathbf{0}) \begin{bmatrix} 0 & e^{-i\mathbf{M}\cdot\mathbf{m}} \\ -e^{i\mathbf{M}\cdot\mathbf{m}} & 0 \end{bmatrix}. \tag{3.143}$$

This suggests that we take as a normalized basis

$$3\, S_{\mathbf{m}}^{\mathbf{M2};1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{m} \in T, \tag{3.144}$$

$$3\, S_{\mathbf{m}}^{\mathbf{M2};2} = \begin{bmatrix} 0 & e^{-i\mathbf{M}\cdot\mathbf{m}} \\ -e^{i\mathbf{M}\cdot\mathbf{m}} & 0 \end{bmatrix}, \quad \mathbf{m} \in T, \tag{3.145}$$

where for clearness we have separated the G^*-irrep label M2 from the multiplicity index m by means of a semicolon.

The generating matrices of $\overline{Q}^{M2}$ are

$$U^{M2}(a) = \mathrm{diag}(1, -1), \tag{3.146}$$

$$U^{M2}(b^2) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \tag{3.147}$$

$$U^{M2}(b''b) = \mathrm{diag}(1, -1), \tag{3.148}$$

$$U^{M2}(c) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{3.149}$$

The matrices (3.146)–(3.149) and $U(q)$, $q \in \{a, b^2, b''b, c\}$, where $U(b^2) = U(b)U(b)$ and $U(b''b) = U(b'')U(b)$, define the operators $T(q)$. The comatrix representation Δ, defined by

$$T(q)S^{M2;m} = \sum_{m'} \Delta_{m',m}(q) S^{M2;m'}, \tag{3.150}$$

is a two-dimensional matrix corepresentation of $\tilde{Q}^{M2}$. Employing (3.118)–(3.121), (3.146)–(3.149), and (3.144) and (3.145) we arrive at the following matrix corepresentation:

$$\begin{aligned} &\Delta(a) = \mathrm{diag}(1, -1), \\ &\Delta(b^2) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \\ &\Delta(b''b) = \mathrm{diag}(1, -1), \\ &\Delta(c) = \mathrm{diag}(1,1). \end{aligned} \tag{3.151}$$

This implies

$$\tilde{Q}^{M2} \cong (C_2 \circledS (C_4 \circledS C_2)) \times C_2, \quad \tilde{Q}_0^{M2} \cong C_2 \circledS (C_4 \circledS C_2). \tag{3.152}$$

The remaining problem that has to be solved is to verify whether $\Delta(q)$, $q \in Q^{M2}$, is an irreducible corepresentation or not. A character test shows that (3.151) is irreducible. This implies that the multiplicity problem is entirely resolved by the auxiliary group $\tilde{Q}^{M2}$.

Due to our general approach we obtain the blocks $S^{N2;m}$, $m = 1,2$ by specifying (2.42) to this case. We define

$$S^{N2;m} = U(b'')S^{M2;m}, \quad m = 1,2, \tag{3.153}$$

which correpsonds to our choice of the coset representative. We have to insert (3.120), (3.144), and (3.145) into (3.153) in order to get

$$3\,S_{\mathbf{m}}^{N2;1} = \begin{bmatrix} e^{i\mathbf{Y}\cdot\mathbf{m}} & 0 \\ 0 & -e^{-i\mathbf{Y}\cdot\mathbf{m}} \end{bmatrix}, \quad \mathbf{m} \in T, \tag{3.154}$$

$$3\,S_{\mathbf{m}}^{N2;2} = \begin{bmatrix} 0 & e^{i\mathbf{X}\cdot\mathbf{m}} \\ e^{-i\mathbf{X}\cdot\mathbf{m}} & 0 \end{bmatrix}, \quad \mathbf{m} \in T. \tag{3.155}$$

The last representative we have to investigate is X2. As the procedure is quite the same as in the foregoing case we merely sketch it. At first we have to find a general solution of (3.127) where $\forall k = \mathrm{X2}$. Again we make an ansatz similar to that in (3.138) and specify the defining equations for $(E\,|\mathbf{t})$ and $(z|\mathbf{0})$, respectively. This leads to identities that are analogous to (3.140) and (3.141). This set of equations yields a two-parameter solution of the form

$$\begin{aligned} &\alpha_{11}(\mathbf{m}) = e^{-i\mathbf{N}\cdot\mathbf{m}}\alpha_{11}(\mathbf{0}), \quad \alpha_{12}(\mathbf{m}) = e^{-i\mathbf{Y}\cdot\mathbf{m}}\alpha_{12}(\mathbf{0}), \\ &\alpha_{21}(\mathbf{m}) = -e^{i\mathbf{Y}\cdot\mathbf{m}}\alpha_{12}(\mathbf{0}), \quad \alpha_{22}(\mathbf{m}) = e^{i\mathbf{N}\cdot\mathbf{m}}\alpha_{11}(\mathbf{0}), \end{aligned} \tag{3.156}$$

where $\alpha_{11}(\mathbf{0})$ and $\alpha_{12}(\mathbf{0})$ are the free parameters. This agrees with $m_{X2} = 2$. So our general solution can be written as

$$\begin{aligned} S_{\mathbf{m}}^{X2} = \alpha_{11}(\mathbf{0}) &\begin{bmatrix} e^{-i\mathbf{N}\cdot\mathbf{m}} & 0 \\ 0 & e^{i\mathbf{N}\cdot\mathbf{m}} \end{bmatrix} \\ &+ \alpha_{12}(\mathbf{0}) \begin{bmatrix} 0 & e^{-i\mathbf{Y}\cdot\mathbf{m}} \\ -e^{i\mathbf{Y}\cdot\mathbf{m}} & 0 \end{bmatrix}. \end{aligned} \tag{3.157}$$

For obvious reasons we choose as an orthonormalized basis

$$3\,S_{\mathbf{m}}^{X2;1} = \begin{bmatrix} e^{-i\mathbf{N}\cdot\mathbf{m}} & 0 \\ 0 & e^{i\mathbf{N}\cdot\mathbf{m}} \end{bmatrix}, \quad \mathbf{m} \in T, \tag{3.158}$$

$$3\,S_{\mathbf{m}}^{X2;2} = \begin{bmatrix} 0 & e^{-i\mathbf{Y}\cdot\mathbf{m}} \\ -e^{i\mathbf{Y}\cdot\mathbf{m}} & 0 \end{bmatrix}, \quad \mathbf{m} \in T. \tag{3.159}$$

The generating matrices of $\overline{Q}^{X2}$ are

$$D^{X2}(a) = U^{X2}(b'') = \mathrm{diag}(1, -1), \tag{3.160}$$

$$U^{X2}(b^2) = U^{X2}(c) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{3.161}$$

Employing the general definition (2.39) of the operators $T(q)$, $q \in \{a, b^2, b'', c\}$, where $U(b^2) = U(b)U(b)$, we establish by means of

$$T(q)S^{X2;m} = \sum_{m'} \Delta_{m',m}(q) S^{X2;m'} \tag{3.162}$$

a two-dimensional matrix corepresentation of Q^{X2}. A straightforward calculation yields

$$\Delta(a) = \Delta(b'') = \mathrm{diag}(1, -1), \tag{3.163}$$

$$\Delta(b^2) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \tag{3.164}$$

$$\Delta(c) = \mathrm{diag}(1,1). \tag{3.165}$$

This gives rise to the operator group

$$\tilde{Q}^{X2} \cong (C_2 \circledS (C_4 \circledS C_2)) \times C_2, \quad \tilde{Q}_0^{X2} \cong C_2 \circledS (C_4 \circledS C_2). \tag{3.166}$$

The remaining task is to investigate whether the matrix corepresentation (3.163)–(3.165) is irreducible or not. Again the character test shows that this corepresentation is irreducible. Accordingly the multiplicity problem is entirely resolved by the auxiliary group $\tilde{Q}^{X2}$.

The last task is to generate the blocks belonging to Y2. This is achieved by defining

$$S^{Y2;m} = U(b)S^{X2;m}, \quad m = 1,2, \tag{3.167}$$

where the choice of the coset representative corresponds to the last line of (3.126). Employing (3.119), (3.158), and (3.159) we arrive at the final result

$$3\,S_{\mathbf{m}}^{Y2;1} = \begin{bmatrix} e^{-i\mathbf{X}\cdot\mathbf{m}} & 0 \\ 0 & e^{i\mathbf{X}\cdot\mathbf{m}} \end{bmatrix}, \quad \mathbf{m} \in T, \tag{3.168}$$

$$3\,S_{\mathbf{m}}^{Y2;2} = \begin{bmatrix} 0 & e^{i\mathbf{N}\cdot\mathbf{m}} \\ -e^{-i\mathbf{N}\cdot\mathbf{m}} & 0 \end{bmatrix}, \quad \mathbf{m} \in T. \tag{3.169}$$

Finally let us briefly summarize our results. The rectangular blocks S^{G3}, S^{G4}; $S^{M2;m}, S^{N2;m}$ with $m = 1,2$ and $S^{X2;m}, S^{Y2;m}$ with $m = 1,2$ compose the 18-dimensional reducing matrix S. The crucial point of our approach is that the blocks $S^{\nu k}$ are symmetry adapted not only with respect to the group G^* but also with respect to the auxiliary groups $\tilde{Q}^{\nu k}$ and the "partner" blocks are fixed by generating relations. The freedom inherent in the generating relations has always been used to choose them in their simplest form. In this example we arrive at a complete resolution of the multiplicity problem by means of the auxiliary groups $\tilde{Q}^{\nu k}$.

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Crossing rules in Cartesian and standard coordinate systems

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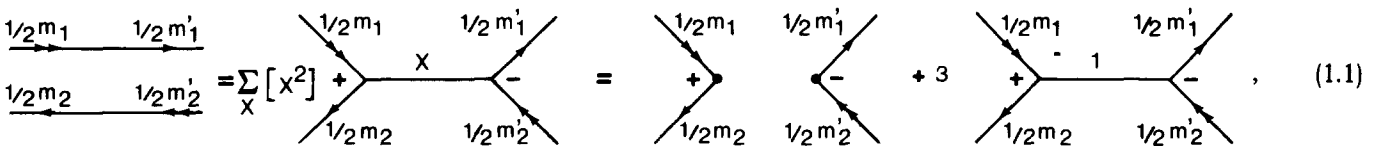
A vectorial and a tensorial crossing rule are defined in Cartesian coordinate systems. Different applications are given. With a particular choice of the standardization coefficient of vectors the same expression of dot and vector products in the standard and Cartesian coordinate systems results. The crossing rules are thus redefined in a standard coordinate system. Applications are obtained in the simplification of some particular "3*nj*" coefficients.

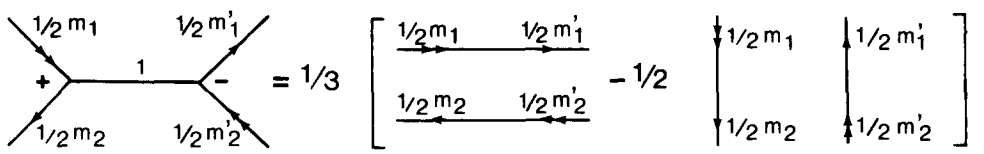
I. INTRODUCTION

The use of the *j*-summation rule[1] gives in some cases a systematic procedure to simplify expressions like "3*nj*" coefficients. The coupling of two spin-$\frac{1}{2}$'s gives, for instance,



(1.1)

and we can thus define the "spin-$\frac{1}{2}$ crossing rule"



(1.2)

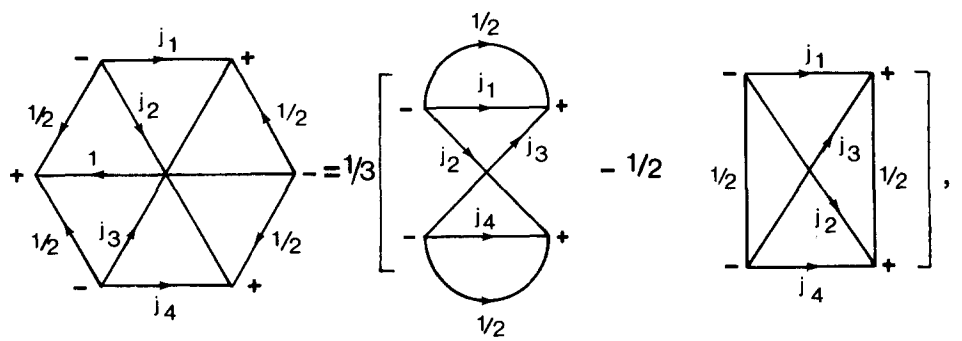
which reads analytically

$$\sum_m \begin{pmatrix} m_1 & \frac{1}{2} & m \\ \frac{1}{2} & m_2 & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{2} & m_2' \\ m & m_1' & \frac{1}{2} \end{pmatrix} = \frac{1}{3}\delta_{m_1 m_1'}\delta_{m_2 m_2'} - \frac{1}{6}\delta_{m_1 m_2}\delta_{m_1' m_2'} . \tag{1.3}$$

Applied to "6*j*" coefficient it gives, for instance,

$$\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & j \end{Bmatrix} = \frac{2}{3}\delta_{j0} - \frac{1}{6}(-)^j \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & j \\ \frac{1}{2} & \frac{1}{2} & j \end{Bmatrix}, \tag{1.4}$$

and with a "9*j*" coefficient it comes out



(1.5)

$$\begin{Bmatrix} j_1 & j_2 & \frac{1}{2} \\ j_3 & j_4 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 1 \end{Bmatrix} = \frac{1}{3}[j_2^{-2}]\delta_{j_2 j_3} \begin{Bmatrix} \frac{1}{2} & j_1 & j_2 \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & j_2 & j_4 \end{Bmatrix} + \frac{1}{6}(-)^{j_2+j_3} \begin{Bmatrix} j_1 & \frac{1}{2} & j_2 \\ j_4 & \frac{1}{2} & j_3 \end{Bmatrix} .$$

The above rule applies to more complicated diagrams and it is thus tempting to search for analog rules for higher spin.

In Cartesian coordinates a well-known vectorial crossing rule exists that represents graphically the summation over an index of the product of two Levi-Civita tensors. It appears that a suitable choice of transformation coefficients of Cartesian coordinates into spherical standard coordinates leads to a vectorial crossing rule and moreover, after some transformations, to

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a tensorial crossing rule in standard basis. Section III is thus devoted to the description of a graphical representation of a Cartesian basis and to some applications of the vectorial crossing rule in such a coordinate system. Section IV concerns the spherical standard coordinate system and the vectorial and tensorial crossing rules. Different applications in the determination of particular "3*nj*" coefficients are given in the last part of this paper.

II. THE CONFIGURATION SPACE

We suppose that the configuration space is spanned by an abstract vector state $|\hat{e}\rangle$, which forms a complete orthogonal system and thus verifies a closure relation like

$$\int |\hat{e}\rangle d\hat{e}\langle\hat{e}| = 1 , \tag{2.1}$$

if the $|\hat{e}\rangle$ state varies continuously over the spanned space. As an example of such a continuous state we usually introduce the solid angle state $|\Omega\rangle$

$$\int |\Omega\rangle d\Omega\langle\Omega| = 1 . \tag{2.2}$$

We know that a projection of the oribital momentum state $|lm\rangle$ on the configuration space spanned by $|\Omega\rangle$ states gives the spherical harmonic functions

$$\langle\Omega|lm\rangle = Y_{lm}(\Omega) , \tag{2.3}$$

which verify the orthonormalization relations

$$\int Y^*_{l'm'}(\Omega) Y_{lm}(\Omega) d\Omega = \int \langle l'm'|\Omega\rangle d\Omega\langle\Omega|lm\rangle = \langle l'm'|lm\rangle = \delta_{ll'}\delta_{mm'} . \tag{2.4}$$

III. THE CARTESIAN COORDINATE SYSTEM

Let $\mathbf{e}_i$ ($i = 1,2,3 = x,y,z$) represent three vectors of unit length along the three mutually perpendicular lines $0x$, $0y$, $0z$, respectively, that are taken as the positive coordinates axes. We introduce Cartesian orthonormal complete states $|1i\rangle = |i\rangle$:

$$\langle i|j\rangle = \delta_{ij}, \quad \sum_i |i\rangle\langle i| = 1 , \tag{3.1}$$

with $i = x,y,z$. The unit $\mathbf{e}_i$ vectors will be the projection of the $|i\rangle$ states onto the $|\hat{e}\rangle$ configuration state:

$$\mathbf{e}_i = \langle\hat{e}|i\rangle = \langle\hat{e}|1i\rangle . \tag{3.2}$$

In a three-dimensional Cartesian system it is not necessary to distinguish between covariant and contravariant components and thus

$$\mathbf{e}_i = \mathbf{e}_i^+ = \langle i|\hat{e}\rangle = \langle 1i|\hat{e}\rangle = \mathbf{e}_i . \tag{3.3}$$

The orthonormalization of the Cartesian unit vectors $\mathbf{e}_i$ now reads as

$$\mathbf{e}_i \cdot \mathbf{e}_j = \int \langle i|\hat{e}\rangle d\hat{e}\langle\hat{e}|j\rangle = \langle i|j\rangle = \delta_{ij} . \tag{3.4}$$

Let $\mathbf{V}$ be a vector and V_i the projection of $\mathbf{V}$ on the coordinate axis. Then

$$\mathbf{V} = \sum_i V_i \mathbf{e}_i = \sum_i \langle\hat{V}|i\rangle\langle i|\hat{e}\rangle = \langle\hat{V}|\hat{e}\rangle = \langle\hat{e}|\hat{V}\rangle , \tag{3.5}$$

where

$$V_i = \langle\hat{V}|i\rangle = V^i = \langle i|\hat{V}\rangle . \tag{3.6}$$

The scalar or dot product is obtained by replacing the $|\hat{e}\rangle$ configuration vector by an actual vector in (3.5):

$$\langle\hat{A}|\hat{B}\rangle = \sum_i \langle\hat{A}|i\rangle\langle i|\hat{B}\rangle = \sum_i A_i B_i = \mathbf{A}\cdot\mathbf{B} . \tag{3.7}$$

We introduce the following graphical representations:

$$\mathbf{e}_i = \mathbf{e}^i \;=\; \hat{e} \longleftarrow 1i , \qquad V_i = V^i \;=\; \hat{V} \longleftarrow 1i . \tag{3.8}$$

The usual summation rule over the i-index[1] leads to the graphical representation of a vector and of a scalar product of two vectors:

$$V = \langle\hat{e}|\hat{V}\rangle = \langle\hat{V}|\hat{e}\rangle = \hat{V} \longleftarrow 1 \longleftarrow \hat{e} , \qquad \langle\hat{A}|\hat{B}\rangle = \langle\hat{B}|\hat{A}\rangle = \mathbf{A}\cdot\mathbf{B} = \hat{A} \longleftarrow 1 \longleftarrow \hat{B} . \tag{3.9}$$

Let us now introduce a graphical representation of the Levi-Civita tensor:

$$\epsilon_{ijk} = \begin{cases} 1, & \text{for an even permutation of } x\,y\,z \text{ indices} , \\ -1, & \text{for an odd permutation of } x\,y\,z \text{ indices} , \\ 0, & \text{otherwise} , \end{cases} \tag{3.10}$$

$$= \quad \begin{array}{l} \text{i} \\ + \longleftarrow \text{k} \\ \text{j} \end{array} . \tag{3.11}$$

We thus get the graphical representation of the vector or cross product:

$$(\mathbf{A}\wedge\mathbf{B}) = \sum_k (\mathbf{A}\wedge\mathbf{B})_k \mathbf{e}_k = \sum_{ijk} A_i B_j \mathbf{e}_k \epsilon_{ijk}$$

$$= \quad \begin{array}{l} \hat{A} \overset{1}{\longleftarrow} \\ \qquad + \longleftarrow 1 \longleftarrow \hat{e} . \\ \hat{B} \overset{1}{\longleftarrow} \end{array} \tag{3.12}$$

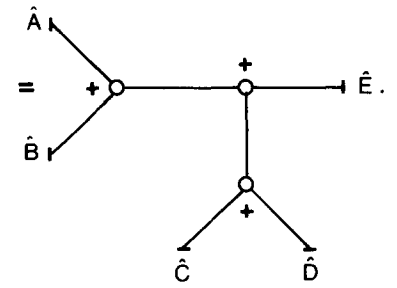
The triple scalar product is obtained by replacing $|\hat{e}\rangle$ by an actual vector in (3.12):

$$(\mathbf{A}\wedge\mathbf{B})\cdot\mathbf{C} = \sum_{ijk} A_i B_j C_k \epsilon_{ijk}$$

$$= \quad \begin{array}{l} \hat{A} \\ \qquad + \longleftarrow \hat{C} . \\ \hat{B} \end{array} \tag{3.13}$$

The graphical representations (3.7) and (3.12), (3.13) allow us to visualize any multiple product of vectors. We get, for instance,

$$P = ((\mathbf{A} \wedge \mathbf{B}) \wedge (\mathbf{C} \wedge \mathbf{D})) \cdot \mathbf{E}$$



(3.14)

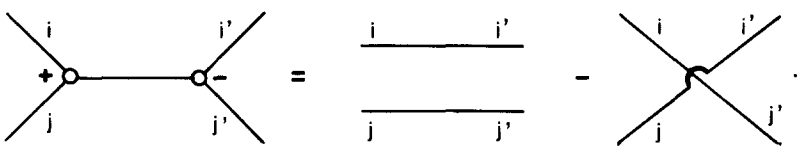
Such a product is expressible in seven different ways corresponding to the different possible separation of its representative diagram:

$$P = ((\mathbf{A} \wedge \mathbf{B}) \wedge (\mathbf{C} \wedge \mathbf{D})) \cdot \mathbf{E} = \mathbf{A} \cdot (\mathbf{B} \wedge ((\mathbf{C} \wedge \mathbf{D}) \wedge \mathbf{E}))$$

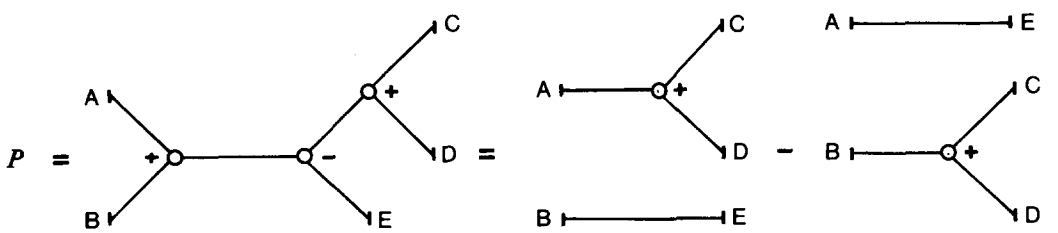
$$= (\mathbf{A} \wedge \mathbf{B}) \cdot ((\mathbf{C} \wedge \mathbf{D}) \wedge \mathbf{E}) = \cdots . \tag{3.15}$$

Let us now define "the vectorial crossing rule" by representing graphically the well-known identity

$$\sum_k \epsilon_{ijk}\epsilon_{i'j'k'} = \delta_{ii'}\delta_{jj'} - \delta_{ij'}\delta_{i'j} , \tag{3.16}$$

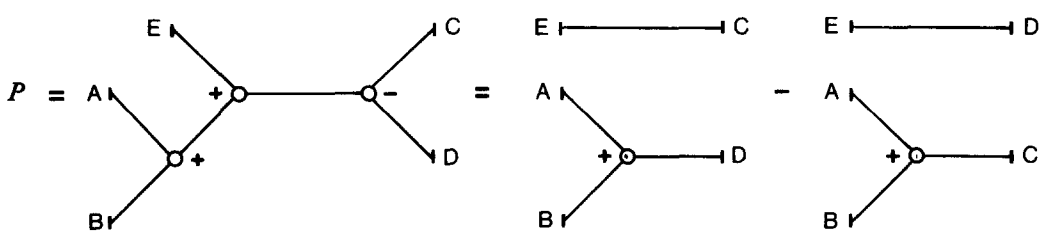


This crossing rule gives an easy simplification of any multiple product of vectors. We get, for instance, with (3.14),



$$= (\mathbf{A} \cdot (\mathbf{D} \wedge \mathbf{C}))(\mathbf{B} \cdot \mathbf{E}) - (\mathbf{A} \cdot \mathbf{E})(\mathbf{B} \cdot (\mathbf{D} \wedge \mathbf{C})) , \tag{3.17}$$

or, if we cut it in a different way,

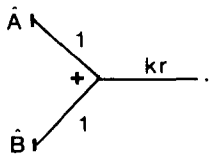


$$= (\mathbf{E} \cdot \mathbf{C})((\mathbf{A} \cdot (B \wedge \mathbf{D})) - (\mathbf{E} \cdot \mathbf{D})((\mathbf{A} \cdot (\mathbf{B} \wedge \mathbf{C})) . \tag{3.18}$$

Let us now consider vectors as rank-1 tensors in the Cartesian coordinate space $A_i = \langle \hat{A} \,|1i\rangle = A_{1i}$ and introduce a "3*jm*" Cartesian coefficient in the coupling of the tensors[2]:

$$C_{kr} = [k] \sum_{st} \begin{pmatrix} 1 & 1 & k \\ s & t & r \end{pmatrix} A_{1s}B_{1t}$$

$$= [k]$$



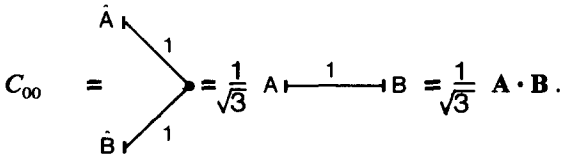
. (3.19)

The analytical expression of Cartesian "3*jm*" coefficients has already been given[2] and one finds the following three products.

(i) The scalar or dot product is

$$C_{00} = \sum_{st} \begin{pmatrix} 1 & 1 & 0 \\ s & t & 0 \end{pmatrix} A_{1s}B_{1t}$$

$$= \frac{1}{\sqrt{3}} \sum_{st} \delta_{st}A_{1s}B_{1t} = \frac{1}{\sqrt{3}} \mathbf{A} \cdot \mathbf{B} , \tag{3.20}$$

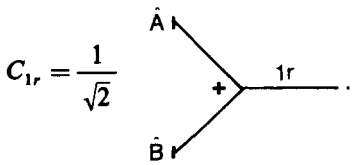


We find in the Cartesian system too, that a pole on a j line takes the $[j^{-1}]$ value.

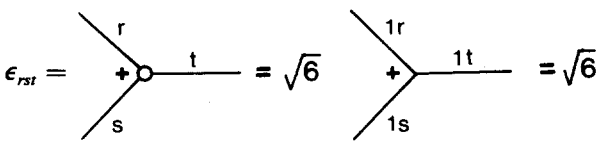
(ii) The vector or cross product is

$$C_{1r} = \sqrt{3}\sum_{st}\begin{pmatrix}1 & 1 & 1\\ s & t & r\end{pmatrix}A_{1s}B_{1t}$$

$$= \frac{1}{\sqrt{2}}\sum_{st}\epsilon_{str}A_{1s}B_{1t} = \frac{1}{\sqrt{2}}(\mathbf{A}\wedge\mathbf{B})_r\,, \tag{3.21}$$

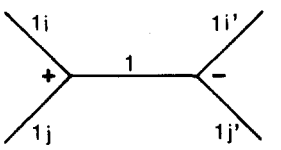


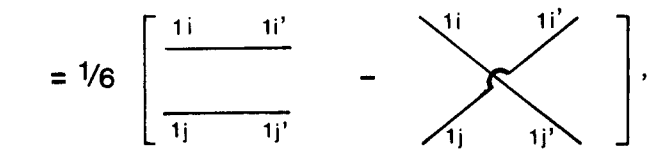
It appears here that the Levi-Civita tensor is proportional to a "3jm" Cartesian coefficient



$$\times\begin{pmatrix}1 & 1 & 1\\ r & s & t\end{pmatrix}. \tag{3.22}$$

With Cartesian "3jm" coefficients the vectorial crossing rule (3.15) now reads





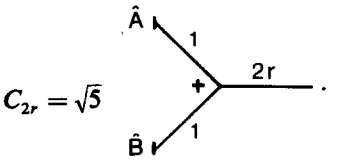
$$\sum_k\begin{pmatrix}1 & 1 & 1\\ i & j & k\end{pmatrix}\begin{pmatrix}1 & 1 & 1\\ i' & j' & k'\end{pmatrix} \tag{3.23}$$

$$= \tfrac{1}{6}[\delta_{ii'}\delta_{jj'} - \delta_{ij'}\delta_{ji'}]\,.$$

(iii) A tensor product is

$$C_{2r} = \sqrt{5}\sum_{st}\begin{pmatrix}1 & 1 & 2\\ s & t & r\end{pmatrix}A_{1s}B_{1t}$$

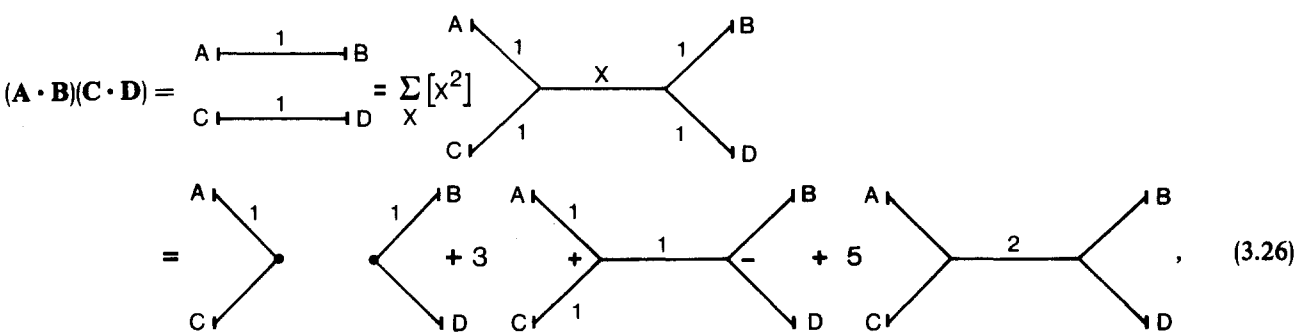
$$= A_rB_r - \frac{1}{3}B_r\sum_s A_s\,, \tag{3.24}$$



The analytical value of the "3jm" Cartesian coefficient is now

$$\begin{pmatrix}1 & 1 & 2\\ s & t & r\end{pmatrix} = \frac{1}{\sqrt{5}}\left(\delta_{rs}\delta_{tr} - \frac{1}{3}\delta_{rr}\delta_{st}\right). \tag{3.25}$$

If we apply the usual j-summation rule to the product of two dot products and use the vectorial crossing rule (3.15) we get a tensorial crossing rule:

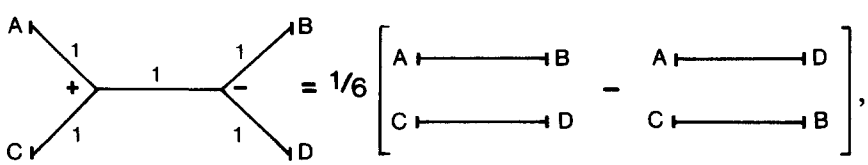


(3.26)

which reads analytically

$$(\mathbf{A}\cdot\mathbf{B})(\mathbf{C}\cdot\mathbf{D}) = \tfrac{1}{3}(\mathbf{A}\cdot\mathbf{C})(\mathbf{B}\cdot\mathbf{D}) + \tfrac{1}{2}(\mathbf{A}\wedge\mathbf{C})\cdot(\mathbf{B}\wedge\mathbf{D}) + T_2(\mathbf{A},\mathbf{C})\cdot T_2(\mathbf{B},\mathbf{D})\,.$$

We use the vectorial crossing rule (3.23) and



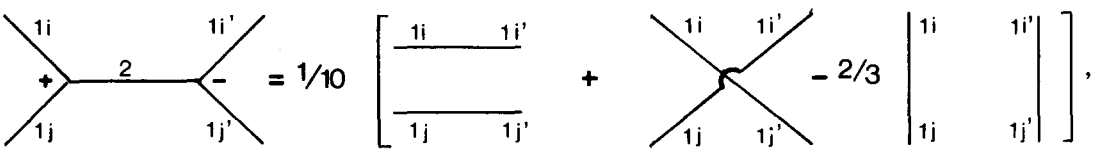
(3.27)

$$(\mathbf{A}\wedge\mathbf{C})\cdot(\mathbf{B}\wedge\mathbf{D}) = (\mathbf{A}\cdot\mathbf{B})(\mathbf{C}\cdot\mathbf{D}) - (\mathbf{A}\cdot\mathbf{D})(\mathbf{B}\cdot\mathbf{C})\,.$$

Bringing this value into (3.25) gives the result

$$T_2(\mathbf{A},\mathbf{C})\cdot T_2(\mathbf{B},\mathbf{D}) = \tfrac{1}{2}(\mathbf{A}\cdot\mathbf{B})(\mathbf{C}\cdot\mathbf{D}) + \tfrac{1}{2}(\mathbf{A}\cdot\mathbf{D})(\mathbf{C}\cdot\mathbf{B}) - \tfrac{1}{3}(\mathbf{A}\cdot\mathbf{C})(\mathbf{B}\cdot\mathbf{D})\,. \tag{3.28}$$

It leads to "the tensorial crossing rule"

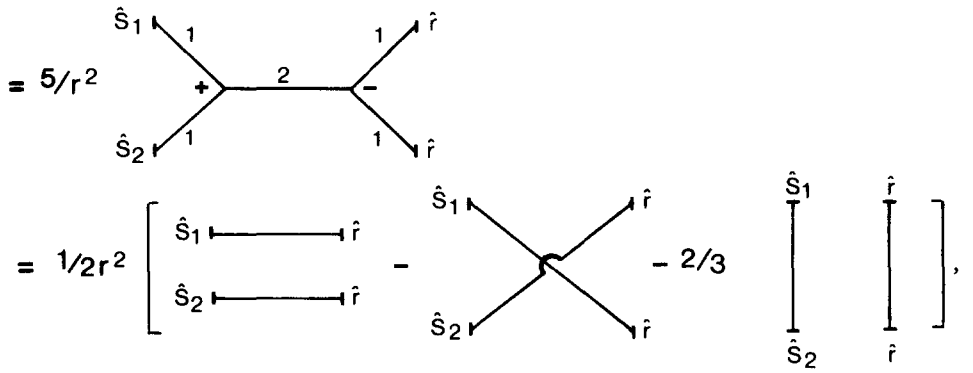


(3.29)

$$\sum_k \begin{pmatrix} 1 & 1 & 2 \\ i & j & k \end{pmatrix}\begin{pmatrix} 1 & 1 & 2 \\ i' & j' & k' \end{pmatrix} = \frac{1}{10}\left[\delta_{ii'}\delta_{jj'} + \delta_{ij'}\delta_{ji'} - \frac{2}{3}\delta_{ij}\delta_{i'j'}\right].$$

A good example of application of the above crossing rule is given with the nuclear tensor force

$$S_{12} = \frac{1}{r^2} T_2(\mathbf{S}_1,\mathbf{S}_2)\cdot T_2(\mathbf{r},\mathbf{r})$$



(3.30)

$$S_{12} = \tfrac{1}{2} r^{-2}\left[(\mathbf{S}_1\cdot\mathbf{r})(\mathbf{S}_2\cdot\mathbf{r}) + (\mathbf{S}_1\cdot\mathbf{r})(\mathbf{S}_2\cdot\mathbf{r}) - \tfrac{2}{3}(\mathbf{S}_1\cdot\mathbf{S}_2)(\mathbf{r}\cdot\mathbf{r})\right]. \tag{3.31}$$

We thus find the well-known expression of the tensor force in Cartesian coordinates to be

$$S_{12} = [(\mathbf{S}_1\cdot\mathbf{r})(\mathbf{S}_2\cdot\mathbf{r})/r^2] - \tfrac{1}{3}(\mathbf{S}_1\cdot\mathbf{S}_2). \tag{3.32}$$

IV. THE STANDARD COORDINATE SYSTEM

We introduce a standard basis spanned by the $|1\mu\rangle$ complete set of orthonormal states:

$$\langle 1\mu|1\mu'\rangle = \delta_{\mu\mu'}, \quad \sum_\mu |1\mu\rangle\langle 1\mu| = 1, \tag{4.1}$$

with $\mu = -1, 0, 1$. Projecting these states onto the configuration space defines the unit vector in the standard basis, we get

$$\mathbf{e}_\mu = \langle\hat{e}|1\mu\rangle = \hat{e} \xrightarrow{1\mu}, \qquad \mathbf{e}^\mu = \mathbf{e}_\mu^+ = (-)^{1-\mu}\mathbf{e}_{-\mu} = \hat{e} \xleftarrow{1\mu}. \tag{4.2}$$

We have now to distinguish between contravariant and covariant compounds of a vector:

$$V_\mu = \langle\hat{V}|1\mu\rangle = \hat{V} \xrightarrow{1\mu}, \qquad V^\mu = V_\mu^+ = (-)^{1-\mu}V_{-\mu} = \hat{V} \xleftarrow{1\mu}. \tag{4.3}$$

It is now clear that any vector may be projected onto its covariant or contravariant components as

$$\begin{aligned}\mathbf{V} = \langle\hat{V}|\hat{e}\rangle &= \sum_\mu \langle\hat{V}|1\mu\rangle\langle 1\mu|\hat{e}\rangle \\ &= \sum_\mu V_\mu e^\mu = \hat{V} \xrightarrow{1} \hat{e} \\ &= \langle\hat{e}|\hat{V}\rangle = \sum_\mu \langle\hat{e}|1\mu\rangle\langle 1\mu|\hat{V}\rangle \\ &= \sum_\mu V^\mu \mathbf{e}_\mu = \hat{e} \xrightarrow{1} \hat{V},\end{aligned} \tag{4.4}$$

and one gets the scalar product of two vectors with

$$\begin{aligned}\langle\hat{A}|\hat{B}\rangle &= \sum_\mu \langle\hat{A}|1\mu\rangle\langle 1\mu|\hat{B}\rangle \\ &= \sum_\mu A_\mu B^\mu = \hat{A} \xrightarrow{1} \hat{B} \\ &= \langle\hat{B}|\hat{A}\rangle = \sum_\mu \langle\hat{B}|1\mu\rangle\langle 1\mu|\hat{A}\rangle \\ &= \sum_\mu B_\mu A^\mu = \hat{B} \xrightarrow{1} \hat{A}.\end{aligned} \tag{4.5}$$

If we express the summation over μ, we get

$$\langle\hat{A}|\hat{B}\rangle = \langle\hat{B}|\hat{A}\rangle = A_{11}B_{1-1} + A_{1-1}B_{11} - A_{10}B_{10}. \tag{4.6}$$

The standardization procedure[3] links spherical standard and Cartesian unit vectors with the relations

$$\mathbf{e}_{10} = C(-i\mathbf{e}_z), \quad \mathbf{e}_{1\pm1} = \pm(C/\sqrt{2})(i\mathbf{e}_x \mp \mathbf{e}_y), \tag{4.7}$$

and we find, with (4.6), that

$$\langle\hat{A}|\hat{B}\rangle = \langle\hat{B}|\hat{A}\rangle = C^2\mathbf{A}\cdot\mathbf{B}. \tag{4.8}$$

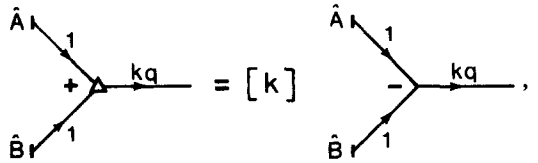
If we compare (4.8) to (3.7) it appears that we must impose $C^2 = 1$ to get an identical definition of the dot product in scalar and spherical standard coordinates.

We thus choose $C = 1$ in the standardization procedure (4.7).

With $A_{1\mu}$ and $B_{1\mu}$ standard components of **A** and **B** vectors (rank-1 tensors) we may define a tensor product as

$$\pi_{kq} = \sum_{\mu\nu} \langle 1\mu\ 1\nu | kq \rangle A_{1\mu} B_{1\nu}$$

$$= [k] \sum_{\mu\nu} \begin{pmatrix} \mu & \nu & k \\ 1 & 1 & q \end{pmatrix} A_{1\mu} B_{1\nu} , \tag{4.9}$$



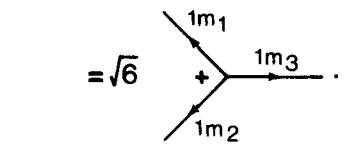
where the usual Clebsch–Gordan and "3*jm*" coefficients have been introduced. One then easily obtains the following tensor components:

(i) $\pi_{00} = (1/\sqrt{3})\,\mathbf{A}\cdot\mathbf{B} = C_{00}$,

(ii) $\pi_{1q} = (1/\sqrt{2})(\mathbf{A}\wedge\mathbf{B})_q = C_{1q}$. (4.10)

It appears that the dot and the vector product of two vectors get the same graphical representation in Cartesian and in standard coordinates. In other words,

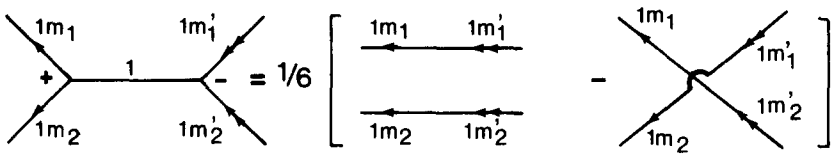
$$\epsilon_{m_1 m_2 m_3} = \sqrt{6} \begin{pmatrix} 1 & 1 & 1 \\ m_1 & m_2 & m_3 \end{pmatrix}$$



(4.11)

In standard coordinates $m_1 m_2 m_3 = 0 \pm 1$ and $m_1 + m_2 + m_3 = 0$, and in Cartesian coordinates $m_1 m_2 m_3 = x\,y\,z$.

We can thus define "the vectorial crossing rule" in any coordinate system:



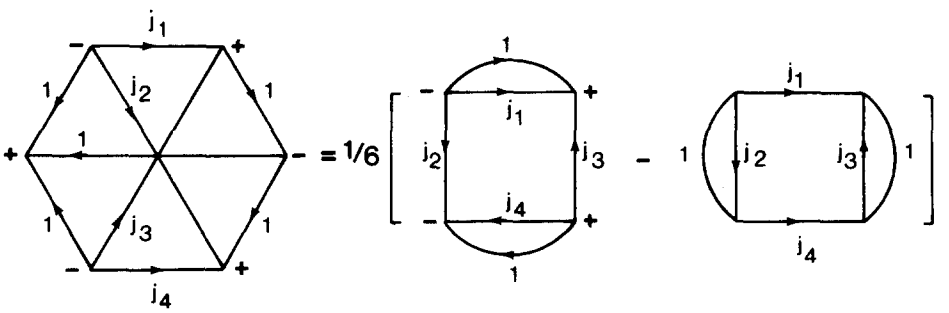
(4.12)

$$\sum_{m_3} \begin{pmatrix} 1 & 1 & 1 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} m_3 & m_1' & m_2' \\ 1 & 1 & 1 \end{pmatrix} = \frac{1}{6} \left[\delta_{m_1 m_1'} \delta_{m_2 m_2'} - \delta_{m_1 m_2'} \delta_{m_2 m_1'} \right] .$$

We can use (4.12) to determine "3*nj*" coefficients. We get, for instance,

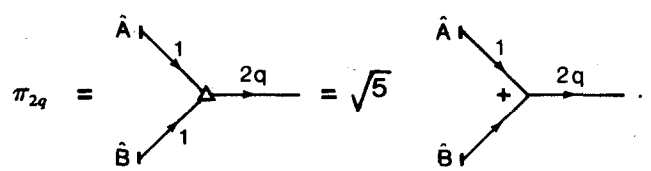
$$\begin{Bmatrix} 1 & 1 & 1 \\ 1 & 1 & j \end{Bmatrix} = -\frac{1}{6} \left[3\delta_{j0} - \{1\ \ 1\ \ j\} \right] , \tag{4.13}$$

while



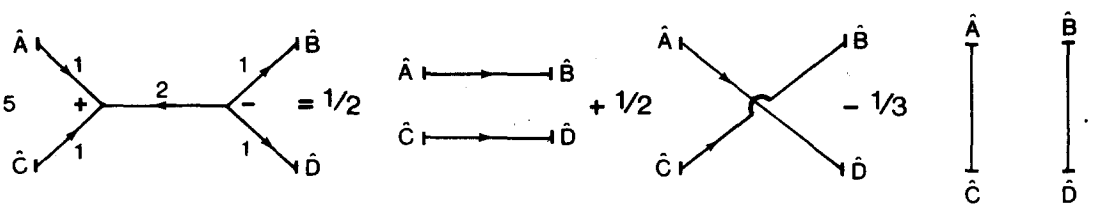
$$= \tfrac{1}{6}[j_2^{-2}]\delta_{j_2 j_3} \{1\ \ j_1\ \ j_2\}\{1\ \ j_2\ \ j_4\} - \tfrac{1}{6}[j_1^{-2}]\delta_{j_1 j_4} \{j_1\ \ j_2\ \ 1\}\{j_1\ \ j_3\ \ 1\} . \tag{4.14}$$

(iii) The rank-2 tensor is obtained with (4.9):



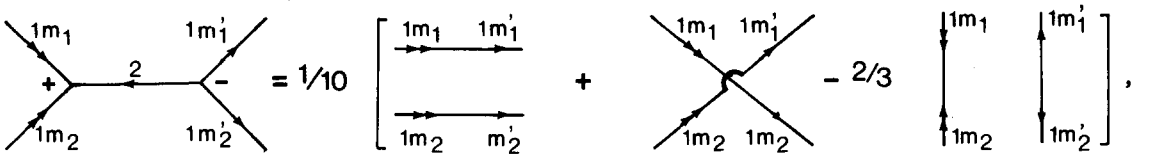
(4.15)

The scalar product (3.28) is easily expressed in standard coordinates:



(4.16)

It leads to "the tensorial crossing rule"



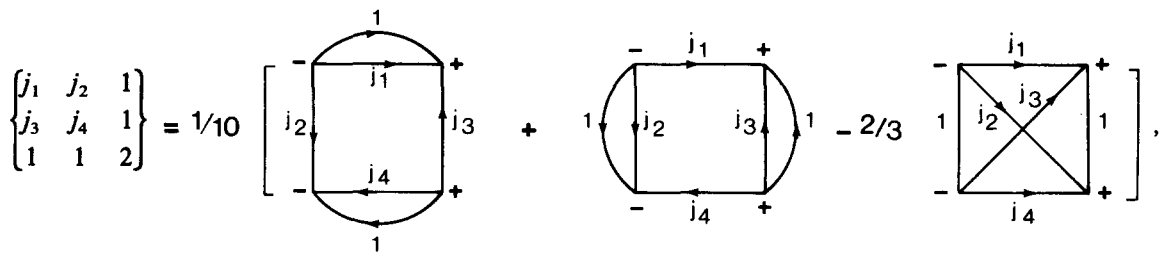
(4.17)

$$\sum_{m_3}\begin{pmatrix} m_1 & m_2 & m_3 \\ 1 & 1 & 2 \end{pmatrix}\begin{pmatrix} 2 & 1 & 1 \\ m_3 & m_1' & m_2' \end{pmatrix} = \tfrac{1}{10}\delta_{m_1 m_1'}\delta_{m_2 m_2'} + \tfrac{1}{10}\delta_{m_1 m_2'}\delta_{m_2 m_1'} - \tfrac{1}{15}(-)^{m_2+m_2'}\delta_{m_1,-m_2}\delta_{m_1'-m_2'}.$$

Such a crossing rule gives analytical expressions of particular "3nj" coefficients. We get, for instance,

$$\begin{Bmatrix} 1 & 1 & 2 \\ 1 & 1 & j \end{Bmatrix} = \frac{3}{10}\delta_{j0} + \frac{1}{5}\left(\frac{1}{2} - \frac{1}{3}(-)^j\right)\{1 \quad 1 \quad j\}, \tag{4.18}$$

while a "9j"gives the analytical value



(4.19)

$$\begin{Bmatrix} j_1 & j_2 & 1 \\ j_3 & j_4 & 1 \\ 1 & 1 & 2 \end{Bmatrix} = \frac{1}{10}[j_2^{-2}]\delta_{j_2 j_3}\{j_1 \quad j_2 \quad 1\}\{j_2 \quad j_4 \quad 1\}$$

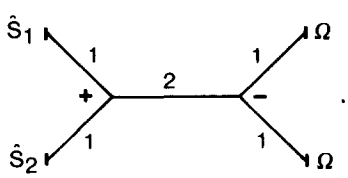
$$+\frac{1}{10}[j_1^{-2}]\delta_{j_1 j_4}(-)^{j_3-j_2}\{j_1 \quad j_2 \quad 1\}\{j_1 \quad j_3 \quad 1\} - \frac{1}{15}(-)^{j_2+j_3}\begin{Bmatrix} j_1 & 1 & j_2 \\ j_4 & 1 & j_3 \end{Bmatrix}. \tag{4.20}$$

Another interesting example consists in expressing the tensor force S_{12} as given in (3.30) and (3.32) in a standard basis. In that case,

$$= r_{1\mu} = -i\sqrt{4\pi/3}\, rY_{1\mu}(\Omega), \tag{4.21}$$

and thus

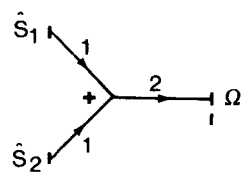
$$S_{12} = -\frac{20\pi}{3}$$



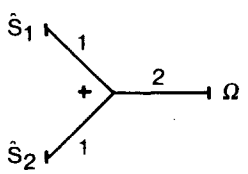
(4.22)

We use the contraction rule of the two spherical harmonics[1] to get

$$S_{12} = -\frac{4\pi}{3}\begin{pmatrix} 1 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix}\frac{[1 \quad 1 \quad 2]}{\sqrt{4\pi}}$$



$$= -\sqrt{\frac{8\pi}{3}}$$



$$= -\sqrt{\frac{8\pi}{3}}\sum_{\mu\nu\lambda} S^{(1)}_{1\mu}S^{(2)}_{1\nu}Y_{2\lambda}(\hat{r})\begin{pmatrix} \mu & \nu & 2 \\ 1 & 1 & \lambda \end{pmatrix}. \tag{4.23}$$

Such an expression of the tensor force is more suitable to handle with the Wigner–Eckart theorem, for instance.

We have thus defined a "spin-$\frac{1}{2}$ crossing rule" in (1.2) or (1.3), a "vectorial crossing rule" in (3.15) or (3.23) or (4.12), and a "tensorial crossing rule" in (3.29) or (4.17). One can probably extend the procedure to higher spin values by a direct summation in Cartesian coordinate systems for integer values of the spin, but the interest of such rules lies essentially in their simplicity.

ACKNOWLEDGMENTS

I am indebted to Dr. J. Meyer and Dr. G. H. Lamot from the Institut de Physique Nucléaire, Lyon for helpful discussions and for carefully reading the manuscript.

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Relation between the supertableaux of the supergroups OSP(2|2) and SU(1|2)

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The classification and the interpretation of the Young supertableaux of the orthosymplectic group OSP (2|2) are given. A comparison is made with the supertableaux of the superunitary group SU(1|2) taking advantage of the isomorphism of the corresponding superalgebras.

I. INTRODUCTION

The simplest orthosymplectic group having both typical and atypical finite-dimensional representations is OSP(2|2). A second interest for this supergroup if the isomorphism of its superalgebra C(2) with the superalgebra of the superunitary group SU(1|2).

The purpose of this paper is an analysis of the Young supertableaux of OSP(2|2). We determine the SO(2)×Sp(2) content of the supertableaux by using the tensor product method. This allows us to connect the supertableaux with representations of C(2). As a result we obtain typical representations and atypical non-fully-reducible representations only. Of course all these representations are self-contragradient.

In the last parts we recall a few results concerning the supertableaux of SU(1|2) and we make the comparison between the two sets of supertableaux associated to isomorphic superalgebras.

II. GENERALITIES

Let V be a graded four-dimensional vector space and G an even bilinear form written in a convenient basis as

$$G=\begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{vmatrix}.$$

We have two possible graduations for V, $\varepsilon_v = \pm 1$, depending if the grade $g_\alpha = 0$ or 1 modulo 2 of the indices

$$\varepsilon_v = +1, \quad g_1 = g_2 = 0, \quad g_3 = g_4 = 1,$$

$$\varepsilon_v = -1, \quad g_1 = g_2 = 1, \quad g_3 = g_4 = 0.$$

The orthosymplectic group OSP(2|2) is the set of graded linear transformations in V leaving invariant the even bilinear form G. Its superalgebra is the set of generators superantisymmetric with respect to G. In Kac's notation this superalgebra is C(2) (see Ref. 1).

The Bose sector of C(2) is the Lie algebra of SU(2) ⊗ Sp(2) or, by isomorphism, of U(1) ⊗ SU(2).

The irreducible representations of C(2) are defined by their highest weight, e.g., by two Kac–Dynkin parameters a_1 and a_2: a_1 is an arbitrary complex number; and a_2 is a nonnegative integer—it is the Sp(2) Dynkin parameter. We shall use the notation

$$\{a_1|a_2\}$$

for an irreducible representation of C(2).

The hidden SO(2) generator k has eigenvalues related to the Kac–Dynkin parameters as follows[2]:

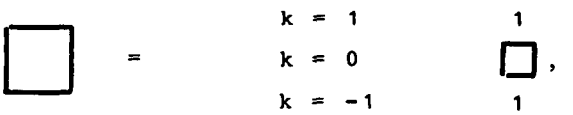
$$k = a_1 - a_2.$$

When the graduation of V is $\varepsilon_v = +1$ we have class I representations, and when it is $\varepsilon_v = -1$ we have class II representations. The simple connection existing between class I and class II representations allows us to restrict from now to class I representations.[3]

Young supertableaux have been defined for the simple classical super groups[3,4] and in particular for the orthosymplectic group OSP(2|2).

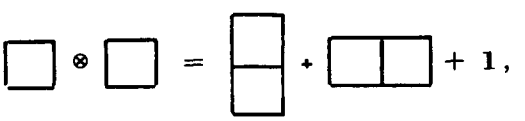
III. METHOD

The method of investigation of the properties of the OSP(2|2) supertableaux is the tensor product method already extensively discussed in previous publications.[5,6] We start with the one box supertableau describing the four-dimensional typical irreducible representation $\{1|0\}$, where the orthosymplectic group OSP(2|2) is defined. The SO(2) ⊗ Sp(2) components of this representation are



where 1 is the singlet representation of Sp(2).

The simplest case is the tensor product of one box by itself and we have



$$4 \times 4 = 8 + 7 + 1$$

where 1 is the zero box supertableaux of OSP(2|2).

The dimensions indicated are computed with the determinant techniques of Balentekin and Bars.[3]

The first supertableau corresponds to a second-rank superantisymmetric tensor and it describes the eight-dimensional adjoint representation $\{2|1\}$.

The supersymmetric subspace of the tensor product $V \otimes V$ contains the invariant one-dimensional subspace associated with the conserved form G. However, a direct calcula-

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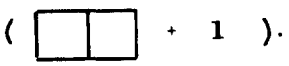
tion[3] shows that this subspace cannot be substracted and the same result holds for any orthosymplectic group OSP(2p|2p). The supersymmetric subspace is then a non-fully-reducible representation of dimension 8 associated to the set of supertableaux



This set will be called a generalized supertableau[5,6] and we use the notation

IV. INTERPRETATION OF THE SUPERTABLEAUX OF OSP(2|2)

The supertableaux of OSP(2|2) have one row and one column of arbitrary length. The class I supertableaux are conveniently parametrized as indicated on Fig. 1 (see Ref. 2). The highest weight of the supertableau κ, ν is given by a Young tableau of Sp(2) with ν boxes and the eigenvalue of the SO(2) generator $k = \kappa$. This highest weight will be denoted by $(\nu + \kappa|\nu)$.

Besides the zero box supertableau 1, which has the highest weight (0|0) and which describes the singlet representation $\{0|0\}$ of OSP(2|2), the atypical supertableaux are those for which the lengths of the row and the column are related by

$$\kappa = 2 + \nu.$$

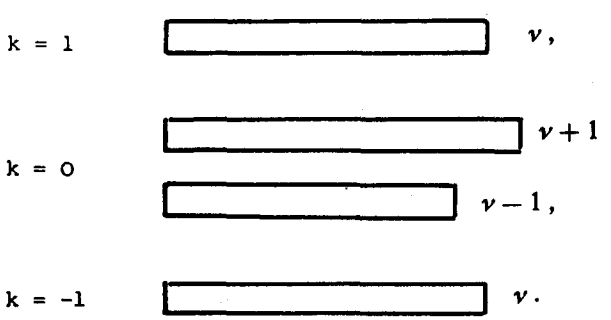
This relation corresponds, for the Kac–Dynkin parameter a_1 of the highest weight, to the atypical value

$$a_1 = 2(1 + a_2).$$

The one-column supertableaux $\kappa = 1$ are all typical and they describe the irreducible representation of OSP(2|2),

$$\{\nu + 1|\nu\}.$$

This representation has, for $\nu \geqslant 1$, four SO(2) ⊗ Sp(2) components distributed in three levels in k,



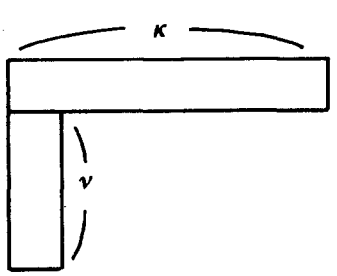


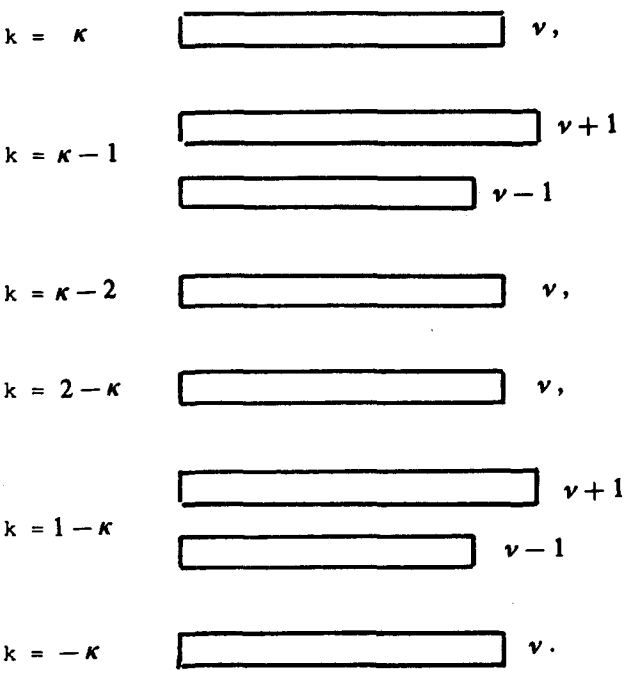
FIG. 1. Supertableau of OSP(2|2).

It is a self-contragradient representation of dimension $4(1 + \nu)$. The case $\nu = 0$ has been considered in Sec. III.

For the supertableaux $\kappa > 1$ we have to take into account the reducibility O(2) ⇒ SO(2) (see Ref. 2). Consider first the typical cases where $\kappa \neq 2 + \nu$. The supertableau describes the direct sum of two irreducible typical representations of OSP(2|2),

$$\{\nu + \kappa|\nu\} \oplus \{\nu + 2 - \kappa|\nu\}.$$

Each of these representations has, for $\nu \geqslant 1$, four SO(2) ⊗ Sp(2) components distributed in three levels in k and the reduction of the supertableau with respect to SO(2) ⊗ Sp(2) is the following:



The two contragradient irreducible representations $\{\nu + \kappa|\nu\}$ and $\{\nu + 2 - \kappa|\nu\}$ have the dimension $4(\nu + 1)$ and the typical supertableau has the dimension $8(\nu + 1)$.

Let us now discuss the atypical case $\kappa = 2 + \nu$. Such supertableaux are easily obtained in the tensor product of a typical supertableau T by the one box supertableau. As a result of the tensor product method we observe the production in pairs (T_1, T_2) of atypical supertableaux with

$$T_1 \Rightarrow \nu + 2, \nu, \quad T_2 \Rightarrow \nu + 1, \ \nu - 1.$$

This pair is called a generalized supertableau and it is noted as in Fig. 2 (see Refs. 5 and 6).

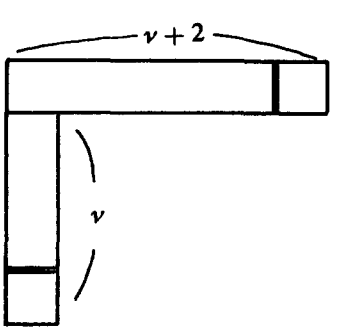


FIG. 2. Generalized supertableau of OSP(2|2).

The case $\nu = 0$ has been discussed in Sec. III.

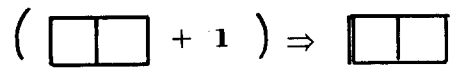
The dimension of the atypical supertableau T_1 as given by the determinant method is[3]

$$8(1+\nu) + (-)^{1+\nu},$$

and for the pair (T_1, T_2) we get the dimension $8(2\nu+1)$.

The two supertableaus T_1 and T_2 cannot be separated and they are associated to non-fully-reducible representations of OSP(2|2) with four atypical components.

For $\nu = 0$ the generalized supertableau introduced in Sec. III,

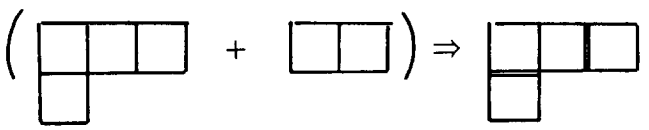


describes the self-contragradient non-fully-reducible representation of dimension 8 of OSP(2|2) whose atypical components are

$$\{2|0\}_3 + 2\{0|0\}_1 + \{0|1\}_3.$$

For $\nu \geqslant 1$ the generalized supertableaux are associated to pairs of contragradient non-fully-reducible representations. We now make precise the atypical components of these representations.

For $\nu = 1$ the generalized supertableau



has the dimension $17 + 7 = 24$ and the two 12-dimensional non-fully-reducible representations are

$$[\{4|1\}_5 + 2\{2|0\}_3 + \{0|0\}_1] \oplus [\{0|2\}_5 + 2\{0|1\}_3 + \{0|0\}_1].$$

For $\nu \geqslant 2$ the atypical components of the supertableaux are

$$[\{2\nu+2|\nu\} + 2\{2\nu|\nu-1\} + \{2\nu-2|\nu-2\}] \oplus [\{0|\nu+1\} + 2\{0|\nu\} + \{0|\nu-1\}].$$

Resume: The set of the supertableaux of OSP(2|2) generated by tensor product from the fundamental representation $\{1|0\}$ of C(2) is conveniently divided into two classes.

(i) Class A: $\nu + \kappa$ is even. It is a subset of the supertableaux generated by the tensor product from the adjoint representation $\{2|1\}$ of C(2). In this set we find typical supertableaux and generalized supertableaux.

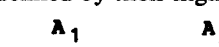
(ii) Class B: $\nu + \kappa$ is odd. It is not a subgroup and it contains only typical supertableaux.

Obviously class A is the factor group of the full set of supertableaux by Z_2.

V. THE SU(1|2) SUPERTABLEAUX

The representations and the supertableaux have been extensively studied[3] and we only briefly here recall a few results for the purpose of comparison.

The superalgebra of the superunitary group SU(1|2) is denoted A(0,1) by Kac and its even part is the Lie algebra of $U(1) \times SU(2)$. The irreducible representations of A(0,1) are defined by their highest weight and denoted



where A_1 is an arbitrary complex number and A_2 a non-negative integer, i.e., a SU(2) Dynkin parameter. The U(1) generator Q has eigenvalues given by

$$Q = A_1 - \tfrac{1}{2}A_2.$$

The two superalgebra C(2) and A(0,1) are isomorphic and the correspondence between the Kac–Dynkin parameters is as follows:

$$A_1 = a_1/2, \quad A_2 = a_2, \quad Q = k/2.$$

The supertableaux of the superunitary group SU(1|2) are constructed by the tensor product of the two contragradient fundamental representations

The corresponding set of involved representations has integer algebraic values for A_1.

It is convenient to classify the SU(1|2) supertableaux in two classes.[5]

(i) Class Δ_0*:* naturally typical supertableaux. We have here typical supertableaux describing typical irreducible representations of SU(1|2) and generalized supertableaux associated to non-fully-reducible representations of SU(1|2) with four atypical components.

(ii) Class Δ_1*:* naturally atypical supertableaux. They are associated to the atypical irreducible representations of SU(1|2).

We shall consider in what follows the class I supertableaux of SU(1|2) by grading the three-dimensional space $V = V_0 + V_1$ of the fundamental representation $\overset{1}{\otimes}\!\!-\!\!\overset{0}{0}$ as

$$\dim V_0 = 1, \quad \dim V_1 = 2.$$

The SU(1|2) supertableaux of the CLASS Δ_0 are characterized by one row and two column parameters for two Kac–Dynkin parameters A_1 and A_2. Therefore we can introduce in Δ_0 a relation of equivalence for supertableaux associated to the same representation of SU(1|2). e.g., having the same dimension and the same $U(1) \otimes SU(2)$ content. Such a relation holds for typical supertableaux and generalized atypical supertableaux.[5] In the examples used in the next section we shall choose the simplest supertableau of the family for illustration.

VI. RELATION BETWEEN THE SUPERTABLEAUX OF OSP(2|2) AND SU(1|2)

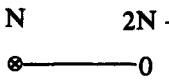
We first observe that the class B supertableaux of OSP(2|2) are associated to representations with a_1 odd and therefore A_1 half-integer. Thus they cannot be related to supertableaux of SU(1|2).

The class A supertableaux of OSP(2|2) describe either typical representations or non-fully-reducible atypical representations of OSP(2|2). Therefore they cannot be related to the atypical irreducible supertableaux of class Δ_1 of SU(1|2).

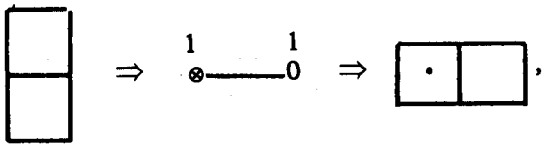
The only possible overlap between the two sets of supertableaux concerns only the class A supertableaux of OSP(2|2) and the class Δ_0 supertableaux of SU(1|2).

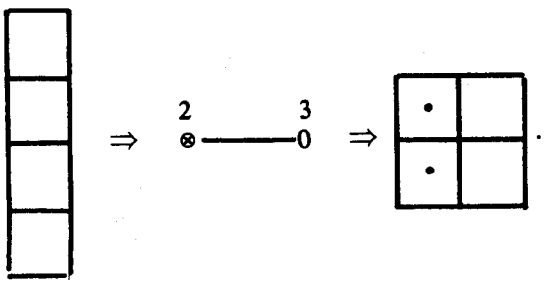
For $\kappa = 1, \nu = 2N - 1$ $(N \geqslant 1)$ the OSP(2|2) supertableau

of highest weight $(2N, 2N-1)$ describes the self-contragradient irreducible typical representation of $A(0,1)$,

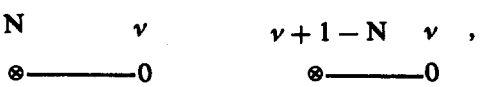


and it is associated to a one-parameter family of equivalent irreducible typical mixed supertableaux of SU(1|2). Let us give the two examples $N=1$ and $N=2$:

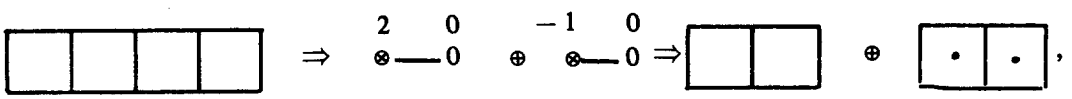


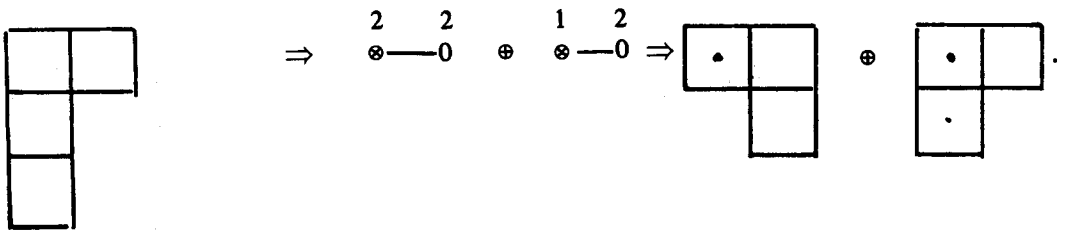


For $\kappa > 1$, $\nu + \kappa = 2N$ typical $(N \geqslant 2,\ N \neq 1+\nu)$ the OSP(2|2) supertableau of highest weight $(2N\,|\nu)$ describes the direct sum of two contragradient irreducible typical representations of $A(0,1)$,



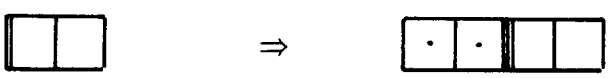
and it is associated to a one-parameter family of equivalent pairs of irreducible typical supertableaux of SU(1|2). Let us give the two examples for $N=2$:





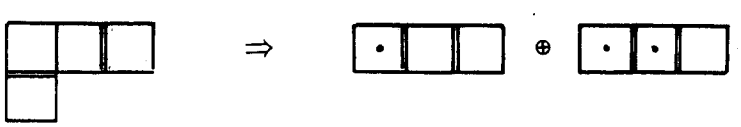
For $\kappa = \nu + 2$ the pair T_1 and T_2 of atypical supertableaux of OSP(2|2) with highest weights $(2\nu+2|\nu)$, $(2\nu|\nu-1)$ is a generalized atypical supertableau and it describes for $\nu \geqslant 1$ the direct sum of two contragradient non-fully-reducible representations of A(0,1) with four atypical components. This generalized atypical supertableau of OSP(2|2) is then associated to a one-parameter family of equivalent pairs of generalized atypical supertableaux of SU(1|2). Let us give three examples for $\nu = 0$, 1, 2.

For $\nu = 0$ we have the eight-dimensional self-contragradient non-fully-reducible representation of A(0,1)



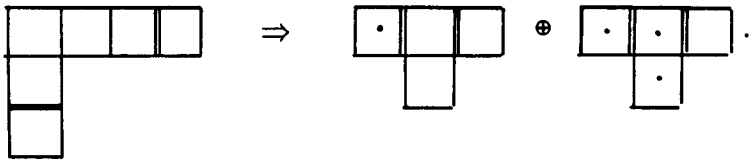
8 8

For $\nu = 1$ we have two 12-dimensional non-fully-reducible representations of A(0,1)



24 12 12

For $\nu = 2$ we have two 20-dimensional non-fully-reducible representations of A(0,1)



40 20 20

For the description of the generalized atypical supertableaux of SU(1|2) see Ref. 5.

VII. CONCLUDING REMARKS

The classification of the Young supertableaux of the orthosymplectic group OSP(2|2) has been made by using two different criteria: (i) the size of the supertableau defined by the value of the parameter κ,

$$\kappa = 0, \quad \kappa = 1, \quad \kappa > 1,$$

and (ii) the structure of the full set of supertableau with the parity of $\nu + \kappa$, the center of the orthosymplectic group OSP(2|2) being isomorphic to Z_2.

These two types of considerations can be extended to the orthosymplectic groups OSP(2|2p) and the results will be given in a later publication.

The isomorphism of the superalgebra C(2) and A(0,1) allows us to control our results by making a comparison with those obtained for the supertableaux of the superunitary group SU(1|2). The analogies and the differences between the two sets of supertableaux have been explained and explicit examples of correspondences have been given.

ACKNOWLEDGMENTS

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Occurrence of secular terms in the Carleman embedding

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Secular terms occur in many perturbative solutions of nonlinear equation systems. In this work, an investigation is made of which cases they may occur in as the result of the application of the linear Carleman embedding to a system of nonlinear equations. The solution for the embedded system is written in a form that makes it convenient to see how these terms originate. Their occurrence for the general case is discussed and the results are exemplified by working out the Hénon–Heiles system.

I. INTRODUCTION

Secular terms appear very often in connection with perturbative expansions of the solution of a system of nonlinear equations. These terms should be avoided when we look for approximate solutions over several revolutions of the system. Otherwise they will cause steadily growing amplitudes with time, in disagreement with the observed motion in the majority of cases. The anharmonic oscillator is a simple system where secular terms do appear if conventional straightforward perturbation expansion is performed.

The concepts of Carleman embedding (CE) and secular terms have been put together in a review article on the CE by Montroll and Helleman.[1] They employ the CE to recover the known exact solution of the logistic equation, and show how it can be used to develop a perturbation theory without secular terms. This last point is illustrated by the analysis of the anharmonic oscillator. Since this work, some attempts have been made to apply the CE to more complex systems. Steeb and Wilhelm,[2] have treated the two-dimensional Lotka–Volterra system in a first-order approximation, with results in agreement with the first term of an expansion of the limit cycle. In the context of the Lorenz model, Andrade and Rauh[3] show that any finite-order approximation given by the CE breaks down at the turbulent threshold.

The present work has been motivated by an analysis of the Hénon–Heiles system.[4,5] We wished to investigate how the CE would work near the transition to chaos in this model. Unlike the case of the Lorenz model, this transition is not associated with a stable fixed point that becomes unstable at a well-defined threshold value of a control parameter. In the Hénon–Heiles model, we have a large region of values of the energy where there are two kinds of coexisting trajectories, namely, those lying on the surface of the two-dimensional tori, and those which are chaotic. We have found that the approximate solutions are always similar, for all values of the energy, without any recognizable structural difference between a chaotic and a regular regime. Moreover, secular terms are present in the approximate solutions of order larger than 1. This behavior, of course, contrasts with the proposals of Montroll and Helleman,[1] who emphasize the absence of secular terms within the framework of the CE. A critical reading of the paper of Montroll and Helleman, however, reveals that the absence of secular terms is not due to the CE itself, but rather to a subtle expansion of the oscillation frequency which is carried out by the authors together with the embedding. Similar expansions of the frequency may be performed without any connection with the CE, and are related to the evaluation of the so-called Poincaré recurrence time.[6,7]

The main purpose of this work is to clear up these points. Also, we present a detailed discussion of the occurrence of secular terms when a given nonlinear system is treated by the CE only, without any extra approximations as in the paper of Montroll and Helleman. We think it is important to discuss the occurrence of the secular terms even if we wish to avoid them. This discussion provides a deeper insight of the method itself, and allows some comparisons between the CE and other methods which show the same kind of problem. In this paper we formally consider an autonomous system of P equations with quadratic nonlinearities and suppose, for the sake of simplicity, that it is written in a coordinate basis with a diagonal linear part. Section II is devoted to developing the formal CE solution of the system into a form which is particularly useful for the discussion of the occurrence of secular terms. This will be accomplished in Sec. III, where we show which terms may appear in each block of the infinite CE time evolution operator. In Sec. IV we illustrate the discussion of the preceding sections by the presentation of some results for the Hénon–Heiles system. Finally, we make some concluding remarks in Sec. V.

II. THE SOLUTION

We consider a P-dimensional system described by the vector $\mathbf{x}(t)$, whose equations of motion may be written as

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x} + B\mathbf{x}^{[2]}, \tag{1}$$

where A and B are constant matrices of order $P \times P$ and $P \times P^2$, moreover A is supposed to be diagonal, and $\mathbf{x}^{[2]} = \mathbf{x} \otimes \mathbf{x}$ is a P^2-dimensional vector, where $\otimes$ denotes the Kronecker product.[2,8] After proceeding with the embedding of the original system, we are led to[2,8]

$$\frac{d}{dt}\begin{pmatrix} \mathbf{x}^{[1]} \\ \mathbf{x}^{[2]} \\ \vdots \\ \mathbf{x}^{[N]} \end{pmatrix} = \begin{pmatrix} A^1 & B^1 & 0 & 0 & \cdots \\ 0 & A^2 & B^2 & 0 & \cdots \\ 0 & 0 & \ddots & \ddots & \\ \vdots & \vdots & & A^N & B^N \end{pmatrix} \begin{pmatrix} \mathbf{x}^{[1]} \\ \mathbf{x}^{[2]} \\ \vdots \\ \mathbf{x}^{[N]} \end{pmatrix}, \tag{2}$$

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or, in shorthand notation

$$\frac{d}{dt}X = MX. \tag{2'}$$

In (2) we have

$$\begin{aligned} &\mathbf{x}^{[N]} = \mathbf{x}^{[N-1]} \otimes \mathbf{x}, \quad \mathbf{x}^{[1]} = \mathbf{x}, \\ &A^N = A^1 \otimes I^{N-1} + I^1 \otimes A^{N-1}, \quad A^1 = A, \\ &B^N = B^1 \otimes I^{N-1} + I^1 \otimes B^{N-1}, \quad B^1 = B, \end{aligned} \tag{3}$$

where I^N indicates the $P^N \times P^N$ identity matrix. Our intention is to write the solution of (2') as

$$X(t) = \exp(Mt)\,X(0) = T\exp(\tilde{M}t)T^{-1}X(0), \tag{4}$$

where T is the matrix which transforms M into its diagonal form $\tilde{M}$. We will write T in terms of its block components denoted by capital indices $T_{L,K}$. The dimension of such a block $T_{L,K}$ is $P^L \times P^K$. Due to the structure of M and to the fact that the A^1 (and hence all A^N) are diagonal matrices we have

$$T_{L,K} = 0, \quad L > K, \quad T_{K,K} = I^K. \tag{5}$$

The blocks of the inverse matrix $T^{-1} = U$ will be denoted by $U_{L,K}$ of order $P^L \times P^K$, and may be easily expressed in terms of the $T_{L,K}$ by

$$U_{L,K} = (-1)^{L+K}\,\mathrm{Det}(T')_{K,L}, \tag{6}$$

where $(T')_{K,L}$ is the matrix obtained from T by elimination of the Kth block line and the Lth block column. Now, $\mathrm{Det}(T')_{K,L}$ indicates a matrix of dimension $P^L \times P^K$ which is obtained by performing matrix multiplications and sums among the blocks of $(T')_{K,L}$ in the same way we calculate the determinant of a matrix. As a matter of fact, (6) is the block equivalent to the well-known expression for the elements of the inverse matrix. In the evaluation of (6) we must pay attention that the order of the factors $T_{L,K}$ in each term must be such that the several matrix multiplications are possible, but the product of an identity block by another identity block (or by a nonsquare block) does not afford them to be compatible in the sense of usual matrix multiplication. For instance, we have

$$\begin{aligned} &U_{L,L} = I^L, \quad U_{L,L+1} = -T_{L,L+1}, \\ &U_{L,L+2} = T_{L,L+1}T_{L+1,L+2} - T_{L,L+2}. \end{aligned} \tag{7}$$

The results above do indicate how we can bring (6) to the simpler form

$$U_{L,L+K} = -\sum_{M=J}^{J+K-1} U_{L,M}T_{M,L+K}. \tag{8}$$

The blocks $T_{L,K}$ and $U_{L,K}$ are to be determined from the condition $\tilde{M} = UMT$, and as we have $\tilde{M}_{L,K} = A^L\delta_{L,K}$ we get

$$A^L\delta_{L,K} = \sum_{M=L}^{K} U_{L,M}A^M T_{M,K} + \sum_{M=J}^{K-1} U_{L,M}B^M T_{M+1,K}. \tag{9}$$

When $L = K$, the above equation becomes an identity; when $L \neq K$, it gives the relations which determine the $T_{L,K}$. Making use of (8) we can reduce (9) to

$$\tilde{M}_{L,K} = \sum_{M=L}^{L+K-1} U_{L,M}\{A^M T_{M,K} - T_{M,K}A^K + B^M T_{M+1,K}\} = 0. \tag{10}$$

Since (10) must be valid for any K, the $T_{M,K}$ will have to satisfy

$$A^M T_{M,K} - T_{M,K}A^K = -B^M T_{M+1,K}. \tag{11}$$

At this point we shall introduce a new notation for the blocks of T and U, which takes into account better the fact that the solution of (11) is dependent of the diagonal the block belongs to. So let

$$T^{L,K} = T_{L,L+K}, \quad U^{L,K} = U_{L,L+K}. \tag{12}$$

With this notation it becomes clearer that (11) gives a solution for the blocks of the K th diagonal in terms of those of the $(K-1)$th diagonal. The components of this block are expressed as

$$T^{L,K}_{m,n} = \sum_j \frac{B^L_{m,j}T^{L+1,K-1}_{j,n}}{A^{L+K}_n - A^L_m}. \tag{13}$$

Now if we successively explicit the $T^{L,K-1}$ in terms of the $T^{L,K-2}$, $T^{L,K-3}$, and so on, we get the general result

$$T^{L,K}_{l_0,l_K} = \sum_{l_1,\ldots,l_{K-1}} \prod_{M=0}^{K-1} \frac{B^{L+M}_{l_M,l_{M+1}}}{A^{L+K}_{l_K} - A^{L+M}_{l_M}}. \tag{14}$$

The next task is to determine the $U^{L,K}_{l_0,l_K}$, starting from (8). We will not deduce it here, but we can easily see that if we insert the expression

$$U^{L,K}_{l_0,l_K} = \sum_{l_1,\ldots,l_{K-1}} \prod_{M=0}^{K-1} \frac{B^{L+M}_{l_M,l_{M+1}}}{A^L_{l_0} - A^{L+M+1}_{l_{M+1}}} \tag{15}$$

together with (14) into (8) we come to an identity.

Now we can finally write down the evolution operator $\exp(Mt)$. Since we are interested in the evolution of the first block component $\mathbf{x}^{[1]} = \mathbf{x}$ of X, we concentrate on the evaluation of the block components $(e^{Mt})_{1,K}$,

$$(e^{Mt})_{1,K} = \sum_{M=1}^{K} T_{1,M}e^{A^M t}U_{M,K}. \tag{16}$$

If we define $(e^{Mt})^{1,K} = (e^{Mt})_{1,K+1}$, and make use of the notation introduced in (12) we get

$$(e^{Mt})^{1,K}_{m,n} = \sum_{M=0}^{K}\sum_j T^{1,M}_{m,j}(e^{A^{M+1}t})_j U^{M,K-M}_{j,n}. \tag{17}$$

Now we insert expressions (14) and (15) into (17) to get the explicit form of the $(e^{Mt})^{1,K}_{l_0,l_K}$

$$(e^{Mt})^{1,K}_{l_0,l_K} = \sum_{M=0}^{K}\left\{\sum_{l_M}\left\{\sum_{l_1,\ldots,l_{M-1}}\prod_{N=0}^{M-1}\frac{B^{N+1}_{l_N,l_{N+1}}}{A^{M+1}_{l_M} - A^{N+1}_{l_N}}\right\}(e^{A^{M+1}t})_{l_M}\left\{\sum_{l_{M+1},\ldots,l_{K-1}}\prod_{N=0}^{K-M-1}\frac{B^{M+N}_{l_{M+N},l_{M+N+1}}}{A^M_{l_M} - A^{M+N+1}_{l_{M+N+1}}}\right\}\right\}. \tag{18}$$

We proceed one step further and bring (18) to a more convenient form for the analysis we will undertake in Sec. III,

$$(e^{Mt})^{1,K}_{l_0,l_K} = \sum_{l_0,\ldots,l_{K-1}} \prod_{N=1}^{K-1} B^{N+1}_{l_N,l_{N+1}} \times \sum_{M=0}^{K} (e^{A^{M+1}t})_{l_M} \prod_{N=0}^{K} \frac{1-\delta_{N,M}}{A^{M+1}_{l_M} - A^{N+1}_{l_N}}, \tag{19}$$

where we consider that

$$\lim_{M\to N} \frac{1-\delta_{N,M}}{A^{M+1}_{l_M} - A^{N+1}_{l_N}} = 1. \tag{20}$$

III. DISCUSSION OF THE SECULAR TERMS

In this section we will discuss the conditions necessary for the secular terms to occur. If we consider (19) we see that it is much like the expansion coming from perturbation theory for the eigenvalues of a perturbed Hamiltonian $H = H_0 + \lambda H'$ in terms of the eigenvalues of H_0. It is well known that this expansion breaks down whenever you have degenerated states. A similar fact happens in (19) when we have

$$A^{M+1}_{l_M} = A^{N+1}_{l_N}. \tag{21}$$

In such a case the denominator in (19) goes to zero. However, due to the presence of the sum in M, we have two (or more) terms in (19) with the same denominator which will cancel each other, leading to an indetermination of the type 0/0 which is responsible for the secular terms. In order to see when (21) may occur, we have to consider that the eigenvalues A^M_m of A^M may be expressed in terms of the eigenvalues A^1_n of A^1 as[4,5]

$$A^M_m = \sum_{n=1}^{P} c_n A^1_n, \quad 0 \leqslant c_n \in \mathbf{N}, \quad \sum_{n=1}^{P} c_n = M. \tag{22}$$

So (22) indicates that (21) will be satisfied for large enough values of M and N provided

$$A^1_m / A^1_n = p/q, \quad p,q \in \mathbf{Z}, \tag{23}$$

for at least one pair of eigenvalues of A^1.

Before we start performing a detailed analysis of the occurrence of secular terms, we make simplifying changes in the notation and consider only the part of (19) that is relevant for the secular terms. So, for a given value for the set $\{l_\nu\}$ in (19) we consider the subset S^q_0 with $q+1$ elements of the set $\{A^{M+1}_{l_M}\}$ such that

$$S^q_0 = \{A^{M+1}_{l_M} | A^{M+1}_{l_M} = a_0\}. \tag{24}$$

We may consider, without loss of generality, that these elements are the $A^{M+1}_{l_M}, M = 0,1,\ldots,q$, and will write henceforth

$$a_m = A^{M+1}_{l_M}. \tag{25}$$

Then the occurrence of secular terms for that particular choice of the $\{l_k\}$ will depend upon

$$Q^q_0 = \sum_{m=0}^{q} e^{a_m t} \prod_{n=0}^{K} \frac{1-\delta_{m,n}}{a_m - a_n}. \tag{26}$$

In (26) it is sufficient to take the sum until $m = q$, since the terms with $m = q+1, q+2,\ldots,K$ do not contribute to the secular terms associated with the set S^q_0.

The evaluation of the Q^q_0 is performed by the usual limit procedures, e.g., by writing $a_n = a_0(1+r_n)$, $n = 1,2,\ldots,q$, and then taking the limit as $r_n \to 0$. As a result of the limit procedure we arrive at the expression

$$Q^q_0 = e^{a_0 t} \sum_{n=q+1}^{K} \frac{1}{a_0 - a_n} \sum_{s=0}^{q} \frac{t^s}{s!} \times \sum_{\substack{n_1,\ldots,n_{q-s}=q+1 \\ n_1>\cdots>n_{q-s}}} \prod_{\alpha=1}^{q-s} \frac{1}{a_{n_\alpha} - a_0}. \tag{27}$$

We verify easily that (27) holds for low values of q, and for larger values we may proceed by induction to show that it is valid overall. This proof, though simple, is too lengthy to justify discussing the details here.

Now we recall the most important features, which indicate the number and the order of the secular terms that appear in any block $(e^{Mt})^{1,K}$. This time-evolution block is given by (19), in which several sums are to be taken over the set of indices $\{l_0,l_1,\ldots,l_K\}$. For each set of values that these indices may assume, we ought to perform another sum over $M = 0,1,\ldots,K$. We determine, for that particular choice of the $\{l_K\}$, the subsets $S^{q_0}_0, S^{q_1}_1, \ldots, S^{q_t}_t$ of the set $\{A^{M+1}_{l_M}, M = 0,1,\ldots,K\}$, such that all $q_n + 1$ eigenvalues belonging to a given $S^{q_n}_n$ are equal. Now in the sum over M we group together all those terms corresponding to the values of M for which the $A^{M+1}_{l_M}$ belong to the same set $S^{q_n}_n$, and call this group of terms $Q^{q_n}_n$. Each of the $Q^{q_n}_n$ will contain secular terms of maximal order t^{q_n}, whose general expression is given by (27). Now the highest-order secular term appearing in (19) for that particular choice of the $\{l_K\}$ is proportional to $t^{\bar{q}}$, where

$$\bar{q} = \max\{q_0,q_1,\ldots,q_t\}. \tag{28}$$

The number of secular terms in $(e^{Mt})^{1,K}$ increases monotonically with the value of K. This block will contain all secular terms which had already appeared for lower K's and also new terms. These are due either to new eigenvalues that become equal, leading to secular terms associated with a new frequency, or to a larger number of equal eigenvalues already present in former blocks, which lead to a higher-order term associated with that frequency.

IV. EXAMPLE

We have undertaken an analysis of the Hénon–Heiles[4,5] model along the lines described in Sec. II and III. Several approximations for the trajectories have been evaluated, by considering different cutoffs of the matrix M. For each cutoff we determined the blocks $(e^{Mt})^{1,K}$, and then approximate the solution. The model we worked with is described by the following Hamiltonian:

$$H(q_1,q_2,p_1,p_2) = \tfrac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2 q_2 - q_2^3/3. \tag{29}$$

This model is nonintegrable and the trajectories in the phase space are qualitatively different, depending upon the energy E of the system. In what follows we restrict the discussion to the cases where $E < \frac{1}{6}$. For energies far lower than $\frac{1}{6}$, the trajectories are confined to tori in the phase space. Increasing

the energy until $E = \frac{1}{6}$ makes the trajectories leave the invariant tori and meander chaotically in the space among those most stable tori, which do exist until $E = \frac{1}{8}$. Despite the difference in the character of the trajectories for different values of E, all of them remain bounded in this range of energy.

If we write the equations of motion for the system described by (29), it turns out that the matrix A^{1}, which gives the linear part of the system is not diagonal, as the previous discussion affords it to be. We change then to a new coordinate basis in order that the matrix A^{1} becomes a diagonal. In this new coordinate basis we have

$$Q_j = 2^{-1/2}(q_j - ip_j), \quad P_j = 2^{-1/2}(q_j + ip_j). \tag{30}$$

The eigenvalues of A^{1} are $\pm i$, each one double degenerate. This indicates, according to (22), that the eigenvalues of A^{M} will be of the form

$$i(M - 2m), \quad m = 0,1,...,M. \tag{31}$$

The nonlinear part is described by the matrices B^{N}, as indicated in (2). It is originated by the cubic terms in the Hamiltonian.

Now we consider several approximations. An sth-order approximation takes into account the first $s+1$ blocks A^{M} and s blocks B^{M}. The zeroth-order approximation is that which considers no informations of the nonlinear part. The trajectories are the same as for the harmonic oscillator, and expressed by trigonometric funtions of t.

The first-order trajectories are still limit cycles, but now they contain harmonic contributions. There is still no secular term at this order, for there is no degeneracy between the eigenvalues of A^{1} and those of A^{2}. We write below the time evolution for q_1 at this approximation

$$\begin{aligned} q_1^{(1)}(t) = q_1^{(0)}(t) &+ (\tfrac{2}{3} q_1^0 q_2^0 + \tfrac{4}{3} p_1^0 p_2^0)\cos t \\ &- \tfrac{2}{3}(p_1^0 q_2^0 + p_2^0 q_1^0)\sin t + \tfrac{1}{3}(q_1^0 q_2^0 - p_1^0 p_2^0)\cos 2t \\ &+ \tfrac{1}{3}(p_1^0 q_2^0 + q_1^0 p_2^0)\sin 2t - (q_1^0 q_2^0 + p_1^0 p_2^0), \end{aligned} \tag{32}$$

where superscript 0 indicates the values of the coordinates at $t = 0$. In terms of the accuracy, this approximation is equivalent to that presented by Steeb[2] for the Lotka–Volterra model.

The second-order approximation gives trajectories which do contain secular terms of the type $t \sin t$ and $t \cos t$. Hence they are not limit cycles, but open orbits which revolute with increasing amplitude. The presence of these terms is due to the occurrence of the cases $A^{1}_{l_0} = A^{3}_{l_2} = \pm i$ in the sums of expression (19). The approximation also includes higher harmonic contributions, as becomes clear in the expression below for the $q_1(t)$ when $q_2^0 = p_2^0 = 0$:

$$\begin{aligned} q_1^{(2)}(t) = q_1^{(1)}(t) &+ \tfrac{1}{48}(q_1^{03} - 3q_1^0 p_1^{02})\cos 3t \\ &+ \tfrac{1}{8}(q_1^{03} + 4q_1^0 p_1^{02})\cos 2t \\ &+ \tfrac{1}{144}(29q_1^{03} - 55q_1^0 p_1^{02})\cos t \\ &- q_1^{03}/3 + \tfrac{5}{12}(q_1^{03} + q_1^0 p_1^{02})t \sin t \\ &+ \tfrac{1}{48}(3p_1^0 q_1^{02} - p_1^{03})\sin 3t \\ &+ \tfrac{1}{8}(2p_1^{03} - p_1^0 q_1^{02})\sin 2t \\ &+ \tfrac{1}{144}(5p_1^{03} + 65p_1^0 q_1^{02})\sin t \\ &- \tfrac{5}{12}(p_1^{03} + p_1^0 q_1^{02})t \cos t. \end{aligned} \tag{33}$$

The next approximation would consider four diagonal blocks. We have not worked out this case explicitly, but we are in a position to indicate which terms it will contain, based on the results of the previous sections. In the case of four blocks, besides those terms already present in (33), there would appear two more terms, which are linked with the cases $A^{2}_{l_1} = A^{4}_{l_3} = 0, \pm 2i$ in (19). Such analysis may be extended to higher-order approximations with the following general result: the blocks $(e^{Mt})^{1,K}$ will contain secular terms of maximal order L, when $K = 2L$ or $K = 2L + 1$.

We should consider two points about the presence of secular terms in the approximate solutions of the Hénon–Heiles system. The first has already been partially referred to in the Introduction; they indicate a growing amplitude, whereas the orbits are bounded for values of $E < \frac{1}{6}$.

The second is connected to other general aspects of the trajectories of the system. They are not limit cycles, and the time interval between two successive intersections with a plane in the phase space oscillates around 2π. If there were no secular terms, the approximate trajectories would be limit cycles with period 2π at any order considered, since all eigenvalues of M are of the form given by (31). That would not agree even qualitatively with the observed picture. So the presence of secular terms seems to be necessary and is, perhaps, the only way this method can display nonperiodicity and other nonlinear features of the solution of the system. An infinite number of such terms will certainly sum up to give the right solution, but as long as we are faced with a finite number of terms, the problems discussed above for the solution (33) will appear.

V. CONCLUSIONS

We have discussed the occurrence of the secular terms in the solution of a system of nonlinear equations using the method of the Carleman embedding without any concomitant perturbation expansion. We have obtained the formal CE solution of the system under consideration and brought it to a form particularly useful for the analysis of the occurrence of secular terms. If we concentrate on the blocks of the type $(e^{Mt})^{1,K}$, which are responsible for the description of the trajectories, we show that these terms will occur whenever we have two (or more) equal eigenvalues which belong to different diagonal blocks A^{L} and A^{N} of the matrix M, with $L,N \leqslant K$.

The occurrence of secular terms in the blocks $(e^{Mt})^{1,K}$ is cumulative, since these blocks, for a given K, will contain all secular terms already present in the blocks with lower K, in addition to new terms. These new terms are due to the fact that either new eigenvalues become equal or the number of equal eigenvalues already present for lower K have increased. Since there is a well-known recurrence relations for the eigenvalues of A^{N} in terms of the eigenvalues of the block A^{1}, it turns out that it is quite simple to see which terms will appear in a given order of approximation of the solution.

We have illustrated the use of the general results obtained in this paper by presenting our early expressions for the approximate solution of the Hénon–Heiles system. The occurrence of secular terms has been explicitly shown for a second-order cutoff, and a general discussion of the presence

of other secular terms for higher-order truncations has been presented.

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On the stability of dense point spectrum for self-adjoint operators

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Let A be a (random) self-adjoint operator with fixed orthonormal eigenvectors, but with independently distributed random eigenvalues. [Typically, for the eigenvalue distributions, A is considered to have a dense point spectrum almost surely (a.s.).] A class of perturbations $\{B\}$ is exhibited such that $A+B$ has only point spectrum a.s. Examples are also constructed, including a rank-one perturbation B, such that $A+\mu B$ has no eigenvalues (for $\mu\neq 0$) a.s., despite A having dense point spectrum a.s.

I. INTRODUCTION

In this paper we wish to make a few remarks about perturbations that preserve the pure point (p.p.) spectrum of self-adjoint operators. Such questions are often of interest in physical problems where one wishes to know, at least qualitatively, what happens to the eigenvalues of some given operator under a weak perturbation. Here, however, we consider the problem from a purely functional analytic point of view. The setting we consider is probabilistic: Let A be a (random) self-adjoint operator with fixed orthonormal eigenvectors, but with independently distributed random eigenvalues. [Typically, for the eigenvalue distributions we consider, A has dense point spectrum almost surely (a.s.).] We exhibit a class of perturbations $\{B\}$ such that $A+B$ has only point spectrum a.s. We also construct examples, including a rank-one perturbation B such that $A+\mu B$ has no eigenvalues (for $\mu\neq 0$) a.s., despite A having dense point spectrum a.s. Aronszajn[1] and Donaghue[2] have constructed self-adjoint operators A with p.p. spectrum and self-adjoint rank-one perturbations B such that $A+\mu B$ has no eigenvalues for $\mu\neq 0$. Our second result extends their theorem to a probabilistic setting and shows that their examples are "typical" rather than exceptional.

Our first theorem (Theorem 2.1) is a result concerning the stability of point spectrum. It can be regarded as an abstract operator version of deeper theorems on the stability of p.p. spectrum in classical and quantum mechanics. Perhaps the most renowned theorem of this type is the Kolmogorov–Arnol'd–Moser (KAM) theorem.[3–5] Suppose one is given a smooth, integrable, classical mechanical system with Hamiltonian H_0. There exist "action-angle" variables[6] such that the trajectories of the system are just translations T_t^{ω} on an N-dimensional torus T^N by the vector ωt, where t is the time, for some $\omega\in\mathbb{R}^N$. Provided ω satisfies certain "nonresonance" conditions (almost every $\omega\in\mathbb{R}^N$ satisfies these conditions), then for sufficiently small, smooth V, there will be trajectories of the system with Hamiltonian H_0+V which lie on some smooth N-dimensional manifold M. Furthermore, if S_t is the flow on M given by solving Hamilton's equations, there is a canonical transformation C: $M\to T^N$ such that $S_t=C^{-1}T_t^{\omega}C$. To see the connection of these results with the preservation of point spectrum, recall that Koopman's lemma implies there are unitary maps U_t^S from $L^2(M,d\lambda)$ into itself and U_t^T from $L_2(T^N,d\lambda)$ into itself (λ is the Liouville measure) given by $(U_t^Sf)(x)=f(S_t(x))$ and $(U_t^Tf)(x)=f(x+\omega t)$. Furthermore one can calculate the spectrum of U_t^T, which consists of the eigenvalues $\{e^{i\nu\omega t}\}_{\nu\in\mathbb{Z}^N}$. On the other hand, we can define a unitary map $V^C: L^2(M,d\lambda)\to L^2(T^N,d\lambda)$ by $(V^Cf)(x)=(f\circ C)(x)$. (The unitarity of V^C follows from the measure-preserving property of canonical transformations.) A little calculation gives $V^CU_t^S=U_t^TV^C$, so U_t^S has the same eigenvalues as U_t^T and in particular it has p.p. spectrum.

The next examples of the p.p. spectrum are random Schrödinger operators.[7,8] In these examples one considers a space of operators $\mathbb{O}$ and defines a probability measure m on $\mathbb{O}$. One also assumes that there is some transformation T acting on $\mathbb{O}$ such that m is invariant with respect to T. Typically, an element in $\mathbb{O}$ is of the form $-\Delta+V$, where Δ is the one-dimensional Laplacian, or its discrete approximation, and V is an element of $L^{\infty}(\mathbb{R})$ or $l^{\infty}(\mathbb{Z})$. The measure m is a probability measure on one of these two spaces, and T is taken to be the translation operator. A more general situation is considered in Ref. 8. One then proves that any $H\in\mathbb{O}$, almost surely (with respect to m) has p.p. spectrum. The existence of the transformation T and the invariance of m with respect to T play an important role in the proof.

The final examples of the p.p. spectrum are Schrödinger operators with limit periodic potentials.[9–12] One considers the operator $H=-\mu\Delta+V$, with μ a small coupling constant, Δ the discrete Laplacian, and V a limit periodic function on $\mathbb{Z}^N$, $N\geqslant 1$. Limit periodic potentials V were constructed such that H had pure point spectrum. The most common examples consist of fixing a function V obeying certain nonresonance conditions, and then finding some function $\hat{V}$ such that $H=-\mu\Delta+\hat{V}$ has spectrum V. A more difficult question is to determine whether or not $H=-\mu\Delta+V$ has p.p. spectrum for some given V. A few examples are known where this question may be answered affirmatively. The method of proof used in the first three of the above studies is to construct a sequence of unitary operators, $\{U_n\}$, such that $U_n^{-1}HU_n$ becomes successively closer and closer to diagonal. The technique is closely related to the methods used to prove the KAM theorem.

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Our second theorem (Theorem 3.1) on "the nonconservation of spectral type," should be contrasted with the theorem of von Neumann and Weyl: Let A be an operator on a separable Hilbert space. Then for any $\epsilon > 0$ there is a $B \in \mathbf{B}_2(\mathbf{H})$ (= Hilbert–Schmidt class) with $\|B\|_2 \in \epsilon$ such that $A + B$ has p.p. spectrum. This result was sharpened by Kuroda[13] who showed that the Hilbert–Schmidt norm could be replaced by any unitarily equivalent cross norm, weaker than the trace norm.

We conclude with a remark concerning Theorem 3.1, which provides examples of rank-one perturbations B such that $A + B$ has a continuous spectrum while A has a p.p. spectrum. The continuous part of $A + B$ must be singular continuous by the theorem of Kato and Rosenblum.[14,15] This result should be contrasted with the theorem of Carey and Pincus[16] who showed that given any self-adjoint operator A with no absolutely continuous spectrum and $\epsilon > 0$, there is $B \in \mathbf{B}_1(\mathbf{H})$ with $\|B\|_1 < \epsilon$ such that $A + B$ has p.p. spectrum.

II. STABILITY OF POINT SPECTRUM

Let $\phi_1, \phi_2, \ldots$, be a fixed orthonormal basis for a Hilbert space $\mathscr{H}$ and let $\lambda_1(\omega), \lambda_2(\omega), \ldots$, be a sequence of independent, identically distributed random variables with continuous distributions. (Here ω denotes a sample space point.) We define the random self-adjoint operator acting on $\mathscr{H}$ by

$$A(\omega) = \sum_{n=1}^{\infty} \lambda_n(\omega) P_n, \tag{2.1}$$

where P_n is the projection onto the one-dimensional subspace corresponding to ϕ_n.

Let B be a bounded self-adjoint operator acting on $\mathscr{H}$, and having the decomposition

$$B = \sum_{n=1}^{\infty} B_n, \tag{2.2}$$

where the B_n's are self-adjoint, act invariantly on the subspace $E_n = \text{span}\{\phi_1, \phi_2, \ldots, \phi_n\}$, and are equal to zero on the orthogonal complement of E_n.

Theorem 2.1: Suppose that there exists a positive sequence $\delta_1, \delta_2, \ldots$, satisfying

(i) $\Sigma_{n=1}^{\infty}\, n \sup_x \text{Prob}(|\lambda_i - x| < \delta_n) < \infty$,

(ii) $\delta_{n-1} < \delta_n - 2\|B_n\|$, $n = 1,2,\ldots$,

(iii) $\Sigma_{n=1}^{\infty} n\|B_n\|/\delta_n < \infty$.

(Here $\|\cdot\|$ denotes the operator norm.) Then the random operator $A + B$ almost surely has pure point spectrum, i.e., $A + B$ has no continuous part, a.s.

Example 2.2: If the eigenvalues $\{\lambda_i\}$ are uniformly distributed on the unit interval, the hypotheses can be sastisfied if $\|B_n\| < c/n^{4+\epsilon}$, for any $c, \epsilon > 0$.

Proof: To fix the notation we set $A_0(\omega) = A(\omega)$, $A_n(\omega) = A(\omega) + \Sigma_{n=1}^{n} B_m$. Each $A_n(\omega)$ obviously has a pure point spectrum. The idea of the proof is to turn on the B_n's successively while controlling the shift in the eigenvalues and the change in the eigenvectors.

Define, inductively, a set of eigenvectors $\{\phi_i^n(\omega)\}$ and eigenvalues $\lambda_i^n(\omega)$ for $A_n(\omega)$. Let $\phi_i^0 = \phi_i$ be the original basis and let $\lambda_i^0(\omega) = \lambda_i$. Assuming that the $\{\phi_i^{n-1}(\omega)\}$ and $\{\lambda_i^{n-1}(\omega)\}$ have been defined, we consider the one-parameter family $A_n(\omega,\epsilon) = A_{n-1}(\omega) + \epsilon B_n$, $0 \leqslant \epsilon \leqslant 1$. For $i > n$ we take $\phi_i^n(\omega) = \phi_i^{n-1}(\omega)\,(= \phi_i^0)$ and $\lambda_i^n(\omega) = \lambda_i^{n-1}(\omega) = \lambda_i^0(\omega)$ (recall that $B_n\,\phi_i^0 = 0$ for $i > n$). For $i \geqslant n$, and thinking for the moment of the eigenfunction $\phi_i^{n-1}(\omega)$ and eigenvalue $\lambda_i^{n-1}(\omega)$ as functions of ϵ, we have that $\lambda_i^{n-1}(\omega,\epsilon)$ [with $\lambda_i^{n-1}(\omega,0) = \lambda_i^{n-1}$] satisfies the differential equation (Feynman–Hellman formula)

$$\frac{d\lambda_i^{n-1}}{d\epsilon} = \langle \phi_i^{n-1}(\omega,\epsilon), B_n\, \phi_i^{n-1}(\omega,\epsilon) \rangle, \tag{2.3}$$

with $\phi_i^{n-1}(\omega,\epsilon)$ an eigenfunction of $A_{n-1}(\omega,\epsilon)$ corresponding to $\lambda_i^{n-1}(\omega,\epsilon)$. Thus we take $\lambda_i^n(\omega) = \lambda_i^{n-1}(\omega,1)$ and note that

$$|\lambda_i^n(\omega) - \lambda_i^{n-1}(\omega)| \leqslant \|B_n\|, \quad 1 \leqslant i \leqslant n, \tag{2.4}$$

even in the case where degeneracy among the first n eigenvalues occurs. Note that this estimate, together with hypotheses (ii) and (iii) of Theorem 2.1, imply that λ_i^n converges as $n \to \infty$. We take $\phi_i^n = \phi_i^{n-1}(\omega, \epsilon = 1)$ to be the corresponding eigenfunction. (We will regularly suppress the dependence of ϕ_i^n and λ_i^n on ω from now on.)

Let $S_n = \{\omega \mid |\lambda_i^n - \lambda_{n+1}^0| > \delta_n, \text{ for all } 1 \leqslant i \leqslant n\}$.

Lemma 2.3: For almost all ω, $\exists\, N(\omega) < \infty$ such that $\omega \in \bigcap_{n > N(\omega)} S_n$.

Proof: The proof is a Borel–Cantelli argument. We have that

$$\sum_{n=1}^{\infty} \text{Prob}(S_n^c) < \sum_{n=1}^{\infty} \sum_{i=1}^{n} \text{Prob}(|\lambda_i^n - \lambda_{n+1}^0| < \delta_n)$$

$$\leqslant \sum_{n=1}^{\infty} n \sup_x \text{Prob}(|x - \lambda_{n+1}^0| < \delta_n) < \infty, \tag{2.5}$$

so that $\omega \in S_n$ for all sufficiently large n, a.s.

Henceforth, ω is fixed, corresponding to a finite $N(\omega)$. We now attack the question of convergence for the eigenfunctions. It is convenient to set $\eta_j = \|B_j\|/\delta_j$. We first establish an estimate for the projections P_i^n corresponding to ϕ_i^n, $i > N(\omega)$.

Lemma 2.4: For $i > N(\omega)$ and $N(\omega) \leqslant n < m$,

$$\|P_i^n - P_i^m\| < 2 \sum_{j > \max(i, n+1)}^{m} \eta_j. \tag{2.6}$$

Proof: We first argue, by induction on n, that for $n \geqslant N(\omega)$, $|\lambda_i^n - \lambda_j^n| > \delta_n$ for $i < j$ with $1 \leqslant i \leqslant n$, $N(\omega) < j \leqslant n + 1$. This is clearly the case for $n = N(\omega)$. Assuming this to be the case for arbitrary n, we have for $n + 1$ that $|\lambda_i^{n+1} - \lambda_j^{n+1}| > \delta_n - 2\|B_{n+1}\| > \delta_{n+1}$ by the Feynman–Hellman formula and (ii) of Theorem 2.1 for $i < j$, $1 \leqslant i \leqslant n$, $N(\omega) < j \leqslant n + 1$. For $1 \leqslant i \leqslant n + 1$, $j = n + 2$ the result holds since $\omega \in S_{n+1}$, which completes the induction step. Since B_{n+1} is the zero operator on $\text{span}\{\phi_{n+2}^0, \phi_{n+3}^0, \ldots\}$, we have, for $N(\omega) < i \leqslant n + 1$,

$$\|P_i^n - P_i^{n+1}\| = \left\| \left(\frac{1}{2\pi i}\right) \oint_{|z-\lambda_i^n|=\delta_n/2} \left(\frac{1}{A_n - z} - \frac{1}{A_{n+1} - z}\right) dz \right\|$$

$$= \left\| \left(\frac{1}{2\pi i}\right) \oint_{|z-\lambda_i^n|=\delta_n/2} \left(\frac{1}{A_n - z} B_{n+1} \frac{1}{A_{n+1} - z}\right) dz \right\|$$

$$\leqslant (1/2\pi) 2\pi(\delta_n/2)(2/\delta_n)\|B_{n+1}\|(\delta_n/2 - \|B_{n+1}\|)^{-1}$$

$$\leqslant 2\eta_{n+1}. \tag{2.7}$$

For $i > n+1$, of course, $P_i^{n+1} = P_i^n$ and the lemma follows.

We proceed to the convergence of the eigenvectors ϕ_i^n for all i.

Lemma 2.5: There exists a subsequence $\{\phi_i^{n_p}\}$, $p = 1,2,...$ of complete orthonormal eigenvectors corresponding to $\{A_{n_p}\}$ such that

$$\lim_{p\to\infty} \phi_i^{n_p} = \phi_i^\infty, \quad i = 1,2,..., \tag{2.8}$$

exists for all i. The $\{\phi_i^\infty\}$ form a complete set of eigenvectors for $A + B$.

Proof: We first consider the question of convergence of the eigenvectors beginning with the case $i = 1,2,...,N(\omega)$. Define

$$P^n = \sum_{i>N(\omega)} P_i^n.$$

Then by Lemma 2.4, for $n < m$,

$$\|P^n - P^m\| < 2\sum_{j>n}^{m} j\eta_j < 2\sum_{n>j}^{\infty} j\eta_j,$$

implying that P^n is Cauchy in the norm topology by (iii) of Theorem 2.1 and hence convergent to a projection P^∞. Let $Q^n = \mathbb{I} - P^n$, $Q^\infty = \mathbb{I} - P^\infty$. [The uniform convergence of Q^n implies that Q^∞ is $N(\omega)$ dimensional.] Set $\psi_i^n = Q^\infty \phi_i^n$. Then the ψ_i^n have norms approaching 1, and are asymptotically orthogonal as $n \to \infty$. It follows that since $Q^\infty \mathscr{H}$ is finite dimensional, we can select a subsequence of ψ_i^n's and hence ϕ_i^n's such that they, along with their eigenvalues λ_i^n, are convergent, $i = 1,...,N(\omega)$.

Lemma 2.4 implies that for $i > N(\omega)$,

$$1 - |\langle \phi_i^n, \phi_i^m \rangle|^2 \leqslant 2\sum_{j>n}^{\infty} \eta_j, \tag{2.9}$$

so that if the phase of ϕ_i^m is chosen appropriately

$$\|\phi_i^n - \phi_i^m\|^2 \leqslant 2 - 2\left(1 - 2\sum_{j>n}^{m} \eta_j\right)^{1/2} = O\left(\sum_{j>n}^{m} \eta_j\right). \tag{2.10}$$

It follows that we can select a subsequence of the $\{\phi_i^n\}$ (possibly taking the n values from among the n_p-values used for the first $N(\omega)$ eigenvectors) such that (redefining the subsequence) (2.8) follows for all i.

The orthogonality of the $\{\phi_i^\infty\}$ is immediate. Let λ_i^∞ be the limit of the eigenvalues λ_i^n. Then for $\operatorname{Im} z \neq 0$

$$\lim_{n_p\to\infty} (A_{n_p} - z)^{-1}\phi_i^{n_p} = (A + B - z)^{-1}\phi_i^\infty = (\lambda_i^\infty - z)^{-1}\phi_i^\infty, \tag{2.11}$$

implying that ϕ_i^∞ is an eigenvector of $A + B$. (Here we have passed to resolvents, since A may be unbounded.)

It remains to show the completeness of the $\{\phi_i^\infty\}$. To do this it suffices to show that for any element $\psi \in \mathscr{H}$ with $\|\psi\| = 1$ the l^2-valued sequence a^{n_p} defined by $a_i^{n_p} = \langle \phi_i^{n_p}, \psi \rangle$ converges in the l^2-norm. Now for any $i > N(\omega)$, and $m \geqslant N(\omega)$,

$$|a_i^m|^2 = \langle \psi, P_i^m \psi \rangle = \langle \psi, P_i^N \psi \rangle + \langle \psi, (-P_i^N + P_i^m)\psi \rangle$$

$$\leqslant |a_i^N|^2 + 2\sum_{j>1}^{\infty} \eta_j \equiv c_i, \tag{2.12}$$

with $a_i^\infty = \langle \phi_i^\infty, \psi \rangle$ satisfying a similar estimate. For $i \leqslant N(\omega)$ let $c_i = 1$. Then the c_i's are summable, since

$$\sum_{i>N(\omega)}^{\infty} \sum_{j>i}^{\infty} \eta_j = \sum_{j>N(\omega)}^{\infty} (j - N(\omega))\eta_j < \sum_{j=1}^{\infty} j\eta_j < \infty, \tag{2.13}$$

by hypothesis (iii) of Theorem 2.1. Consequently

$$\lim_{p\to\infty} \|a^{n_p} - a^\infty\|_{l^2}^2 = \lim_{p\to\infty} \sum_i |a_i^{n_p} - a_i^\infty|^2 = 0, \tag{2.14}$$

by the dominated convergence theorem with dominating sequence $\{4c_i\}$. This completes the proof of the lemma and hence the theorem.

III. INSTABILITY OF POINT SPECTRUM

In this section we prove a theorem and provide some examples concerning instability of point spectrum. The operator $A = A(\omega)$ is the same as in Sec. II; the eigenvalues however need not be independent nor continuously distributed. We do require that $\operatorname{Prob}(\lambda_i = \lambda_j) = 0$ for $i \neq j$, i.e., that the eigenvalues are almost surely not equal.

Theorem 3.1: Let $0 < \delta < 1$ and let $\{\epsilon_n\}$ and $\{M_n\}$ be positive real- and integer-valued sequences, respectively, with $\epsilon_n \to 0$ and $M_n \to \infty$, with the M_n's strictly monotone. Suppose that for some bounded subset $I \subset \mathbb{R}$ ($\mathbb{R}$ is the set of real numbers),

(i) $$\sum_{n=1}^{\infty} \epsilon_n^{-1} \sup_{x\in I} \operatorname{Prob}(|\lambda_i - x| \geqslant \epsilon_n, \text{ for all } i,\ M_{n-1} < i \leqslant M_n) < \infty,$$

(ii) $$\sum_{n=1}^{\infty} \epsilon_n^{-2} M_n^{-1-\delta} = \infty.$$

Then there exists a fixed rank-one perturbation B such that $A+\mu B$ has no eigenvalue in I for all $\mu \neq 0$, a.s.

Remark 3.2: The perturbation B can be taken to be of the form $B\psi = \langle \chi,\psi\rangle\chi$ with χ having Fourier coefficients $\chi_n = \langle \phi_n,\chi\rangle = n^{-(1+\delta)/2}$.

Corollary 3.3: Suppose that $I = \cup_m I_m$ is a countable union of bounded sets $\{I_m\}$ for each of which the hypotheses of Theorem 3.1 are satisfied. (In particular, δ and the respective sequences $\{\epsilon_n\}$ and $\{M_n\}$ need not be the same for each I_m.) Then there exists a fixed rank-one perturbation such that $A+\mu B$ has no eigenvalues in I.

We postpone the proof of the theorem and omit the proof of the corollary. We first consider the examples.

Example 3.4: Assume that the eigenvalues are independent and uniformly distributed in [0,1]. Let $I=[0,1]$, $\epsilon_n = e^{-n}$, $M_n = \exp(2n/(1+\delta))$. Then

$$\sup_{x\in I} \text{Prob}(|\lambda_i - x| \geq \epsilon_n, \quad \text{for all } i,\ M_{n-1} < i \leq M_n)$$
$$= (1-\epsilon_n)^{M_n - M_{n-1}}$$
$$\sim \exp(-(1-e^{-2/(1+\delta)})e^{n(1-\delta)/(1+\delta)}), \tag{3.1}$$

for large n, which is clearly summable against ϵ_n^{-1} so that hypotheses (i) and (ii) of Theorem 3.1 are readily seen to be satisfied. The conclusion is that there exists a B such that $A+\mu B$ has no eigenvalue in [0,1] a.s. By the remark, B may be taken to be of the form $B\psi = \langle\chi,\psi\rangle\chi$ with $\chi_n = \langle\chi,\phi_n\rangle = n^{-(1+\delta)/2}$. If B is decomposed $B = \Sigma_k B_k$ with $B_k\psi = \Sigma' \chi_n\chi_m\langle\phi_n,\psi\rangle\phi_n$, where the sum extends over n and $m \leq k$ and n or $m = k$, then $\|B_k\| = O(n^{-(1+\delta)/2})$. This decay estimate on B_k should be compared with that in example 2.2. Since A and $A+\mu B$ have the same essential spectrum, it follows that $A+\mu B$ has continuous spectrum in [0,1] and only isolated eigenvalues outside [0,1].

Example 3.5: Assume that the eigenvalues are independently distributed with distributions absolutely continuous with respect to Lebesgue measure. Assume (primarily for reasons of simplicity) that the density $f(x)$ is symmetric about the origin and decreases monotonically, $0 < x \to \infty$. (For example, the eigenvalues may be normally distributed.) Then there is a perturbation B such that $A+\mu B$ has no eigenvalues, a.s. Here, we take $I_m = [-m,m]$ and the ϵ_n's and M_n's as in the previous example, the same for each m, and apply the corollary. The probability estimate needed for hypothesis (i) of theorem 3.1 now takes the form

$$\sup_{x\in I_m} \text{Prob}(|\lambda_i - x| \geq \epsilon_n, \quad \text{for all } i,\ M_{n-1} < i \leq M_n)$$
$$\leq (1 - f(m)\epsilon_n)^{M_n - M_{n-1}}$$
$$\sim \exp(-f(m)(1-e^{-2/(1+\delta)})e^{n(1-\delta)/(1+\delta)}), \tag{3.2}$$

for n large. Since $\mathbf{R} = \cup_m I_m$ the result follows.

Proof of Theorem 3.1: for $x \in I$, set

$$A_n(x) = \{\omega \mid |\lambda_i - x| \leq \epsilon_n, \quad \text{for all } i,\ M_{n-1} < i \leq M_n\} \tag{3.3}$$

and

$$A_n = \{\omega \mid \text{for some } x \in I\ |\lambda_i - x| \geq 2\epsilon_n, \quad \text{for all } i, \quad M_{n-1} < i \leq M_{n-1}\}. \tag{3.4}$$

Then, since I is a bounded set, there exists a constant c, independent of n, such that

$$A_n \subseteq \bigcup_{1\leq i\leq c/\epsilon_n} A_n(x_{i,n}), \tag{3.5}$$

for some suitably chosen set of points $x_{1,n}, x_{2,n}, \ldots, x_{p_n,n} \in I$ with $p_n < c/\epsilon_n$. By hypothesis (i) of Theorem 3.1,

$$\sum_{n=1}^{\infty} \text{Prob}(A_n) < \sum_{n=1}^{\infty} \text{Prob}(\cup A_n(x_{i,n}))$$
$$< c \sum_{n=1}^{\infty} \epsilon_n^{-1} \sup_x \text{Prob}(A_n(x)) < \infty, \tag{3.6}$$

so that by Borel–Cantelli, almost surely there is an $N(\omega) < \infty$ such that for all $x \in I$ there is an i, $M_{n-1} < i \leq M_n$ with $|\lambda_i - x| < 2\epsilon_n$ for each $n > N(\omega)$.

Let B be the perturbation defined in Remark 3.2, and suppose to the contrary that there is an eigenvector $\psi(\omega)$ satisfying $(A(\omega)+\mu B)\psi = x\psi$. If $B\psi = 0$, then

$$\langle\chi,\psi\rangle = \sum{}' a_n \langle\chi,\phi_n\rangle = \sum_n a_n n^{-(1+\delta)/2} = 0, \tag{3.7}$$

with the sum extending over two or more terms, and with the corresponding ϕ_n's having $\lambda_n = x$. By assumption, the eigenvalues λ_n are nondegenerate a.s. so this cannot happen. Hence $B\psi \neq 0$. For this case, $\psi = \mu\langle\chi,\psi\rangle(x-A)^{-1}\chi$, which is also impossible since thre is some i, $M_{n-1} < i \leq M_n$, with $|\lambda_i - x| < 2\epsilon_n$ and so

$$\|(x-A)^{-1}\chi\|^2 = \sum_m |\lambda_m - x|^{-2} m^{-1-\delta}$$
$$> \sum_{n > N(\omega)} 4\epsilon_n^{-2} M_n^{-1-\delta} = \infty. \tag{3.8}$$

Thus $A+\mu B$ has no eigenvector with eigenvalue in I, a.s.

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Factorization of systems of differential equations

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It is shown that the classical Infeld–Hull factorization method can be extended to coupled systems of second-order equations. A complete solution of the factorization equations in two dimensions is given and a partial enumeration of factorizable systems is made.

I. INTRODUCTION

As is well known, the classical factorization method of Infeld and Hull[1] plays an outstanding role in the theory[2,3] and applications[4] of the special functions of mathematical physics. The essence of the method is the reduction of

$$y'' + r(x,m)\,y + \lambda y = 0, \tag{1.1}$$

for some values of the parameter m, into first-order equations. Solutions for other values of m can be found then by successive applications of the raising and lowering operators.

In view of the effectiveness of this method, it is not surprising that several authors attempted to generalize and extend the method in various contexts.[5–8] Our objective in this paper is, therefore, to show that this classical method can be extended to coupled systems of second-order equations. Although the application of this extension to specific physical systems will not be considered here, we wish to point out that the coupled systems of Schrödinger equations appear in various physical contexts[9,10] and several authors sought to decouple such systems by means of Darboux transformations.[11,12] The factorization method, however, provides a different approach and new classes of coupled systems that are amenable to analytic treatment.

The plan of the paper is as follows: In Sec. II we discuss the factorization method for coupled systems in R^n and derive the basic equations. In Sec. III we restrict ourselves to two-dimensional systems and solve in full generality the factorization equations. In Sec. IV we demonstrate that there exist factorizable systems whose factorization kernel has no one-dimensional analog. Finally, in Sec. V we present a partial list of factorizable equations in R^2.

It should be remarked, however, that some of the "algebra" in this paper was carried out by using MACSYMA.

II. FACTORIZATION OF SYSTEMS

Following the classical factorization technique, we say that a system of second-order differential equations

$$\underline{y}'' + R(x,m)\underline{y} + \lambda \underline{y} = 0, \quad \underline{y} \in R^n, \quad R(x,m) \in M(n) \tag{2.1}$$

can be factored if it is possible to replace it by both of the following systems

$$H^-_{m+1} H^+_m \underline{y}(\lambda,m) = [\lambda - L(m+1)]I\underline{y}(\lambda,m), \tag{2.2}$$

$$H^+_{m-1} H^-_m \underline{y}(\lambda,m) = [\lambda - L(m)]I\underline{y}(\lambda,m), \quad L(m) \in R, \tag{2.3}$$

where

$$H^+_m = K(x,m+1) - \frac{d}{dx} I, \tag{2.4}$$

$$H^-_m = K(x,m) + \frac{d}{dx} I, \tag{2.5}$$

$K(x,m)$ is a $n \times n$ matrix, and I is the $n \times n$ identity matrix.

To find out for which $R(x,m)$ the system (2.1) can be factored we carry out explicitly the multiplications of H^+ and H^- in (2.2) and (2.3) using (2.1). We obtain

$$K^2(x,m+1) + K'(x,m+1) + L(m+1)I = -R(x,m), \tag{2.6}$$

$$K^2(x,m) - K'(x,m) + L(m)I = -R(x,m), \tag{2.7}$$

and hence

$$K^2(x,m+1) - K^2(x,m) + K'(x,m+1) + K'(x,m) = [L(m) - L(m+1)]I. \tag{2.8}$$

To determine those matrices $K(x,m)$ that satisfy this equation, we examine three possible forms for the dependence of this matrix on m.

A. $K(x,m) = K_0(x) + mK_1(x)$

From (2.8) this ansatz leads to

$$(m+1)^2(K_1^2 + K_1') + (m+1)(K_0K_1 + K_1K_0 + 2K_0') - m^2(K_1^2 + K_1') - m(K_0K_1 + K_1K_0 + 2K_0') = (L(m) - L(m+1))I. \tag{2.9}$$

Following the same argument as in Ref. 1, we conclude from (2.9) that

$$K_1' + K_1^2 = -a^2 I, \tag{2.10}$$

$$2K_0' + K_0K_1 + K_1K_0 = \begin{cases} -caI, & a \neq 0, \\ bI, & a = 0, \end{cases} \tag{2.11}$$

and

$$L(m) = \begin{cases} m^2a^2 + ca, & a \neq 0, \\ -bm, & a = 0. \end{cases} \tag{2.12}$$

In Sec. III we shall consider some explicit solutions of the system (2.10) and (2.11) in the two dimensions.

B. $K(x,m) = K_0(x) + mK_1(x) + (1/m)K_2(x)$

Substituting this form of $K(x,m)$ in (2.8) we obtain

$$[(m+1)^2(K_1^2 + K_1') + (m+1)(2K_0' + K_1K_0 + K_0K_1) + [1/(m+1)](K_2' + K_2K_0 + K_0K_2) + K_2^2/(m+1)^2] - [\text{same terms with } m] = (L(m) - L(m+1))I. \tag{2.13}$$

Hence we infer that

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$$K_2^2 = \gamma_1 I, \tag{2.14}$$

$$K_2' + K_2K_0 + K_0K_2 = \gamma_2 I, \tag{2.15}$$

$$2K_0' + K_1K_0 + K_0K_1 = \gamma_3 I, \tag{2.16}$$

$$K_1' + K_1^2 = -a^2 I. \tag{2.17}$$

Obviously, this system reduces to (2.10) and (2.11) if we set $K_2 = 0$, however, we observe that nontrivial solutions with $K_2 \neq 0$ are also possible if we let K_2 be a matrix with constant entries, $K_0 = 0$, while K_1 satisfies Eq. (2.17). Furthermore, since (2.17) and (2.10) are the same it follows, then, that the two-dimensional solutions for K_1, which will be derived in Sec. III, essentially provide a solution for the form of $K(x,m)$ under consideration.

C. $K(x,m) = K_0(x) + mK_1(x) + m^2K_2(x)$

Substitution of this form of K in (2.8) leads, after some simple algebraic manipulations, to the following system;

$$K_2^2 = \gamma_1 I, \tag{2.18}$$

$$2K_2' + 3\{K_1,K_2\} = \gamma_2 I, \tag{2.19}$$

$$K_1' + \{K_0,K_2\} + K_1^2 = \gamma_3 I, \tag{2.20}$$

$$2K_0' - \tfrac{1}{2}\{K_1,K_2\} + \{K_0,K_1\} = \gamma_4 I, \tag{2.21}$$

where $\{A,B\} = AB + BA$ and γ_i, $i = 1,...,4$ are constants. We observe that in contrast to the scalar case[1] one can not deduce from these equations that $K_2 \neq 0$ leads to a trivial system of coupled equations, viz. $R(x,m)$ is a matrix with constant entries. In fact, we shall show in Sec. IV that contrary to the negative results in one dimension, the systems (2.14)–(2.17) and (2.18)–(2.21) admit solutions with $K_0 \neq 0$ and $K_2 \neq$ const, respectively, in two dimensions. Consequently, these kernels and their corresponding factorizable systems have no analog in one dimension.

III. FACTORIZATION OF SYSTEMS IN TWO DIMENSIONS

Although we derived the factorization equations (2.10) and (2.11) in R^n the number of coupled scalar equations which have to be solved to compute the entries of K_0,K_1 increases rapidly with n. Due to this, we shall restrict ourselves in this section (and the rest of this paper) to systems in two dimensions. Our objective in this section is, therefore, to show that a complete closed form solution for K_0, K_1 is available when $n = 2$. The solutions we find will depend on several arbitrary parameters, which demonstrates that in principle the factorization method is applicable to a large class of systems. From a practical point of view, however, these general expressions are rather cumbersome and one must set several of these parameters to zero in order to bring them to a more manageable (and presentable) form. This task will be carried, however, in Sec. IV where a partial enumeration of factorizable systems in two dimensions will be given.

A. Calculation of K_1

Letting

$$K_1 = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \tag{3.1}$$

and using (2.10) we obtain the following system of equations

$$\alpha' + \alpha^2 + \beta\gamma = -a^2, \tag{3.2}$$

$$\delta' + \delta^2 + \beta\gamma = -a^2, \tag{3.3}$$

$$\beta' + \beta(\alpha + \delta) = 0, \tag{3.4}$$

$$\gamma' + \gamma(\alpha + \delta) = 0. \tag{3.5}$$

Subtracting (3.3) from (3.2) and introducing

$$\mu = \alpha - \delta, \quad \nu = \alpha + \delta, \tag{3.6}$$

we obtain

$$\mu' + \nu\mu = 0. \tag{3.7}$$

From (3.4), (3.5), and (3.7) we see that β, γ, and μ satisfy the same first-order differential equation and we have

$$\mu = c_1 J, \quad \beta = c_2 J, \quad r = c_3 J, \tag{3.8}$$

where

$$J = \exp\left(-\int \nu(x)dx\right).$$

To compute ν we add Eqs. (3.2) and (3.3) and use (3.8) to obtain

$$\nu' + \frac{\nu^2}{2} + \rho \exp\left(-2\int \nu(x)dx\right) = -2a^2, \tag{3.9}$$

where $\rho = c_1^2/2 + 2c_2c_3$. We now show that Eq. (3.9) can be solved in full generality. To this end, we first substitute (assuming $\rho \neq 0$)

$$w = \exp\left(\frac{1}{2}\int \nu(x)dx\right) \tag{3.10}$$

to obtain

$$2w'' = -\frac{d}{dw}\left(a^2w^2 - \frac{\rho}{2}w^{-2}\right). \tag{3.11}$$

Multiplying (3.11) by w' and using the chain rule, we obtain after integration

$$w' = [(\rho/2)w^{-2} - a^2w^2 + c_4]^{1/2}, \tag{3.12}$$

where c_4 is an integration constant. Finally, we introduce $z = w^2$, which yields

$$x = c_5 + \frac{1}{2}\int \frac{dz}{(\rho/2 - a^2z^2 + c_4z)^{1/2}}, \tag{3.13}$$

where the last integral can be evaluated explicitly in terms of elementary functions.[13] After some algebra this yields

$$\nu = \begin{cases} \dfrac{2ah\cos 2a(x - c_5)}{h\sin 2a(x - c_5) + c_4}, & h \neq 0, \quad \rho \neq 0, \quad (3.14) \\ \dfrac{4a^4}{c_4 \exp[2a^2(x - c_5)] + 2a^2}, & h = 0, \quad \rho \neq 0, \quad (3.15) \end{cases}$$

where $h = \sqrt{2a^2\rho + c_4^2}$. When $\rho = 0$, Eq. (3.9) reduces to a Ricatti equation (equivalent to the equation obtained for K_1 in Ref. 1 for one differential equation) whose solutions are

$$\nu_1(x) = 2a\cot(ax + \phi), \quad \nu_2(x) = 2ia, \quad a \neq 0, \tag{3.16}$$

$$\nu_3(x) = 0, \quad \nu_4(x) = 2/(x + c_7), \quad a = 0. \tag{3.17}$$

The expressions for $J(x)$ which correspond to these $\nu(x)$ are not hard to obtain and will be omitted for brevity. (Some of these will be computed, whenever necessary, in Sec. IV.)

B. Calculation of K_0

Letting

$$K_0 = \begin{pmatrix} r & s \\ p & q \end{pmatrix}, \tag{3.18}$$

and using (2.11), (3.1), and (3.8) we obtain the following system of equations:

$$2r' + 2\alpha r + J(c_2 p + c_3 s) = -ca, \tag{3.19}$$

$$2s' + (\alpha + \delta)s + c_2 J(r + q) = 0, \tag{3.20}$$

$$2p' + (\alpha + \delta)p + c_3 J(r + q) = 0, \tag{3.21}$$

$$2q' + 2\delta q + J(c_2 p + c_3 s) = -ca. \tag{3.22}$$

(When $a = 0$, $-ca$ is replaced in these equations by b.)

Although Eqs. (3.19)–(3.22) represent a coupled system of equations we now show that they always can be solved analytically and the solution can be expressed explicitly in terms of J and its integrals. To verify this assertion we have to consider, however, several cases.

1. $c_1 \neq 0$, $c_2 c_3 \neq 0$, and $\rho \neq 0$ (the "general case")

To begin with we multiply (3.20) and (3.21) by c_3 and c_2, respectively, and add and subtract the resulting equations. This yields

$$2N' + (\alpha + \delta)N + 2c_2 c_3 JS = 0, \tag{3.23}$$

$$2M' + (\alpha + \delta)M = 0, \tag{3.24}$$

where

$$M = c_3 s - c_2 p, \quad N = c_3 s + c_2 p, \quad S = r + q. \tag{3.25}$$

Adding and subtracting (3.19) and (3.22) we obtain

$$2A' + (\alpha + \delta)A + c_1 JS = 0, \tag{3.26}$$

$$2S' + (\alpha + \delta)S + J(c_1 A + 2N) = -2ca. \tag{3.27}$$

Multiplying (3.23) by c_1 and (3.26) by $2c_2 c_3$ and subtracting, leads to

$$2T' + (\alpha + \delta)T = 0, \tag{3.28}$$

where $T = 2c_2 c_3 A - c_1 N$. Multiplying (3.26) by c_1 and (3.23) by 2 and adding yields

$$2H' + (\alpha + \delta)H + 2\rho JS = 0, \tag{3.29}$$

where $H = c_1 A + 2N$. Finally, introducing $W = (2\rho)^{1/2} S = kS$ in Eqs. (3.27) and (3.29) and adding and subtracting the resulting equations we obtain

$$2X' + (\alpha + \delta + kJ)X = -2cak, \tag{3.30}$$

$$2Y' + (\alpha + \delta - kJ)Y = -2cak, \tag{3.31}$$

where $X = H + W$, $Y = W - H$. Equations (3.24), (3.28), (3.30), and (3.31) form a decoupled system of equations which is equivalent to the original system. The explicit solution of the new system is given by

$$M = c_8 J^{1/2}(x), \quad T = c_9 J^{1/2}(x), \tag{3.32a}$$

$$X = J^{1/2}(x) L^{-1}(x) \left[c_{10} - 2cak \int J^{-1/2}(x) L(x)\, dx \right], \tag{3.32b}$$

$$Y = J^{1/2}(x) L(x) \left[c_{11} - 2cak \int J^{-1/2}(x) L^{-1}(x)\, dx \right], \tag{3.32c}$$

where $L(x) = \exp((k/2)\int J(x)\, dx)$.

The backward transformation from these functions to the original s, p, r, and q is given by

$$r = [(k - c_1)Y + (k + c_1)X + 4T]/4k^2,$$

$$q = [(k + c_1)Y + (k - c_1)X - 4T]/4k^2,$$

$$s = -[c_2 c_3 (Y - X) + c_1 T - k^2 M]/2c_3 k^2,$$

$$p = -[c_2 c_3 (Y - X) + c_1 T + k^2 M]/2c_2 k^2.$$

When any of the constants c_1, $c_2 c_3$, or ρ is equal to zero the solution of the system (3.19)–(3.22) is easier to obtain than in the general case. We discuss now briefly each of these situations.

2. $c_2 c_3 = 0$ (ρ, c_1 arbitrary)

If (let us say) $c_2 = 0$, Eq. (3.20) can be solved for s and (since $c_2 = 0$) Eqs. (3.19) and (3.22) can then be solved for r and q. Equation (3.21) can be solved, then, for p since r and q are known

3. $c_1 = 0$, $c_2 c_3 \neq 0$ ($\rho \neq 0$)

We proceed as in case 1 up to Eqs. (3.26) and (3.27). Since $c_1 = 0$, Eq. (3.26) can be solved for A. The remaining two equations, (3.23) and (3.27), can then be solved by introducing $W = kS$ and adding and subtracting these equations.

4. $\rho = 0$, $c_1 \neq 0$, $c_2 c_3 \neq 0$

In this instance we can proceed as in case 1 up to Eq. (3.28). Since T is proportional to H, Eq. (3.27) can then be solved for S, and using this result we can solve Eq. (3.23).

IV. SOME SPECIAL FACTORIZATIONS IN TWO DIMENSIONS

In this section we discuss solutions to the systems (2.14)–(2.17) and (2.18)–(2.21) in two dimensions. Our primary objective is to show that there exist solutions to these systems with $K_0 \neq 0$ and $K_2 \neq 0$ (respectively) which lead to new classes of factorizable systems of equations in contrast to the one-dimensional case. However, for the sake of brevity we shall omit the proofs of our statements, but will provide them in a separate publication elsewhere.

We divide our discussion into two cases. In the first part we consider the aforementioned systems with $\gamma_1 \neq 0$, while in the second we let $\gamma_1 = 0$.

A. $\gamma_1 \neq 0$

Theorem 1: (1) In two dimensions, if $\gamma_1 \neq 0$, then the only solution to the system (2.18)–(2.21) is the trivial solution where K_0, K_1, and K_2 are matrices with constant entries.

(2) Similarly, if $\gamma_1 \neq 0$ and $\gamma_2 \neq 0$, then the only solution to the system (2.14)–(2.17) is the trivial solution.

Theorem 2: In two dimensions, if $\gamma_1 \neq 0$, $\gamma_2 = 0$, and $\gamma_3 = 0$, then there exist nontrivial solutions to (2.14)–(2.17) with $K_0 \neq 0$.

One particular class of nontrivial solutions which satisfies the conditions of Theorem 2 is given by

$$K_0 = J^{1/2} \begin{pmatrix} 0 & d_2 \\ d_3 & 0 \end{pmatrix}, \quad K_2 = \begin{pmatrix} q_1 & 0 \\ 0 & -q_1 \end{pmatrix}, \tag{4.1}$$

and K_1 is the general solution of (2.17) (which was discussed in Sec. III) subject to the condition $c_2 d_3 + c_3 d_2 = 0$.

B. $\gamma_1 = 0$

The general form of K_2 in this case is

$$K_2 = \begin{pmatrix} q_1(x) & q_2(x) \\ q_3(x) & -q_1(x) \end{pmatrix}, \quad q_1^2 + q_2 q_3 = 0. \tag{4.2}$$

However, to simplify the following discussion, we consider only the forms

$$K_2 = b(x)\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = b(x)A,$$
$$K_2 = b(x)\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = b(x)B. \tag{4.3}$$

For each of these forms of K_2 there exist nontrivial solutions for the systems (2.14)–(2.17) and (2.18)–(2.21).

Theorem 3: The system (2.14)–(2.17) in two dimensions admits nontrivial solutions with $\gamma_1 = \gamma_2 = 0$, $K_2 = b(x)A$ or $b(x)B$, and $K_0 \neq 0$.

The general form of the solution for the second case [$K_2 = b(x)B$] is given by

$$K_0 = \begin{pmatrix} r & s \\ s & r \end{pmatrix}, \quad K_1 = \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix} \tag{4.4}$$

where α, β, r, s, and b must satisfy the equations

$$b' + 2rb = 0, \quad \beta' + 2\alpha\beta = 0, \quad \alpha' + \alpha^2 + \beta^2 = -a^2,$$
$$s' + \alpha s + \beta r = 0, \quad 2r' + 2\alpha r + 2\beta s = \gamma_3. \tag{4.5}$$

Theorem 4: The system (2.18)–(2.21) in two dimensions has nontrivial solutions with (1) $\gamma_1 = \gamma_2 = 0$, $K_2 = b(x)A$, and (2) $\gamma_1 = \gamma_2 = \gamma_4 = 0$, $K_2 = b(x)B$.

The general form of the solution for the second case of this theorem is given by

$$K_1 = \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}, \quad K_0 = \begin{pmatrix} r & s \\ -s & -r \end{pmatrix} \tag{4.6}$$

where α, β, r, s, and b satisfy

$$b' + 3\alpha b = 0, \quad \beta + 2\alpha\beta = 0,$$
$$\alpha' + \alpha^2 + \beta^2 + 2b(r - s) = \gamma_3, \tag{4.7}$$
$$2r' + 2\alpha r = \alpha b, \quad 2s' + 2\alpha s = \alpha b.$$

V. PARTIAL ENUMERATION OF FACTORIZABLE SYSTEMS IN TWO DIMENSIONS

In Sec. IV we saw that the analytic expressions for the entries of K_0 and K_1 contain several parameters and thereby lead to a large class of factorizable kernels $R(x,m)$. From a practical point of view one must set, therefore, some of these parameters to zero in order to obtain tractable expressions. We shall, therefore, assume in the following that either $K = K_0 + mK_1$ or $K = mK_1 + K_2/m$ with $c_1 = c_2 = c_3 = 0$, and give a complete enumeration of factorizable systems in two dimensions under these assumptions. (The resulting six classes are the two-dimensional analogs of those in Ref. 1.)

Furthermore, as final examples we shall present two special classes of factorizable systems which are related to those discussed in Sec. IV.

Using Eqs. (3.1)–(3.8) and (3.19)–(3.22) we see immediately that the entries of K_0 and K_1 are given by the following expressions:

$$\alpha = \delta = \nu/2, \quad \beta = \gamma = 0, \tag{5.1}$$
$$r = J^{1/2}\left[d_1 - \frac{ca}{2}\int J^{-1/2}\,dx\right], \tag{5.2}$$
$$q = J^{1/2}\left[d_2 - \frac{ca}{2}\int J^{-1/2}\,dx\right], \tag{5.3}$$
$$s = d_3 J^{1/2}, \quad p = d_4 J^{1/2}. \tag{5.4}$$

(When $a = 0$, one has to replace $-ca$ by b.)

Evaluating these expressions explicitly for each of the possible forms of $\nu(x)$ as given by (3.16) and (3.17), and letting

$$R(x,m) = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix}, \tag{5.5}$$

we obtain the following formulas. [In (a), (b), (c), and (d) we assume that $K = K_0 + mK_1$, while in (e) and (f) we let $K = mK_1 + (1/m)K_2$.]

(a) $\nu = 2a\cot(ax + \phi)$.

$$L(m) = ma(ma + c),$$
$$K_1 = a\cot(ax + \phi)I,$$
$$K_0 = \frac{1}{2\sin(ax + \phi)} \times \begin{pmatrix} c\cos(ax + \phi) + 2d_1 & 2d_3 \\ 2d_4 & c\cos(ax + \phi) + 2d_2 \end{pmatrix},$$
$$R_{11} = -\frac{1}{4\sin^2(ax + \phi)}\{c^2\cos^2(ax + \phi) + 4d_1[a(2m + 1) + c]\cos(ax + \phi) + 4am[a(m + 1) + c] + 2ac + 4(d_1^2 + d_3 d_4)\},$$
$$R_{21} = -\frac{d_4}{\sin^2(ax + \phi)} \times \{[a(2m + 1) + c]\cos(ax + \phi) + d_1 + d_2\},$$
$$R_{12} = -\frac{d_3}{\sin^2(ax + \phi)} \times \{[a(2m + 1) + c]\cos(ax + \phi) + d_1 + d_2\},$$
$$R_{22} = -\frac{1}{4\sin^2(ax + \phi)}\{c^2\cos^2(ax + \phi) + 4d_2[a(2m + 1) + c]\cos(ax + \phi) + 4am[a(m + 1) + c] + 2ac + 4(d_2^2 + d_3 d_4)\}.$$

(b) $\nu = 2/(x + c_7)$.

$$L(m) = -bmI, \quad K_1 = \frac{1}{x + c_7}I,$$
$$K_0 = \frac{1}{x + c_7} \times \begin{pmatrix} [bx(x + 2c_7) + 4d_1]/4 & d_3 \\ d_4 & [bx(x + 2c_7) + 4d_2]/4 \end{pmatrix}.$$

Due to the length of the expressions we present R only when $c_7 = 0$:

$$R_{11} = -\left[\frac{b^2x^2}{16} + \frac{(m+d_1)(m+d_1+1)+d_3d_4}{x^2} + \frac{b}{4}(2d_1 - 2m - 1)\right],$$

$$R_{21} = -d_4\left(\frac{b}{2} + \frac{d_1+d_2+2m+1}{x^2}\right),$$

$$R_{12} = -d_3\left(\frac{b}{2} + \frac{d_1+d_2+2m+1}{x^2}\right),$$

$$R_{22} = -\left[\frac{b^2x^2}{16} + \frac{(m+d_2)(m+d_2+1)+d_3d_4}{x^2} + \frac{b}{4}(2d_2 - 2m - 1)\right].$$

(c) $\nu = 0$.

$$L(m) = -bmI,$$

$$K_0 = \begin{pmatrix} bx/2 + d_1 & d_3 \\ d_4 & bx/2 + d_2 \end{pmatrix}, \quad K_1 = 0,$$

$$R_{11} = -(bx + 2d_1)^2/4 + b(m + \tfrac{1}{2}) - d_3d_4,$$

$$R_{21} = -d_3(d_1 + d_2 + bx),$$

$$R_{12} = -d_4(d_1 + d_2 + bx),$$

$$R_{22} = -(bx + 2d_2)^2/4 + b(m + \tfrac{1}{2}) - d_3d_4.$$

(d) $\nu = 2ia$. Following Ref. 1 we replace ia by a, c by $-ic$, and add $-a^2c^2I$ to $L(m)$. We obtain

$$L(m) = -a^2(m+c)^2I, \quad K_1 = aI,$$

$$K_0 = e^{-ax}\begin{pmatrix} \frac{2d_1 - ce^{ax}}{2} & d_3 \\ d_4 & \frac{2d_2 - ce^{ax}}{2} \end{pmatrix},$$

$$R_{11} = c(2a+1)[4ma + (2a-1)c] + 4d_1e^{-ax}[c - a(2m+1)] - 4e^{-2ax}(d_3d_4 + d_1^2),$$

$$R_{21} = -e^{-2ax}d_4\{e^{ax}[a(2m+1) - c] + d_1 + d_2\},$$

$$R_{12} = e^{-2ax}d_3\{e^{ax}[a(2m+1) - c] + d_1 + d_2\},$$

$$R_{22} = c(2a+1)[4ma + (2a-1)c] + 4d_2e^{-ax}[c - a(m+1)] - 4e^{-2ax}(d_3d_4 + d_1^2).$$

As to the next two factorizations, where

$$K = mK_1 + m^{-1}K_2,$$

it follows immediately from (2.14) and the assumption that K_2 is a matrix with constant entries that

$$K_2 = \begin{pmatrix} q_1 & q_2 \\ q_3 & -q_1 \end{pmatrix}$$

and $q_1^2 + q_2q_3 = \gamma_1$. Using this relationship and Eqs. (2.11) and (2.13) we obtain the following.

(e) $\nu = 2a\cot(ax + \phi)$.

$$L(m) = m^2a^2 - \frac{\gamma_1}{m^2},$$

$$K_1 = a\cot(ax+\phi)I, \quad K_0 = 0,$$

$$R_{11} = -\left[\frac{a^2m(m+1)}{\sin^2(ax+\phi)} + 2aq_1\cot(ax+\phi)\right],$$

$$R_{21} = -2aq_3\cot(ax+\phi),$$

$$R_{12} = -2aq_2\cot(ax+\phi),$$

$$R_{22} = -\left[\frac{a^2m(m+1)}{\sin^2(ax+\phi)} - 2aq_1\cot(ax+\phi)\right].$$

(f) $\nu = 2/(x + c_7)$.

$$L(m) = -\gamma_1/m^2,$$

$$k_1 = \frac{1}{x+c_7}I, \quad K_0 = 0,$$

$$R_{11} = -\frac{2q_1(x+c_7) + m(m+1)}{(x+c_7)^2},$$

$$R_{12} = -\frac{2q_2}{x+c_7},$$

$$R_{22} = \frac{2q_1(x+c_7) - m(m+1)}{(x+c_7)^2}, \quad R_{21} = -\frac{2q_3}{x+c_7}.$$

SF-A: This class of special factorizable (SF) systems corresponds to those described by Theorem 2. To satisfy the condition $c_2d_3 + c_3d_2 = 0$ we let $c_2 = c_3 = 0$. Furthermore we set $\alpha = \delta$. The form of the matrices K_0 and K_2 is given by Eq (4.1) and $K_1 = \alpha I$ where

$$\alpha' + \alpha^2 = a^2. \tag{5.6}$$

[We replace here, and in the following example, $-a^2$ by a^2 in (2.17).] Using the special solution $\alpha = a$ for α we find then that

$$L(m) = -(\gamma_1/m + m^2a^2)$$

and

$$R_{11} = -(e^{-2ax}/m)[m(2aq_1e^{2ax} + d_2d_3) + (d_2q_3 + d_3q_2)e^{ax}],$$

$$R_{12} = -ae^{-ax}[2q_2e^{ax} + d_2(2m+1)],$$

$$R_{21} = -ae^{-ax}[2q_3e^{ax} + d_3(2m+1)],$$

$$R_{22} = (e^{-2ax}/m)[m(2aq_1e^{2ax} - d_2d_3) - (d_2q_3 + d_3q_2)e^{ax}].$$

SF-B: These factorizable systems correspond to those obtained from Theorem 3 with $K_2 = b(x)A$ and $s = p = r + q = \gamma_3 = 0$, $\alpha = \delta$. Under these conditions one infers that the general form for $L(m)$ and the matrices K_0, K_1, and K_2 is

$$L(m) = -a^2m^2,$$

$$K_0 = \begin{pmatrix} r & 0 \\ 0 & -r \end{pmatrix}, \quad K_1 = \begin{pmatrix} \alpha & \beta \\ 0 & \alpha \end{pmatrix}, \quad K_2 = bA,$$

where b is a constant. The differential equations for α, β, and r are

$$\alpha' + \alpha^2 = a^2, \quad \beta' + 2\alpha\beta = 0,$$
$$r' + \alpha r = 0,$$

i.e.,

$$\beta = c_2 J, \quad r = d_1 J^{1/2}.$$

Using $\alpha = a$ as a solution for α we obtain for $R(x,m)$

$$R_{11} = -e^{-2ax}\{d_1[(2m+1)ae^{ax} + d_1] + bc_2\},$$
$$R_{12} = -2m(m+1)ac_2 e^{-2ax},$$
$$R_{21} = -2ab,$$
$$R_{22} = e^{-2ax}\{d_1[(2m+1)ae^{ax} - d_1] - bc_2\}.$$

To solve these factorizable systems of equations we have to consider them at the top (or bottom) of the ladder in m where $\lambda = L(m+1)$ and, therefore, $\underline{y}(\lambda,m)$ must satisfy

$$H_m^+ \underline{y}(\lambda,m) = \left(K(x,m+1) - \frac{d}{dx} I\right)\underline{y}(\lambda,m) = 0. \tag{5.7}$$

(We note that the proof that H^+ and H^- are raising and lowering operators follows exactly as in the scalar case.[1]) Equation (5.6) represents a coupled system of first-order equations which can be reduced by elimination to two uncoupled second-order equations for each of the components of $\underline{y}$ (and then solved by standard techniques). The explicit form of these solutions and the investigation of their properties will be deferred, however, to another publication.

VI. CONCLUSIONS

In this paper we generalized the classical factorization method to systems of coupled second-order equations and enumerated in Sec. IV some of these systems in two dimensions. In view of the close relationship between the special functions of mathematical physics and the factorization method it is perhaps appropriate to consider the solutions of factorizable systems in n dimensions as "generalized special functions." The properties and Lie algebraic contents of such factorizable systems deserve further investigation.

From a physical point of view these factorizable systems might be useful as exactly solvable models for physical systems which are represented by coupled Schrödinger equations. The exact solution of these factorizable equations could then lead to a better insight and understanding of the more realistic models for these physical systems.

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Some practical observations on the predictor jump method for solving the Laplace equation

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The best conditions for the application of the predictor jump (PJ) method in the solution of the Laplace equation are discussed and some practical considerations for applying this new iterative technique are presented. The PJ method was remarked on in a previous article entitled "A new way for solving Laplace's problem (the predictor jump method)" [J. M. Vega-Fernández, J. F. Duque-Carrillo, and J. J. Peña-Bernal, J. Math. Phys. **26**, 416 (1985)].

I. INTRODUCTION

In our previous article,[1] we described a new method with substantial advantages over any other iterative technique for solving Laplace's problem and problems of this type. The predictor jump (PJ) method, which converges faster than any other, gets its name from the jump made over the iterations required by other methods when a certain condition is satisfied. This condition is that a parameter, which we denote as $EQ^{(k}$ (the ratio between the errors of iterations k and $k-1$), satisfies

$$|EQ^{(k} - EQ^{(k-1}| < \epsilon'. \tag{1}$$

If ϵ' is chosen small enough, then the parameter can be taken as roughly constant.

If m is the first iteration for which condition (1) is satisfied, and if one takes

$$EQ^{(m} = EQ^{(m+1} = \cdots = \alpha = \text{const}, \tag{2}$$

then

$$\phi_i^{(\infty} = \phi_i^{(m+1} + [\phi_i^{(m+1} - \phi_i^{(m}]\,[\alpha/(1-\alpha)]. \tag{3}$$

This expression gives the value of the solution of $\nabla^2\phi = 0$ at each point i as a function of the values of ϕ_i for two successive iterations, m and $m+1$.

II. CONDITION FOR USING THE PJ METHOD

Equation (1) is a necessary, and generally sufficient, condition for the successful application of the PJ method. Nevertheless, later on we will look at circumstances when the method may not work correctly despite condition (1) being satisfied.

In a given problem, the point at which condition (1) is reached depends only upon the value of ω, the overrelaxation factor. In general, the conventional method that supplies the best convergence to the solutions of Laplace's problems is the successive overrelaxation (SOR) method.[2] In the algorithm for its resolution, a factor of overrelaxation called ω is introduced, so that

$$\phi_i^{(k+1} = \phi_i^{(k} + \frac{\omega}{a_{ii}}\left[bi - \sum_{j=1}^{i-1} a_{ij}\cdot\phi_j^{(k+1} - \sum_{j=1}^{N} a_{ij}\cdot\phi_j^{(k}\right], \tag{4}$$

where the terms a_{ij} and b_i are the elements of the matrices of coefficients and the independent terms, respectively. These elements appear as a result of using the Laplace equation in a central finite difference.

In Fig. 1, $EQ^{(k}$ is plotted against the number of iterations for different values of ω. The instability of the parameter $EQ^{(k}$ is seen to increase with greater values of ω until, as in Fig. 1(d), the solution is arrived at before condition (1) is fulfilled, and the PJ method is not used.

It is also clear from the figures that the parameter $EQ^{(k}$ reaches a stable value more quickly when ω is around unity, and that this value is closer to 1 for larger ω.

III. BEST CONDITIONS FOR THE APPLICATION OF THE PJ METHOD

Equation (3) gives the exact solution, if the parameter $EQ^{(k}$ remains exactly constant from the mth iteration. In practice, the parameter is not constant but is treated as if it were so, as long as Eq. (1) is satisfied. So, it is reasonable to expect that the smaller the value set for ϵ', the closer $\phi_i^{(\infty}$, given by the PJ method, will be to the exact value.

This expected behavior is indeed seen, as shown in Figs. 2 and 3 where $\log E^{(k}$ is plotted against the number of iterations for $\omega = 1.5$.

If ϵ' is set at a small value, more iterations are needed for Eq. (1) to be satisfied, and although the PJ method gives values very close to the final solution, the number of jumps (predictions) made in the process of iteration will be smaller than if ϵ' had been set at a higher value. It is therefore impossible to say beforehand whether the smallest number of iterations needed to solve the problem will result from a smaller or larger choice of ϵ'.

The accuracy of a prediction is sensitive to the value of α in Eq. (3). With a fixed ϵ', and error δ of 10^{-3} in the value of α gives rise to an maximum error in the $\alpha/(1-\alpha)$ term (in absolute value) of 0.016 06 if $\alpha = 0.75$, and of 2.6315 if $\alpha = 0.98$.

Therefore, as can be seen in Fig. 1, small values of ω (close to unity) have the advantage of stabilizing the parameter $EQ^{(k}$ rapidly, however, this same stable value has the

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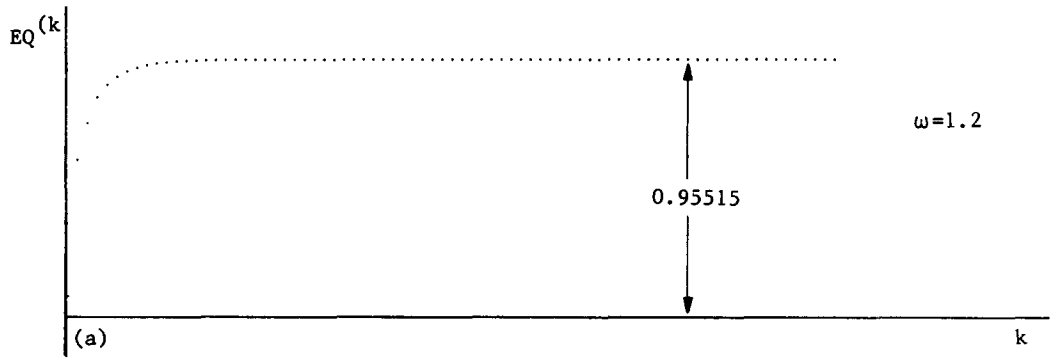


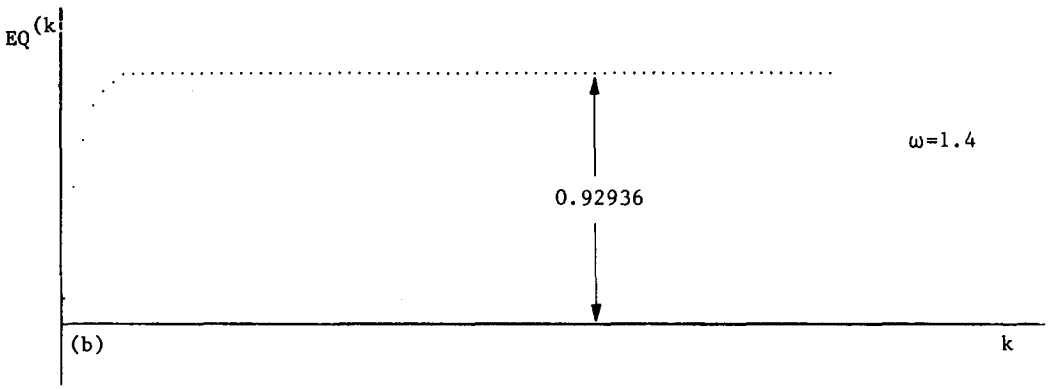
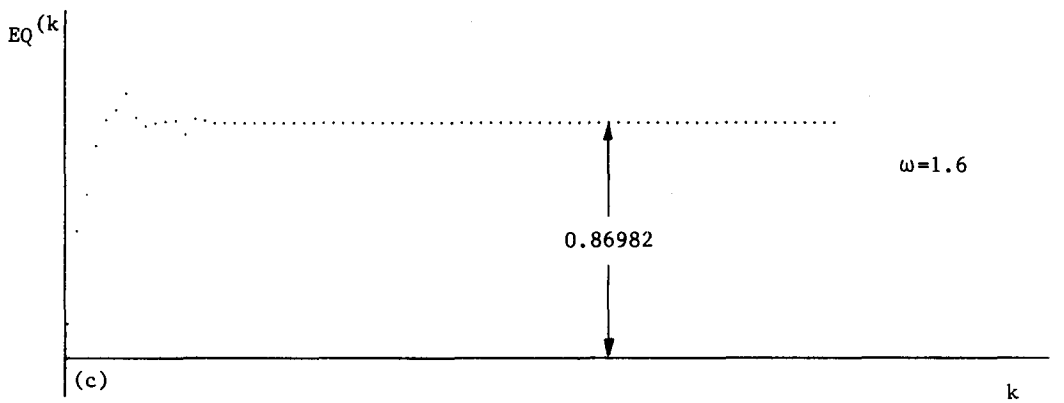
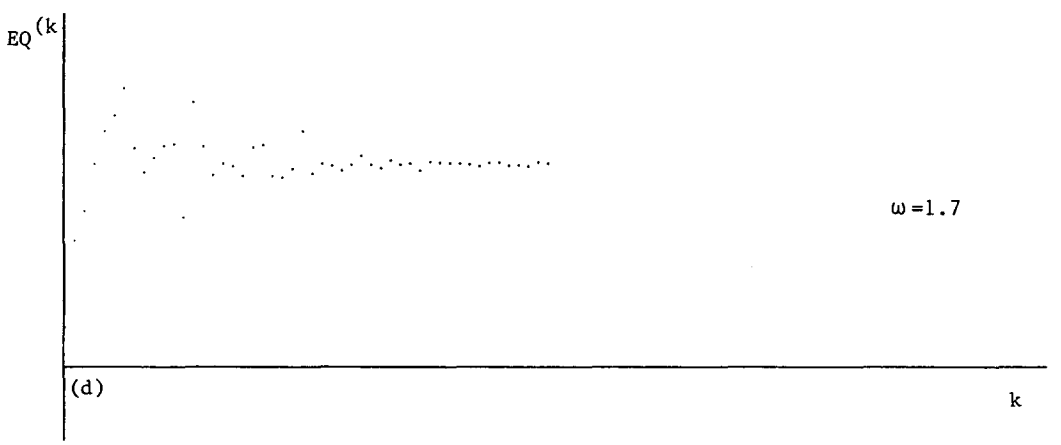


FIG. 1. The parameter $EQ^{(k}$ plotted against the number of iterations for different values of ω.





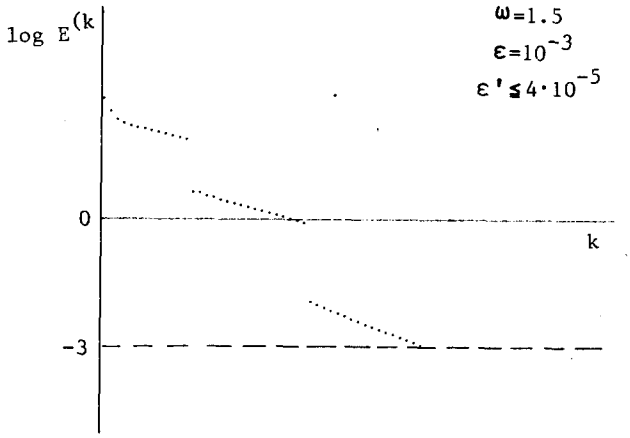


FIG. 2. The log $E^{(k}$ plotted against the number of iterations for $\omega = 1.5$. The iterative process finishes when $E^{(k} < \epsilon$.

disadvantage of being close to unity. On the other hand, larger values of ω have the inconvenience of a slower stabilization of $EQ^{(k}$, but the advantage of the resulting stable value being further from unity.

There are no values of ω that will give the ideal situation (a stable value of $EQ^{(k}$ far from unity and a rapid approach to this value) for applying the PJ method.

Experience has taught us to adopt a compromise solution, in the sense that, instead of fixing ϵ' before beginning to resolve the problem, the value of ϵ' is a function of $EQ^{(k}$. Thus, for a value of $EQ^{(k}$ close to 1, ϵ' should be smaller than if $EQ^{(k}$ were farther from 1 for the same degree of accuracy in the predictions.

We get an expression for ϵ' in the following way: As we observed above, Eq. (3) gives us the solution at every point if the parameter $EQ^{(k}$ becomes constant and equal to α for all iterations starting with the mth. As this value of α is unknown in practice, the value of $EQ^{(k}$ is taken for α and used in Eq. (3), giving

TABLE I. Extension to two and three dimensions.

System	One-dimensional a_1 points	Two-dimensional $a_1 \cdot a_2$ points	Three-dimensional $a_1 \cdot a_2 \cdot a_3$ points
Memory requirement (words)	Vector dimension a_1 and one scratch variable	Matrix dimension $a_1 \cdot a_2$ and one scratch vector of a_1 words	Matrix dimension $a_1 \cdot a_2 \cdot a_3$ and one scratch matrix dimension $a_1 \cdot a_2$

$$\phi_i^{(\infty}(\mathrm{PJ}) = \phi_i^{(m+1} + [\phi_i^{(m+1} - \phi_i^{(m}]\,[EQ^{(m}/(1 - EQ^{(m})]. \tag{5}$$

If δ is the error in taking $EQ^{(m}$ instead of the true value, then

$$\alpha = EQ^{(m} + \delta. \tag{6}$$

Substracting Eq. (5) from Eq. (3) term by term for each of the N points of the problem gives

$$\mu = A \cdot \left[\frac{\alpha}{1-\alpha} - \frac{EQ^{(m}}{1 - EQ^{(m}}\right], \tag{7}$$

where

$$\mu = \sum_{i=1}^{N} |\phi_i^{(\infty} - \phi_i^{(\infty}(PJ)|$$

and

$$A = \sum_{i=1}^{N} |\phi_i^{(m+1} - \phi_i^{(m}|.$$

Equations (6) and (7) give, on substitution,

$$\delta = \frac{(\mu/A)(1 - EQ^{(m})^2}{1 + (\mu/A)(1 - EQ^{(m})}. \tag{8}$$

This is an expression for δ given a certain prediction error μ. One is interested in knowing the value of ϵ', and it appears reasonable to take as an approximation

$$\epsilon' \cong a\delta. \tag{9}$$

We have assigned empirically the value 0.02 to a. It does not matter if Eq. (9) is not totally correct, since the only effect

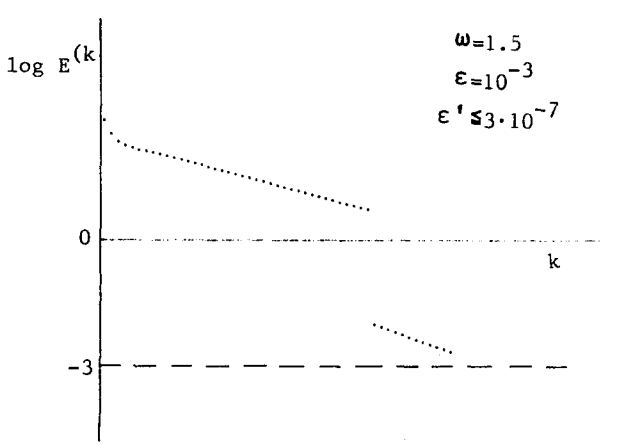


FIG. 3. The log $E^{(k}$ plotted against the number of iterations for $\omega = 1.5$.

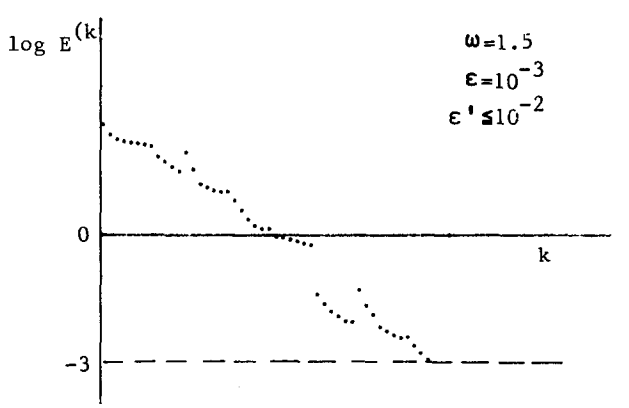


FIG. 4. Some incorrect predictor jumps appear when log $E^{(k}$ is plotted against the number of iterations.

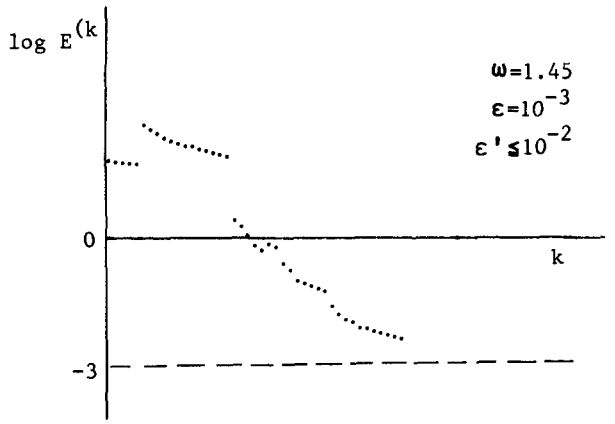


FIG. 5. Some incorrect predictor jumps appear when $\log E^{(k}$ is plotted against the number of iterations.

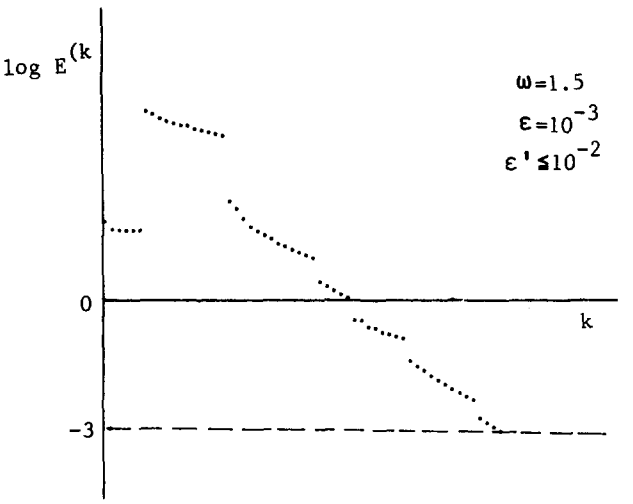


FIG. 7. An erroneous predictor jump.

will be to give an error of prediction that does not coincide with the set value μ, but is nevertheless close to it.

IV. THE PJ METHOD IN PRACTICE

In this section we shall discuss some practical considerations for applying the PJ method that we remarked on in the previous article.

There are two apparently negative aspects of the PJ method over other iterative methods. First, to make a prediction using Eq. (3) one needs the values ϕ_i from two consecutive iterations. This appears equivalent to having to open up two matrices of unknowns in order to store the values of the function for iterations m and $m+1$, respectively. Second, the computation time for one iteration is greater than for any other method, since at the end of an iteration it appears necessary to transfer the contents of one matrix to the other in case Eq. (1) is satisfied on the next iteration and Eq. (3) will have to be used. This is, however, obviated easily in the following way. At the end of iteration k, Eq. (1) is checked and if it is satisfied, the matrix transfer is made. After the next iteration, $k+1$, Eq. (3) is applied, using $EQ^{(k+1)}$ for α, which is better than $EQ^{(k}$ anyway, because the stability of this parameter increases with each iteration. In this way, the average time per iteration is practically the same as that for other methods.

Let us now return to the first point and see how it is possible to use only one of the two matrices, even though later on we will look at the advantages of using two matrices.

For simplicity, let us consider the Laplace equation in one direction. First, the value $\phi_i^{(k}$ is calculated at each point i using

$$\phi_i^{(k} = (\phi_{i-1}^{(k} + \phi_{i+1}^{(k-1})/2.$$

Then one checks to see if Eq. (1) is satisfied. If m is the first iteration for which this condition is fulfilled, then one calculates not only $\phi_i^{(m+1}$ at each point i, but $\phi_i^{(\infty}$ from Eq. (3). The value of $\phi_i^{(\infty}$ is transferred to the matrix of variables after having calculated $\phi_{i+1}^{(m+1}$, so that the forecast value $\phi_i^{(\infty}$ is stored in a scratch variable location until $\phi_{i+1}^{(m+1}$ has been calculated for the next point $i+1$.

This argument is extendable to two or three dimensions as shown in Table I. However, although one is able to get away with using just one matrix in this way, let us look now at the reason the use of two matrices is preferable as long as the available computer memory allows it. There are cases when the prediction may be incorrect in the sense that the

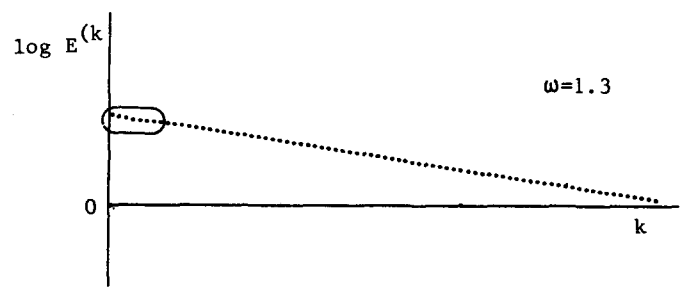


FIG. 6. Arbitrary initial value conditions give rise to this behavior of $\log E^{(k}$ versus number of iterations.

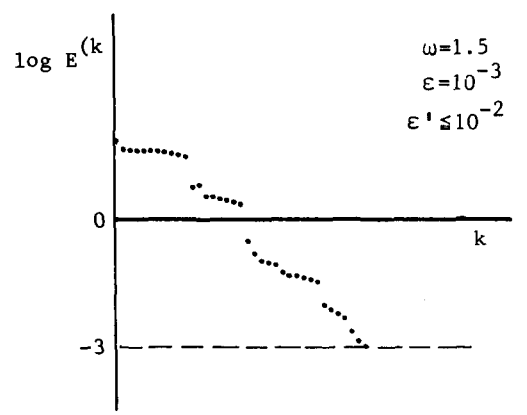


FIG. 8. The erroneous predictor of Fig. 7 is rejected.

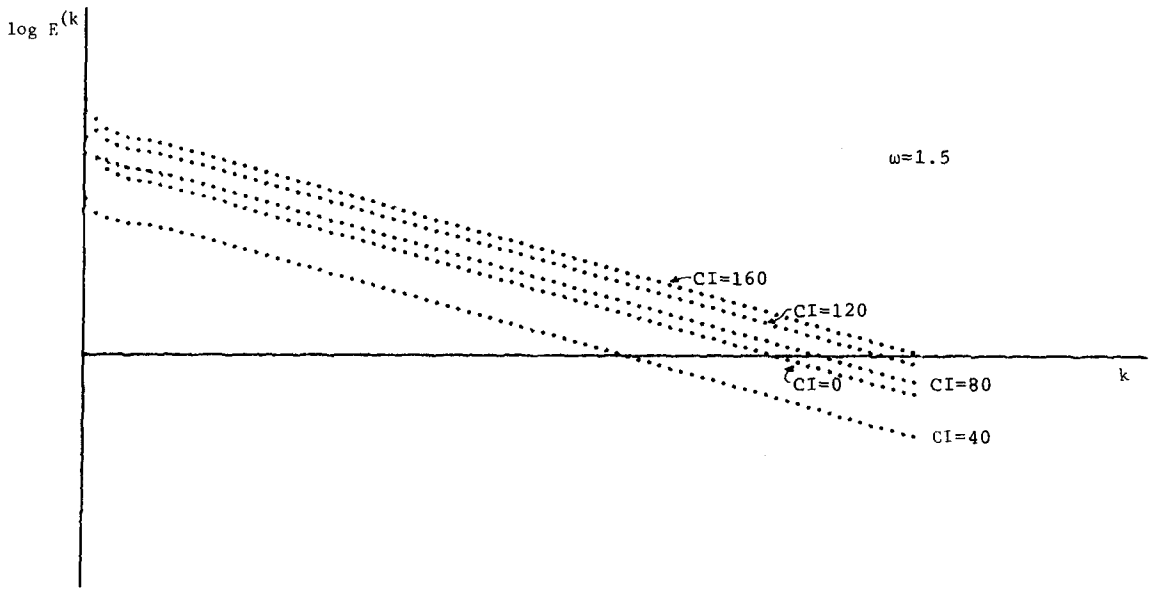


FIG. 9. The SOR method for different values of the initial condition with overrelaxation factor $\omega = 1.5$.

output error of the PJ method is greater than the input error. In Figs. 4 and 5, where $\log E^{(k}$ is plotted against the number of iterations, there appear some incorrect predictor jumps.

Examples of possible causes of these problems may be seen in the case where ω is chosen high enough to impede the stabilization of $EQ^{(k}$ [Fig. 1(d)] and where, accidentally, there are consecutive iterations that satisfy Eq. (1), or, in the case of arbitrary initial conditions that give rise to a behavior of $\log E^{(k}$ versus number iterations like those seen in Fig. 6, where entry into the PJ method is likely to occur in the region marked.

With two matrices of variables, one is able to reject any incorrect predictor jump and let the system evolve normally as if nothing had happened. Given that the values $\phi_i^{(m+1}$ are stored in the matrix of variables, and the values $\phi_i^{(m}$ in the other matrix (which we could call the auxiliary matrix) at the moment of calculating a prediction using Eq. (3), it is enough to store in a scratch location the value $\phi_i^{(m}$ when $\phi_i^{(\infty}$ is going to be calculated, and store $\phi_i^{(m+1}$ in the auxiliary matrix. On the following iteration $m+2$, which is carried out using the predicted values that have been stored in the primary matrix, the error $E^{(m+2}$ is compared with $E^{(m+1}$. If the output error $E^{(m+2}$ is less than the input error $E^{(m+1}$, the prediction was correct and the system continues its evolution. Otherwise the values $\phi_i^{(m+1}$, stored in the auxiliary matrix, are transferred to the primary matrix of unknowns and iteration $m+2$ is carried out using these values, thus rejecting the incorrect prediction.

An erroneous predictor jump is shown in Fig. 7, representing $\log E^{(k}$ versus number of iterations. Figure 8 is the same case with the erroneous prediction rejected.

In short, when two matrices are used, it is possible to reject the incorrect predictions so that the PJ method can be applied without any type of precautions.

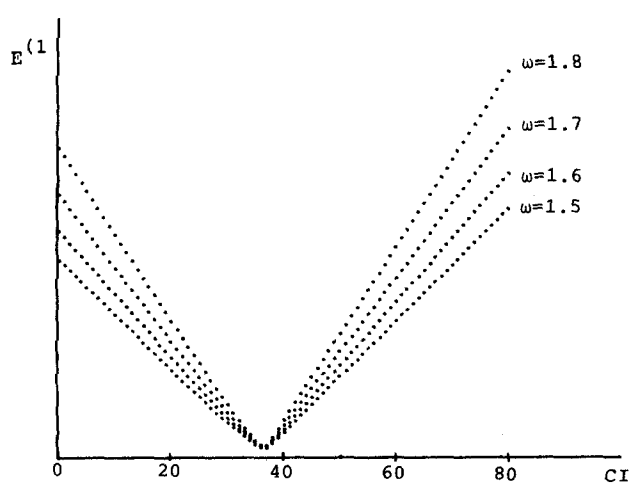


FIG. 10. The relation between the initial error $E^{(1}$ and the initial condition for different values of ω.

V. INFLUENCE OF THE INITIAL CONDITIONS

Figure 9 has been obtained by applying the SOR method for different values of the initial condition with the same value of the overrelaxation factor ($\omega = 1.5$).

This figure states first that the parameter $EQ^{(k}$, which coincides with the slope of the straight lines, is independent of the initial condition values. Second, it can be observed that knowing the initial condition that originates the smallest value of the initial error, $E^{(1}$ is an advantage, because in such a way the solution is reached sooner. Nevertheless this best value for the initial condition is difficult to obtain. Figure 10

shows the relation between the initial error $E^{(1}$ and the initial condition for different values of ω.

The way we have chosen to try to obtain this best value is as follows. For two very high values of the initial condition, the equation of one of the straight lines is calculated; this calculation is repeated for the other two very small values and another equation is obtained. The intersection of both straight lines is approximately the initial condition that originates the minimum value of the initial error.

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Tree graphs and the solution to the Hamilton–Jacobi equation

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A combinatorial method is used to construct solutions of the Hamilton–Jacobi equation. An exact expression for Hamilton's principal function S is obtained for classical systems of finitely many particles interacting via a certain class of time-dependent potentials. If x, p, and t are the position, momentum, and time variables for N point particles of mass m, it is shown that Hamiltonians of the form $H(x,p,t) = (1/2m)p^2 + v(x,t)$ have complete integrals S that are analytic functions of the inverse mass parameter m^{-1} in a punctured disk about the origin. If $v(x,t)$ is bounded, C^∞ in the x variable, and has controlled x-derivative growth, then the coefficients of the Laurent expansion of S about $m^{-1} = 0$ may be expressed in terms of gradient structures associated with tree graphs. This series expansion for $S(x,t;y,t_0)$ converges absolutely, and uniformly for all x, y for time displacements $|t - t_0| < T \equiv 2K^{-1}(m/eU)^{1/2}$, where K and U are bounds associated with the space derivatives of the potential. For $|t - t_0| < T$, the classical path (from any initial space-time configuration y,t_0 to any final configuration x,t) induced by S is unique, passes through no conjugate points, and furnishes the action functional with a strong minimum. The local solution S given above may be used to obtain the classical trajectories for arbitrarily large times.

I. INTRODUCTION

In this paper we construct an explicit solution to the Hamilton–Jacobi equation. Consider a nonrelativistic classical system composed of N point particles each having mass m and interacting via smooth bounded pair potentials. The Hamiltonian for such a system has the general form

$$H(x,p,t) = (1/2m)p^2 + v(x,t), \tag{1.1}$$

where $t \in \mathbf{R}$ is the time variable. The vectors $x,p \in \mathbf{R}^d$ denote the positions and momenta of all N particles. For particles moving in three dimensions, $d = 3N$. The function $v(x,t)$ is the total potential energy of the system at time t associated with configuration x. Given $H(x,p,t)$ the related Hamilton–Jacobi equation is

$$\frac{\partial}{\partial t} S(x,t;y,t_0) + \frac{1}{2m} |\nabla_x S(x,t;y,t_0)|^2 + v(x,t) = 0, \tag{1.2}$$

where y,t_0 represents $d + 1$ independent free parameters.

The Hamilton–Jacobi equation is a nonlinear partial differential equation in $d + 1$ dimensions, so obtaining solutions is a nontrivial task. This is particularly true in the general problem considered here where one cannot expect that $v(x,t)$ will have symmetry properties that would permit the study of (1.2) by the method of separation of variables. We investigate (1.2) by considering solutions that take the form

$$S(x,t;y,t_0) = \frac{m}{2} \frac{(x-y)^2}{t-t_0} - \Phi(x,t;y,t_0), \tag{1.3}$$

where Φ is a bounded real-valued function that admits a series representation in the variable m^{-1},

$$\Phi(x,t;y,t_0) = \sum_{n=0}^{\infty} m^{-n} A_n(x,t;y,t_0), \tag{1.4}$$

for some coefficients A_n. The function Φ will be found to depend on v and have the property that Φ vanishes if $v = 0$. In this latter case, (1.3) becomes the solution of the Hamilton–Jacobi equation that describes free particle motion (with constant velocity) from initial configuration y,t_0 to final configuration x,t. It will turn out that A_n assumes the form of a parametric integral in $n + 1$ dimensions whose integrand has a structure determined by the sum of all labeled tree graphs that can be formed on the vertex set $\{1,2,\ldots,n+1\}$. It will be shown that the series (1.4) is uniformly and absolutely convergent for all x,y and for $t - t_0$ restricted to some finite time interval containing the origin. Furthermore, we prove that $S(x,t;y,t_0)$ is the action (Hamilton's principal function) for the trajectory of $H(x,p,t)$ that travels from y,t_0 to x,t.

Motivation for the study of $S(x,t;y,t_0)$ and some initial technical insight is provided by the WKB[1,2] approximation for the kernel of the time-evolution operator in quantum mechanics. To avoid unnecessary complications in this discussion assume temporarily that v is a static potential $v(x,t) = v(x)$ and choose the initial time $t_0 = 0$. Let us denote by $\hat{H}$ the quantum Hamiltonian operator associated with (1.1). Then $\hat{H}$ is the self-adjoint extension in $L^2(\mathbf{R}^d)$ of the quadratic elliptic differential operator

$$H_{(x)} = -q\,\Delta_x + v(x), \tag{1.5}$$

where Δ_x is the Laplacian in $\mathbf{R}^d$. In terms of Planck's constant $\hbar$, q is the quantum scale factor $\hbar^2/2m$. For an appropriately smooth potential, let $U(x,y;it/\hbar)$ be the fundamental solution of Schrödinger's equation[3]

$$i\hbar \frac{\partial}{\partial t} U(x,y;\frac{it}{\hbar}) = H_{(x)} U(x,y;\frac{it}{\hbar})$$

that satisfies the delta-function initial condition

$$U(x,y;it/\hbar) \to \delta(x-y) \quad \text{as } t \to 0,$$

where U is the coordinate space kernel of $\exp(it\hat{H}/\hbar)$. The standard form of the WKB approximation, to lowest order in $\hbar$, is the approximation

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$$U(x,y;it/\hbar)\approx(2\pi i\hbar)^{-d/2}$$
$$\times\sum_k\left|\det\left[-\frac{\partial^2}{\partial x_i\,\partial y_j}S_k(x,t;y,0)\right]\right|^{1/2}$$
$$\times\exp\left[i\left\{\frac{1}{\hbar}S_k(x,t;y,0)-\frac{\pi}{2}M_k\right\}\right]. \quad (1.6)$$

Here the sum extends over classical paths q_k from y to x taking time t, and S_k is the action defined by the path q_k:

$$S_k(x,t;y,0)=\int_0^t d\tau\left[\frac{m}{2}\,|\,\dot q_k(\tau)|^2-v(q_k(\tau))\right]. \quad (1.7)$$

The integer M_k is the Morse index of the path q_k that is determined by how many caustics the path q_k transverses and their orders.[1] If the space-time coordinate end points $y,0$ and x,t are close enough together then typically there is only one path joining them and the right-hand side of (1.6) reduces to a single term. Clearly the actions $S_k(x,t;y,t_0)$ play a key role in determining the behavior of the WKB approximation. For this reason it is of interest to solve the Hamilton–Jacobi equation and to obtain an explicit expression for the action.

A semiclassical approximation that differs from the WKB approach is the Wigner–Kirkwood[4,5] approximation for the coordinate space kernel of the operator $e^{-\beta\hat H}$, $\beta>0$. If β is the inverse temperature of a system, $e^{-\beta\hat H}$ is the unnormalized canonical density operator. Let $U(x,y;\beta)$ be the coordinate space kernel of $e^{-\beta\hat H}$. The Wigner–Kirkwood semiclassical approximation results from a $q\to 0$ uniform (in x,y) asymptotic expansion of $U(x,y;\beta)$ (see Refs. 6 and 7). In particular, the general study[6] of the Wigner–Kirkwood approximation shows it is related to a linked graph description of $U(x,y;\beta)$. In this representation the kernel admits the factorization

$$U(x,y;\beta)=(4\pi\beta q)^{-d/2}e^{-|x-y|^2/4\beta q}F(x,y;\beta). \quad (1.8)$$

The factor preceding F is the free diffusion kernel associated with $e^{-\beta\hat H_0}$, where $H_0=-q\Delta_x$. Here F is a smooth bounded function that is unity if $v=0$ and for $v\neq 0$ approaches unity as $\beta\to 0$.

The graphical representation of interest provides an expansion of $\log F(x,y;\beta)$, and is in fact a coupling constant expansion. Replace $v(x)$ by $\lambda v(x)$ in (1.5) (where λ is real); then one has

$$\log F(x,y;\beta)=\sum_{n=1}^{\infty}\lambda^n L_n(x,y;\beta,q). \quad (1.9)$$

The formula (determined in Ref. 6) for L_n is

$$L_n(x,y;\beta,q)=\sum_{\mathscr{G}_n}\sum_{p=0}^{\infty}(-1)^n\frac{2^s\beta^{n+p+s}q^{p+s}}{n!p!}\int_{I^n}d^n\xi$$
$$\times\prod_{i>j}^{n}\frac{1}{l_{ij}!}(b_{ij})^{l_{ij}}(c_n)^p v(\vec\xi_1)v(\vec\xi_2)\cdots v(\vec\xi_n). \quad (1.10)$$

The notation used in (1.10) is as follows. The b_{ij} and c_n are differential operators,

$$b_{ij}=\phi(\xi_i,\xi_j)D_i\cdot D_j,\quad c_n=\sum_{i=1}^{n}(1-\xi_i)\xi_i D_i\cdot D_i,$$

where D_i denotes a gradient operator in $\mathbb{R}^d$ that acts only upon the potential function whose argument contains the index i, as follows: for $i\in\{1,2,\ldots,n\}$,

$$D_i v(\vec\xi_1)\cdots v(\vec\xi_n)\equiv v(\vec\xi_1)\cdots(\nabla v)(\vec\xi_i)\cdots v(\vec\xi_n).$$

The coefficient function ϕ is the one-dimensional Green's function,

$$\phi(\xi_i,\xi_j)=\min(\xi_i,\xi_j)[1-\max(\xi_i,\xi_j)].$$

The symbol $\vec\xi_i$ is the linear path in $\mathbb{R}^d$ from y to x:

$$\vec\xi_i=y+\xi_i(x-y),\quad \xi_i\in[0,1]\equiv I.$$

Further, the $d^n\xi$ integration is the multiple integral

$$\int_{I^n}d^n\xi=\int_0^1 d\xi_1\int_0^1 d\xi_2\cdots\int_0^1 d\xi_n.$$

The sum indicated by $\mathscr{G}_n$ is the sum over all distinct connected graphs on n labeled vertices. For a given connected graph, if vertices i and j are linked ($\{i,j\}$ is a member of the edge set) then l_{ij} is summed from 1 to ∞. If i and j are not linked, $l_{ij}=0$. Finally

$$s=\sum_{i>j\geq 1}^{n}l_{ij}.$$

In order to compare the forms of (1.8) and the WKB representation (1.6), set $\beta=it/\hbar$, $q=\hbar^2/2m$. Then formally one has (after restoring λ to 1)

$$U\left(x,y;\frac{it}{\hbar}\right)=\frac{1}{(2\pi i\hbar t/m)^{d/2}}\exp\left\{\frac{i}{\hbar}\frac{m}{2t}|x-y|^2\right.$$
$$\left.+\sum_{n=1}^{\infty}L_n\left(x,y;\frac{it}{\hbar},\frac{\hbar^2}{2m}\right)\right\}.$$

Using (1.10) and collecting powers of $\hbar$, t, and m yields

$$L_n(x,y;it/\hbar,\hbar^2/2m)$$
$$=\sum_{\mathscr{G}_n}\sum_{p=0}^{\infty}\frac{(i\hbar)^{p+s_+-1}}{n!p!}\frac{t^{2n+s_++p-1}}{2^p m^{n+s_++p-1}}\int_{I^n}(\cdots), \quad (1.11)$$

where the integral is the same as in (1.10) and $s_+=s-(n-1)\geq 0$ is the increment of s above its minimum value of $n-1$ for a connected graph. All the $\hbar$ dependence of L_n appears in the factor $\hbar^{p+s_+-1}$. With (1.11) the sum over n of L_n can be reorganized to read

$$\sum_{n=1}^{\infty}L_n\left(x,y;it/\hbar,\frac{\hbar^2}{2m}\right)=\sum_{n=0}^{\infty}(i\hbar)^{n-1}\Phi_n(x,t;y,0),$$

where the Φ_n are independent of $\hbar$. Here Φ_0 is the contribution to the exponential factor of $U(x,y;it/\hbar)$ that is proportional to $\hbar^{-1}$. Equation (1.11) requires that all the contributions to Φ_0 must have $s_+=p=0$. This means the graphs in $\mathscr{G}_n$ contributing to Φ_0 must have $n-1$ links and so are tree graphs.[8] In fact,

$$\Phi_0(x,t;y,0)=\sum_{n=1}^{\infty}\frac{t^{2n-1}}{m^{n-1}}\frac{1}{n!}\sum_{\mathscr{G}_n|\text{trees}}\int_{I^n}(\cdots). \quad (1.12)$$

Thus the graph representation of the time evolution kernel takes the form

$$U(x,y;it/\hbar)=(2\pi i\hbar t/m)^{-d/2}$$
$$\times\exp\left\{\frac{i}{\hbar}\left[\frac{m}{2t}|x-y|^2-\Phi_0\right]+\Phi_1+O(\hbar)\right\}. \quad (1.13)$$

If (1.13) and the WKB approximation (1.6) are to be consis-

tent in the limit $\hbar \to 0$, then (1.3) should follow with $\Phi = \Phi_0$. The graphical analysis leading to the derivation of (1.9) and (1.12) is formal and the nature of the convergence properties of these series is not yet known. Nevertheless this heuristic line of reasoning provides us with an explicit series expression for Φ that through Eq. (1.3) yields a candidate solution of the Hamilton–Jacobi equation in the autonomous case. The generalization of this series to include the effects of a time-dependent potential is straightforward and will be given in the next section.

One merit of our tree graph constructive representation of the complete integral of the Hamilton–Jacobi equation is that many detailed dynamical properties of the Hamiltonian system (1.1) can be established with elementary analytical methods. That such a graphical expansion of the solution to the Hamilton–Jacobi equation should exist has been noted by Marinov[9] and Voros.[10] The assumption of a common mass m for all particles is made purely for notational convenience. The general kinetic energy operator for an N-body system with distinct masses m_i, $i \in 1 \sim N$, can always be brought into the Hamiltonian form (1.1) by a scale transformation of the particle coordinates.

The plan of this paper is as follows. Section II studies the series expansion (1.4). Explicit expressions for A_n are determined from a recurrence relation and the convergence properties of the series are determined. The fact that (1.3) and (1.4) constitute a complete integral of the Hamilton–Jacobi equation is established in Sec. III. The final section characterizes the dynamical behavior of the system and analyzes the behavior of the fixed-end-point variational problem. For $t - t_0$ in a fixed time interval $(0,T)$ it is proved that all classical paths are free of conjugate points, and that the variational problem defined by the action functional has only a strong minimum. The Appendix contains the tree graph proof of the explicit form the coefficients A_n take.

II. THE INVERSE MASS EXPANSION

This section investigates the natural recurrence relations associated with the inverse mass power series expansion of a solution to the Hamilton–Jacobi equation. It is established that the coefficient functions A_n have a multiple integral representation with an integrand determined by tree graphs. Finally we conjecture an explicit solution of the form (1.3) and (1.4) and determine its convergence properties.

First we characterize the class of potentials $v(x,t)$ to be employed. Basically these allowed potentials are real valued, C^∞ in x, C^1 in t, and have bounded derivatives of controlled growth. Let $\mathbf{N}$ denote the positive and $\mathbf{W}$ the non-negative integers. If $\alpha \in \mathbf{W}^d$ is a multi-index and $l \in \mathbf{W}$, then we use the notation

$$(\nabla^\alpha \partial^l v)(x,t) = \nabla_x^\alpha \left(\frac{\partial}{\partial t}\right)^l v(x,t).$$

Definition 1: Let $\Gamma \subseteq \mathbf{R}$ be an open (possibly infinite) interval and let $L \in \mathbf{W}$. A continuous potential v: $\mathbf{R}^d \times \Gamma \mapsto \mathbf{R}$ is said to be in the class $\mathscr{A}(\Gamma,L)$ if the following hold.

(i) Each partial derivative of v that contains at most L derivations with respect to the time argument exists and is continuous on $\mathbf{R}^d \times \Gamma$.

(ii) v is bounded,

$$\|v\| \equiv \sup\{|v(x,t)| \mid (x,t) \in \mathbf{R}^d \times \Gamma\} < \infty.$$

(iii) There exist finite non-negative constants U, B, and K (depending on v) such that whenever $\alpha \in \mathbf{W}^d$, $l \in \{0,1,\ldots,L\}$ and $|\alpha| + l > 0$ one has

$$\|\nabla^\alpha \partial^l v\| \leqslant U B^l (K/\sqrt{d})^{|\alpha|}.$$

The class $\mathscr{A}(\Gamma,L)$ is a real vector space. If $L < L'$ then $\mathscr{A}(\Gamma,L) \supseteq \mathscr{A}(\Gamma,L')$. It is simple to verify that if $v \in \mathscr{A}(\Gamma,L)$ and $t \in \Gamma$ is fixed, then $v(\cdot,t)$ is a real-analytic function on $\mathbf{R}^d$. Throughout the remainder of the paper it is assumed that $v \in \mathscr{A}(\Gamma,L)$ with $L \geqslant 1$ and this hypothesis will not always be written out.

Suppose a solution $S(x,t;y,t_0)$ of (1.2) admits the m^{-1} series expansion given by (1.3) and (1.4). Now if we formally substitute (1.3) and (1.4) into (1.2) we find that the coefficients of powers of m must satisfy the recurrence relation

$$\left[(2n-1) + (t-t_0)\frac{\partial}{\partial t} + (x-y)\cdot\nabla_x\right] a_n(x,t;y,t_0)$$
$$= \delta_{n,1} v(x,t) + \frac{1}{2}\sum_{k=1}^{n-1} \binom{n}{k} (\nabla_1 a_k \cdot \nabla_1 a_{n-k})(x,t;y,t_0), \tag{2.1}$$

where

$$A_n(x,t;y,t_0) = \frac{(t-t_0)^{2n+1}}{(n+1)!} a_{n+1}(x,t;y,t_0). \tag{2.2}$$

Here ∇_i is the gradient with respect to the ith vector argument of a_k. The sum on the right of (2.1) is absent if $n = 1$. The factor $\binom{n}{k}$ is the binomial coefficient and $\delta_{n,1}$ the Kronecker delta.

In formula (1.10) (for the static case $\partial v = 0$) the parametrized linear path $\vec{\xi}$ from y to x played a key role. For time-dependent potentials we extend the idea of linear path to include the time variable. Specifically, the path in $\mathbf{R}^d \times \Gamma$ from (y,t_0) to (x,t) is denoted

$$\tilde{\xi} = (y + \xi(x-y),\ t_0 + \xi(t-t_0))$$
$$= (\vec{\xi},\ t_0 + \xi(t-t_0)), \quad \xi \in I = [0,1].$$

Since $\mathbf{R}^d \times \Gamma$ is convex, it always contains $\tilde{\xi}$.

Our first observation is that the recurrence relation (2.1) has an integral equivalent.

Lemma 1: Let $n \in \mathbf{N}$ and $\{a_k\}_{k=1}^n$ be a sequence of continuously differentiable functions a_k: $(\mathbf{R}^d \times \Gamma)^2 \mapsto \mathbf{R}$. Then $\{a_k\}_1^n$ satisfies (2.1) if and only if $\{a_k\}_1^n$ satisfies the recursive integral identity

$$a_1(x,t;y,t_0) = \int_I d\xi\, v(\tilde{\xi}) \quad (n=1),$$

$$a_n(x,t;y,t_0) = \frac{1}{2}\sum_{k=1}^{n-1} \binom{n}{k} \int_I d\xi\, \xi^{2n-2} (\nabla_1 a_k \cdot \nabla_1 a_{n-k})(\tilde{\xi};y,t_0)$$

$$(n \geqslant 2). \tag{2.3}$$

Proof: Suppose (2.1) is satisfied and $n \geqslant 2$. Replace (x,t) with $\tilde{\xi}$ in (2.1) and notice that

$$\xi \frac{d}{d\xi} a_n(\tilde{\xi};y,t_0) = \xi(x-y)\cdot\nabla_1 a_n(\tilde{\xi};y,t_0) + \xi(t-t_0)(\partial_1 a)(\tilde{\xi};y,t_0)$$

and $\xi(x-y) = \vec{\xi} - y$. Multiplying (2.1) by ξ^{2n-2} one finds

$$\frac{d}{d\xi}\left[\xi^{2n-1} a_n(\tilde{\xi};y,t_0)\right] = \xi^{2n-2}\frac{1}{2}\sum_{k=1}^{n-1}\binom{n}{k}(\nabla_1 a_k \cdot \nabla_1 a_{n-k})(\tilde{\xi};y,t_0).$$

Integrating over $\xi \in I$ we obtain (2.3). A similar argument applies if $n = 1$.

Conversely, let (2.3) be satisfied. Replace (x,t) throughout by $\bar{\lambda}$ where $\lambda \in I$, and multiply by λ^{2n-1}. Change the integration variable to $\gamma = \lambda\xi$, differentiate with respect to λ, and set $\lambda = 1$. □

Our next step is to introduce a formula for $a_n(x,t;y,t_0)$ suggested by expansion (1.12). In order to do so it is helpful to review the notation used to describe tree graphs. A labeled tree T on $n \in \mathbb{N}$ vertices is the ordered pair $T = (V(T), E(T))$; $V(T)$ is the vertex set of T, and consists of n distinct natural numbers, the vertex labels; and $E(T)$ is the edge set over $V(T)$ of T, and consists of $n-1$ unordered pairs of distinct elements of $V(T)$, unless $n = 1$ where $E(T) = \emptyset$. Each element $i \in V(T)$ must appear in at least one pair in $E(T)$. The elements of $E(T)$ are called links.

If we fix a vertex set V, then the symbol $\mathcal{T}V$ will denote the set of all labeled trees on V. According to Cayley's theorem,[8] if V has n elements there are n^{n-2} trees in $\mathcal{T}V$. If $f: \mathcal{T}V \to A$, where A is a vector space, then the notation

$$\sum_{T \in \mathcal{T}V} f(T)$$

means to sum over all trees in $\mathcal{T}V$.

If $\beta \in E(T)$, then the notation $\beta = \{i_\beta, j_\beta\}$ $[i_\beta, j_\beta \in V(T)]$ will be understood consistently to imply $i_\beta < j_\beta$. For example, if $i = i_\beta, j = j_\beta$ in the formula for b_{ij} it is helpful to think of b_{ij} as a function of the link $\{i_\beta, j_\beta\}$. Specifically

$$b_\beta \equiv \phi(\xi_{i_\beta}, \xi_{j_\beta}) D_{i_\beta} \cdot D_{j_\beta}.$$

Here (as in Sec. I) the D_i is a differential operator that only acts on the potential v whose argument contains the index i. Thus D_i is the gradient with respect to the position variable $\vec{\xi}_i$ of the appropriate potential v.

We often encounter vertex sets which consist of the first n natural numbers, so it is convenient to introduce the abbreviation

$$V_n \equiv 1 \sim n \equiv \{1,2,\ldots,n\}.$$

Definition 2: For $n \in \mathbb{N}$ define the functions a_n: $(\mathbb{R}^d \times \Gamma)^2 \mapsto \mathbb{R}$ by the following "tree sums":

$$a_1(x,t;y,t_0) \equiv \int_I d\xi\, v(\tilde{\xi}), \tag{2.4}$$

$$a_n(x,t;y,t_0) \equiv \int_{I^n} d^n\xi \sum_{T \in \mathcal{T}V_n} \left[\prod_{\beta \in E(T)} b_\beta\right] \prod_{p=1}^{n} v(\tilde{\xi}_p), \tag{2.5}$$

for $(n > 1)$.

The following examples will be helpful in understanding these formulas. For $n = 1$, (2.4) is a special case of (2.5) if we take the empty product to be unity.

For $n = 2$, there is one tree T on two vertices. It is $T = (V_2, \{1,2\})$ and may be identified with the planar graph

T = ① —— ②

Hence,

$$a_2(x,t;y,t_0) = \int_0^1 d\xi_1 \int_0^1 d\xi_2\, \phi(\xi_1,\xi_2)(\nabla v)(\tilde{\xi}_1)\cdot(\nabla v)(\tilde{\xi}_2).$$

For $n = 3$, there are three different trees; each associated with a different planar graph, i.e.,

T_1 = ① —— ② —— ③ , T_2 = ① —— ③ —— ② ,

T_3 = ② —— ① —— ③ .

The tree T_1 contributes a term in the Σ_T of

$$\int_{I^3} d^3\xi\, \phi(\xi_1,\xi_2)\phi(\xi_2,\xi_3)(D_1 \cdot D_2)(D_2 \cdot D_3)v(\tilde{\xi}_1)v(\tilde{\xi}_2)v(\tilde{\xi}_3).$$

A change of labels in fact shows that the contributions of T_1, T_2, and T_3 to $a_3(x,t;y,t_0)$ are identical. So the value of a_3 is three times the above integral.

For $n \geq 4$, not all trees have the same topological structure and so a complete reduction of the sum to a single multiple integral will not occur. It should be evident now how all the a_n are determined, and that they are once continuously differentiable.

The main result of this section is the following.

Proposition 1: The functions $a_n: (\mathbb{R}^d \times \Gamma)^2 \mapsto \mathbb{R}$ defined by (2.4) and (2.5) satisfy the recurrence relation (2.1) for all $n \geq 1$.

Proof: Because of its substantial length we place the proof in the appendix. There it is shown (Lemma 11) that if the a_n are given by (2.4) and (2.5), then the recursive integral identity (2.3) is obeyed. By Lemma 1 it follows that recurrence relation (2.1) is satisfied. □

Given the determination of the coefficients a_n in Definition 2, we define a function Φ, which will turn out to be proportional to the part of Hamilton's principal function S, due to the interaction v [cf. (1.3)]. In the static potential case this function Φ is identical with the Φ_0 provided by formula (1.12).

Definition 3: Let $v \in \mathcal{A}(\Gamma,1)$ and select a fixed value $t_0 \in \Gamma$. Set

$$T = (2/K)(m/eU)^{1/2} \tag{2.6}$$

and label an interval of the time axis by $\Omega \equiv \Omega(\Gamma,T,t_0) \equiv (t_0 - T, t_0 + T) \cap \Gamma$. Define the function $\Phi(\cdot,\cdot;\cdot,t_0)$: $\mathbb{R}^d \times \Omega \times \mathbb{R}^d \mapsto \mathbb{R}$ by the series

$$\Phi(x,t;y,t_0) \equiv \sum_{n=1}^{\infty} \frac{(t-t_0)^{2n-1}}{m^{n-1} n!} a_n(x,t;y,t_0). \tag{2.7}$$

We summarize the convergence properties of this series.

Lemma 2: Let $v \in \mathcal{A}(\Gamma,1)$, $t_0 \in \Gamma$.

(i) For each fixed $t \in \Omega$, series (2.7) converges absolutely and uniformly for $(x,y) \in \mathbb{R}^d$. If t is restricted to a compact subset of Ω the convergence is also uniform in t.

(ii) For fixed $x,t;y,t_0$ in the domain of Φ, series (2.7) defines an analytic function of the inverse mass in the complex disk $|m^{-1}| < 4(eU)^{-1}K^{-2}(t-t_0)^{-2}$.

(iii) In the static case ($\partial v = 0$, $\Gamma = \mathbb{R}$) coefficients a_n are independent of t, t_0 and so for fixed $x, y \in \mathbb{R}^d$ and $m > 0$, series (2.7) defines an analytic function of time displacement in the complex disk $|t - t_0| < T$.

(iv) If $t \in \Omega$ is fixed, Φ is a C^∞ function of $(x,y) \in \mathbb{R}^{2d}$. In fact if $\alpha, \alpha' \in \mathbb{W}^d$, $l, l' \in \{0,1\}$, and $l + l' \leqslant 1$, then

$$(\nabla_1^\alpha \nabla_2^{\alpha'} \partial_1^l \partial_2^{l'} \Phi)(x,t;y,t_0)$$

$$= \sum_{n=1}^{\infty} \frac{1}{m^{n-1} n!} \left(\frac{\partial}{\partial t}\right)^l \left(\frac{\partial}{\partial t_0}\right)^{l'} [(t - t_0)^{2n-1} \times (\nabla_1^\alpha \nabla_2^{\alpha'} a_n)(x,t;y,t_0)], \tag{2.8}$$

where the series (2.8) has the same properties (i)–(iii) above as does series (2.7).

Proof: These results are evident consequences of the tree sum definition (2.4) and (2.5) of a_n and the requirement $v \in \mathscr{A}(\Gamma, 1)$. For example, using Cayley's theorem, the fact that $2(n-1)$ gradients occur in $\Pi_{\beta \in E(T)} b_\beta$ for $T \in \mathscr{T} V_n$, and $0 \leqslant \phi(\xi_i, \xi_j) \leqslant \frac{1}{4}$, we obtain the bound

$$|a_n(x,t;y,t_0)| \leqslant n^{n-2} U^n (K^2/4)^{n-1},$$

$$n \geqslant 2, \quad (x,y) \in \mathbb{R}^{2d}.$$

This implies (i). Then (ii) and (iii) are immediate. Similarly, (iv) follows from the smoothness of v and the estimate (for $n \in \mathbb{N}$, $|\alpha + \alpha'| + l + l' \neq 0$)

$$|\nabla_1^\alpha \nabla_2^{\alpha'} \partial_1^l \partial_2^{l'} a_n| \leqslant n^{n-2} (K^2/4)^{n-1} (K/\sqrt{d})^{|\alpha+\alpha'|} \times B^{l+l'} n^{|\alpha+\alpha'|+l+l'} U^n. \tag{2.9}$$

□

III. THE COMPLETE INTEGRAL

The detailed behavior of the function $S(x,t;y,t_0)$ and its relation to the Hamiltonian is considered in this section. In particular it is proved that S is a complete integral of the Hamilton–Jacobi equation. The associated Jacobian determinant is defined together with its continuity equation. For sufficiently small positive time displacements it is shown that this determinant is uniformly continuous in all its arguments and is positive.

Let the Hamiltonian H: $\mathbb{R}^{2d} \times \Gamma \mapsto \mathbb{R}$ be given by (1.1). The associated Hamilton–Jacobi equation is

$$\frac{\partial}{\partial \tau} \mathscr{S}(q,\tau) + H(q, \nabla_q \mathscr{S}(q,\tau), \tau) = 0, \tag{3.1}$$

where q is the position coordinate in $\mathbb{R}^d$, and $\mathscr{S}$: $\mathbb{R}^d \times \Gamma \mapsto \mathbb{R}$. A class of solutions to (3.1) of particular importance is the complete integral.

Definition 4: A function $\mathscr{S}$: $G \subseteq \mathbb{R}^{2d+1} \mapsto \mathbb{R}$ will be called a *complete integral* of the Hamilton–Jacobi equation if (i) G is a region (a connected open set); (ii) $\mathscr{S}(q,\tau;Q)$ depends continuously on d independent parameters $Q = (Q_1, Q_2, \ldots, Q_d)$ lying in some (nonempty) region $G_Q \subseteq \mathbb{R}^d$; (iii) $\mathscr{S}(q,\tau;Q)$ is continuously differentiable with respect to q and τ; and (iv) $\mathscr{S}$ is a solution of (3.1).

Consider the function S given by the following.

Definition 5: For each $v \in \mathscr{A}(\Gamma, 1)$, let $\omega \equiv \omega(\Gamma, T, t_0) \equiv \Omega \cap (t_0, \infty)$ and $\Phi(x,t;y,t_0)$ be the function given by the series (2.7). Define $S(\cdot,\cdot;\cdot,t_0)$: $\mathbb{R}^d \times \omega \times \mathbb{R}^d \mapsto \mathbb{R}$ by

$$S(x,t;y,t_0) = \frac{m}{2(t - t_0)} |x - y|^2 - \Phi(x,t;y,t_0). \tag{3.2}$$

We first show that S is a solution of (3.1).

Theorem 1: Let $v \in \mathscr{A}(\Gamma, 1)$, $t_0 \in \Gamma$ and suppose the Hamiltonian $H(x,p,t)$ is given by (1.1). The map

$$(x,t,y) \mapsto S(x,t;y,t_0)$$

is a complete integral of the Hamilton–Jacobi equation (3.1) with region $G = \mathbb{R}^d \times \omega \times \mathbb{R}^d$.

Proof: It is apparent that conditions (i)–(iii) of Definition 4 are satisfied. Note that the d independent parameters are given by the vector $y \in \mathbb{R}^d$. It remains to show that $S(x,t;y,t_0)$ is a solution of the Hamilton–Jacobi equation. Direct calculation yields

$$\frac{\partial}{\partial t} S(x,t;y,t_0) + H(x, \nabla_x S(x,t;y,t_0), t)$$

$$= -\frac{\partial}{\partial t} \Phi - \frac{1}{t - t_0} (x - y) \cdot \nabla_x \Phi + \frac{1}{2m} |\nabla_x \Phi|^2 + v(x,t). \tag{3.3}$$

Lemma 2 makes it permissible to substitute series (2.7) for Φ, differentiate term-by-term, and to evaluate $|\nabla_x \Phi|^2$ by the Cauchy product. Collecting common powers of m^{-1}, we find that the coefficient of $-[(t - t_0)^2/m]^{n-1}/n!$ is

$$\left[(2n-1) + (t - t_0) \frac{\partial}{\partial t} + (x - y) \cdot \nabla_x\right] a_n(x,t;y,t_0) - v(x,t) \delta_{n,1} - \frac{1}{2} \sum_{k=1}^{n-1} \binom{n}{k} (\nabla_1 a_k \cdot \nabla_1 a_{n-k})(x,t;y,t_0), \tag{3.4}$$

where the sum is taken to be zero if $n = 1$. But since the a_k are defined by the tree sums (2.4) and (2.5) it follows from Proposition 1 that the coefficient (3.4) vanishes identically. Thus the right-hand side of (3.3) vanishes, proving the theorem. □

We observe that our construction of S, and Theorem 1, would also be valid if potential v and mass parameter m were allowed to be complex valued in the Hamilton–Jacobi partial differential equation (1.2).

In view of the fact that S is a complete integral we can continue the investigation of S and the classical dynamics it implies by appealing to Jacobi's theorem. First note that the Jacobian matrix[11,12] is constructed from the elements $(i,j \in 1 \sim d)$

$$M_{ij}(x,t;y,t_0) \equiv -\frac{\partial}{\partial y_i} \frac{\partial}{\partial x_j} S(x,t;y,t_0) = \frac{m}{t - t_0} \delta_{ij} + \frac{\partial}{\partial y_i} \frac{\partial}{\partial x_j} \Phi(x,t;y,t_0),$$

and has determinant D: $\mathbb{R}^d \times \omega \times \mathbb{R}^d \mapsto \mathbb{R}$,

$$D(x,t;y,t_0) \equiv \det M(x,t;y,t_0).$$

We now fix some initial time $t_0 \in \Gamma$ for the remainder of the discussion. For brevity, we will understand S to be $S(\cdot,\cdot;\cdot,t_0)$ and similarly for D. With this terminology, we can state the famous result of Jacobi.

Theorem 2: Suppose S is a complete integral of the Hamilton–Jacobi equation. Suppose further that the second partials,

$$\frac{\partial^2 S}{\partial x_i\,\partial y_j},\quad \frac{\partial^2 S}{\partial x_i\,\partial t},\quad \frac{\partial^2 S}{\partial y_i\,\partial t},\quad i,j\in 1\sim d,$$

exist and are continuous.

For $p_0,y\in\mathbf{R}^d$, let $q(\tau)\equiv q(\tau;y,t_0,p_0)$ be a solution to

$$-(\nabla_2 S)(q,\tau;y,t_0)=p_0 \tag{3.5}$$

defined by the implicit function theorem in a region where $D(q,\tau;y,t_0)\neq 0$. Let $p(\tau)\equiv p(\tau;y,t_0,p_0)$ be given [whenever $q(\tau)$ exists] by

$$p(\tau)\equiv(\nabla_1 S)(q(\tau),\tau;y,t_0). \tag{3.6}$$

Then $q(\cdot)$, $p(\cdot)$ satisfy Hamilton's equations

$$\dot q(\tau)=(\nabla_2 H)(q(\tau),p(\tau),\tau),$$

$$\dot p(\tau)=-(\nabla_1 H)(q(\tau),p(\tau),\tau).$$

Proof: See Refs. 13–15. □

We proceed by deriving a number of technical results that facilitate the application of Jacobi's theorem. Most of these technical results aid us in applying the implicit function part of the theorem in order to define $q(\tau)$ as the solution of (3.5).

Lemma 3: Given $\sigma\in(0,1)$ let $t(\sigma)=(1+c/\sigma)^{-1/2}T$, where $c=2\sqrt{2/\pi}$. Then

$$\left|\frac{t-t_0}{m}\frac{\partial}{\partial x_i}\frac{\partial}{\partial y_j}\Phi(x,t;y,t_0)\right|<\frac{\sigma}{d}, \tag{3.7}$$

for all $i,j\in 1\sim d$, $x,y\in\mathbf{R}^d$, and $t\in(t_0,t_0+t(\sigma))\cap\Gamma\subseteq\omega$.

Proof: Estimate (3.7) follows by applying bound (2.9) to the series (2.8). □

An important consideration that occurs when applying the implicit function theorem to solve (3.5) for the classical path $q(\cdot)$ is the behavior of the range of $-\nabla_2 S$. For example, if the value p_0 is not assumed by $-(\nabla_2 S)(q,\tau;y,t_0)$ as q varies through $\mathbf{R}^d$ and τ varies through ω for fixed y, then (3.5) is empty and so does not define a function $q(\cdot)$. The range of $-\nabla_2 S$ is characterized by the following statement.

Lemma 4: Given any $y,p_0\in\mathbf{R}^d$ and $t\in(t_0,t_0+t(\sigma))\cap\Gamma$, the equation

$$-(\nabla_2 S)(x,t;y,t_0)=p_0, \tag{3.8}$$

has a unique solution for $x\in\mathbf{R}^d$. Consequently,

$$-(\nabla_2 S)(\mathbf{R}^d\times\omega\times\mathbf{R}^d)\equiv\text{Range}(-\nabla_2 S)=\mathbf{R}^d.$$

Proof: Equation (3.8) suggests we examine a function $F\colon\mathbf{R}^d\to\mathbf{R}^d$ defined by

$$F(x)=y+\frac{t-t_0}{m}p_0-\frac{t-t_0}{m}(\nabla_2\Phi)(x,t;y,t_0). \tag{3.9}$$

Of course, F depends parametrically on y,p_0,t, and t_0. We first show F is a contraction mapping of $\mathbf{R}^d$ into $\mathbf{R}^d$. If $x,x'\in\mathbf{R}^d$ are arbitrary, then (3.9) implies

$$F(x)-F(x')=[(t-t_0)/m]\,[(\nabla_2\Phi)(x',t;y,t_0)-(\nabla_2\Phi)(x,t;y,t_0)].$$

Apply Taylor's formula to the jth component of F and use the Schwartz inequality. One finds

$$|F_j(x)-F_j(x')|\leqslant|x-x'|\,|\nabla F_j(x+\lambda_j(x'-x))|$$

for some $\lambda_j\in(0,1)$. Since $t-t_0<t(\sigma)$, estimate (3.7) is valid and

$$|\nabla F_j(x'')|<\sigma/\sqrt{d},$$

for all $x''\in\mathbf{R}^d$. Computing the Euclidean norm for the difference of F gives

$$|F(x)-F(x')|<\sigma|x-x'|.$$

Since $\sigma<1$, F is a contraction mapping. By the contraction principle[16] it possesses a unique fixed point $x^*\in\mathbf{R}^d$, that is, $F(x^*)=x^*$. Since $t\neq t_0$ this can be rearranged to give

$$[m/(t-t_0)](x^*-y)+(\nabla_2\Phi)(x^*,t;y,t_0)=p_0,$$

so that x^* is a solution of (3.8). □

We conclude this section by investigating the basic properties of the determinant D. In particular we determine the region in x,y, and t where D cannot have a zero.

Lemma 5: If $t\in\omega$ the determinant D satisfies the following continuity equation:

$$\mathbf{D}_x\cdot[(\mathbf{D}_2 H)(x,\mathbf{D}_x S(x,t;y,t_0),t)D(x,t;y,t_0)]+\frac{\partial}{\partial t}D(x,t;y,t_0)=0, \tag{3.10}$$

for all x,y.

Proof: This is a consequence of the fact that S is a complete integral in region G of the Hamilton–Jacobi equation and has partials up to third order which are continuous, provided they contain at most one time derivative [cf. Lemma 2, (iv)]. See Refs. 11 and 12. □

Lemma 6: Let $[t_1,t_2]\subset\omega$. The determinant D is uniformly continuous on the restricted domain $\mathbf{R}^d\times[t_1,t_2]\times\mathbf{R}^d$.

Proof: Due to the algebraic nature of the determinant, D is a finite sum of finite products. Differentiation of $D(x,t;y,t_0)$ with respect to t or components of x,y can be carried out term by term. The resulting factors are uniformly bounded on the domain $\mathbf{R}^d\times[t_1,t_2]\times\mathbf{R}^d$ since t is bounded away from t_0 and t_0+T [see (2.8) and (2.9)]. It follows that there exists a finite constant C such that

$$|\nabla_z D(z,t_0)|<C,\quad z\in\mathbf{R}^d\times[t_1,t_2]\times\mathbf{R}^d,$$

where $z=(x,t,y)$. Applying Taylor's theorem and Schwartz' inequality to D (noting the restricted domain is convex) one finds

$$|D(z,t_0)-D(z',t_0)|\leqslant C|z-z'|,\quad z,z'\in\mathbf{R}^d\times[t_1,t_2]\times\mathbf{R}^d.$$

Thus D is uniformly continuous in this allowed range of x,t,y. □

If the determinant $D(x,t;y,t_0)$ is nonvanishing the implicit function theorem tells us that (3.5) has a local C^1 solution for x in terms of t,y,t_0, and p_0. So, it is helpful to establish conditions that guarantee that $D\neq 0$. We first note $D>0$ if $t\in(t_0,t_0+t(\sigma))\cap\Gamma$. To see this, recall the definition

$$D(x,t;y,t_0)=(m/(t-t_0))^d\det(1+A), \tag{3.11}$$

where A is the $d\times d$ matrix with elements

$$A_{ij}=\frac{t-t_0}{m}\frac{\partial}{\partial x_j}\frac{\partial}{\partial y_i}\Phi(x,t;y,t_0).$$

But these are just the quantities estimated in (3.7), so we obtain the following bound on the operator norm of the linear transformation A:

$$\|A\| < \left(\sum_{i,j=1}^{d} |A_{ij}|^2 \right)^{1/2} < \sigma < 1.$$

This bound is x,y uniform, and for all $t \in (t_0, t_0 + t(\sigma)) \cap \Gamma$. It follows that $1 + A$ is invertible, hence $D \neq 0$ in this region. In fact a simple argument involving the Jordan normal form of a matrix and the Neumann series for $(1 + A)^{-1}$ leads to the estimate

$$D(x,t;y,t_0) > (m/(t - t_0))^d (1 - \sigma)^d,$$
$$t \in (t_0, t_0 + t(\sigma)) \cap \Gamma, \quad x,y \in \mathbf{R}^d.$$

Given the existence of an interval $(t_0, t_0 + t(\sigma))$ such that D is bounded away from zero uniformly (in x,y), it is useful to define the largest time interval with this property. We call the right end point t_J of this largest interval the *Jacobi time* (relative to t_0).

Definition 6: Let the domain of D and S be $Z = \mathbf{R}^d \times \omega \times \mathbf{R}^d$. Define the sets Λ and $\Pi_t(\Lambda)$ to be

$$\Lambda \equiv \{ z \in Z \mid D(z,t_0) = 0 \},$$

$$\Pi_t(\Lambda) \equiv \{ t \in \omega \mid (x,t,y) \in \Lambda, \text{ for some } (x,y) \in \mathbf{R}^{2d} \}.$$

If $\Lambda = \emptyset$, then set $t_J = \sup \omega$, otherwise set $t_J = \inf \Pi_t(\Lambda)$.

Notice that Z, t_J, Λ, and $\Pi_t(\Lambda)$ all depend on the choice of t_0; $\Lambda = D^{-1}\{0\}$ is the null set of D and $\Pi_t(\Lambda)$ is its projection onto the time axis. From the definition of the Jacobi time one has $t_J \geqslant \sup[(t_0, t_0 + t(\sigma)) \cap \Gamma]$. In the next section we will show that the optimal result $t_J = \sup \omega$ holds.

IV. CLASSICAL PATHS, UNIQUENESS, AND THE VARIATIONAL PRINCIPLE

By systematic application of Jacobi's theorem we shall derive many of the dynamical properties of the Hamiltonian system (1.1). This section will establish the uniqueness properties of the classical paths, prove the absence of conjugate points and demonstrate that the fixed-end-point variational problem has only one extremum if $t_0 < t < t_J$.

Consider first the behavior of the solutions to (3.5).

Lemma 7: For each $y, p_0 \in \mathbf{R}^d$, Eq. (3.5) has a C^1 solution $q(\tau; y, t_0, p_0)$ for all $\tau \in (t_0, t_J)$. Furthermore

$$\lim_{\tau \to t_0^+} q(\tau; y, t_0, p_0) = y, \tag{4.1}$$

$$\frac{\partial q}{\partial \tau}(t_0^+; y, t_0, p_0) = \frac{p_0}{m}. \tag{4.2}$$

Proof: Choose $\sigma \in (0,1)$ such that $t(\sigma) \in (0, t_J - t_0)$ as in Lemma 3. Lemma 4 implies there is a (unique) solution $q(\tau; y, t_0, p_0)$ for each $\tau \in (t_0, t_0 + t(\sigma))$. Since $-\nabla_2 S$ is a C^1 mapping and since $D(q,\tau; y, t_0) \neq 0$ for $\tau \in (t_0, t_J)$, we may apply the implicit function theorem[16] in the neighborhood of this solution. Thus it follows that $q(\tau; y, t_0, p_0)$ is C^1 and may be extended in τ to the time interval (t_0, t_J).

To establish (4.1) note that (3.5) may be written as

$$[m/(\tau - t_0)][q(\tau; y, t_0, p_0) - y]$$
$$= -(\nabla_2 \Phi)(q(\tau; y, t_0, p_0), \tau; y, t_0) + p_0.$$

The boundedness of $-\nabla_2 \Phi + p_0$ as $\tau \to t_0^+$ implies (4.1). The fact that $-(\nabla_2 \Phi)(q,\tau; y, t_0)$ vanishes uniformly (in q) as $\tau \to t_0^+$ gives (4.2). □

We now turn to the uniqueness aspects of the classical paths $q(\tau)$. So far we know from Lemma 4 that $q(\tau)$ is unique if $\tau \in (t_0, t_0 + t(\sigma)) \cap \Gamma$. We extend this range of uniqueness to the interval (t_0, t_J) and remark that in due course it will be proved that $t_J = \sup \omega$. The term *classical path* will denote a C^2 function $q: (a,b) \subseteq \mathbf{R} \to \mathbf{R}^d$ that satisfies Newton's equation

$$m \frac{d^2}{d\tau^2} q(\tau) = -\nabla v(q(\tau), \tau).$$

Proposition 2: Let $y, p_0 \in \mathbf{R}^d$ and $q(\tau) \equiv q(\tau; y, t_0, p_0)$ be the solution of (3.5) given in Lemma 7. Then $q(\cdot)$ is a classical path with the following properties.

(i) Initial value uniqueness. Let $(\tilde{q}, \tilde{p})$: $\Gamma \to \mathbf{R}^{2d}$ be the unique solution to Hamilton's equations, with $\tilde{q}(t_0) = y$ and $\tilde{p}(t_0) = p_0$. Then

$$\tilde{q}(\tau) = q(\tau), \quad \tau \in (t_0, t_J).$$

Hence $q(\cdot)$ is the unique solution to (3.5).

(ii) Two-end-point uniqueness. Consider any two distinct classical paths q_i: $(t_0, t_J) \to \mathbf{R}^d$ $(i = 1,2,\ q_1 \neq q_2)$ emanating from the same initial point y:

$$q_i(t_0^+) = y, \quad i = 1,2.$$

Then these paths do not intersect:

$$q_1(\tau) \neq q_2(\tau), \quad \tau \in (t_0, t_J).$$

(iii) Completeness. As (y, p_0) varies throughout $\mathbf{R}^{2d}$ the unique solutions $q(\tau)$ to (3.5) exhaust all possible classical paths.

Proof: By Theorems 1 and 2 and the fact that $D(q,\tau; y, t_0) \neq 0$ for $q,\tau,y \in \mathbf{R}^d \times (t_0, t_J) \times \mathbf{R}^d$ we find that $q(\tau)$ and $p(\tau) = \nabla_1 S(q(\tau),\tau; y, t_0)$ solve Hamilton's equations

$$\dot{q}(\tau) = (1/m)p(\tau), \quad \dot{p}(\tau) = -\nabla v(q(\tau),\tau).$$

These imply $q(\cdot)$ is a classical path. Lemma 7 shows $q(t_0^+) = y$ and $p(t_0^+) = m\dot{q}(t_0^+) = p_0$.

(i) Writing $\tilde{z} = (\tilde{q}, \tilde{p})$, Hamilton's equations take the form

$$\frac{d\tilde{z}}{d\tau} = (\nabla_2 H, -\nabla_1 H)(\tilde{z}(\tau),\tau).$$

For potentials $v \in \mathcal{A}(\Gamma, 1)$ one may verify the hypothesis of Theorem 6.1.4 of Ref. 17 and conclude that there is a unique solution $\tilde{z}$: $\Gamma \to \mathbf{R}^{2d}$ subject to the initial condition $\tilde{z}(t_0) = (y, p_0)$. Hence $q = \tilde{q}$.

If there were another solution q' to (3.5) it must agree with q on $(t_0, t_0 + t(\sigma)) \cap \Gamma$, so $(q', m\dot{q}')$ solves Hamilton's equations and $q' = q$.

(ii) Assuming the contrary, there exists $\tau^* \in (t_0, t_J)$ such that $q_1(\tau^*) = q_2(\tau^*)$, and therefore

$$-\nabla_2 S(q_1(\tau^*),\tau^*; y, t_0) = -\nabla_2 S(q_2(\tau^*),\tau^*; y, t_0). \tag{4.3}$$

Since $(q_i, m\dot{q}_i)$ solve Hamilton's equations $(i = 1,2)$, (i) implies that they satisfy (3.5) in the form

$$-\nabla_2 S(q_i(\tau),\tau; y, t_0) = m\dot{q}_i(t_0^+) \quad (i = 1,2, \quad \text{all } \tau).$$

Choosing $\tau = \tau^*$, (4.3) implies $\dot{q}_1(t_0^+) = \dot{q}_2(t_0^+)$. Then by (i) we must have $q_1 = q_2$. This contradicts that q_1 and q_2 are distinct.

(iii) This follows from (i) and Lemma 4. □

Notice that the fixed-end-point trajectory problem is solved by a special choice of p_0. Set

$$p_0 = p_0(x,t;y,t_0) \equiv -(\nabla_2 S)(x,t;y,t_0), \tag{4.4}$$

where $t \in (t_0,t_J)$. Then the unique classical path

$$q(\tau;x,t;y,t_0) \equiv q(\tau;y,t_0,p_0(x,t;y,t_0)) \tag{4.5}$$

provided by the solution of (3.5) with p_0 given by (4.4) runs from y at $\tau = t_0$ to x at time $\tau = t$. That $q(t) = x$ is verified by checking that this endpoint is indeed a solution of (3.5).

A second observation of interest concerns orbital periods in the case of a static potential $\partial v = 0$. A *closed orbit* $(q(\cdot),p(\cdot))$ is a periodic solution of Hamilton's equations, i.e., there is a least positive time T_0 such that $(q(\cdot),p(\cdot))$ are translation invariant $(q(\tau),p(\tau)) = (q(\tau+T_0),p(\tau+T_0))$, all τ. Consider a closed orbit $(q(\cdot),p(\cdot))$. One possibility is that the orbit be trivially "periodic" in the sense that $p(\tau) = 0$ for all τ. In this case the path $q(\tau) = x_0$, a constant, and x_0 corresponds to a point of equilibrium for the system, i.e., $\nabla v(x_0) = 0$. (Also a least $T_0 > 0$ fails to exist.)

If the orbit is not trivial, then there is a time, say $\tau = 0$, where $p_0 \equiv p(0) \neq 0$. Let $y = q(0)$ and consider two distinct paths emanating from y; one being the original orbit path, and the other having initial momentum $-p(0) \neq p_0$. Since the Hamiltonian is time-reversal invariant, the second path follows the trace of q in the reverse direction relative to the first. Because the orbit is closed, the two paths must intersect at time $t^* = T_0/2$. Proposition 2(i) implies $t^* \geqslant T$. So we have the conclusion that every (nontrivial) closed orbit has period $T_0 \geqslant 2T$.

Returning to the case of the time-dependent potential, the next objective is to optimize the region of validity of these results by proving that $t_J = \sup \omega$. The following lemma and proposition achieve this goal.

Lemma 8: For all $(x,t,y) \in \mathbb{R}^d \times (t_0,t_J) \times \mathbb{R}^d$, the Jacobian determinant has the representation

$$D(x,t;y,t_0) = \left(\frac{m}{t-t_0}\right)^d \exp\left\{\frac{1}{m}\int_{t_0}^{t} d\tau \times (\Delta_1\Phi)(q(\tau;x,t;y,t_0),\tau;y,t_0)\right\}. \tag{4.6}$$

Proof: Let (x,t,y) be given. Define N: $\mathbf{R}^d \times (t_0,t) \to \mathbf{R}$ by

$$N(q,\tau) = ((\tau - t_0)/m)^d D(q,\tau;y,t_0).$$

The estimates

$$(1-\sigma)^d \leqslant ((\tau - t_0)/m)^d D(q,\tau;y,t_0) \leqslant (1+\sigma)^d$$

valid for all $q, y \in \mathbb{R}^d$, $\tau \in (t_0, t_0 + t(\sigma)) \cap \Gamma$ imply, as $\sigma \to 0^+$, that

$$\lim_{\tau \to t_0^+} N(q,\tau) = 1$$

uniformly in q and y. In terms of N, the continuity equation of Lemma 5 reads

$$\frac{\partial N}{\partial \tau}(q,\tau) + \frac{1}{m}(\nabla_1 S)(q,\tau;y,t_0)\cdot(\nabla N)(q,\tau) = (1/m)N(q,\tau)(\Delta_1\Phi)(q,\tau;y,t_0).$$

Since $t_0 < \tau < t < t_J$, $N(q,\tau) > 0$ and we may divide by N to obtain

$$\frac{\partial}{\partial \tau}\log N + \frac{1}{m}\nabla_1 S \cdot \nabla_1 \log N = \frac{1}{m}\Delta_1\Phi.$$

Take q to be the classical path $q(\tau) \equiv q(\tau;x,t;y,t_0)$ defined in (4.5). Observe from Jacobi's theorem that the velocity, $\dot{q}(\tau)$, of this trajectory is $(1/m)\nabla_1 S(q(\tau),\tau;y,t_0)$. So we have

$$\frac{d}{d\tau}\log N(q(\tau),\tau) = \frac{1}{m}\Delta_1\Phi(q(\tau),\tau;y,t_0).$$

Integrating over $\tau \in (t_0,t)$ gives (4.6). □

Combining representation (4.6) with the uniform continuity of D implies that $D(x,t;y,t_0) > 0$ if $t \in \omega$. In terms of the notation of Definition 6 we obtain the following.

Proposition 3: $\Lambda = \varnothing$ (or $t_J = \sup \omega$).

Proof: We show the assumption $\Lambda \neq \varnothing$ leads to a contradiction. If $\Lambda \neq \varnothing$, then $t_J \in \omega$ and for all $\delta > 0$

$$(t_J - \delta, t_J + \delta) \cap \Pi_t(\Lambda) \neq \varnothing. \tag{4.7}$$

Fix δ small enough so that

$$t_0 < t_J - \delta \equiv t_1 < t_J + \delta \equiv t_2 < \sup \omega. \tag{4.8}$$

Let

$$C = \sup\{(1/m)|\Delta_x\Phi(x,t;y,t_0)| \;|\; x,y \in \mathbb{R}^d, \quad t \in [t_0,t_J]\}.$$

Lemma 2, part (iv) implies $C < \infty$. Define ϵ to be

$$\epsilon = \tfrac{1}{2}(m/(t_J - t_0))^d e^{-(t_J - t_0)C}.$$

From the uniform continuity of D (Lemma 6) there exists a $\delta_\epsilon > 0$ satisfying $\delta_\epsilon \leqslant \delta$ and such that

$$|D(x,t;y,t_0) - D(x',t';y',t_0)| < \epsilon, \tag{4.9}$$

if $|(x,t,y) - (x',t',y')| < \delta_\epsilon$ and $t,t' \in [t_1,t_2]$. By (4.7) there exists a point $(x',t',y') \in \Lambda$ at which D is zero, with

$$t' \in (t_J - \delta_\epsilon/2, t_J + \delta_\epsilon/2).$$

Setting $x = x'$ and $y = y'$, (4.9) becomes the upper bound

$$|D(x',t;y',t_0)| < \tfrac{1}{2}(m/(t_J - t_0))^d e^{-(t_J - t_0)C}, \tag{4.10}$$

for all $t \in (t_J - \delta_\epsilon/2, t_J + \delta_\epsilon/2)$. But if $t \in (t_J - \delta_\epsilon/2, t_J)$, then D has representation (4.6), which in turn implies the lower bound

$$|D(x',t;y',t_0)| \geqslant (m/(t-t_0))^d e^{-(t-t_0)C} \geqslant (m/(t_J - t_0))^d e^{-(t_J - t_0)C}. \tag{4.11}$$

Bound (4.10) is in contradiction with bound (4.11). Thus $\Lambda = \varnothing$. □

Proposition 3 lets us apply Jacobi's theorem in order to find all solutions of Hamilton's equations for time displacements less than T. However, by an iterative application of Jacobi's theorem we can obtain the solution to Hamilton's equations for all times $t > t_0$. This is done as follows.

For simplicity we assume the potential $v(x,t)$ is defined for all t, i.e., $\sup \Gamma = \infty$. Let $y^{(0)}$, $p^{(0)}$ be the arbitrary initial position and momentum at time t_0 of a classical path Q: $[t_0,\infty) \to \mathbb{R}^d$. We choose some $t \in (0,T)$ and let $n \equiv [(\tau - t_0)/t]$ be the greatest integer less than $(\tau - t_0)/t$.

The trajectory Q,P (solution to Hamilton's equations) corresponding to path Q is then defined recursively for all $\tau > t_0$;

$$Q(\tau) \equiv q(\tau;y^{(n)},t_0 + nt,p^{(n)}),$$

$$P(\tau) \equiv (\nabla_1 S)(Q(\tau),\tau;y^{(n)},t_0 + nt),$$

$$y^{(l)} \equiv q(t_0 + lt;y^{(l-1)},t_0 + (l-1)t,p^{(l-1)}) = Q(t_0 + lt),$$

$$p^{(l)} \equiv (\nabla_1 S)(y^{(l)},t_0 + lt,y^{(l-1)},t_0 + (l-1)t) = P(t_0 + lt),$$

where $l \in \mathbf{N}$.

The reason this works is because the implicit function theorem can always be used to define $q(\cdot\,; y^{(l)}, t_0 + lt, p^{(l)})$ for any values of $Q(t_0 + lt), P(t_0 + lt)$ that may happen to evolve along the trajectory. These values are then regarded as new initial values for the next segment of the trajectory.

The action which appears in the WKB approximation is the time integral of the Lagrange function. If $q(\tau)$ is the classical path defined in (4.5) the Lagrangian action (Hamilton's principal function) is defined to be

$$S_L(x,t;y,t_0) \equiv \int_{t_0}^{t} d\tau\, L(q(\tau),\dot{q}(\tau),\tau). \tag{4.12}$$

The integrand here is the Lagrange function associated with the Hamiltonian (1.1),

$$L(q,\dot{q},\tau) = \tfrac{1}{2}m\dot{q}^2 - v(q,\tau).$$

It is known that S_L is a solution of the Hamilton–Jacobi equation (1.2). We demonstrate that S_L is identical with the function $S(x,t;y,t_0)$ defined by (3.2) provided $t \in \omega$.

Proposition 4: $S_L(x,t;y,t_0) = S(x,t;y,t_0)$ for all $(x,t,y) \in Z$.

Proof: Start with formula (4.12) where $q(\tau)$ is the unique classical path from $q(t_0) = y$ to $q(t) = x$, i.e., the path defined by (4.5). Jacobi's theorem gives us

$$\dot{q}(\tau) = (1/m)(\nabla_1 S)(q(\tau),\tau;y,t_0).$$

Insert this identity into the integrand of (4.12) and use the Hamilton–Jacobi equation for S. One finds

$$S_L(x,t;y,t_0) = \int_{t_0}^{t} d\tau[\,-(\partial_1 S)(q(\tau),\tau;y,t_0) - 2v(q(\tau),\tau)\,].$$

Expressing the first term of the integrand as a total derivative with respect to τ, via

$$(\partial_1 S)(q(\tau),\tau;y,t_0) = \frac{d}{d\tau} S(q(\tau),\tau;y,t_0) - m|\dot{q}(\tau)|^2,$$

leads to

$$S_L(x,t;y,t_0) = -S(q(\tau),\tau;y,t_0)\Big|_{\tau=t_0}^{t} + 2\int_{t_0}^{t} d\tau\, L(q(\tau),\dot{q}(\tau),\tau),$$

or

$$S_L(x,t;y,t_0) = S(x,t;y,t_0) - \lim_{\tau\to t_0^+} S(q(\tau),\tau;y,t_0).$$

From the properties of $q(\tau)$ and Φ it is easily seen that the limit vanishes. □

We conclude our analysis by discussing the implications of our solution of the Hamilton–Jacobi equation for the fixed end-point variational problem. Fix $(x,t,y) \in Z$ and let $D(J)$ be a class of functions appropriate for the domain of a functional. The action functional J: $D(J) \to \mathbf{R}$ is defined by

$$J[Q] = \int_{t_0}^{t} d\tau\, L(Q(\tau),\dot{Q}(\tau),\tau), \tag{4.13}$$

where the domain of J is $D(J) = \{Q\colon [t_0,t] \to \mathbf{R}^d \mid Q$ piecewise smooth, $Q(t_0) = y$, $Q(t) = x\}$. Each smooth element $Q^* \in D(J)$, where the first variation[13] of J vanishes, is an *extremal*. The associated $Q^*(\tau)$ is a solution of the Euler–Lagrange equations. In favorable circumstances an extremal may be a local minimum of the functional. The nature of the minimum is characterized by the norm associated with it.

For piecewise-smooth functions Q on $[t_0,t]$ define two norms by

$$||Q||_0 \equiv \sup_{\tau\in[t_0,t]} |Q(t)|,$$

$$||Q||_1 \equiv ||Q||_0 + \sup_{\tau} |\dot{Q}(\tau)|.$$

In the $||\cdot||_1$ norm the supremum is taken only over the values of $\tau \in [t_0,t]$ where the derivative exists. An extremal $Q^* \in D(J)$ is a *strong local minimum* if there exists an $\epsilon > 0$ such that

$$J[Q^*] < J[Q], \tag{4.14}$$

for all $Q \in D(J)$ satisfying

$$||Q - Q^*||_0 < \epsilon.$$

On the other hand, $J[Q]$ is said to have a *weak local minimum* at Q^* if (4.14) is valid for $Q \in D(J)$ obeying

$$||Q - Q^*||_1 < \epsilon.$$

Of course, if Q^* is a strong minimum it is also a weak minimum.

In general terms establishing whether or not an extremal is a minimum requires proving that the second variation of $J(Q)$ at $Q = Q^*$ is positive and this in turn is determined in large part by the absence of conjugate points. More precisely,[13] given a classical path q: $[t_0,t] \to \mathbf{R}^d$, a point $\tau_F \in (t_0,t]$ is said to be *conjugate* to t_0 if there exists a sequence $\{q_n\}$ of neighboring classical paths satisfying

$$q_n(t_0) = q(t_0), \quad q_n(\tau_n) = q(\tau_n), \tag{4.15}$$

where

$$0 < ||q_n - q||_0 \to 0, \quad \tau_n \to \tau_F, \quad \text{as } n \to \infty.$$

Lemma 9: For each $(y,p_0) \in \mathbf{R}^{2d}$, let $q(\cdot\,; y,t_0,p_0)$ be the classical path defined by (3.5). Then $q(\cdot\,; y,t_0,p_0)$ has no point conjugate to t_0 in the interval ω.

Proof: Equation (4.15) requires the existence of two distinct classical paths q and q_n that have the same initial position y and the same final position for $\tau = \tau_n \to \tau_F$. But by Proposition 2 this is impossible if $\tau_F \in \omega$. □

This technical result enables us to establish the character of the stationary points of the functional $J[\cdot]$.

Theorem 3: Let $v \in \mathscr{A}(\Gamma,2)$ and $t_0 \in \Gamma$. For each $(x,t,y) \in Z$ the associated functional $J[\cdot]$ has only one extremal $Q^* \in D(J)$. Furthermore if q is the classical path defined by (4.5) then $Q^* = q(\cdot\,; x,t; y,t_0)$ and this extremal furnishes J with a strong minimum.

Proof: Our theorem takes $v \in \mathscr{A}(\Gamma,2)$ as its hypothesis, rather than $v \in \mathscr{A}(\Gamma,1)$, in order that the Lagrange function $L(q,\dot{q},\tau)$ is sufficiently differentiable[18] to ensure the applicability of standard results from the calculus of variations to be used below.

Each extremal Q^* is a solution of the Euler–Lagrange equations that has initial point y, final point x. Proposition 2 shows that there is only one such classical path and this unique path is $Q^*(\cdot) = q(\cdot\,; x,t; y,t_0)$, where q is defined in (4.5).

Sufficient conditions for a strong local minimum are established in Refs. 13 and 14. The first three of these four conditions are as follows.

(i) $q(\cdot)$ is a classical path.

(ii) The $d \times d$ matrix, $K(q(\tau),\dot{q}(\tau),\tau)$ defined by

$$\frac{\partial}{\partial \dot{q}_i}\frac{\partial}{\partial \dot{q}_j} L(q(\tau),\dot{q}(\tau),\tau), \quad i,j \in 1 \sim d,$$

is positive definite for $\tau \in [t_0,t]$.

(iii) The path $q(\cdot)$ has no point conjugate to $\tau = t_0$ in $[t_0,t]$.

Jacobi's theorem assures us that (i) is valid. Lemma 9 guarantees that (iii) is fulfilled; (ii) is an immediate consequence of definition of the Lagrangian.

Let E be the Weierstrass function defined by the time-dependent Lagrange function $L(q,\dot{q},\tau)$. For $Q,\dot{Q},z \in \mathbb{R}^d$

$$E(\tau,Q,\dot{Q},z) \equiv L(Q,z,\tau) - L(Q,\dot{Q},\tau) - (z-\dot{Q})\cdot(\nabla_2 L)(Q,\dot{Q},\tau).$$

Upon using the Taylor series remainder formula, this can also be written

$$E(\tau,Q,\dot{Q},z) = \tfrac{1}{2}(z-\dot{Q})\cdot K(Q,\dot{Q}+\theta(z-\dot{Q}),\tau)(z-\dot{Q}),$$

for some value of $\theta \in (0,1)$. The fourth condition needed to establish a strong local minimum is the following.

(iv) The E-function $E(\tau,Q,\dot{Q},z) \geqslant 0$ in a region of $\tau,Q,\dot{Q}$ space containing $\{(\tau, q(\tau),\dot{q}(\tau)) | \tau \in [t_0,t]\}$ for all $z \in \mathbb{R}^d$.

Noting that K is m times the unit matrix for all arguments, one has

$$E(\tau,Q,\dot{Q},z) = \tfrac{1}{2}m|z-\dot{Q}|^2 \geqslant 0.$$

Thus condition (iv) is obeyed. □

APPENDIX: TREE COMBINATORICS

The purpose of this Appendix is to prove Proposition 1. First we make a few additions to our notations for trees and their combinatorics. For a given $k \in \mathbb{N}$, let J_k be a k-element vertex set chosen from the set $\{1,2,\ldots,n+1\}$. There are $\binom{n+1}{k}$ such different possible choices and the sum over all these possibilities we denote by Σ_{J_k}. Also, given J_k the associated complement will be taken as

$$J_k^c = \{1,2,\ldots,n+1\} \setminus J_k.$$

Suppose β is some element of the edge set for a given tree $(V(T),E(T))$. If β is removed from the edge set $E(T)$ the tree is broken into two disjoint subtrees T_1^β, T_2^β satisfying

$$V(T) = V(T_1^\beta) \cup V(T_2^\beta), \quad E(T) = E(T_1^\beta) \cup E(T_2^\beta) \cup \{\beta\},$$
$$i_\beta \in V(T_1^\beta) \quad \text{and} \quad j_\beta \in V(T_2^\beta).$$

Finally we let $\mathcal{T}$ indicate the set of all labeled trees formed over finite subsets of $\mathbb{N}$.

Lemma 10 (tree grafting): Let $n \in \mathbb{N}$, and A be a vector space. Suppose $f: \mathcal{T}^2 \times \mathbb{N}^2 \to A$ is a function symmetric in its first two and last two arguments

$$f(T',T'';l,m) = f(T'',T';l,m) = f(T',T'';m,l);$$

i.e., f is a function of an unordered pair of trees and an unordered pair of vertex labels. Then

$$\frac{1}{2}\sum_{k=1}^{n}\sum_{J_k}\sum_{T_1 \in \mathcal{T}J_k}\sum_{T_{21} \in \mathcal{T}J_k^c}\sum_{r \in J_k}\sum_{q \in J_k^c} f(T_1,T_2;r,q) = \sum_{T \in \mathcal{T}V_{n+1}}\sum_{\beta \in E(T)} f(T_1^\beta,T_2^\beta;i_\beta,j_\beta). \tag{A1}$$

Proof: We show that (i) sums of pairs of terms on the left-hand side occur as a single term on the righ-hand side, and conversely, (ii) every term on the right side occurs as a pair of terms on the left-hand side.

(i) On the left-hand side fix an arbitrary term in the sum:

$$k = l \in V_n, \quad J_l, \quad T_1 = T_1^* \in \mathcal{T}J_l, \quad T_2 = T_2^* \in \mathcal{T}J_l^c,$$
$$r = r^* \in J_l, \quad q = q^* \in J_l^c.$$

However, when $k = n+1-l$, there will exist a partner to this term for which $J_{n+1-l} = J_l^c$ and

$$T_1 = T_2^* \in \mathcal{T}J_{n+1-l} = \mathcal{T}J_l^c,$$
$$T_2 = T_1^* \in \mathcal{T}J_{n+1-l}^c = \mathcal{T}J_l,$$
$$r = q^* \in J_{n+1-l}, \quad q = r^* \in J_{n+1-l}^c.$$

We note these partners are always different terms in the left-hand sum. If $l \neq n+1-l$, then they arise from different terms in the $\Sigma_{k=1}^n$ sum. Whereas if $l = (n+1)/2$, then because T_1 and T_2 are trees on disjoint vertex sets (J_l,J_l^c), the partners arise from complementary choices of J_k in the sum Σ_{J_k}.

The sum of the two partner terms is

$$\tfrac{1}{2}f(T_1^*,T_2^*;r^*,q^*) + \tfrac{1}{2}f(T_2^*,T_1^*;q^*,r^*) = f(T_1^*,T_2^*;r^*,q^*) \tag{A2}$$

by the symmetry of f. Now T_1^* and T_2^* are two disjoint trees that can be grafted together by the link $\beta = \{r^*,q^*\}$ because $r^* \in J_l = V(T_1^*)$ and $q^* \in J_l^c = V(T_2^*)$. That is we can define a tree T by

$$V(T) = V(T_1^*) \cup V(T_2^*) = J_l \cup J_l^c = V_{n+1},$$
$$E(T) = E(T_1^*) \cup E(T_2^*) \cup \{r^*,q^*\},$$

so that $T \in \mathcal{T}V_{n+1}$ and $\beta \in E(T)$. Appealing to the symmetry of f in the event $r^* > q^*$, we find that sum $f(T_1^*,T_2^*;r^*,q^*)$ of the left-hand side partner terms will occur on the right-hand side of (A1).

(ii) Let $T \in \mathcal{T}V_{n+1}$ and $\beta \in E(T)$ be given on the right side of (A1) with T_1^β and T_2^β the disjoint trees defined by removing link β. Since all possible disjoint vertex sets, trees on them, and vertex label pairs between them are summed over on the left-hand side of (A1) there will exist a term where

$$k = (\text{cardinality of } V(T_1^\beta)) \in V_n,$$
$$J_k = V(T_1^\beta), \quad J_k^c = V(T_2^\beta),$$
$$T_1 = T_1^\beta, \quad T_2 = T_2^\beta, \quad r \in \beta, \quad q \in \beta \setminus \{r\},$$

and as in (i) this term will have a partner. □

We remark that in the case where $A = \mathbb{R}$ and $f = 1$ (the unit constant function) then (A1) is a known result (cf. Ref. 8, p. 53). The basic content of Proposition 1 is given by the following.

Lemma 11: The functions $a_n: (\mathbb{R}^d \times \Gamma)^2 \to \mathbb{R}$, defined by (2.4) and (2.5) satisfy the recurrence relation (2.3) for all $n \geqslant 1$.

Proof: We use induction to implement the proof. The definition of a_1 shows the recurrence relation is valid for

$n=1$. Now assume that (2.3) is valid for all a_m, $1\leq m<n$, where a_m is defined by the tree sums (2.4) and (2.5). Let W be the integral

$$W\equiv\sum_{k=1}^{n}\frac{1}{2}\binom{n+1}{k}\int_I d\xi\,\xi^{2n}(\nabla_1 a_k\cdot\nabla_1 a_{n+1-k})(\tilde{\xi};y,t_0). \tag{A3}$$

We must show

$$W=\int_{I^{n+1}} d^{n+1}\xi\sum_{T\in\mathscr{T}V_{n+1}}\prod_{\beta\in E(T)}b_\beta\prod_{p=1}^{n+1}v(\tilde{\xi}_p), \tag{A4}$$

or equivalently we must show that W is a tree sum over the vertex set V_{n+1}. Using (2.4) and (2.5) for $m<n$ gives

$$W=\sum_{k=1}^{n}\frac{1}{2}\binom{n+1}{k}\int_I d\xi\,\xi^{2n}\left[\nabla_{\vec{\xi}}\int_{I^k}d^k\xi\sum_{T\in\mathscr{T}V_k}\prod_{\beta\in E(T)}b_\beta\prod_{p=1}^{k}v(y+\xi_p(\vec{\xi}-y),t_0+\xi\xi_p(t-t_0))\right]$$
$$\cdot\left[\nabla_{\vec{\xi}}\int_{I^{n+1-k}}d^{n+1-k}\xi\sum_{T'\in\mathscr{T}V_{n+1-k}}\prod_{\beta'\in E(T')}b_{\beta'}\prod_{p'=1}^{n+1-k}v(y+\xi_{p'}(\vec{\xi}-y),t_0+\xi\xi_{p'}(t-t_0))\right].$$

For potentials in the class $\mathscr{A}(\Gamma,1)$ we can differentiate with respect to $\vec{\xi}$ inside the integrals. The $\nabla_{\vec{\xi}}$ may then act on any of the factors v. Relabel the integration variables $\xi_{p'}$ in the second [ ] factor above $\xi_1\to\xi_{k+1},\ldots,\xi_{n+1-k}\to\xi_{n+1}$, then the two multiple integrals may be written as one giving

$$W=\sum_{k=1}^{n}\frac{1}{2}\binom{n+1}{k}\int_I d\xi\,\xi^{2n}\int_{I^{n+1}}d^{n+1}\xi$$
$$\times\left\{\sum_{T\in\mathscr{T}V_k}\sum_{T'\in\mathscr{T}k+1\sim n+1}\prod_{\beta\in E(T)}b_\beta\prod_{\beta'\in E(T')}b_{\beta'}\right.$$
$$\left.\times\left(\sum_{r=1}^{k}\sum_{q=k+1}^{n+1}\xi_r\xi_q D_r\cdot D_q\right)\prod_{p=1}^{n+1}v([\xi\xi_p]^{\sim})\right\}.$$

The notation for the argument of the potential is the usual abbreviation $[\xi\xi_p]^{\sim}=(y+\xi\xi_p(x-y),t_0+\xi\xi_p(t-t_0))$, and the symbol $k+1\sim n+1$ denotes the vertex set $\{k+1,\ldots,n+1\}$. The overall factor $\binom{n+1}{k}$ may be absorbed by summing over all distinct k-element vertex sets J_k, which may be chosen from V_{n+1}, so

$$W=\sum_{k=1}^{n}\frac{1}{2}\int_I d\xi\,\xi^{2n}\int_{I^{n+1}}d^{n+1}\xi$$
$$\times\sum_{J_k}\sum_{T\in\mathscr{T}J_k}\sum_{T'\in\mathscr{T}J_k^c}\prod_{\beta\in E(T)}b_\beta$$
$$\times\prod_{\beta'\in E(T')}b_{\beta'}\sum_{r\in J_k}\sum_{q\in J_k^c}\xi_r\xi_q D_r\cdot D_q\prod_{p=1}^{n+1}v([\xi\xi_p]^{\sim}).$$

We may remove all the ξ dependence in the potentials by the change of variables $\xi_p\to\xi_p/\xi$ ($p\in V_{n+1}$). Each factor ϕ in a b_β will contribute one multiplicative factor of ξ^{-1} due to this change of variables. The altered integration region becomes

$$\int_0^1 d\xi\int_{[0,\xi]^{n+1}}d^{n+1}\xi=\int_{I^{n+1}}d^{n+1}\xi\int_M^I d\xi,$$

where $M=\max\{\xi_1,\ldots,\xi_{n+1}\}$. Thus W may be written as

$$W=\sum_{k=1}^{n}\frac{1}{2}\int_{I^{n+1}}d^{n+1}\xi\left\{\int_M^1 d\xi\,\xi^{-2}\right.$$
$$\times\sum_{J_k}\sum_{T\in\mathscr{T}J_k}\sum_{T'\in\mathscr{T}J_k^c}\left[\prod_{\beta\in E(T)}\xi_\beta^{<}\left(1-\frac{\xi_\beta^{>}}{\xi}\right)D_{i_\beta}\cdot D_{j_\beta}\right]$$
$$\times\left[\prod_{\beta'\in E(T')}\xi_{\beta'}^{<}\left(1-\frac{\xi_{\beta'}^{>}}{\xi}\right)D_{i_{\beta'}}\cdot D_{j_{\beta'}}\right]$$
$$\left.\times\sum_{r\in J_k}\sum_{q\in J_k^c}\xi_r\xi_q D_r\cdot D_q\prod_{p=1}^{n+1}v(\tilde{\xi}_p)\right\},$$

where $\xi_\beta^{<}(\xi_\beta^{>})$ is the smallest (greatest) value of the pair ξ_{i_β}, ξ_{j_β}.

Observe that the integrand $\{\int_M^1 d\xi\ldots\}$ is symmetric under the pair exchange $l\leftrightarrow m$ of any two labels $l,m\in V_{n+1}$. To see this notice that M and the product of the v's have this property. Next consider any fixed term J_k in Σ_{J_k}. If $l,m\in J_k$ (or $l,m\in J_k^c$) then $l\leftrightarrow m$ at most exchanges the identification of two trees in $\mathscr{T}J_k$ (or $\mathscr{T}J_k^c$). But all trees in $\mathscr{T}J_k$ (or $\mathscr{T}J_k^c$) are summed over, so the sum is invariant under the exchange $l\leftrightarrow m$. Alternately if $l\in J_k$ and $m\in J_k^c$, then $l\leftrightarrow m$ just interchanges two terms in the Σ_{J_k} sum, i.e., $J_k\leftrightarrow(J_k\setminus\{l\})\cup\{m\}$ and $J_k^c\leftrightarrow(J_k^c\setminus\{m\})\cup\{l\}$.

Since the integrand is permutation invariant the integral may be ordered:

$$\int_{I^{n+1}}d^{n+1}\xi=(n+1)!\int_{0<\xi_1<\cdots<\xi_{n+1}<1}\cdots\cdots\int d^{n+1}\xi$$
$$\equiv(n+1)!\int_<^1 d^{n+1}\xi.$$

With this ordering implemented, note that

$$M=\xi_{n+1},\quad \xi_\beta^{<}=\xi_{i_\beta},\quad \xi_\beta^{>}=\xi_{j_\beta}.$$

Thus we arrive at

$$W=(n+1)!\int_<^1 d^{n+1}\xi\int_{\xi_{n+1}}^1 d\xi\,\xi^{-2}\left\{\sum_{k=1}^{n}\frac{1}{2}\sum_{J_k}\sum_{T\in\mathscr{T}J_k}\sum_{T'\in J_k^c}\sum_{r\in\mathscr{T}J_k}\sum_{q\in J_k^c}\left[\prod_{\beta\in E(T)}\xi_{i_\beta}\left(1-\frac{\xi_{j_\beta}}{\xi}\right)D_{i_\beta}\cdot D_{j_\beta}\right]\right.$$
$$\left.\times\left[\prod_{\alpha\in E(T')}\xi_{i_\alpha}\left(1-\frac{\xi_{j_\alpha}}{\xi}\right)D_{i_\alpha}\cdot D_{j_\alpha}\right]\xi_r\xi_q D_r\cdot D_q\right\}\prod_{p=1}^{n+1}v(\tilde{\xi}_p).$$

To the terms in $\{\cdots\}$ we apply Lemma 10 with A chosen to be the vector space of differential operators and f to be

$$f=f(T,T';r,q)\equiv\left[\prod_{\beta\in E(T)}\cdots\right]\left[\prod_{\alpha\in E(T')}\cdots\right]\xi_r\xi_q D_r\cdot D_q,$$

where the square brackets are those given immediately above. This f has all the required properties for Lemma 10 (note the D_j's commute). Thus, after some rearrangement, W may be written as

$$W=(n+1)!\int_<^1 d^{n+1}\xi\sum_{T\in\mathcal{T}V_{n+1}}\left(\prod_{\alpha\in E(T)}\xi_{i_\alpha}D_{i_\alpha}\cdot D_{j_\alpha}\right)\times\prod_{p=1}^{n+1}v(\tilde{\xi}_p)\sum_{\beta\in E(T)}\xi_{j_\beta}\left\{\int_{\xi_{n+1}}^1 d\xi\,\xi^{-2}\times\prod_{\gamma\in E(T)\setminus\{\beta\}}\left(1-\frac{\xi_{j_\gamma}}{\xi}\right)\right\}. \tag{A5}$$

The ξ integral is now elementary and straightforward calculation shows the curly bracket term becomes

$$\{\cdots\}=\sum_{\mu=0}^{n-1}\frac{(-1)^\mu}{\mu+1}(\xi_{n+1}^{-(\mu+1)}-1)\times\sum_{\alpha\subset E(T)\setminus\{\beta\}}^{(\mu)}\xi_{j_{\alpha(1)}}\cdots\xi_{j_{\alpha(\mu)}}.$$

The sum $\Sigma^{(\mu)}$ and notation α require explanation. First of all, when $\mu=0$, $\Sigma^{(0)}\equiv 1$. Otherwise, $\alpha\equiv\{\alpha(1),\ldots,\alpha(\mu)\}\subseteq E(T)\setminus\{\beta\}$ denotes a set of μ distinct elements $\alpha(i)\in E(T)\setminus\{\beta\}$ and the $\Sigma^{(\mu)}$ specifies a sum over all possible distinct sets α of this type.

Performing the summation and a few simple manipulations gives

$$\sum_{\beta\in E(T)}\xi_{j_\beta}\{\cdots\}=\sum_{\mu=0}^{n-1}(\xi_{n+1}^{-(\mu+1)}-1)(-1)^\mu\sum_{\alpha\subset E(T)}^{(\mu+1)}\xi_{j_{\alpha(1)}}\cdots\xi_{j_{\alpha(\mu+1)}}=\prod_{\beta\in E(T)}(1-\xi_{j_\beta})-\prod_{\beta\in E(T)}\left(1-\frac{\xi_{j_\beta}}{\xi_{n+1}}\right).$$

As β runs through $E(T)$ there is at least one link with $j_\beta=n+1$, so the last product vanishes. Returning to (A5) we see that it takes the form

$$W=(n+1)!\int_<^1 d^{n+1}\xi\times\sum_{T\in\mathcal{T}V_{n+1}}\left[\prod_{\alpha\in E(T)}\xi_{i_\alpha}(1-\xi_{j_\alpha})D_{i_\alpha}\cdot D_{j_\alpha}\right]\prod_{p=1}^{n+1}v(\tilde{\xi}_p).$$

Note that the differential operator in the square bracket is b_α. Observing that the integrand is invariant under permutation of the labels on $\xi_1,\xi_2,\ldots,\xi_{n+1}$, we may remove the order restriction and integrate over the $(n+1)$-dimensional unit cube giving (A4). □

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Symmetries and integrability of the cylindrical Korteweg–de Vries equation

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The direct scheme to test integrability of a given nonlinear equation proposed by Chen, Lee, and Liu is tested on the cylindrical Korteweg–de Vries equation. The explicit dependence on t of this equation does not present any real difficulties. Constants of motion and symmetries are found readily and the Lax operators for the scattering problem constructed accordingly.

I. INTRODUCTION

A given nonlinear evolution equation

$$u_t = K(u,u_x,u_{xx},\ldots,x,t) \tag{1}$$

is deemed integrable if (1) can be rewritten as an operator equation

$$L_t = [A,L], \tag{2}$$

where L depending on u is a spectral operator for wave functions $\psi(x,t)$ such that

$$L\psi = \lambda\psi. \tag{3}$$

The operator A also depending on u, governs the time evolution of the function ψ such that

$$\psi_t = A\psi. \tag{4}$$

Equations (3) and (4) are compatible if and only if u satisfies Eq. (2) and hence Eq. (1).

The linearization of Eq. (1) can be written as

$$\phi_t = K'(\phi), \tag{5}$$

where

$$K'(\phi) = \frac{d}{d\epsilon} K(u+\epsilon\phi)\Big|_{\epsilon=0},$$

and its adjoint equation is

$$\psi_t + K'^{+}(\psi) = 0, \tag{6}$$

where K'^{+} is the adjoint operator of K' defined by

$$\langle K'(\phi),\psi\rangle = \langle \phi,K'^{+}(\psi)\rangle, \tag{7}$$

and

$$\langle \phi,\psi\rangle = \int_{-\infty}^{+\infty} \phi(x)\psi(x)dx \tag{8}$$

is the inner product in the Hilbert space. From Eqs. (4) and (6) we then identify $-K'^{+} \equiv A$.

It is well known[1] that if T_n is a constant density of Eq. (1), then the functional derivative of the constant $\overline{T}_n = \int_{-\infty}^{+\infty} T_n(u)dx$ with respect to $u(x,t)$ is a solution of Eq. (6). That is,

$$\frac{d}{dt}\left(\frac{\delta\overline{T}_n(u)}{\delta u}\right) + K'^{+}\left(\frac{\delta\overline{T}_n(u)}{\delta u}\right) = 0. \tag{9}$$

Among the solutions $\psi_n = \delta\overline{T}_n/\delta u$ of Eq. (6), the linear recursion operator R, such that

$$\psi_{n+1} = R\psi_n, \tag{10}$$

can be shown to satisfy

$$R_t = [A,R], \tag{11}$$

and therefore it is taken to be the spectral operator L in Eq. (2).

So far this scheme has been applied successfully to many equations with coefficients independent of x and t. In this paper, we would like to extend the case to the cylindrical Korteweg–de Vries (cKdV) equation, which has an explicit t-dependent coefficient.

II. SYMMETRIES OF THE cKdV EQUATION

The cylindrical KdV equation is written as

$$u_t + 6uu_x + u_{xxx} + u/2t = 0. \tag{12}$$

Its linearized equation is

$$\phi_t = K'(u)\phi = (-6u_x - 6uD_x - D_x^3 - 1/2t)\phi; \tag{13}$$

therefore

$$K'^{+} = 6uD_x + D_x^3 - 1/2t. \tag{14}$$

Equation (6) becomes

$$\psi_t + 6u\psi_x + \psi_{xxx} - \psi/2t = 0. \tag{15}$$

When $u = 0$, Eq. (15) has a solution

$$\psi = t^{1/2}\exp(k^3t - kx). \tag{16}$$

The standard approach is to assume $\psi = t^{1/2}\exp(k^3t - kx + \int_{-\infty}^{x} T\,dx)$ to be a solution of Eq. (15) for large $|k|$. Substituting it into Eq. (15), and expanding

$$T = \sum_{n=0}^{\infty} k^{-n}T_n, \tag{17}$$

we obtain a nonlinear recursion relation for T_n,

$$\int^{x} T_{n,t}\,dx - 6u\delta_{n+1,0} + 6uT_n + T_{n,xx} - 3T_{n+1,x} + 3\sum_{i=0}^{n} T_iT_{n-i,x} + 3T_{n+2} - 3\sum_{i=0}^{n+1} T_iT_{n+1-i} + \sum_{i=0}^{n}\sum_{j=0}^{n-i} T_iT_jT_{n-i-j} = 0. \tag{18}$$

From (18) we immediately obtain

$$\begin{aligned} &T_0 = 0, \quad T_1 = 2u, \quad T_2 = 2u_x, \\ &T_3 = 2u^2 + 2u_{xx} + (1/3t)D^{-1}u, \\ &T_4 = 2u_{xxx}8uu_x + 2u/3t, \\ &T_5 = (1/2t)[D^{-1}(2u^2 + (1/3t)D^{-1}u)] + (2/3t)uD^{-1}u \\ &\quad + (1/t)u_x + 10u_x^2 + 12uu_{xx} + 2u_{xxxx} + 4u^3, \end{aligned} \tag{19}$$

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where

$$D^{-1}=\int_{-\infty}^{x}\cdot\,dx.$$

These T_n's are not yet the conserved densities of Eq. (1). From the recursion relation (19) we obtain instead an equation for $\int_{-\infty}^{x} T_1\,dx$

$$\frac{d}{dt}\left(\int_{-\infty}^{x} T_1\,dx\right)=-6u^2-2u_{xx}-\frac{1}{2t}\left(\int_{-\infty}^{x} T_1\,dx\right). \tag{20}$$

Supposing u and its nth partial derivative with respect to x $(n=1,\ 2,...)$ vanish when $|x|\to\infty$, then in the limit $x\to+\infty$ we have

$$\frac{d}{dt}\overline{T}_1=-\frac{1}{2t}\overline{T}_1. \tag{21}$$

We thus obtain a constant of motion C_1 as

$$C_1=t^{1/2}\overline{T}_1=t^{1/2}\int_{-\infty}^{+\infty}2u\,dx. \tag{22}$$

A sequence of constants of motion are obtained this way. We now list the first seven of them:

$$\begin{aligned}
&\frac{d}{dt}\overline{T}_1=-\frac{1}{2t}\overline{T}_1,\quad \overline{T}_2=0,\\
&\frac{d}{dt}\overline{T}_3=-\frac{3}{2t}\overline{T}_3,\quad \overline{T}_4=\frac{1}{3}t^{-3/2}C_1,\\
&\frac{d}{dt}\overline{T}_5=-\frac{5}{2t}\overline{T}_5+\frac{C_1^2}{24t^3},\quad \overline{T}_6=\frac{3}{2}t^{-5/2}C_3,\\
&\frac{d}{dt}\overline{T}_7=-\frac{7}{2t}\overline{T}_7+\frac{31}{72}t^{-7/2}C_1+\frac{C_1C_3}{4t^4},
\end{aligned} \tag{23}$$

and

$$\begin{aligned}
C_1&=t^{1/2}\overline{T}_1=t^{1/2}\int_{-\infty}^{\infty}2u\,dx,\quad C_2=0,\\
C_3&=t^{3/2}\overline{T}_3=t^{3/2}\int_{-\infty}^{+\infty}\left[2u^2+\frac{1}{3t}D^{-1}u\right]dx,\\
C_4&=t^{3/2}\overline{T}_4=C_1/3,\\
C_5&=t^{5/2}\overline{T}_5-(C_1^2/12)t^{1/2}\\
&=t^{5/2}\int_{-\infty}^{+\infty}\left[\frac{1}{t}D^{-1}u^2\right.\\
&\qquad\left.+\frac{1}{6t^2}D^{-2}u+2uu_{xx}+4u^3\right]dx,\\
C_6&=t^{5/2}\overline{T}_6=\tfrac{3}{2}C_3,\\
C_7&=t^{7/2}\overline{T}_7-\tfrac{31}{72}C_1t-\tfrac{1}{2}C_1C_3t^{1/2}\\
&=t^{7/2}\int_{-\infty}^{+\infty}\left[\frac{5}{12t^2}D^{-2}\left(2u^2+\frac{1}{3t}D^{-1}u\right)\right.\\
&\qquad+\frac{5}{6t}D^{-1}(4u^3+2uu_{xx})\\
&\qquad\left.+(10u^2u_{xx}+2u_{xx}^2+10u^4)+\frac{5u}{36t^2}\right]dx.
\end{aligned} \tag{24}$$

We see from (24) that the even-numbered constants are not independent. From (22) and (24) we get

$$\begin{aligned}
\psi_1&=\frac{\delta C_1}{\delta u}=2t^{1/2},\\
\psi_3&=\frac{\delta C_3}{\delta u}=t^{3/2}\left(4u-\frac{x}{3t}\right),\\
\psi_5&=\frac{\delta C_5}{\delta u}=t^{5/2}\left[\frac{x^2}{12t^2}-\frac{2xu}{t}+12u^2+4u_{xx}\right],\\
\psi_7&=\frac{\delta C_7}{\delta u}\\
&=t^{7/2}\left[\frac{5}{12}\left(\frac{-x^3}{18t^3}+\frac{6x^2u+1}{3t^2}\right)-\frac{10}{3t}(3xu^2+xu_{xx}\right.\\
&\qquad\left.+u_x)+(40u^3-40uu_{xx}+20u_x^2+4u_{xxxx})\right].
\end{aligned} \tag{25}$$

They can be verified directly as solutions of Eq. (15). We also note that if ϕ is a solution of Eq. (15), then $(1/t)\phi_x$ is a solution of Eq. (13). They are also called symmetries.[2–4] The first three of these classical symmetries

$$K_i=(1/t)\left(\frac{d}{dx}\right)(\psi_{2i+1}),\quad i=0,\ 1,\ 2$$

are given as follows:

$$\begin{aligned}
K_0&=t^{1/2}(4u_x-1/3t),\\
K_1&=t^{3/2}\left(\frac{x}{6t^2}-\frac{2u+2xu_x}{t}+24uu_x+4u_{xxx}\right),\\
K_2&=t^{5/2}[4(10u^3+10uu_{xx}+5u_x^2+u_{xxxx})x]\\
&\qquad-\tfrac{5}{72}(x^2/t^3)+(5/6t^2)(2xu+x^2u_x)\\
&\qquad-(10/3t)(3u^2+6xuu_x+xu_{xxx}+2u_{xx}).
\end{aligned} \tag{26}$$

On the other hand, three new symmetries can be found as

$$\begin{aligned}
\tau_0&=3t^{-1/2}K_0+A_0=12u_x,\\
\tau_1&=\tfrac{3}{2}xt^{-1/2}K_0+3t^{-1/2}K_1+A_1\\
&=12t(u_{xxx}+6uu_x)-2u-4xu_x,\\
\tau_2&=\frac{3}{2}xt^{-1/2}K_1+3t^{-1/2}K_2+A_2\\
&=12t^2(u_{xxxx}+5u_x^2+10uu_{xx}+10u^3)_x\\
&\qquad-t(12u_{xx}+14u^2+8xu_{xxx}+48xuu_x\\
&\qquad-4u_xD^{-1}u)+\tfrac{4}{3}xu+\tfrac{4}{3}x^2u_x-\tfrac{1}{3}D^{-1}u,
\end{aligned} \tag{27}$$

with

$$\begin{aligned}
&A_0=t^{-1},\quad A_1=4u-4xu_x,\\
&A_2=t[16u^2-24xuu_x-4xu_{xxx}+8u_{xx}+4u_xD^{-1}u]\\
&\qquad+(\tfrac{1}{6}x^2u_x-\tfrac{2}{3}xu-\tfrac{1}{3}D^{-1}u)-x^2/24t.
\end{aligned}$$

These symmetries satisfy a graded Lie algebra

$$\begin{aligned}
&[K_m,K_n]=0,\quad [K_m,\tau_n]=2(2m+1)K_{m+n-1},\\
&[\tau_m,\tau_n]=4(m-n)\tau_{m+n-1},\quad m,n=0,1,2,
\end{aligned} \tag{28}$$

where the Lie product for two symmetries F and G is defined by[2] $[F,G]=F'[G]-G'[F]$.

III. LAX SPECTRAL OPERATOR FOR cKdV EQUATION

We now present two methods to derive the Lax spectral operator L.

A. Use of the scheme in CLL[1]

Equation (25) suggests that they are connected by the recursion operator

$$L = L^0 + L^1,$$

where

$$L_0 = L|_{u=0}. \tag{29}$$

In order to determine L^0, we set $u = 0$ first and obtain

$$A^0 = A|_{u=0} = 1/2t - D_x^3 \tag{30}$$

and

$$\psi_1^0 = 2t^{1/2}, \quad \psi_3^0 = -\tfrac{1}{3}xt^{1/2},$$
$$\psi_5^0 = \tfrac{1}{12}x^2t^{1/2},$$
$$\psi_7^0 = -\tfrac{5}{216}x^3t^{1/2} + \tfrac{5}{36}t^{3/2}, \tag{31}$$

where

$$\psi_i^0 = \psi_i|_{u=0}.$$

In general, we obtain from (4) and (31)

$$\psi_{2n+1}^0 = \sum_{m=0}^{[n/3]} (-1)^{n-m} \frac{2(2n-1)!!}{6^n(n-3m)!} \frac{1}{m!} x^{n-3m} t^{1/2+m}, \tag{32}$$

where $[x]$ is the integral part of x.

From (21) and (32) we obtain

$$L^0 = tD_x^2 - x/3 + \tfrac{1}{6}D^{-1}, \tag{33}$$

such that[1]

$$L^0\psi_{2n+1}^0 = \psi_{2n+3}^0. \tag{34}$$

Following Ref. 1, we will now derive L^1. Let u be small, i.e., $u = \epsilon q$. At first order in ϵ, Eq. (12) has the solution

$$q^0 = \sum_m \frac{1}{\sqrt{t}} q_m^0 e^{-mx+m^3t}$$

and Eq. (15) has the solution

$$\psi^0 = \sum_l \sqrt{t}\ \psi_l^0 e^{-lx+l^3t},$$

where q_m^0, ψ_l^0 are arbitrary constant amplitudes.

The leading term in Eq. (2) is

$$[A^0, L^1]\psi^0 + [A^1, L^0]\psi^0 = L_t^1\psi^0, \tag{35}$$

with

$$A^1 = -6q^0D_x. \tag{36}$$

In order to determine L^1, set

$$L^1\psi^0 = \sum_{l,m} \left(A(l,m,t) \frac{q_m^0}{\sqrt{t}} \right) \sqrt{t}\ \psi_l^0 e^{-(m+l-x+(l^3+m^3)t}. \tag{37}$$

Substituting (30), (33), and (36) into (35) we obtain an equation for $A(l, m, t)$,

$$A(l,m,t) - (1/2t)A(l,m,t) - 3ml(l+m)A(l,m,t) = (2l+m)/(l+m) - 6lm(2l+m)t; \tag{38}$$

therefore

$$A(l,m,t) = 2t(2l+m)/(l+m) = 2t[2 - m/(l+m)] \tag{39}$$

and

$$L^1 = 2t[2u - D^{-1}u_x]. \tag{40}$$

Finally, we obtain

$$L = t[D_x^2 + 4u - 2D^{-1}u_x] - \tfrac{1}{3}x + \tfrac{1}{6}D^{-1}. \tag{41}$$

B. A scheme utilizing the new symmetry τ_2

We can see from (28) that

$$[K_m, \tau_2] = 2(2m+1)K_{m+1}. \tag{42}$$

This implies that τ_2 is related to the recursion operators (42) L^+ that generate all the K symmetries. A direct relation is easily obtained as[5]

$$L^+ = \tau_2' + D_x\tau_2' + D^{-1}. \tag{43}$$

From (27) and (43) we obtain

$$L^+ = \{t(D_x^2 + 4u + 2u_xD^{-1}) - \tfrac{1}{6}D^{-1} - \tfrac{1}{3}x\}. \tag{44}$$

It can be verified directly that

$$L^+K_i = K_{i+1}, \quad L^+\tau_i = \tau_{i+1}, \quad i = 0,1. \tag{45}$$

IV. LIE ALGEBRA

We now define

$$\tau_3 = L^+\tau_2. \tag{46}$$

Then we have by direct calculation

$$[\tau_3, \tau_0] = 12\tau_2, \quad [\tau_3, K_0] = -2K_2. \tag{47}$$

It is compatible with (28).

We now define K_m's and τ_m's ($m \geq 3$) as follows:

$$K_{m+1} \equiv [1/2(2m+1)][K_m, \tau_2], \quad m \geqslant 2, \tag{48}$$

$$\tau_{m+1} \equiv [1/4(m-2)][\tau_m, \tau_2], \quad m \geqslant 3. \tag{49}$$

We then obtain two series of symmetries K_n's and τ_n's. They constitute an infinite-dimensional Lie algebra expressed by (28). As a matter of fact, Eq. (28) can be combined into a single formula as the following[6]:

$$[\sigma_n^m, \sigma_s^r] = 4[r(n+\tfrac{1}{2}) - m(s+\tfrac{1}{2})]\ \sigma_{n+s-1}^{m+r-1}, \tag{50}$$

for

$$m,r = 0,1 \quad n,s = 0,1,2,\ldots,$$

where

$$\sigma_s^0 \triangleq K_s, \quad \sigma_n^1 \triangleq \sigma_n.$$

V. ALTERNATIVE FORM OF THE SPECTRAL OPERATOR

Substituting (41) into (3) and taking its derivative with respect to x, we get, together with (15),

$$\psi_{xxx} + (2u_x - 1/6t)\psi + (4u - x/3t)\psi_x = \lambda/t\psi_x, \tag{51}$$

$$\psi_t + 6u\psi_x + \psi_{xxx} - \psi/2t = 0. \tag{52}$$

This is the sought-after spectral problem for the cKdV equation. We now show that it is equivalent to the following eigenvalue problem used[7,8] previously to solve the cKdV equation:

$$\Phi_{xx} + u\Phi - (x/12t) + \lambda/4t)\Phi = 0, \tag{53}$$

$$\Phi_t + (x/3t + 2u + \lambda/t)\Phi_x - (1/6t + u_x)\Phi = 0. \tag{54}$$

Set

$$\psi_x = \phi, \tag{55}$$

$$\phi_x = (x/6t - 2u + \lambda/2t)\psi + \xi, \tag{56}$$

$$\xi_x = (x/6t - 2u + \lambda/2t)\phi. \tag{57}$$

Equations (51) and (52) can be written in the following matrix form:

$$\frac{d}{dx}\begin{pmatrix}\psi\\ \phi\\ \xi\end{pmatrix} = M\begin{pmatrix}\psi\\ \phi\\ \xi\end{pmatrix} \tag{58}$$

and

$$\frac{d}{dt}\begin{pmatrix}\psi\\ \phi\\ \xi\end{pmatrix} = N\begin{pmatrix}\psi\\ \phi\\ \xi\end{pmatrix}, \tag{59}$$

where

$$M = A + (x/6t - 2u + \lambda/2t)B, \tag{60}$$

$$N = (1/3t + 2u_x)C - (x/3t + 2u + \lambda/t)A + [2u_{xx} - (2u + x/3t + \lambda/t)(x/6t - 2u + \lambda/2t)]B. \tag{61}$$

The 3×3 matrices A, B, and C are given by

$$A = \begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}, \tag{62}$$

$$B = \begin{pmatrix}0 & 0 & 0\\ 1 & 0 & 0\\ 0 & 1 & 0\end{pmatrix}, \tag{63}$$

$$C = \begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}. \tag{64}$$

They satisfy the following algebra:

$$[A, B] = C, \quad [A,C] = -A, \quad [B,C] = B, \tag{65}$$

where the Lie bracket for two matrices F and G is defined by $[F,G] = FG - GF$.

Now we introduce 2×2 matrix representations of A, B, and C as follows:

$$A_1 = \frac{\sqrt{2}}{2}\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}, \tag{66}$$

$$B_1 = \frac{\sqrt{2}}{2}\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}, \tag{67}$$

$$C_1 = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{68}$$

They also satisfy (65).

Put

$$M_1 = A_1 + (x/6t - 2u + \lambda/2t)B_1, \tag{69}$$

$$N_1 = (1/3t + 2u_x)C_1 - (x/3t + 2u + \lambda/t)A_1 + [2u_{xx} - (2u + x/3t - 2u\lambda/2t)]B_1. \tag{70}$$

We see that (53) and (54) are just the scattering problem

$$\frac{d}{dx}\begin{pmatrix}\Phi\\ \Sigma\end{pmatrix} = M_1\begin{pmatrix}\Phi\\ \Sigma\end{pmatrix}, \tag{71}$$

$$\frac{d}{dt}\begin{pmatrix}\Phi\\ \Sigma\end{pmatrix} = N_1\begin{pmatrix}\Phi\\ \Sigma\end{pmatrix}. \tag{72}$$

Indeed (51) and (52) can be derived from (53) and (54) directly by setting $\psi = \Phi^2$.

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Positivity and unimodality as stabilizers of the analytic extrapolation of a function known with errors

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Positivity and unimodality hypotheses on an unknown function $\chi_1(x)$ confer Stieltjes character to another function $H_1(z)$, known in a discrete set of real points and affected by errors caused by experimental measurements, and impose constraints on the coefficients of its formal expansion which limit the universe of approximant functions, so acting as stabilizers of the analytic extrapolation. The type I Padé approximants, built with the coefficients of the formal expansion, provide rigorous bounds on the function in the cut complex plane. The application of a Stieltjes–Chebyshev technique allows approximations to the function, even on the cut, to be obtained. The physical problem of $K^{\pm} p$ forward elastic scattering is approached by the previous method, and bounds on the coupling constant and real part of the amplitude are found.

I. INTRODUCTION

An application of analyticity, analytic extrapolation, has been widely used in high energy physics: Once experimental data on an analytic function have been measured in a certain domain of the complex plane, a fitting procedure is designed in order to interpolate the data, and the resulting parametrization is extrapolated to regions where no data have been obtained yet, or, in some cases, where data are not physically accessible.

However, the fact that the functional values are not exactly known, but rather are subject to errors coming from the experimental measurements, makes the predictive power of analytic extrapolation by itself null. It can be shown[1] that one can construct an analytic function which, in the region where there are experimental data, fits them well, but outside that region can take arbitrarily preassigned values in points of its analytic domain. In other words, there is an arbitrary number of parametrizations which, while agreeing in the experimental region, give absolutely different results when extrapolated to other regions. This fact, known as instability in analytic extrapolation, forces the search for other properties of functions (besides analyticity), which act as stabilizers of the analytic extrapolation in such a way that small perturbations in the data region do not give rise to very different predictions outside the experimental region.

Several methods exist for stabilization of the analytic extrapolation. We shall use two properties of the functions, positivity and unimodality, which allow the use of the bounding and convergence properties of Padé approximants and the properites of the sequences of Hausdorff moments, to produce a stable extrapolation.

In Sec. II the bounding properties of Padé approximants on Stieltjes functions are discussed and the Gronwall transformation, which allows the determination of the coefficients of the formal series expansion, is introduced. In Sec. III the constraints imposed on the coefficients by the positivity property are presented, and the same thing is done in Sec. IV with those imposed by unimodality. In Sec. V the extrapolation to the poles is discussed. In Sec. VI Stieltjes–Chebyshev techniques are used to obtain an approximation to the function on the cut, and in Sec. VII the physical problem of $K^{\pm} p$ forward elastic scattering is approached.

II. STIELTJES FUNCTIONS, PADÉ APPROXIMANTS, AND THE GRONWALL TRANSFORMATION

We shall consider the problem of extrapolating from the values

$$G_0(z_j) \pm G_0^e(z_j), \quad j = 1,...,p,$$
$$z_j \text{ real}, \quad z_j > -\epsilon_i, \quad \forall i,j, \tag{2.1}$$

of the function

$$G_0(z) = \sum_{i=1}^{k} \frac{R_i}{\epsilon_i + z} + H(z),$$
$$\epsilon_m > \epsilon_n \text{ for } m > n, \quad \epsilon_i, R_i \text{ real}, \tag{2.2}$$

where $H(z)$ is a Stieltjes function with convergence radius R,

$$H(z) = \int_0^{1/R} \frac{d\psi(u)}{1+zu}, \quad \psi(u) \in \uparrow\beta\,[0,1/R\,], \tag{2.3}$$

to the poles region, $-\epsilon_i$, in order to calculate the residues R_i of the function $G_0(z)$ in $z = -\epsilon_i$.

Let us consider, without loss of generality, $R = 1$, and see how we can get the values of the residues R_i.

Let us first transform the function $G_0(z)$ into

$$G_1(z) = \frac{G_0(z)(z+\epsilon_1) - G_0(z)(z_1+\epsilon_1)}{z - z_1}. \tag{2.4}$$

It can be easily seen that $G_1(z)$ is of the form

$$G_1(z) = \sum_{i=2}^{k} \frac{R_i'}{\epsilon_i + z} + H_1(z), \tag{2.5}$$

where $H_1(z)$ is again a Stieltjes function with convergence radius R. Now

$$H_1(z) = \int_0^{1/R} \frac{\chi_1(u)}{1+uz}\,du, \tag{2.6}$$

where

$$\chi_1(u) = \chi(u)(1-\epsilon_1 u)/(1+x_1 u) \geqslant 0 \quad \text{in } [0,1/R\,], \tag{2.7}$$

and

$$R_i' = R_i(\epsilon_i - \epsilon_1)/(\epsilon_1 + x_1). \tag{2.8}$$

Continuing this pole absorption process as far as necessary, one eventually gets

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$$G_k(z) = \frac{G_{k-1}(z)(z+\epsilon_k) - G_{k-1}(z_k)(z_k+\epsilon_k)}{z - z_k} = H_k(z), \tag{2.9}$$

where now $H_k(z)$ is a pure Stieltjes function, free of poles, with a weight function

$$\chi_k(u) = \prod_{i=1}^{k} \frac{1-\epsilon_i u}{1+z_i u}, \quad \chi(u) \geqslant 0, \quad u \in [0, 1/R\,]. \tag{2.10}$$

In what follows we shall assume, for the sake of simplicity, that there is a single pole in $-\epsilon_1 = -z_\Lambda$ with residue R_1, and consequently we shall work with the Stieltjes function $H_1(z)$ from Eq. (2.6), but the more general case is straightforward.

The formal expansion of $H_1(z)$ is

$$H_1(z) = \sum_{j=0}^{\infty} h_j (-z)^j, \tag{2.11}$$

where

$$h_j = \int_0^{1/R} x^j \chi_1(x)\, dx \tag{2.12}$$

are the moments of the function $\chi_1(x)$. Equation (2.11) is called the Stieltjes series expansion of the function $H_1(z)$. Accordingly, the two following statements are equivalent: (i) There exists a solution to the moments problem (2.12), i.e., a function $\chi_1(x) \geqslant 0$ in $[0, 1/R\,]$ exists such that h_i are its moments; and (ii) $H_1(z)$ is a Stieltjes function with convergence radius R.

If $R = 1$, the moments problem (2.12) is known in the literature as the Hausdorff problem.[2] In that case $H_1(z)$ is analytic in the complex plane cut on the real axis $]-\infty, -R\,]$, and its series expansion (2.11) agrees with the function for $|z| < R$.

In the case $R = 0$ the formal series (2.11) is asymptotic around the origin and $H_1(z)$ is analytic in the plane cut on $]-\infty, 0]$. In this case the moment problem is known as the Stieltjes problem.

The formal series expansion (2.11) does not allow the calculation of the Stieltjes function $H_1(z)$ outside its convergence circle, and even for $|z| < R$ the convergence can be very slow, and for $R = 0$ it converges nowhere. Conversely, the Padé approximants constructed with the coefficients of the formal series expansion for this kind of function do converge very fast to the exact value of the function

$$H_1(z) = \int_0^{1/R} \frac{\chi_1(x)\, dx}{1+xz}$$

in any point of its analyticity domain.[3]

More precisely, we shall use the following theorem to obtain lower and upper bounds to the value of $H_1(z)$ for real z from a certain number of coefficients of the formal expansion of $H_1(z)$.

Theorem 2.1[3]: Let $H_1(z)$ be a Stieltjes series with convergence radius R, then

$$[M/M\,]^c \leqslant H_1(z) \leqslant [M/M\,], \quad z \geqslant 0, \tag{2.13}$$

$$[M/M+1] \leqslant H_1(z) \leqslant [M/M+1]^c, \tag{2.13'}$$

where

$$[L/M\,] = \frac{P_L^{(J)}(z)}{Q_M^{(J)}(z)}, \quad J = L - M, \tag{2.14}$$

is the Padé approximant of the formal series and P_L and Q_M are polynomials of degree L and M, respectively, whose coefficients are constructed from those of the series imposing

$$H_1(z) - [L/M\,] = O(z^{L+M+1}). \tag{2.15}$$

Here, $[M/M\,]^c$ and $[M/M+1]^c$ are the complementary Padé approximants to $[M/M\,]$ and $[M/M+1]$, which are calculated imposing the convergence radius to be R besides (2.15). We have

$$[M/M\,]^c = \frac{P_M^{(0)}(z) Q_M^{(-1)}(-R) + (z/R) P_{M-1}^{(-1)}(z) Q_M^{(0)}(-R)}{Q_M^{(0)}(z) Q_M^{(-1)}(-R) + (z/R) Q_M^{(-1)}(z) Q_M^{(0)}(-R)}, \tag{2.16}$$

$$[M/M+1]^c = \frac{P_M^{(-1)}(z) Q_{M+1}^{(-1)}(-R)}{Q_{M+1}^{(-1)}(z) Q_M^{(0)}(-R) + (z/R) Q_M^{(0)}(z) Q_{M+1}^{(-1)}(-R)}. \tag{2.17}$$

When $-R < z < 0$ the sense of the inequality (2.13) changes, and that of (2.13') holds.

Our problem is now to obtain from the data $H_1(z_i) \pm H_1^e(z_i)$, z_i real, the series expansion of $H_1(z)$ in order to apply the previous theorem.

We now discuss the Gronwall transformation.[2,4] The formal series expansion of $H_1(z)$ is divergent in most of the points where H_1 is known, therefore one cannot determine the coefficients by a fit of the series to the known values.

Instead, we transform the cut z plane into the unit circle $|s| < 1$ by means of the conformal transformation

$$s = (\sqrt{1+z} - 1)/(\sqrt{1+z} + 1) \tag{2.18}$$

which unfolds the cut in the z plane into the unit circumference, and the z_i values that range from -0.3 to 11.73 map into a real interval close to the origin from $s = -0.076$ to 0.56.

The function $G(z) = H_1(z)\sqrt{1+z}$, having the same analytical properties as $H_1(z)$, can be expanded in series in s as follows:

$$G(z(s)) = \sum_{i=0}^{\infty} g_i s^i, \tag{2.19}$$

and its coefficients g_i can be determined by fitting the experimental values $G(z_i)$ with errors $G^e(z_i)$ by the least squares method. The importance of these coefficients g_i lies in that they are related to the coefficients h_i of the series expansion of $H_1(z)$ by the remarkable formula, obtained by Gronwall

$$h_p = 4^{-p}\sum_{r=0}^{p}\binom{2p}{p-r}g_r(-1)^r, \tag{2.20}$$

which allows us, once the first p coefficients are known, to calculate the first p coefficients of the expansion (2.11).

The advantage the present procedure has over any other possible conformal transformation is that the h_i's so determined are the coefficients of a Stieltjes series or, in other words, the moments of a positive function.

Conversely, in Sec. III we shall introduce the constraints the coefficients h_i must fulfill because they are moments of a positive function.

III. CONSTRAINTS IMPOSED BY POSITIVITY

Given a sequence $\{h_n\}$ we shall say that the moments problem has a solution in the set of nondecreasing bounded variation functions in the interval $[a,b]$, $\mu(x) \in \uparrow\beta[a,b]$, if a function $\mu(x)$ belonging to that set exists, satisfying

$$h_n = \int_a^b x^n\, d\mu(x), \quad n = 0,1,\ldots . \tag{3.1}$$

In the case where $\mu(x)$ is differentiable, (3.1) reads

$$h_n = \int_a^b x^n \chi(x) dx, \quad n = 0,1,\ldots , \tag{3.2}$$

where $\chi(x) = \mu'(x) \geqslant 0$ in $[a,b]$, the latter being the case of interest to us.

Several moments problems are considered according to the interval $[a,b]$: Hamburger's problem for the interval $]-\infty,\infty[$ and Stieltjes's for $[0,\infty[$. By the appropriate linear transformation one can go from the finite problem in $[0,1]$, the Hausdorff problem, to the problem in any other finite interval $[a,b]$.

In each case the corresponding name is given to the sequence of moments.

The conditions to be satisfied by the h_n in order that a function $\mu(x) \in \uparrow\beta[a,b]$ exists, which has h_n as moments, are[2] given in the following theorem.

Theorem 3.1: A necessary condition for the existence of a solution to the Hamburger problem is that, for all $n \geqslant 0$,

$$H_n^0(h) \geqslant 0, \tag{3.3}$$

where the $H_n^m(h)$ are known as the Hankel determinants, defined by

$$H_n^m(h) = \begin{vmatrix} h_m & h_{m+1} & \cdots & h_{m+n} \\ h_{m+1} & h_{m+2} & \cdots & h_{m+n+1} \\ \vdots & & & \\ h_{m+n} & h_{m+n+1} & \cdots & h_{m+2n} \end{vmatrix}. \tag{3.4}$$

We shall say that $\{h_i\} \in \mathrm{MH}$ is a sequence of Hamburger moments.

Theorem 3.2: A necessary condition for a solution to the Stieltjes problem to exist is that, for all $n \geqslant 0$,

$$H_n^0(h) \geqslant 0, \quad H_n^1(h) \geqslant 0. \tag{3.5}$$

We shall say that $\{h_i\} \in \mathrm{MS}$ is a sequence of Stieltjes moments.

Theorem 3.3: A necessary and sufficient condition for the Hausdorff problem to have a solution is

$$h_p \equiv \Delta_p^0 \geqslant 0, \quad p = 0,1,\ldots$$
$$\Delta_p^m \equiv \Delta_p^{m-1} - \Delta_{p+1}^{m-1} \geqslant 0, \quad m = 1,2,\ldots , \quad p = 0,1,\ldots . \tag{3.6}$$

Such a sequence is said to be totally monotonic, $\{h_i\} \in \mathrm{TM}$.

In the Hausdorff case the solution is unique; the moment problem is said to be determined.

The following properties of a TM sequence will be used.

Theorem 3.4: If $\{h_n\} \in \mathrm{TM}$, then $\{h_n\}_{n>k} \in \mathrm{TM}$ for k fixed.

Theorem 3.5: If $\{h_n\}_{n>0} \in \mathrm{TM}$ then $\{\Delta_p^k\}_{p>0} \in \mathrm{TM}$ for k fixed.

Obviously, if $\{h_n\} \in \mathrm{TM}$ then $\{h_n\} \in \mathrm{MS}$, since one can take the function μ constant outside $[0,1]$, and conversely, if $\{h_n\}$ is convergent and $\{h_n\} \in \mathrm{MS}$, then $\{h_n\} \in \mathrm{TM}$. From this it follows that (3.5) applies also to totally monotonic sequences.[5]

In the case of $\mu(x)$ taking an infinity of values in the pertinent interval, i.e., $\mu(x)$ is not a step function, which would yield rational Stieltjes functions, the inequalities in Theorems 3.1 and 3.2 become strict and the conditions become necessary and sufficient. In such a case (in the Stieltjes case, for instance), $\{h_n\}_{n>0}$ and $\{h_n\}_{n>1}$ are said to be definite positive sequences.

In the case of a Hausdorff moment sequence we have the following theorem.

Theorem 3.6: If $\{h_n\}_{n>0}$ is a Hausdorff moment sequence with $\mu(x)$ taking an infinity of values $\mu(x) \in \uparrow\beta[0,1]$ V_i, then $\{h_n\}_{n>0}$ is a definite positive sequence, i.e.,

$$H_n^0 > 0, \quad \forall_n .$$

It follows from Theorems 3.6 and 3.4. that

$$H_n^k(h) > 0, \quad k = 1,2,\ldots , \quad n = 0,1,\ldots , \tag{3.7}$$

and that when we use Theorem 3.5, Eq. (3.7) also applies to $\{\Delta_p^k\}_{p>0}$ sequences, with fixed k

$$H_n^m(\Delta^k) > 0, \quad m,n = 0,1,\ldots , \tag{3.8}$$

where

$$H_n^m(\Delta^k) = \begin{vmatrix} \Delta_m^k & \Delta_{m+1}^k & \cdots & \Delta_{m+n}^k \\ \Delta_{m+1}^k & \Delta_{m+2}^k & \cdots & \Delta_{m+n+1}^k \\ \vdots & \vdots & & \vdots \\ \Delta_{m+n}^k & \Delta_{m+n+1}^k & \cdots & \Delta_{m+2n}^k \end{vmatrix}. \tag{3.9}$$

In our case, h_i being determined from experimental data with errors, we shall use (3.8) to obtain bounds that the h_i should satisfy if they are the moments of a positive function. In this way, using the Hankel determinants of the first line, $\Delta_p^0 = h_p$, we get lower bounds for the coefficient h_p, given the previous $h_0,\ldots,h_{p-1}$,

$$H_0^m(h) > 0 \Rightarrow h_m > 0,$$

$$H_1^m(h) > 0 \Rightarrow h_{m+2} > \frac{(h_{m+1})^2}{h_m} > 0,$$

$$H_2^m(h) > 0 \Rightarrow h_{m+4} > \left(h_{m+3}\begin{vmatrix} h_m & h_{m+2} \\ h_{m+1} & h_{m+3} \end{vmatrix} - h_{m+2}H_1^{m+1}\right)(H_1^m)^{-1},$$
$$m = 0,1,\ldots , \tag{3.10}$$

and so forth.

As more coefficients are obtained, more and tighter bounds are obtained. One gets upper bounds for h_m in terms of $h_0,\ldots,h_{m-1}$ taking Hankel determinants of Δ^1, which give lower bounds of Δ^1_m in terms of $\Delta^1_0,\ldots,\Delta^1_{m-1}$

$$H_0^m(\Delta^1)>0 \Rightarrow \Delta^1_m>0, \quad m=0,1,\ldots, \quad \Delta^0_m-\Delta^0_{m+1}>0,$$
$$H_1^m(\Delta^1)>0 \Rightarrow \Delta^1_{m+2}>\frac{(\Delta_{m+1})^2}{\Delta^1_m}, \tag{3.11}$$
$$m=0,1,\ldots, \quad h_{m+3}<h_{m+2}-\frac{(h_{m+1}-h_{m+2})^2}{h_m-h_{m+1}}.$$

The same procedure as with rows 1 and 2 can be followed with the rest of the rows of table Δ^k_m [See Eq. (3.6)], yielding lower bounds for Δ^k_m with increasing m, which translate into lower bounds for h_m when k is even, and upper bounds for h_m when k is odd.

A subroutine has been designed which, given the m first coefficients $\Delta^0_0,\ldots,\Delta^0_{m+1}$, calculates the tighest possible lower and upper bounds for the next coefficient to be one of a Stieltjes series with non-null convergence radius.

In Sec. IV the conditions to be satisfied by the moments of the function $\chi_1(x)$ are sought when, besides being positive in $x\in[0,1]$, the function is supposed to have a unique maximum in a position $\beta\in[0,1]$. This condition will be referred to as unimodality.

IV. CONDITIONS IMPOSED BY UNIMODALITY

Let $\beta\in[0,1]$ be, then, the position of the maximum of $\chi_1(x)$. We shall call $\chi_1(x)$ unimodal if it satisfies

$$\begin{aligned}&\chi_1'(x)\geqslant 0, \quad x<\beta,\\ &\chi_1'(x)=0, \quad x=\beta,\\ &\chi_1'(x)\leqslant 0, \quad x>\beta.\end{aligned} \tag{4.1}$$

The function $\Phi'(x)=(\beta-x)\chi_1'(x)$ is positive in $[0,1]$ and its moments are related to those of $\chi_1(x)$ in the following way:

$$\mu_\nu=\int_0^1 x^\nu\Phi'(x)\,dx=(\nu+1)h-\beta\nu h_{\nu-1}, \quad \nu\neq 0, \tag{4.2}$$
$$\mu_0=h_0-\beta\chi_1(0),$$

where μ_ν, being the moments of a positive function, form a totally monotonic sequence, for which the positivity property of the Hankel determinants $H_n^m(\Delta^k)$ applies, Δ^k being the table constructed with the μ_ν:

$$\begin{array}{ccccccc}\Delta^0_0=\mu_0 & & \Delta^0_1=\mu_1 & & \Delta^0_2=\mu_2 & & \Delta^0_3=\mu_3 \quad \cdots\\ & \Delta^1_0 & & \Delta^1_1 & & \Delta^1_2 & \cdots\\ & & \Delta^2_0 & & \Delta^2_1 & \cdots & \\ & & & \Delta^3_0 & \cdots & & \end{array} \tag{4.3}$$

The inequalities so obtained for the μ_ν turn into inequalities in the h_ν, some of which are more restrictive than those obtained previously with positivity alone.

The most restrictive conditions that can be obtained with three coefficients are

$$h_0>\beta\chi_1(0), \quad \frac{\beta h_0}{2}<h_1<\frac{(\beta+1)h_0-\beta\chi_1(0)}{2}, \tag{4.4}$$

$$2\beta h_1+\frac{(2h_1-\beta h_0)^2}{h_0-\beta\chi_1(0)}<3, \quad h_2<2(\beta+1)h_1-\beta h_0. \tag{4.5}$$

The previous inequalities and those obtained as more coefficients are available, being necessary and sufficient conditions for μ_ν being moments of a weight function, can be used in two ways: (a) assuming we know n moments, discuss whether the associated function is unimodal or not, and what is the allowed range for β, and (b) assume that the weight function is unimodal with β in a certain range and discuss the necessary conditions the moments must satisfy.

We shall follow the second procedure, using the conditions from Eqs. (4.4) and (4.5) to constrain the values of the coefficients h_i candidates to representing our data faithfully, consequently limiting the number of possible functions fitting the data, and so obtaining a stable result when extrapolating to the poles, as will be seen in the applications.

Once of the coefficients h_i of the series expansion of $H_1(z)$ are known, the Padé approximants $[M-1/M]$ and $[M/M]$ are built.

V. EXTRAPOLATION TO THE POLES REGION: RESIDUES

The bounding properties of the type I Padé approximants on the Stieltjes function $H_1(z)$ [see Eq. (2.6)] on the real axis $]-1,\infty[$, produce, once the absorption is reversed, bounds on the residue of the function $H_0(z)$ in the position $-z_\Lambda$ of the pole

$$H_0(z)=\frac{R_1}{z+z_\Lambda}+\int_0^1\frac{\chi(x)\,dx}{1+xz}. \tag{5.1}$$

According to Theorem 2.1, the $[M/M]$ and $[M/M+1]$ Padé approximants and their complementary ones satisfy

$$\begin{aligned}&0<[M/M]<[M/M+1]<H_1(z)\\ &<[M/M+1]^c<[M/M]^c,\\ &z<0,\end{aligned} \tag{5.2}$$

which, in terms of $H_0(z)$, related to $H_1(z)$ by the absorption in z_1,

$$H_1(z)=[H_0(z)(z+z_\Lambda)-H_0(z)(z_1+z_\Lambda)]/(z-z_1), \tag{5.3}$$

becomes, with $z_1>0>z>-z_\Lambda$,

$$\begin{aligned}&[M/M]_{H_0}>[M/M+1]_{H_0}>H_0(z)\\ &>[M/M+1]^c_{H_0}>[M/M]^c_{H_0}.\end{aligned} \tag{5.4}$$

Also, for $z_1>0>-z_\Lambda>z$, all inequalities changing sense,

$$[M/M]_{H_0} < [M/M+1]_{H_0} < H_0(z)$$
$$< [M/M+1]^c_{H_0} < [M/M]^c_{H_0}. \quad (5.5)$$

with

$$[L/M]_{H_0} = \{[L/M](z-z_1) + T_1\}/(z+z_\Lambda) \quad (5.6)$$

and

$$T_1 = H_0(z_1)(z_1 + z_\Lambda). \quad (5.7)$$

All these approximants to $H_0(z)$ have, then, a pole at $-z_\Lambda$, as does $H_0(z)$ itself.

The situation is illustrated in Fig. 1, where the negative sign of the residue of H_0 has been taken into account.

Calculating from (5.6) and its counterpart for $[L/M]^c_{H_0}$ the residues V^L_M and ${}^cV^L_M$ of the approximants $[L/M]_{H_0}$ and $[L/M]^c_{H_0}$, respectively, one has the bounds on the negative residue of the function $H_0(z)$ on the pole at $z = -z_\Lambda$,

$${}^cV^0_0 < {}^cV^0_1 < {}^cV^1_1 < \cdots < R_1 < \cdots < V^1_1 < V^0_1 < V^0_0. \quad (5.8)$$

Each couple of inequalities requires one more coefficient in the expansion of $H_1(z)$, so with h_0, ${}^cV^0_0 < R_1 < V^0_0$, and with h_0 and h_1, ${}^cV^0_0 < {}^cV^0_1 < R_1 < V^0_1 < V^0_0$.

Let us finish this section with a comment on an alternative or complementary use of the function $H_1(z)$. The same kind of inequalities can be obtained from the type II Padé approximants[3] built from values of $H_1(z)$ at different points $z_1, z_2, \ldots$.

More precisely, the necessary and sufficient conditions for n points to belong to a Stieltjes function provide n en-

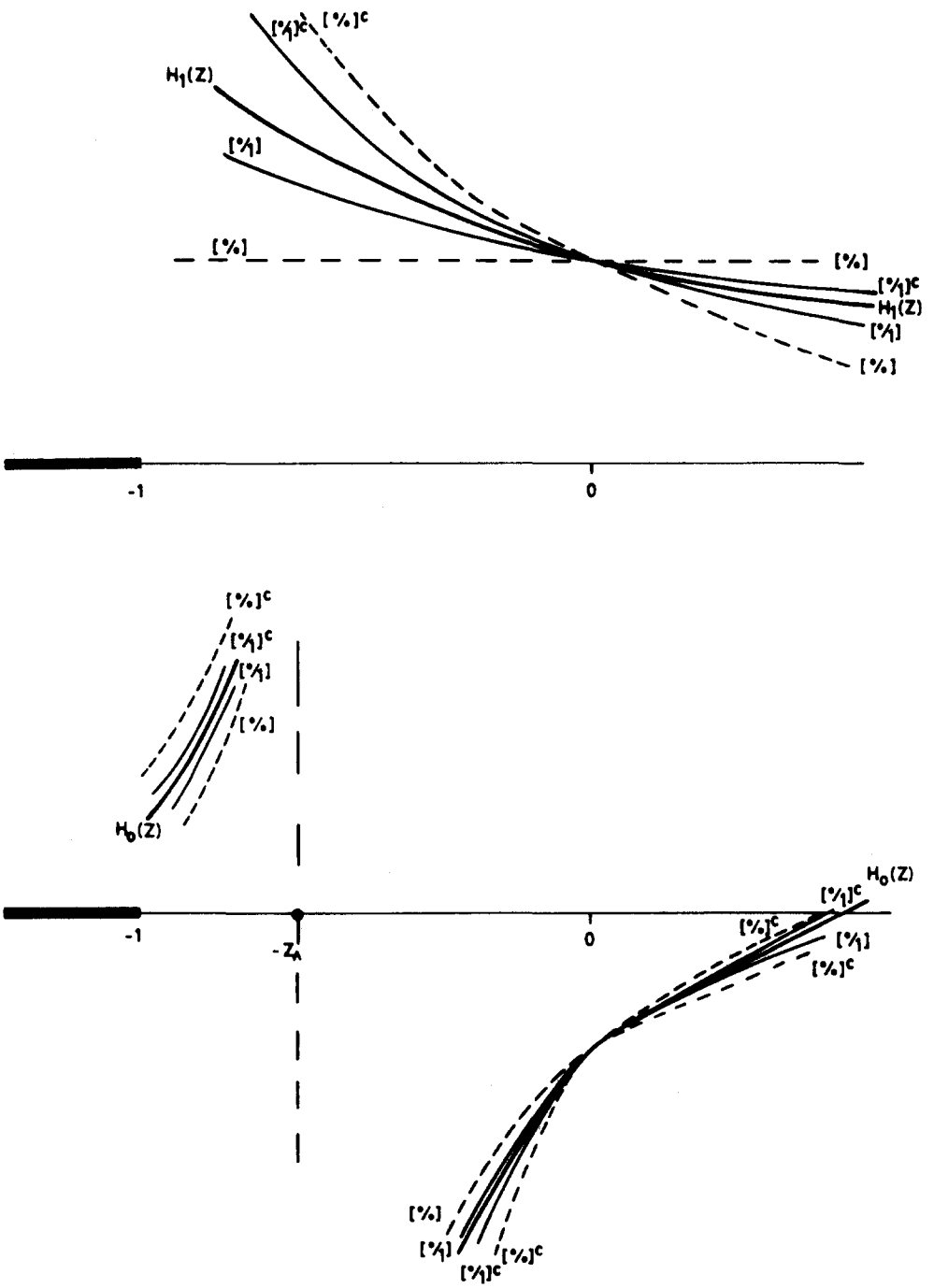

FIG. 1. The upper figure shows the bounding properties of the Padé approximants to the Stieltjes function $H_1(z)$ for $z > -1$. The lower figure shows how the transformed approximants to the function $H_0(z)$ bound ever more tightly the negative residue of the pole $-z_\Lambda$.

cased inequalities for the residue of H_0, R_1. The drawback of the method is that there is no unique set of points satisfying the conditions, but rather many sets which satisfy them separately, but not when joined together. The method followed in this report, based on the series expansion of H_1 and type I Padé approximants seems to us advantageous in that it uses a unique set of points. (See Sec. VII.)

VI. EXTRAPOLATION TO THE REAL CUT

In order to obtain an approximation to the weight function $\chi_1(x)$ closely related to the imaginary part of $H_1(z)$ on the cut $]-\infty, -1]$, we need to invert the moments $h_0, h_1, \ldots, h_n$ calculated in the fitting procedure.

Even if the number of calculated moments is insufficient to obtain a faithful approximation to $\chi_1(x)$ we can again use the constraints imposed by positivity and unimodality on the coefficients of the formal expansion of $H_1(z)$ [See Eq. (3.9)] to obtain upper ($\{h^u_{n+i}\}_{i>0}$) and lower ($\{h^1_{n+i}\}_{i>0}$) moment sequences allowed by the mentioned hypotheses

		$h^u_{n+2}\cdots$
	h^u_{n+1}	
$h_0, h_1, \ldots, h_n$		
	h^1_{n+1}	
		$h^1_{n+2}\cdots$

(6.1)

In this case we have to check if the results with both sequences are compatible.

Stieltjes–Chebyshev techniques are used to obtain approximations to the distribution function[6,7]

$$\psi_1(x) = \int_0^x \chi_1(x')dx' \tag{6.2}$$

and to the weight function $\psi_1(x)$ in the form of histogram approximations, thanks to the orthogonality properties of the Padé denominators with respect to the weight function $\chi_1(x)$.[2,3]

More precisely, Chebyshev inequalities provide upper and lower bounds on the vaues of $\psi_1(x)$ at positions related to the Padé poles by means of the positive residues of the approximants.[7]

Indeed, the approximant $[n-1/n]$ to $H_1(z)$ can be written as

$$[n-1/n] = \frac{P^{(-1)}_{n-1}(z)}{Q^{(-1)}_n(z)} = \sum_{p=1}^{n} \frac{f_p^{(n)}}{1+z\epsilon_p^{(n)}}, \tag{6.3}$$

with $f_p^{(n)}$ and $\epsilon_p^{(n)}$ related to the residues and poles of the approximants

$$[n-1/n] = \sum_{p=1}^{n} \frac{f_p^{*(n)}}{z+\epsilon_p^{*(n)}}, \quad f_p^{*(n)} > 0, \tag{6.4}$$

by

$$\epsilon_p^{(n)} = 1/\epsilon_p^{*(n)}, \quad f_p^{(n)} = f_p^{*(n)}\epsilon_p^{(n)}. \tag{6.5}$$

Since $\epsilon_p^{*(n)} \in [1, \infty]$, this implies $\epsilon_p^{(n)} \in [0,1]$ and $f_p^{(n)} > 0$. In view of (3.2), $d\psi(x) = \chi_1(x)dx$ can be approximated by

$$d\psi_s^{(n)}(x) = \sum_{p=1}^{n} f_p^{(n)}\delta(x-\epsilon_p^{(n)})dx, \tag{6.6}$$

which yields a step approximation $\psi_s^{(n)}$ to $\psi(x)$,

$$\psi_s^{(n)}(x) = 0, \quad 0 \leqslant x < \epsilon_1^{(n)},$$

$$\psi_s^{(n)}(x) = \sum_{p=1}^{j} f_p^{(n)}, \quad \epsilon_j^{(n)} < x < \epsilon_{j+1}^{(n)}, \quad j = 1, \quad n-1, \tag{6.7}$$

$$\psi_s^{(n)}(x) = \sum_{p=1}^{n} f_p^{(n)} = h_0, \quad \epsilon_n^{(n)} < x, \quad \epsilon_i < \epsilon_j, \quad \text{for } i<j,$$

providing bounds for the distribution function $\psi(x)$ in points $\epsilon_p^{(n)}$, $p = 1,2,\ldots,n$, such that

$$\psi_s^{(n)}(\epsilon_i^{(n)} - 0) \leqslant \psi_s^{(m)}(\epsilon_i^{(n)} - 0) \leqslant \psi(\epsilon_i^{(n)}) \leqslant \psi_s^{(m)}(\epsilon_i + 0) \leqslant \psi_s^{(n)}(\epsilon_i + 0), \quad m > n. \tag{6.8}$$

An approximation to $\chi_1(x)$, $\chi_s^{(n)}(x)$, is obtained from the slopes of the segments joining the midpoints of the discontinuities of $\psi_s^{(n)}(x)$.

Satisfactory as the Stieltjes distributions and weights are in many aspects, it is desirable to have continuous approximations to $\psi_1(x)$ and $\chi_1(x)$ at any point $x \in [0,1]$. It is convenient in this connection to consider approximations to the formal expansion of $H_1(z)$ having a prespecified pole at an arbitrary position on the cut $]-\infty, -1]$.[3,8] The denominators of these new approximants are related to the quasiorthogonal polynomials associated with the distribution function $\psi_1(x)$.[8]

The interpolation of the midpoints of the discontinuities of the histogram approximations to $\psi_1(x)$, having an arbitrary spectral point in [0,1], produce a continuous approximation to $\psi_1(x)$. An approximation to $\chi_1(x)$ is obtained by differentiating the approximation to $\psi_1(x)$.

The Cauchy integral formula allows us to obtain the real part of $H_1(z)$ on the cut using the $\chi_1(x)$ approximations.

VII. APPLICATION TO THE $K^{\pm}p$ FORWARD ELASTIC SCATTERING AMPLITUDE

The $K^{\pm}p$ forward elastic scattering amplitude can be represented by two analytic functions of the complex laboratory kaon energy ω, $F_{\pm}(\omega)$, related by the crossing property erty

$$F_{\pm}(\omega) = F_{\mp}(-\omega), \tag{7.1}$$

which allows the reduction of the description to only one function, $F_-(\omega)$.

The function satisfies the Schwartz reality condition

$$F_-(\omega^*) = F^*_-(\omega), \tag{7.2}$$

and is supposed to be asymptotically polynomically bounded.

Unitarity predicts the analytic structure of $F_-(\omega)$ consisting of two poles at the (unphysical) values ω_Λ and ω_Σ, corresponding to the K^-p system having the mass of the hyperons Λ and Σ, respectively, a left-hand cut going from $-m_K$ to $-\infty$ (K^+p scattering), and a right-hand cut from $\omega_{\Lambda\pi}$ to ∞ (K^-p scattering). The latter cut has an unphysical region from $\omega_{\Lambda\pi}$ (the unphysical energy corresponding to the K^-p system having the invariant mass $m_\Lambda + m_\pi$) to $\omega = m_K$. The unphysical region, experimentally inaccesible to the K^-p channel, and dominated by the Y^*_{1405} resonance, is mainly responsible for the discrepancies in the determination of the residues in the Λ and Σ poles, or in the reduced

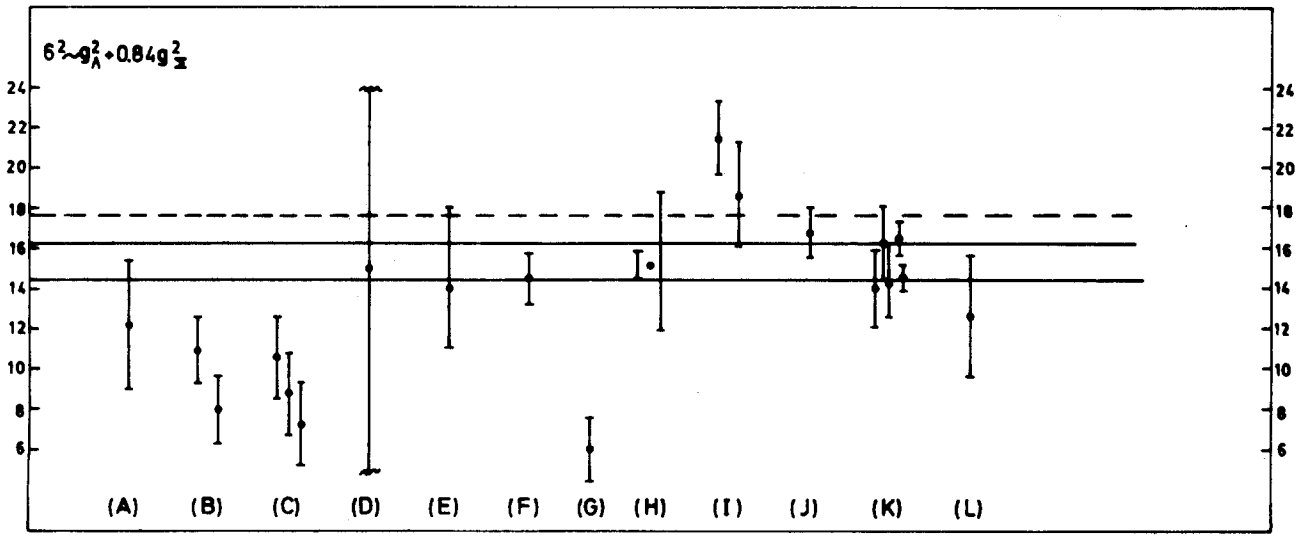

FIG. 2. Comparison of our bounds with other determinations of G^2. The dashed line indicates the upper bound imposed by positivity, the continuous one indicates the one imposed by adding unimodality. The lower bound is common to both casees. The bars indicate the values obtained by other authors for G^2: (A) Queen *et al.* 1969,[9] (B) Perrin and Woolcock, 1969,[10] (C) Martin and Perrin, 1970,[11] (D) Dumbrais *et al.*, 1971,[12] (E) Chao and Pietarinen, 1971,[13] (F) López and Yndurain, 1973,[14] (G) Sznajder-Hald *et al.*, 1973,[15] (H) Cruz and Mabres, 1974,[16] (I) Baillon *et al.*, 1976,[17] (J) Martin, 1976,[18] (K) Di Claudio *et al.* 1979,[19] (L) Atkin *et al.* 1981.[20]

pole, as explained later. Figure 2 shows the wide range of extrapolations for the residues.[9–20]

By applying Cauchy's integral theorem one can write a dispersion relation,[21] once subtracted at $\omega = \omega_0$,

$$\frac{\operatorname{Re} F_\pm(\omega)}{\omega-\omega_0} = \frac{\operatorname{Re} F_\pm(\omega_0)}{\omega-\omega_0} \mp \sum_Y \frac{X_Y}{(\omega_Y \pm \omega)(\omega_Y \pm \omega_0)} \pm \frac{P}{\pi}\int_{m_K}^{\infty} \frac{\operatorname{Im} F_+(\omega')\,d\omega'}{(\omega' \mp \omega)(\omega' \mp \omega_0)} \mp \frac{P}{\pi}\int_{\omega_{\Lambda\pi}}^{\infty} \frac{\operatorname{Im} F_-(\omega')\,d\omega'}{(\omega' \pm \omega)(\omega' \mp \omega_0)}, \quad Y = \Lambda, \Sigma. \tag{7.3}$$

Then we define a discrepancy function[20] as

$$\Delta_-(\omega) = \frac{1}{\pi}\int_{\omega_{\Lambda\pi}}^{m_K} \frac{\operatorname{Im} F_-(\omega')d\omega'}{(\omega'-\omega_0)(\omega'-\omega)} + \sum_Y \frac{X_Y}{(\omega_Y-\omega)(\omega_Y-\omega_0)}, \quad Y = \Lambda, \Sigma, \tag{7.4}$$

which has the structure of (2.2) if we assume the integrand to be singly signed within the integration range. This is essentially the positivity hypothesis, supported by low energy parametrizations.[22]

The dispersion relation can be written in the form

$$\Delta_-(\omega) = \frac{\operatorname{Re} F_-(\omega) - \operatorname{Re} F_-(\omega_0)}{\omega-\omega_0} + \frac{P}{\pi}\int_{m_K}^{\infty} \frac{\operatorname{Im} F_+(\omega')d\omega'}{(\omega'+\omega)(\omega'+\omega_0)} - \frac{P}{\pi}\int_{m_K}^{\infty} \frac{\operatorname{Im} F_-(\omega')d\omega'}{(\omega'-\omega)(\omega'-\omega_0)}, \tag{7.5}$$

which allows the evaluation of $\Delta_-(\omega)$ in those points where $\operatorname{Re} F_\pm(\omega)$ has been measured. Now, Δ_- is known, with errors, in 218 points, 119 on the K^+p cut and 99 on the K^-p cut. (See Fig. 3.)

The integrals in (7.5) are evaluated using the optical theorem, which relates $\operatorname{Im} F_\pm$ with the experimentally

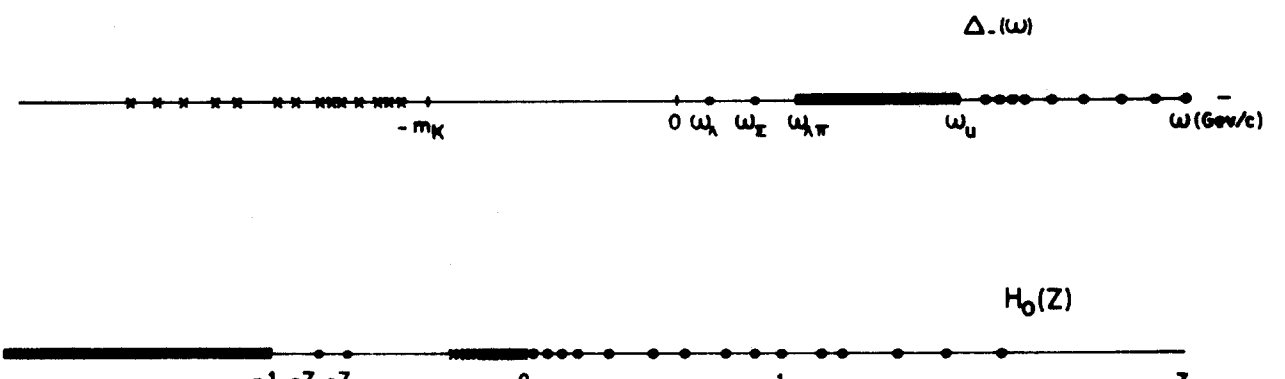

FIG. 3. Analytic structure of the Δ_- discrepancy function in the kaon laboratory energy plane ω and of the function H_0 in the transformed plane $z = (\omega - \omega_{\Lambda\pi})/(\omega - m_K)$. Crosses and closed circles indicate the experimental zone in the K^+p and K^-p regions, respectively, and their location in the z plane.

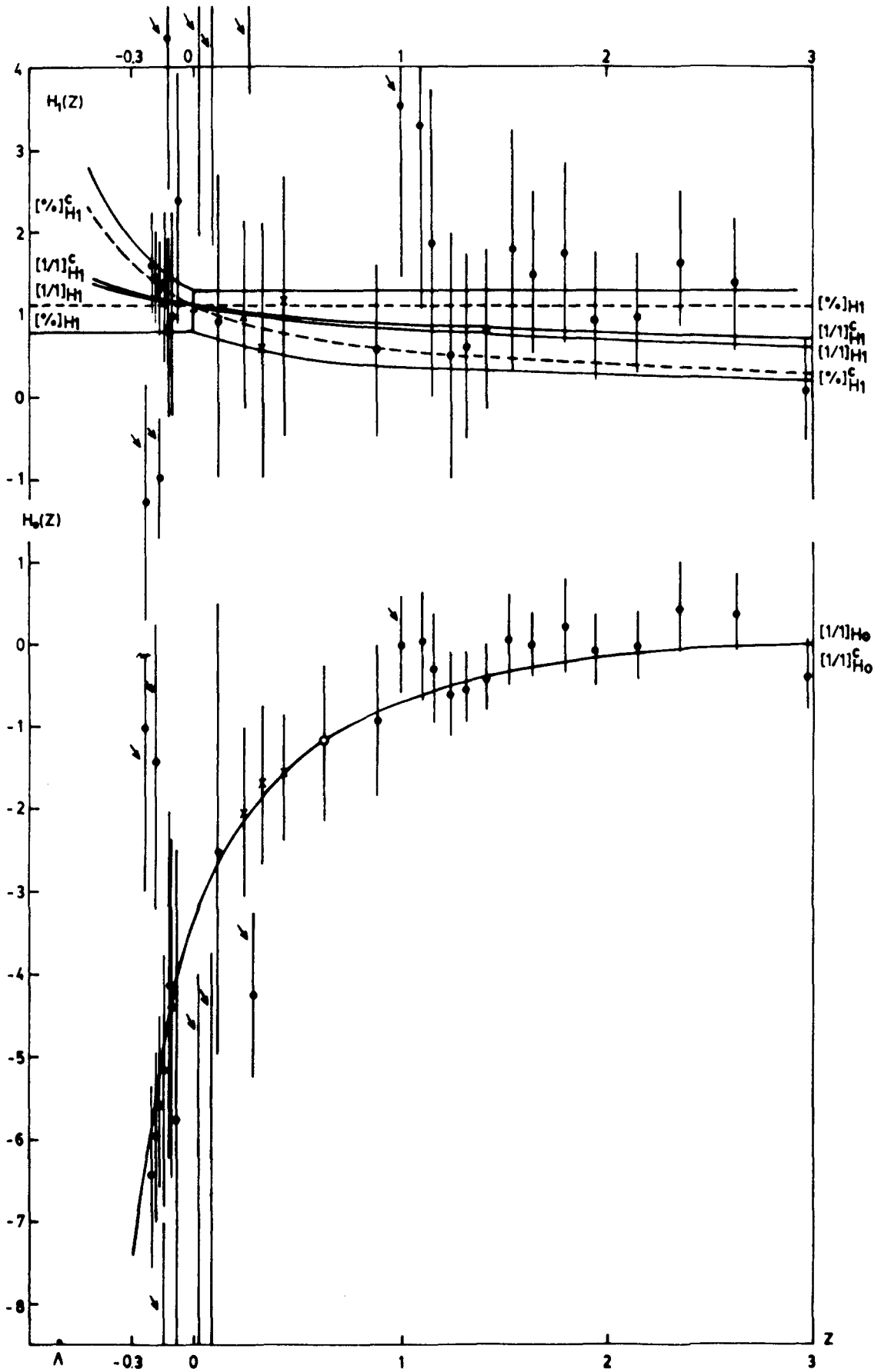

FIG. 4. "Experimental" points of the function $H_1(z)$ with the region allowed by $h_0 \pm 2h_0^c$. The points marked with an arrow have been excluded from the fits. In the lower part, the same experimental points, plus the absorption point, for $H_0(z)$, together with the approximation. The blank point is the absorption point and points marked with "×" are the alternative absorption points.

measured total $K^{\pm} p$ cross section.

Conventionally, the residues X_Y in (6.4) are parametrized as

$$X_Y = G_Y^2[(m_Y - m_p)^2 - m_K^2]/4m_p^2, \tag{7.6}$$

where G_Y is the so-called coupling constant, which we shall reduce to an effective coupling constant of a single Λ pole to account for both physical poles Λ, Σ,

$$G^2 = G_\Lambda^2 + 0.84\, G_\Sigma^2. \tag{7.7}$$

The values for G^2 extrapolated by several authors range from 6 to 22, giving a measure of the instability in the analytic extrapolation referred to above (Fig. 2).

By means of the transformations

$$x(\omega') = \frac{\omega' - m_K}{\omega_{\Lambda\pi} - m_K}, \quad z(\omega) = \frac{m_K - \omega_{\Lambda\pi}}{\omega - m_K}, \tag{7.8}$$

the discrepancy function is turned into

$$H_0(z) = -\frac{\Delta_-(z)}{z} = \int_0^1 \frac{\chi(x)\,dx}{1+zx} + \frac{R_\Lambda(m_K - \omega_{\Lambda\pi})}{1+zx_\Lambda}, \tag{7.9}$$

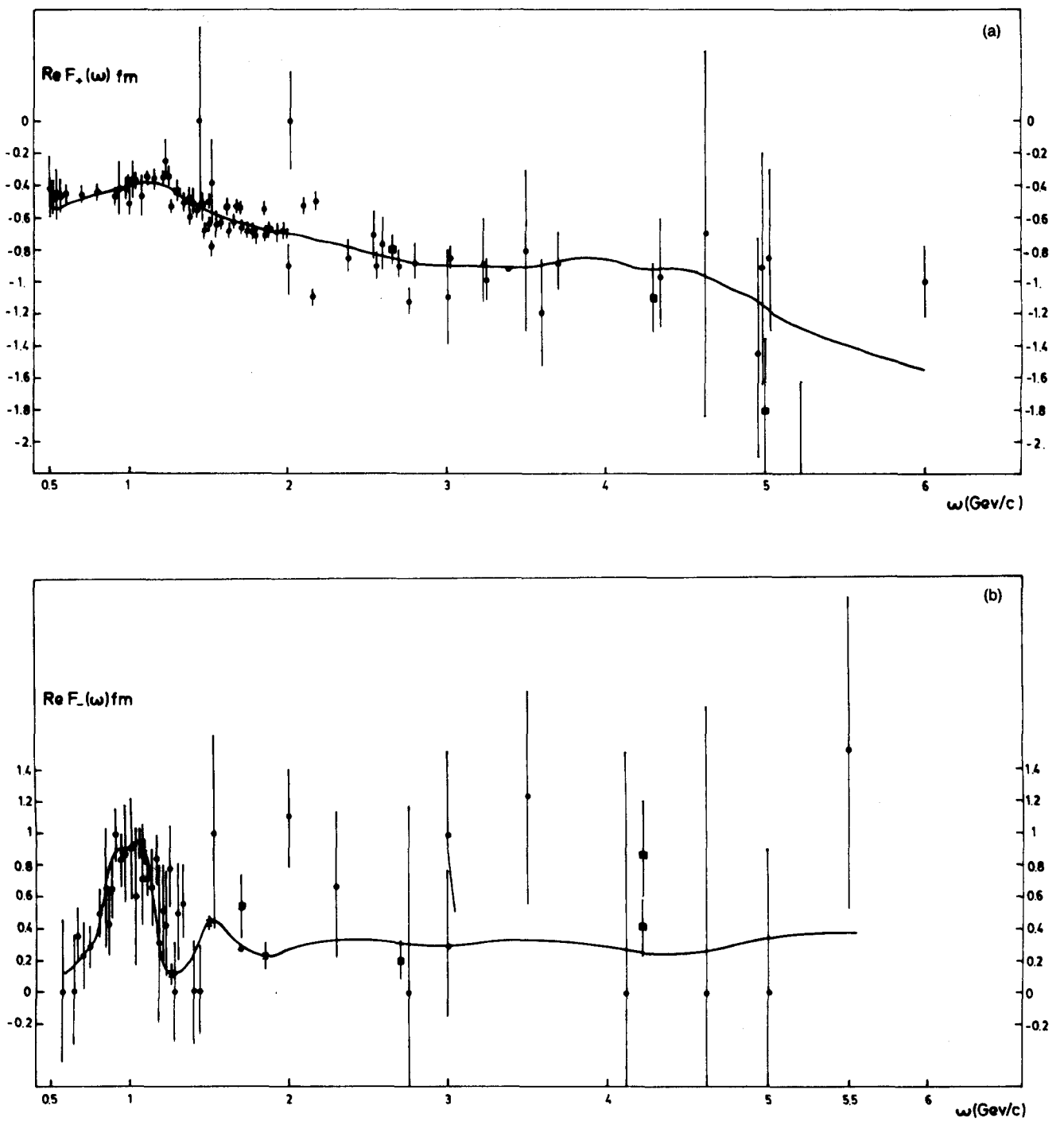

FIG. 5. Real parts of the K^+p and K^-p amplitudes against ω. The continuous line is the result of our calculation. Points marked with a bold square are those measured with Coulomb interference. Points marked with $\times$ are the absorption points.

where

$$\chi(x) = \operatorname{Im} F_-(\omega')/\pi(\omega' - \omega_0), \quad \omega_0 < \omega_{\Lambda\pi}, \tag{7.10}$$

with $\chi(x) \geqslant 0$ for $x \in [0,1]$ as a consequence of the positivity hypothesis, $\operatorname{Im} F_-(\omega') \geqslant 0$, $\omega' \in [\omega_{\Lambda\pi}, m_k]$. Also $R_\Lambda = X_\Lambda/(\omega_\Lambda - \omega_0)$, and the position of the effective pole is now

$$-z_\Lambda = (-x_\Lambda)^{-1} = (m_K - \omega_{\Lambda\pi})/(\omega_\Lambda - m_K)$$
$$= -0.650\,44.$$

The analytic structure of $H_0(z)$ is shown in Fig. 3.

The only remaining effective pole has been absorbed by choosing an absorption point, and that has been done in four different ways, all of them producing coherent extrapolations.

Fifty-four experimental points have been rejected, being incompatible with the positivity hypothesis, as made evident by the fact that all 54 points, with their error bars, lie outside the corridor formed by the Padé approximants $[0/0] = h_0 \pm 2h_0^e$ and $[0/0]^c = (h_0 \pm 2h_0^e)/(1+z)$, as shown in Fig. 4.

The bounds for the coupling constant produced by the positivity hypothesis are

$$14.4 < G^2 < 17.8. \tag{7.11}$$

When the unimodality hypothesis is added, expressing the fact that $\operatorname{Im} F_-(\omega)$ in the unphysical region is dominated by the Y^*_{1405} resonance, which produces a pronounced peak, the bounds are reduced to

$$14.4 < G^2 < 16.3. \tag{7.12}$$

The limits, compared with previous determinations, are shown in Fig. 2.

When the 54 points inconsistent with positivity are taken into account, the values obtained for the coupling constant lie below the lower bounds in (7.11) and (7.12), which might give a clue to some low determinations shown in Fig. 2.

The real parts of the forward elastic $K^\pm p$ amplitude have been calculated [using (7.5)] up to $k = 300$ GeV/c, and are shown in Fig. 5. In particular the value

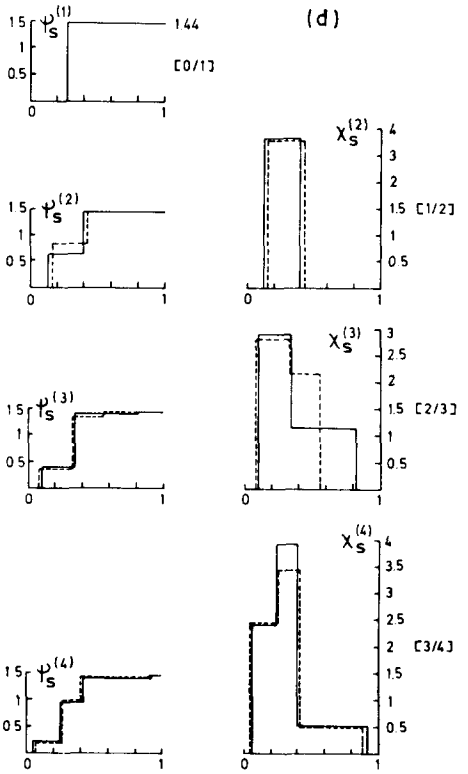

FIG. 7. The succesive approximations $\psi_s^{(n)}$ and $\chi_{(s)}^{(n)}$ to the distribution $\psi(x)$ and function $\chi_1(x)$ generated by the approximants $[n-1/n]$ are shown. The continuous line is the upper moment sequence approximation, and the dashed line is the lower one.

$\operatorname{Re} F_\pm(0) = D(0) = -2.8$ fm has been obtained, in agreement with its most recent determination.[23]

The consistency of the calculated real parts has been checked by using them in the absorption points, and the stability of the extrapolation has been confirmed by repeating the calculation after randomly perturbing the experimental values of the real parts according to their errors.

Taking advantage of the fact that the Padé approximants are valid for complex z, the position of the complex conjugate zeros of the amplitude (Fig. 6) has been found to be

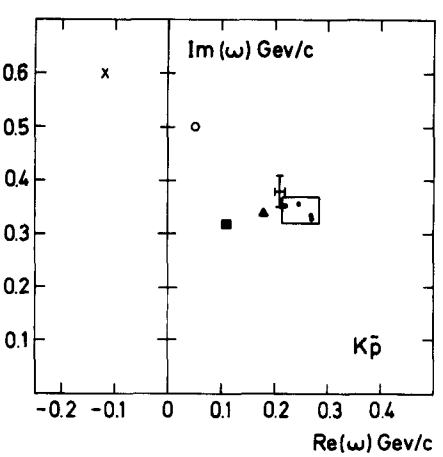

FIG. 6. Positions of the complex-conjugated zeros, on the upper semiplane, of the $K^- p$ scattering amplitude. The marks ×, ○, ■, ▲, and + refer, respectively, to the determinations carried out by Atkin[20], Dumbrais 1972,[24] López,[14] Dumbrais 1978,[25] Dumbrais 1980.[26] The rectangle and their interior points are the allowed region and the values obtained in this work.

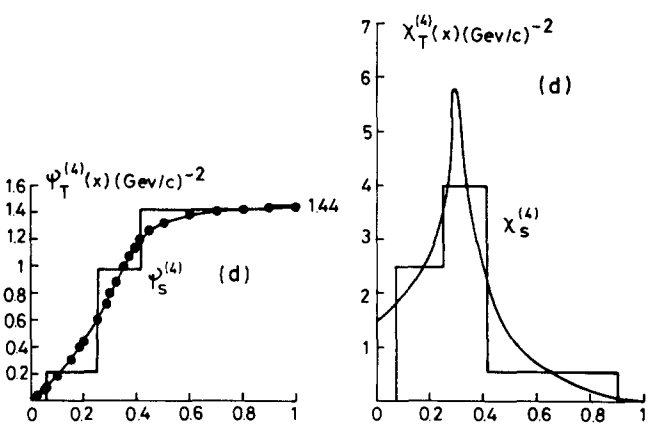

FIG. 8. The left-hand figure shows the interpolation of the Chebyshev values obtained when varying the pole position in the interval [0,1]. The histogram is the [3/4] approximation. The right-hand figure shows the approximation $\chi_T^{(4)}(x)$ obtained by differentiating the previous interpolation, together with the histogram approximation.

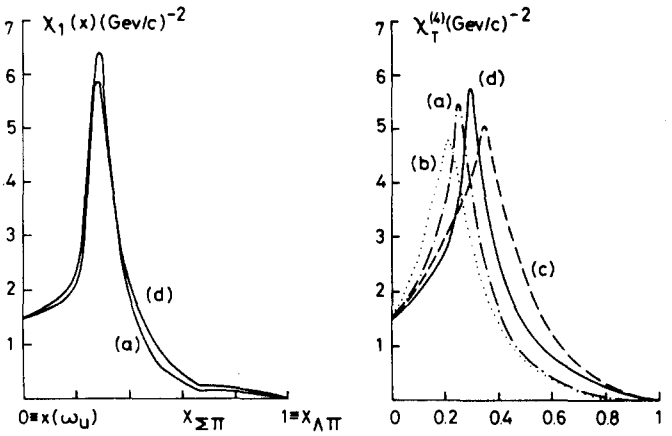

FIG. 9. Comparison of the weight functions obtained by our extrapolation in the four cases (right) with the result of an effective range K matrix analysis.[8]

$$(0.245 \pm 0.035, \quad \pm 0.345 \pm 0.025). \tag{7.13}$$

We have also obtained approximations to the weight function, $\chi_1(x)$ related to Im $F_-(\omega')$ in the form (7.10).

Figure 7 shows the Stieltjes histogram approximations $\psi_s^{(n)}(x)$, n = 1,2,3,4, calculated with 2,4,6,8 moments, respectively, and also the Stieltjes weight histograms $\chi_s^{(n)}(x)$, calculated from the former by means of the slopes of the straight-line segments connecting the succesive Stieltjes values of $\psi_s^{(n)}(x)$, giving a first idea of the shape of $\chi_1(x)$ in one of the absorption cases.

Figure 8 shows the continuous approximations $\psi_T^{(4)}(x)$ and $\chi_T^{(4)}(x)$ calculated, varying the position of one of the spectral points of the histogram distributions.

Figure 9 compares the results obtained, using a low energy model,[18] for $\chi_1(x)$ with ours, depending only on experimental data and therefore being model independent.

Lastly, Fig. 10 shows the real part of the amplitude in the unphysical cut obtained with the calculated values of G^2 and the approximations for $\chi_1(x)$.

In particular a range from -1.075 to -0.865 fm is obtained for the real part of the amplitude at the elastic K^-p threshold, agreeing with other low-energy model-dependent determinations of this parameter.[18,27]

More details on the physical applications of the method can be found in Ref. 28.

Our extrapolation method used to obtain the previous results can be applied to other functions of physical interest with analytic structure similar to that of the K^-p amplitude, like the $K^\pm n$ amplitude, form factors, and structure functions.

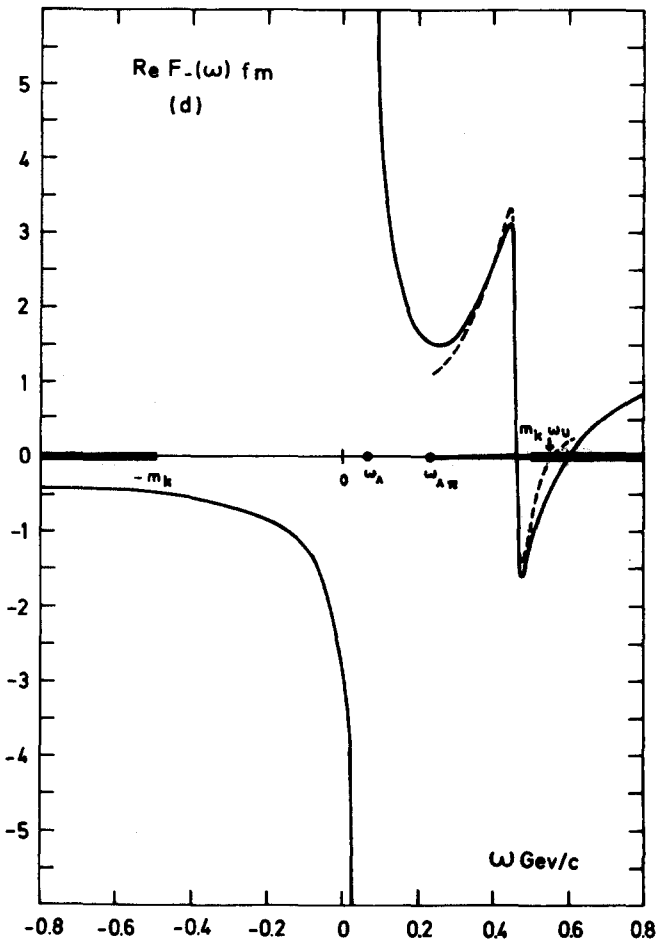

FIG. 10. Real part of the $F_-(\omega)$ amplitude on the unphysical cut. The continuous line is our result [case (d)] and the dashed line is the real part obtained from a low energy parametrization.[18]

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Some algebras of unbounded operators in an indefinite inner product vector space

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A general theory of unbounded representations of *-algebras in the Krein space is formulated. Following the corresponding theory of unbounded representations in the Hilbert space, the connection between states and representations, properties of covariant representations, the notion of irreducibility, and decomposition into irreducible parts are discussed.

I. INTRODUCTION

In the algebraic approach to quantum field theory (QFT) with an indefinite inner product (IIP), developed in our previous works,[1,2] the necessity of consideration of some class of *-algebras represented by unbounded operators in IIP vector space, arises in a natural way. Since the general theory of unbounded representations does not cover this class, one should try to generalize some well-known results of the standard theory to this indefinite inner product case. The aim of the present work is to carry out such generalization for so-called J^*-representations in the Krein space. Using some ideas and results of Powers[3] and Borchers and Yngvason,[4] we examine in detail the following problems: (1) what is the natural extension of the notion of cyclicity of representation to the case of J^*-representation; (2) how can we construct a cyclic J^*-representation starting from some state on the algebra; (3) in what sense is a J^*-representation covariant; (4) how can we introduce the notion of irreducibility; and (5) is it possible to obtain some kind of decomposition of the J^*-representation into irreducible parts?

The article is organized as follows. In Sec. II, after the short introduction of elementary concepts from the theory of IIP spaces, we study some properties of unbounded operators in the Krein space (closability, relation between adjoints with respect to different inner products, essential self-adjointness, etc.). In Sec. III we introduce the notion of a J^*-representation of a *-algebra and other algebraic concepts connected with it (α-cyclic representation and α-cyclic vector, G-covariant representation, α-positive state). We show that α-cyclic J^*-representations can be generated by some state on the algebra that is not positive, but instead satisfies another condition—α-positivity. As in the standard case, a G-invariant state yields a G-covariant representation, but in contrast to the usual Gelfand–Naimark–Segal (GNS) construction the group G is represented by (generally) unbounded operators. Finally, following Ref. 3, we construct several closed extensions of a given J^*-representation and show how this construction works in the case of a G-covariant representation. Section IV contains the explicit construction of the algebra of unbounded operators in the Fock–Krein space. This algebra has all the properties of the so-called Op J^*-algebra (i.e., the algebra of operators generated by some J^*-representation). We show by this example the existence of the J^*-representation itself and illustrate all features of the general theory. In Sec. V we analyze the notion of irreducibility of the J^*-representation. Our definition of the so-called α-irreducibility seems to be the natural generalization of the corresponding definition from the theory of unbounded representations in the Hilbert space, since in the case of a representation generated by the α-positive state, α-irreducibility is equivalent to the extremality of the state. We show also how to generalize the concept of reducing subspaces and construct (following again Ref. 3) the class of J^*-representations for which α-irreducibility is equivalent to the nonexistence of nontrivial reducing subspaces. Finally, in Sec. VI we apply the results of general analysis of the problem of decomposition of unbounded representation performed in Ref. 4 to our case and conclude that every α-cyclic, strongly continuous, J^*-representation of a separable nuclear topological algebra can be decomposed into α-irreducible parts.

II. INDEFINITE INNER PRODUCT SPACES AND OPERATORS

In this section we collect some facts concerning the theory of indefinite inner product space (for more details see the book of Bognar[5] and the work of Jadczyk[6]). We prove also some elementary properties of linear operators in an indefinite inner product space.

A. Indefinite inner product space

Let E be a vector space with an inner product $\langle\ ,\ \rangle$. If the quantity $\langle x, x\rangle$, $x \in E$ may be positive, negative, or zero, a pair $(E, \langle\ ,\ \rangle)$ is called the *indefinite inner product space*. If $\langle\ ,\rangle$ is nondegenerate and

$$E = E^+ \oplus E^-, \quad E^\pm = \{x \in E: \ \langle x, x\rangle \gtrless 0\}, \tag{2.1}$$

then $(E, \langle\ ,\ \rangle)$ is called the *decomposable indefinite inner product space*. Let $P^\pm E = E^\pm$. Let us define the *fundamental symmetry* I of E as

$$I = P^+ - P^- \tag{2.2}$$

[$J(E)$ will denote the set of all fundamental symmetries of E]. For every $I \in J(E)$, we have

(A) $I^{-1} = I$,

(B) $\langle Ix, y\rangle = \langle x, Iy\rangle$,

(C) $(x, y)_I = \langle x, Iy\rangle$ is positive definite.

We can also introduce *the I-norm*

$$\|x\|_I = (x, x)_I^{1/2}. \tag{2.3}$$

One can check that for every $x, y \in E$

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$$|\langle x, y\rangle| \leqslant \|x\|_I \|y\|_I, \tag{2.4}$$

for any $I \in J(E)$.

B. Krein space

If for every $I \in J(E)$ the I-inner product $(\ ,\ )_I$ turns E into the Hilbert space, the indefinite inner product space $(E, \langle\ ,\ \rangle)$ will be called the Krein space.[7] [We will use the following notation: $(\mathscr{K}, \langle\ ,\ \rangle)$ will denote the Krein space and $\mathscr{K}_I$ the corresponding Hilbert space for $I \in J(\mathscr{K})$.]

Let $\mathscr{F} \subset \mathscr{K}$ be a subset of the Krein space $\mathscr{K}$. Let us define

$$\mathscr{F}^{\perp} = \{x \in \mathscr{K}:\ \langle x, y\rangle = 0,\ \forall\, y \in \mathscr{F}\}, \tag{2.5}$$

$$\mathscr{F}^{\perp_{(I)}} = \{x \in \mathscr{K}:\ (x, y)_I = 0,\ \forall\, y \in \mathscr{F}\}. \tag{2.6}$$

It is easy to show that the following relations hold:

$$(I\mathscr{F})^{\perp} = \mathscr{F}^{\perp_{(I)}}, \quad (I\mathscr{F})^{\perp_{(I)}} = \mathscr{F}^{\perp}, \tag{2.7}$$

$$\mathscr{F}^{\perp} = I\mathscr{F}^{\perp_{(I)}}, \quad \mathscr{F}^{\perp_{(I)}} = I\mathscr{F}^{\perp}, \tag{2.8}$$

and as a consequence of (2.7) and (2.8),

$$(I\mathscr{F})^{\perp} = I\mathscr{F}^{\perp}, \quad (I\mathscr{F})^{\perp_{(I)}} = I\mathscr{F}^{\perp_{(I)}}. \tag{2.9}$$

Using these relations we obtain the following result.

Lemma 2.1: Let $\mathscr{F} \subset \mathscr{K}$. The closure $\overline{\mathscr{F}}$ of $\mathscr{F}$ in the Krein space topology is equal to $\mathscr{F}^{\perp\perp}$.

Proof: For a fixed $I \in J(\mathscr{K})$, $\mathscr{K}_I$ is a Hilbert space, so $\overline{\mathscr{F}} = \mathscr{F}^{\perp_{(I)}\perp_{(I)}}$. On the other hand,

$$\mathscr{F}^{\perp\perp} = (I\mathscr{F}^{\perp_{(I)}})^{\perp} = I(I\mathscr{F}^{\perp_{(I)}})^{\perp_{(I)}}$$

$$= II\,\mathscr{F}^{\perp_{(I)}\perp_{(I)}} = \mathscr{F}^{\perp_{(I)}\perp_{(I)}}.$$

Thus $\overline{\mathscr{F}} = \mathscr{F}^{\perp\perp}$.

C. Linear operators in the Krein space

Let A be a densely defined linear operator in $\mathscr{K}$ with the domain $D(A)$. Now we define the adjoint A^* with respect to the indefinite inner product $\langle\ ,\ \rangle$:

$$D(A^*) = \{x \in \mathscr{K}:\ \forall\, y \in D(A)\ \exists\, z \in \mathscr{K}:$$

$$\langle x, Ay\rangle = \langle z, y\rangle\}, \tag{2.10}$$

$$A^*x = z, \quad \text{for } x \in D(A^*).$$

[In the following $A^{*_{(I)}}$ will denote the adjoint of A with respect to the I-inner product $(\ ,\ )_I$.] One can simply prove the following lemma.

Lemma 2.2: $x \in D(A^*)$ iff for every $y \in D(A)$ there is $k > 0$ such that

$$|\langle x, Ay\rangle| \leqslant k\,\|y\|_I$$

[for any $I \in J(\mathscr{K})$].

Lemma 2.3: For every $I \in J(\mathscr{K})$, $ID(A^*) = D(A^{*_{(I)}})$.

Proof: Let $x \in ID(A^*)$, then $x = I\tilde{x}$ for $\tilde{x} \in D(A^*)$. Since

$$|(x, Ay)_I| = |(I\tilde{x}, Ay)_I| = |\langle \tilde{x}, Ay\rangle| \leqslant k\,\|y\|_I,$$

$x \in D(A^{*_{(I)}})$. Let now $x \in D(A^{*_{(I)}})$. Since

$$|\langle Ix, Ay\rangle| = |(x, Ay)_I| \leqslant k_1\|y\|_I,$$

$Ix \in D(A^*)$ and $x \in ID(A^*)$.

Proposition 2.1: A densely defined operator A in the Krein space $\mathscr{K}$ is closable iff $D(A^*)$ is dense in $\mathscr{K}$.

Proof: Assume that A is closable in the Krein space topology. It means that A is closable as an operator in the Hilbert space $\mathscr{K}_I$ for any $I \in J(\mathscr{K})$. Hence $D(A^{*_{(I)}})$ is dense in $\mathscr{K}_I$. Since

$$D(A^*)^{\perp} = (ID(A^{*_{(I)}}))^{\perp} = D(A^{*_{(I)}})^{\perp_{(I)}} = \{0\},$$

$D(A^*)$ is dense $[D\ \overline{(A^*)} = D(A^*)^{\perp\perp}]$. Suppose now that $D(A^*)$ is dense in $\mathscr{K}$. Since

$$D(A^{*_{(I)}})^{\perp_{(I)}} = (ID(A^*))^{\perp_{(I)}} = D(A^*)^{\perp} = \{0\},$$

$D(A^{*_{(I)}})$ is dense in $\mathscr{K}_I$ and A is closable.

Lemma 2.4: Let A be a densely defined operator in the Krein space $\mathscr{K}$. Suppose that for a fixed $I \in J(\mathscr{K})$, $ID(A) \subset D(A)$. Then $(AI)^{*_{(I)}} = A^*I$.

Proof: First we have to check that $D((AI)^{*_{(I)}}) = D(A^*I)$. Let $x \in D((AI)^{*_{(I)}})$ and $y \in D(A)$. Since

$$|\langle Ix, AIy\rangle| = |(x, AIy)_I| \leqslant k\,\|y\|_I = k\,\|Iy\|_I,$$

$Ix \in D(A^*)$ [because $Iy \in D(A)$] and $x \in ID(A^*)$. Similarly we can show that $ID(A^*) = D(A^*I) \subset D((AI)^{*_{(I)}})$. Let now $x \in D((AI^{*_{(I)}}) = D(A^*I) = ID(A^*)$:

$$((AI)^{*_{(I)}}x, y)_I = (x, AIy)_I.$$

On the other hand,

$$(x, AIy)_I = \langle Ix, AIy\rangle = \langle A^*Ix, Iy\rangle = (A^*Ix, y)_I.$$

Hence

$$((AI)^{*_{(I)}}x, y)_I = (A^*Ix, y)_I,$$

for every $y \in D(A)$.

Proposition 2.2: Suppose that A is a symmetric, densely defined linear operator in the Krein space $\mathscr{K}$ such that $ID(A) \subset D(A)$ for some $I \in J(\mathscr{K})$. If the operator AI is essentially $*_{(I)}$-self-adjoint, then A is essentially $*$-self-adjoint.

Proof: We show that $ID((AI)^{*_{(I)}*_{(I)}}) = D(A^{**})$. Indeed, let $x \in D((AI)^{*_{(I)}*_{(I)}})$. Then, for every $y \in D((AI)^{*_{(I)}}) = D(A^*I)$,

$$|(x, (AI)^{*_{(I)}}y)_I| \leqslant k\,\|y\|_I,$$

so

$$|\langle Ix, A^*Iy\rangle| = |(x, (AI)^{*_{(I)}}y)_I| \leqslant k\,\|Iy\|_I.$$

Hence $Ix \in D(A^{**})$ and $ID((AI)^{*_{(I)}*_{(I)}}) \subset D(A^{**})$. If $D((AI)^{*_{(I)}*_{(I)}}) = D((AI^{*_{(I)}})$ then, since

$$D(A^{**}) = ID((AI)^{*_{(I)}*_{(I)}}), \quad D(A^*) = ID((AI)^{*_{(I)}}),$$

we obtain $D(A^{**}) = D(A^*)$.

III. J^*-REPRESENTATIONS OF TOPOLOGICAL $*$-ALGEBRAS[1,2]

A. Definition of the J^*-representation

Let $\mathscr{A}$ be a topological $*$-algebra. If $\mathrm{aut}_*(\mathscr{A})$ denotes the set of all continuous $*$-automorphisms of $\mathscr{A}$, let $j(\mathscr{A}) \subset \mathrm{aut}_*(\mathscr{A})$ be the set of elements α satisfying $\alpha^2 = \mathrm{id}$. Then $(\pi, D(\pi), \{I_\pi(\alpha):\ \alpha \in j(\pi)\})$ is called a J^*-representation of $\mathscr{A}$ if we have the following.

(A) π: $\mathscr{A}\to \mathrm{op}(D(\pi))$ is a mapping of $\mathscr{A}$ into the set of linear operators on $D(\pi)$. Here $((D(\pi), \langle\ ,\ \rangle_\pi)$ is a nondegenerate indefinite inner product space such that (A1) for every $A\in\mathscr{A}$, $\pi(A)D(\pi)\subset D(\pi)$; (A2) for every $A, B\in\mathscr{A}$, $\lambda,\mu\in\mathbb{C}$, and $X\in D(\pi)$, $\pi(AB)X=\pi(A)\pi(B)X$, $\pi(\lambda A+\mu B)X=\lambda\pi(A)X+\mu\pi(B)X$; and (A3) for every $A\in\mathscr{A}$ and $X, Y\in D(\pi)$, $\langle X,\pi(A)Y\rangle_\pi=\langle\pi(A^*)X, Y\rangle_\pi$.

(B) $j(\pi)\subset j(\mathscr{A})$ and $I_\pi(\alpha)$: $D(\pi)\to D(\pi)$ has the properties

$$I_\pi(\alpha)^2=1,\quad \langle I_\pi(\alpha)X, Y\rangle_\pi=\langle X, I_\pi(\alpha)Y\rangle_\pi,$$

and $(X, Y)_\alpha:=\langle X, I_\pi(\alpha)Y\rangle_\pi$ is positive definite.

(C) for every $\alpha\in j(\pi)$, $A\in\mathscr{A}$, and $X\in D(\pi)$,

$$\pi(\alpha(A))X=I_\pi(\alpha)\pi(A)I_\pi(\alpha)X.$$

Remarks: (A) Let

$$\mathscr{K}_{\pi,\alpha}:=\overline{D(\pi)}^{\|\cdot\|_\alpha}[\,\|X\|_\alpha=(X,X)_\alpha^{1/2}]$$

and $\langle\ ,\ \rangle_\alpha$ be the extension of $\langle\ ,\ \rangle_\pi$ to $\mathscr{K}_{\pi,\alpha}$. A pair $(\mathscr{K}_{\pi,\alpha}, \langle\ ,\ \rangle_\alpha)$ is the Krein space.

(B) If $\alpha,\beta\in j(\pi)$ and $\alpha\neq\beta$, the norms $\|\ \|_\alpha$ and $\|\ \|_\beta$ are not generally equivalent (see Sec. IV for an example).

(C) $\pi(\mathscr{A})$ is the example of the Op I^*-algebra discussed by Dadashyan and Horujy.[8]

Suppose that there is defined the representation $\{\tau_g\}$ of the topological group G:

$$g\to\tau_g\in \mathrm{aut}_*(\mathscr{A}). \tag{3.1}$$

The J^*-representation is *G-covariant* if there exists a family $\{U_g^{(\pi)}:\ g\in G\}$ of linear operators with the following properties: (A) for every $g\in G$, $U_g^{(\pi)}$: $D(\pi)\to D(\pi)$; (B) for every $g\in G$ and $X, Y\in D(\pi)$,

$$\langle U_g^{(\pi)}X, U_g^{(\pi)}Y\rangle_\pi=\langle X, Y\rangle_\pi;$$

(C) for every $A\in\mathscr{A}$, $g\in G$, and $X\in D(\pi)$,

$$\pi(\tau_g(A))X=U_g^{(\pi)}\pi(A)\,U_g^{(\pi)*}X;$$

(D) for every $g_1, g_2\in G$ and $X\in D(\pi)$,

$$U_{g_1}^{(\pi)}U_{g_2}^{(\pi)}X=U_{g_1g_2}^{(\pi)}X;$$

and (E) the mapping $g\to\langle X, U_g^{(\pi)}Y\rangle_\pi$ is continuous.

The representation $(\pi, D(\pi), \{I_\pi(\alpha):\ \alpha\in j(\pi)\})$ is *α-cyclic* $[\alpha\in j(\pi)]$ if there is a vector $\Omega_\pi\in D(\pi)$ such that (A) $\pi(\mathscr{A})\Omega_\pi$ is dense in $\mathscr{K}_{\pi,\alpha}$, and (B) $I_\pi(\alpha)\Omega_\pi=\Omega_\pi$.

B. States and GNS construction

For an α-cyclic J^*-representation, the functional ω_π, defined by

$$\omega_\pi(A)=\langle\Omega_\pi, \pi(A)\Omega_\pi\rangle_\pi, \tag{3.2}$$

has the properties

$$\begin{aligned}&\text{(A)}\quad \omega_\pi\circ\alpha=\omega_\pi,\\ &\text{(B)}\quad \text{for every } A\in\mathscr{A},\quad \omega_\pi(\alpha(A^*)A)\geqslant 0.\end{aligned} \tag{3.3}$$

It suggests the following definition: A functional ω on $\mathscr{A}$ is *α-positive* if there exists such $\alpha\in j(\mathscr{A})$ that ω satisfies (3.3). If ω is α-positive, then $P_\omega:=\{\alpha\in j(\mathscr{A}):\ \omega$ is α-positive$\}$. Thus ω is an α-positive state if $\omega(\mathbf{1})=1$.

Theorem 3.1: Let ω be an α-positive and G-invariant state on $\mathscr{A}$. Assume that for every $A, B\in\mathscr{A}$ the mapping $g\to\omega(A\,\tau_g(B))$ is continuous. Then there exists G-covariant representation $(\pi_\omega, D_\omega, \{I_\omega(\alpha):\ \alpha\in P_\omega\})$ of $\mathscr{A}$ with the family $\{U_g^{(\omega)}:\ g\in G\}$. It is α-cyclic for every $\alpha\in P_\omega$. Moreover, for every $g\in G$,

$$U_g^{(\omega)}:\ \mathscr{K}_{\omega,\alpha}\to\mathscr{K}_{\omega,\alpha_g}\quad(\alpha_g=\tau_g\circ\alpha\circ\tau_g^{-1})$$

is the unitary operator between Hilbert spaces $\mathscr{K}_{\omega,\alpha}$ and $\mathscr{K}_{\omega,\alpha_g}$.

Proof: Let $N_\omega=\{A\in\mathscr{A}:\ \omega(BA)=0,\ \forall\, B\in\mathscr{A}\}$. Let

$$D_\omega=\mathscr{A}/N_\omega.$$

If we put

$$\langle X_A^\omega, X_B^\omega\rangle_\omega=\omega(A^*B)$$

(where X_A^ω denotes the equivalence class in D_ω containing $A\in\mathscr{A}$), we obtain an indefinite inner product space $(D_\omega, \langle\ ,\ \rangle_\omega)$. Next we define

$$\begin{aligned}&\pi_\omega(A)X_B^\omega=X_{AB}^\omega,\\ &I_\omega(\alpha)X_A^\omega=X_{\alpha(A)}^\omega,\\ &U_g^{(\omega)}X_A^\omega=X_{\tau_g(A)}^\omega.\end{aligned}$$

It is easy to check that $(\pi_\omega, D_\omega, \{I_\omega(\alpha):\ \alpha\in P_\omega\})$ so defined is a J^*-representation. It is G-covariant and α-cyclic with an α-cyclic vector $\Omega=X_{\mathbf{1}}^\omega$. Since

$$\begin{aligned}(U_g^{(\omega)}X_A^\omega, U_g^{(\omega)}X_B^\omega)_{\alpha_g}&=\omega(\alpha_g\circ\tau_g(A^*)\circ\tau_g(B))\\ &=\omega(\alpha(A^*)B)=(X_A^\omega, X_B^\omega)_\alpha,\end{aligned}$$

U_g^ω can be extended to the unitary mapping between $\mathscr{K}_{\omega,\alpha}$ and $\mathscr{K}_{\omega,\alpha_g}$.

C. Closed extensions of the J^*-representation

Theorem 3.2: Let $(\pi_\omega, D_\omega, \{I_\omega(\alpha):\ \alpha\in P_\omega\})$ be a G-covariant J^*-representation of $\mathscr{A}$ defined by some α-position state ω. For every $\alpha\in P_\omega$ there exists a J^*-representation $(\pi_{\omega,\alpha}, D_{\omega,\alpha}, \{I_\omega(\alpha)\})$ (an *α-closed extension* of it) defined as follows:

$$D_{\omega,\alpha}=\bigcap_{A\in\mathscr{A}}D(\overline{\pi_\omega(A)}^\alpha), \tag{3.4}$$

$$\pi_{\omega,\alpha}(A)X=\overline{\pi_\omega(A)}^\alpha X,\quad X\in D_{\omega,\alpha} \tag{3.5}$$

($\overline{T}^\alpha$ denotes the closure of T in the norm $\|\cdot\|_\alpha$). This J^*-representation has the following properties.

(A) For every $A\in\mathscr{A}$, $\pi_{\omega,\alpha}(A)$ is closed in $\mathscr{K}_{\omega,\alpha}$.

(B) $D_{\omega,\alpha}$ is complete in the topology defined by seminorms

$$\|X\|_{S,\alpha}=\sum_{A\in S}\|\pi_{\omega,\alpha}(A)X\|_\alpha$$

(S is a finite set of elements of $\mathscr{A}$).

(C) Let $(\pi_{\omega,\alpha_g}, D_{\omega,\alpha_g}, \{I_\omega(\alpha_g)\})$ be an α_g-closed extension of $(\pi_\omega, D_\omega, \{I_\omega(\alpha):\alpha\in P_\omega\})$ for some fixed $g\in G$. Then $U_g^{(\omega)}$: $D_{\omega,\alpha}\to D_{\omega,\alpha_g}$ and

$$U_g^{(\omega)}\pi_{\omega,\alpha}(A)X=\pi_{\omega,\alpha_g}(\tau_g(A))\,U_g^{(\omega)}X. \tag{3.6}$$

Proof: Since $D(\pi_\omega(A)^*)\supset D(\pi_\omega(A^*))=D_\omega$, $D(\pi_\omega(A)^*)$ is dense in $\mathscr{K}_{\omega,\alpha}$ (for every $\alpha\in P_\omega$) and, by Proposition 2.1, $\pi_\omega(A)$ is closable for every $A\in\mathscr{A}$. Hence, we can define $D_{\omega,\alpha}$ and $\pi_{\omega,\alpha}$. Similarly as in Ref. 3 one can show that $(\pi_{\omega,\alpha}, D_{\omega,\alpha})$ is a $*$-representation of $\mathscr{A}$. Now we complete the proof that $(\pi_{\omega,\alpha}\ D_{\omega,\alpha}, \{I_\omega(\alpha)\})$ ia a J^*-representation. First we show that $I_\omega(\alpha)D_{\omega,\alpha}\subset D_{\omega,\alpha}$. Let $X\in D_{\omega,\alpha}$.

There exists the sequence $\{X_n\}, X_n \in D_\omega$, such that $X_n \to X$ in $\mathscr{H}_{\omega,\alpha}$ and for every $A \in \mathscr{A}$, $\pi_\omega(A) X_n \to \overline{\pi_\omega(A)}^\alpha X$. Let $Y = I_\omega(\alpha) X$. For $Y_n = I_\omega(\alpha) X_n$ we have $Y_n \to Y$. Since

$$\pi_\omega(A) Y_n = \pi_\omega(A) I_\omega(\alpha) X_n = I_\omega(\alpha)\pi_\omega(\alpha(A)) X_n,$$

there exists the limit

$$\lim_n \pi_\omega(A) Y_n = Z \in \mathscr{H}_{\pi,\alpha}.$$

But $\pi_\omega(A)$ is closable, so $\overline{\pi_\omega(A)}^\alpha Y = Z$ and $Y \in D_{\omega,\alpha}$. It is easy to check that for every $X, Y \in D_{\omega,\alpha}$,

$$\langle \pi_{\omega,\alpha}(\alpha(A^*)) X, I_\omega(\alpha) Y\rangle_\alpha = \langle X, I_\omega(\alpha)\pi_{\omega,\alpha}(A) Y\rangle_\alpha. \quad (3.7)$$

Using the fact that $\pi_{\omega,\alpha}$ is a $*$-representation, from (3.7) we obtain

$$\pi_{\omega,\alpha}(\alpha(A)) I_\omega(\alpha) X = I_\omega(\alpha)\pi_{\omega,\alpha}(A) X.$$

Since point (A) is obvious and the proof of (B) is contained in Ref. 3, we have to show only point (C).

Let $X_n \to X$ in $\mathscr{H}_{\omega,\alpha}$ and $\pi_\omega(A) X_n \to \overline{\pi_\omega(A)}^\alpha X$. As $U_g^{(\omega)} X_n \to U_g^{(\omega)} X$ in $\mathscr{H}_{\omega,\alpha_g}$, the limit $\lim_n \pi_\omega(A) U_g^{(\omega)} X_n$ exists in $\mathscr{H}_{\omega,\alpha_g}$ and

$$\overline{\pi_\omega(A)}^{\alpha_g} U_g^{(\omega)} X = \lim_n \pi_\omega(A) U_g^{(\omega)} X_n.$$

Thus $U_g^{(\omega)} X \in D_{\omega,\alpha_g}$ for $X \in D_{\omega,\alpha}$ and

$$\begin{aligned} U_g^{(\omega)} \pi_{\omega,\alpha}(A) X &= \lim_n U_g^{(\omega)} \pi_\omega(A) X_n \\ &= \lim_n \pi_\omega(\tau_g(A)) U_g^{(\omega)} X_n \\ &= \pi_{\omega,\alpha_g}(\tau_g(A)) U_g^{(\omega)} X. \end{aligned}$$

IV. Op J^*-ALGEBRA GENERATED BY FIELD OPERATORS IN FOCK–KREIN SPACE

A. Tensor product of Krein spaces[9]

Let $(\mathscr{K}_1, \langle , \rangle_1)$ and $(\mathscr{K}_2, \langle , \rangle_2)$ be two Krein spaces. For a fixed $I_1 \in J(\mathscr{K}_1)$ and $I_2 \in J(\mathscr{K}_2)$ let us define

$$I = I_1 \otimes I_2. \quad (4.1)$$

For $\mathscr{K}_1 \otimes \mathscr{K}_2$ (tensor product in the sense of Hilbert spaces) we define

$$\langle x, y\rangle = (x, Iy). \quad (4.2)$$

Here, $(\mathscr{K}_1 \otimes \mathscr{K}_2, \langle , \rangle)$ is the Krein space, which we call the tensor product of Krein spaces. As one can easily check, such a defined tensor product of Krein spaces does not depend on the choice of $I_1 \in J(\mathscr{K}_1)$ and $I_2 \in (\mathscr{K}_2)$.

B. Direct sum of Krein spaces

Let $\{(\mathscr{K}_\gamma, \langle , \rangle_\gamma): \gamma \in A\}$ be a family of Krein spaces. Let us fix the sequence $\{I_\gamma: \gamma \in A\}$, $I_\gamma \in J(\mathscr{K}_\gamma)$. Then $\mathscr{K}^{\{I_\gamma\}}$ is the set of all sequences $\{X_\gamma: \gamma \in A\}, X_\gamma \in \mathscr{K}_\gamma$ satisfying

$$\sum_\gamma \|X_\gamma\|^2_{I_\gamma} < \infty. \quad (4.3)$$

If $X = \{X_\gamma\}$, $Y = \{Y_\gamma\}$, and $X, Y \in \mathscr{K}^{\{I_\gamma\}}$, then we define

$$\langle X, Y\rangle_{\{I_\gamma\}} = \sum_\gamma \langle X_\gamma, Y_\gamma\rangle_\gamma. \quad (4.4)$$

The space $(\mathscr{K}^{\{I_\gamma\}}, \langle , \rangle_{\{I_\gamma\}})$ with the topology defined by the norm

$$\|X\|^2_{\{I_\gamma\}} = \sum_\gamma \|X_\gamma\|^2_{I_\gamma} \quad (4.5)$$

will be called a *direct sum of Krein spaces* $\{(\mathscr{K}_\gamma, \langle , \rangle_\gamma): \gamma \in A\}$ *defined by the sequence* $\{I_\gamma: \gamma \in A\}$ and will be denoted by $\Sigma_\gamma^{\{I_\gamma\}} (\mathscr{K}_\gamma, \langle , \rangle_\gamma)$.

C. Fock–Krein space

Now let us consider the family of Krein spaces $(\mathscr{K}_n, \langle , \rangle_n): n = 0,1,2,...$, with $\mathscr{K}_n = \overset{n}{\otimes} \mathscr{K}$, $\mathscr{K}_0 = \mathbb{C}$, and $\langle \cdot, \cdot\rangle_n = (\cdot, \overset{n}{\otimes} I\cdot)_n$ (where $\mathscr{K}$ is the "one-particle" Krein space and $(\ ,\ )_n$ is the inner product in the Hilbert space $\overset{n}{\otimes} \mathscr{K}$). Also let us fix the sequence $\{I_n: n = 0,1,2,...\}$ with $I_0 = \mathbf{1}$, $I_n = \overset{n}{\otimes} I$, $I \in J(\mathscr{K})$. The direct sum

$$\Gamma_I(\mathscr{K}) = \sum_n^{\{I_n\}} (\mathscr{K}_n, \langle , \rangle_n) \quad (4.6)$$

we call *Fock–Krein space defined* by $I \in J(\mathscr{K})$. If $S_0 = 1$, $S_n = (1/n!) \Sigma_{\sigma \in P_n} \sigma$ (P_n the permutation group of n elements), then we define

$$\mathscr{K}_n^+ = S_n \mathscr{K}_n$$

and

$$\Gamma_I(\mathscr{K}) = \sum_n^{\{I_n\}} (\mathscr{K}_n^+, \langle , \rangle_n). \quad (4.7)$$

Let $\Gamma_0(\mathscr{K}) \subset \Gamma_I(\mathscr{K})$ be the set of sequences $X = \{X_n: n = 0,1,2,...\}$ containing only a finite number of X_n different from 0, then

$$\Gamma_I(\mathscr{K}) = \overline{\Gamma_0(\mathscr{K})}^{\|\cdot\|_{\{I_n\}}}. \quad (4.8)$$

For any $\tilde{I} \in J(\mathscr{K})$ such that $\tilde{I} \neq I$, we can define $\Gamma_{\tilde{I}}(\mathscr{K})$ as before, and also

$$\Gamma_{\tilde{I}}(\mathscr{K}) = \overline{\Gamma_0(\mathscr{K})}^{\|\cdot\|_{\{\tilde{I}_n\}}}. \quad (4.9)$$

For every $X_1, X_2 \in \Gamma_0(\mathscr{K})$, we have

$$\langle X_1, X_2\rangle_{\{\tilde{I}_n\}} = \langle X_1, X_2\rangle_{\{I_n\}} \quad (4.10)$$

and

$$(X_1, X_2)_{\{\tilde{I}_n\}} = (X_1, \Gamma(I\tilde{I}) X_2)_{\{I_n\}} \quad (4.11)$$

[$\Gamma(I\tilde{I})$ means the second quantization of $I\tilde{I}$].

Lemma 4.1: If $\tilde{I} \neq I$, the operator $\Gamma(I\tilde{I})$ defined on $\Gamma_0(\mathscr{K})$ is unbounded.

Proof: We first show that if $\tilde{I} \neq I$ then $\|I\tilde{I}\|_I > 1$ (see Ref. 6). For a fixed $I \in J(\mathscr{K})$, $\mathscr{K}_I$ is the Hilbert space and $B(\mathscr{K}_I)$ is the C^*-algebra with respect to the involution $A \to A^{*(I)} = IA^*I$, $I\tilde{I}$ is the positive self-adjoint element of $B(\mathscr{K}_I)$, and

$$\|I\tilde{I}\|_I = \sup\{|\lambda|: \lambda \in \mathrm{sp}(I\tilde{I})\}.$$

Since $(I\tilde{I})^{-1} = I(I\tilde{I})I$, if $\lambda \in \mathrm{sp}(I\tilde{I})$ then $\lambda^{-1} \in \mathrm{sp}(I\tilde{I})$. Thus $\|I\tilde{I}\|_I > 1$ when $\tilde{I} \neq I$. Thus, if $\tilde{I} \neq I$, $\Gamma(I\tilde{I})$ must be unbounded.[10]

Corollary 4.1: If $\tilde{I} \neq I$ the norms $\|\cdot\|_{\{\tilde{I}_n\}}$ and $\|\cdot\|_{\{I_n\}}$ defined on $\Gamma_0(\mathscr{K})$ are not equivalent.

D. Abstract field operators[11]

For every $F \in \mathscr{K}$ we define

$$b^-(F): \overset{n}{\otimes} \mathscr{K} \to \overset{n-1}{\otimes} \mathscr{K}$$

as

$$b^-(F) X_1 \otimes \cdots \otimes X_n = \langle F, X_1 \rangle X_2 \otimes \cdots \otimes X_n,$$
$$b^-(F) \mathscr{K}_0 = 0, \tag{4.12}$$

and

$$b^+(F): \overset{n}{\otimes} \mathscr{K} \to \overset{n+1}{\otimes} \mathscr{K}$$

as

$$b^+(F) X_1 \otimes \cdots \otimes X_n = F \otimes X_1 \otimes \cdots \otimes X_n. \tag{4.13}$$

If $N = \Gamma(\mathbf{1})$ and $S \upharpoonright \mathscr{K}_n = S_n$, we can define

$$a^-(F) = (N+1)^{1/2} b^{-1}(F),$$
$$a^+(F) = S b^+(F)(N+1)^{1/2}. \tag{4.14}$$

Then, the Segal field operator

$$\Phi_S(F) = 2^{-1/2}[a^-(F) + a^+(F)] \tag{4.15}$$

has the following properties: (A) $\Phi_S(F)$ is closable; (B) if $F_n \to F$ in $\mathscr{K}$, $\Phi_S(F_n) X \to \Phi_S(F) X$ in $\Gamma_I(\mathscr{K})$; (C) $\Omega_F = \{1,0,0,\ldots\} \in \Gamma_0(\mathscr{K})$ is a $\Gamma(I)$-cyclic vector, i.e., the set $\{\Phi_S(F_1) \cdots \Phi_S(F_n)\, \Omega_F: n = 1,2,\ldots\}$ is total in $\Gamma_I(\mathscr{K})$ and $\Gamma(I)\, \Omega_F = \Omega_F$; (D) $[\Phi_S(F_1), \Phi_S(F_2)] X = i \operatorname{Im} \langle F_1, F_2 \rangle X$; and (E) $\Phi_S(F)$ is essentially self-adjoint in $\Gamma_I(\mathscr{K})$.

E. Representation of a symmetry group

Suppose that the symmetry group G is represented by unitary operators $\{T_g: g \in G\}$ in the "one-particle" Krein space $\mathscr{K}$. Since, in general, $\|T_g\|_I > 1$, $U_g = \Gamma(T_g) \upharpoonright \Gamma_0(\mathscr{K})$ is unbounded. On the other hand, since $\Gamma(T_g)\Gamma(I)\Gamma(T_g)^* = \Gamma(T_g I T_g^{-1}) = \Gamma(I_g)$, we have that

$$U_g: \Gamma_I(\mathscr{K}) \to \Gamma_{I_g}(\mathscr{K}) \tag{4.16}$$

and U_g is the unitary mapping between two different Hilbert spaces. The properties of the family $\{U_g: g \in G\}$ can be summarized as follows: For every $g \in G$,

(A) $U_g: \Gamma_0(\mathscr{K}) \to \Gamma_0(\mathscr{K})$,

(B) $U_g: \Gamma_I(\mathscr{K}) \to \Gamma_{I_g}(\mathscr{K})$,

(C) $U_g: \Phi_S(F)\, U_g^* X = \Phi_S(T_g F) X$.

F. Properties of the Op J^*-algebra generated by field operators

Let $\mathscr{A}_F$ be the set of polynomials with complex coefficients over the set $\{\Phi_S(F): F \in \mathscr{K}\}$. Then $\mathscr{A}_F$ has the following properties.

(A) For every $A \in \mathscr{A}_F$, $A: \Gamma_0(\mathscr{K}) \to \Gamma_0(\mathscr{K})$.

(B) $\mathscr{A}_F$ is a $*$-algebra of operators in $\Gamma_0(\mathscr{K})$.

(C) $\Gamma_0(\mathscr{K})$ is dense in each Fock–Krein space $\Gamma_I(\mathscr{K})$, $I \in J(\mathscr{K})$. If $\tilde{I} \neq I$ then $\Gamma_{\tilde{I}}(\mathscr{K}) \setminus \Gamma_0(\mathscr{K}) \neq \Gamma_I(\mathscr{K}) \setminus \Gamma_0(\mathscr{K})$.

(D) For every $I \in J(\mathscr{K})$ there is a $*$-automorphism α_I of $\mathscr{A}_F$ defined by the extension of the formula

$$\alpha_I(\Phi_S(F)) = \Phi_S(IF),$$

where α_I is implemented by the operator $\Gamma(I)$ defined in $\Gamma_I(\mathscr{K})$.

(E) $\mathscr{A}_F$ is G-covariant, i.e., there exists the family $\{U_g: g \in G\}$ of operators in $\Gamma_0(\mathscr{K})$ implementing the group of $*$-automorphisms

$$\tau_g(\Phi_S(F)) = \Phi_S(\tau_g F).$$

If $\alpha_I \circ \tau_g \neq \tau_g \circ \alpha_I$, U_g is unbounded and

$$U_g: \Gamma_I(\mathscr{K}) \to \Gamma_{I_g}(\mathscr{K}).$$

(F) $\mathscr{A}_F$ is α_I-cyclic for every $I \in J(\mathscr{K})$, with a α_I-cyclic vector Ω_F. From these properties, $(\mathscr{A}_F, \Gamma_0(\mathscr{K}), \{\Gamma(I): I \in J(\mathscr{K})\})$ can be thought of as a J^*-representation of some abstract field algebra. Let us look at the state corresponding to this representation:

$$\omega_F(A) = \langle \Omega_F, A\, \Omega_F \rangle. \tag{4.17}$$

Functional (4.17) is α_I-positive for every $I \in J(\mathscr{K})$, so $P_{\omega_F} \simeq J(\mathscr{K})$. As was shown in Ref. 6, the set $J(\mathscr{K})$ has the following structure: for every pair $I_1, I_2 \in J(\mathscr{K})$ there exists $I_{2,1} \in J(\mathscr{K})$ such that $I_2 = I_{2,1} \cdot I_1 \cdot I_{2,1}$. Thus, for every $\alpha_{I_1}, \alpha_{I_2} \in P_{\omega_F}$ [not necessarily lying on the same orbit in $j(\mathscr{A}_F)$ with respect to the group G] there is the mapping $V_{2,1}$ satisfying

(A) $V_{2,1}: \Gamma_0(\mathscr{K}) \to \Gamma_0(\mathscr{K})$,

(B) $\langle V_{2,1} X, V_{2,1} Y \rangle_{\{I_{2n}\}} = \langle X, Y \rangle_{\{I_{1n}\}}$,

(C) $V_{2,1}\, \Gamma(I_1) = \Gamma(I_2)\, V_{2,1}$,

(D) $V_{2,1}: \Gamma_{I_1}(\mathscr{K}) \to \Gamma_{I_2}(\mathscr{K})$.

V. IRREDUCIBILITY OF J^*-REPRESENTATIONS

In this section we study the notion of irreducibility of some J^*-representations. We introduce the so-called α-irreducibility property that seems to be the natural one in the case of J^*-representations. As it turns out, in the case of GNS representation, α-irreducibility is equivalent to the extremality of the α-positive state. Moreover, for the so-called self-adjoint J^*-representations, our notion of irreducibility is equivalent to the intuitive property of nonexistence of nontrivial subrepresentations.

A. α-irreducibility of J^*-representations

Let $(\pi, D(\pi), \{I_\pi(\alpha): \alpha \in j(\pi)\})$ be a J^*-representation of a $*$-algebra $\mathscr{A}$. For a fixed $\alpha \in j(\pi)$ we define the following weak commutant:

$$(\pi)'_{\omega,\alpha} = \{\hat{B} \in B(\mathscr{K}_{\pi,\alpha}): \langle X, \hat{B}\pi(A)\, Y \rangle_\alpha = \langle \pi(A^*) X, \hat{B} Y \rangle_\alpha\}$$
$$\cap \{\hat{B} \in B(\mathscr{K}_{\pi,\alpha}): \langle X, \hat{B} I_\pi(\alpha)\, Y \rangle_\alpha = \langle I_\pi(\alpha) X, \hat{B} Y \rangle_\alpha\}. \tag{5.1}$$

We say that the J^*-representation is α-irreducible if $(\pi)'_{\omega,\alpha} = \{\lambda \mathbf{1}: \lambda \in \mathbb{C}\}$.

Remark: In this general case, irreducibility of a given J^*-representation depends on the choice of $\alpha \in j(\pi)$. When the GNS representation is G-covariant, then for $\alpha, \beta \in j(\pi)$ such that $\beta = \tau_g \circ \alpha \circ \tau_g^{-1}$ for some $g \in G$, there exists the isomorphic mapping

$$M_{\beta,\alpha}: (\pi_\omega)'_{\omega,\alpha} \to (\pi_\omega)'_{\omega,\beta}, \tag{5.2}$$

defined by

$$M_{\beta,\alpha}(\hat{B}) = U_g^{(\omega)}\,\hat{B}\,U_g^{(\omega)*}, \tag{5.3}$$

and for such α and β, the notion of irreducibility is unique. Suppose now, that the structure of the set $j(\mathscr{A})$ is such as in the case of a field algebra (Sec. IV F), i.e., for every α, $\beta \in j(\mathscr{A})$ there exists $\gamma \in j(\mathscr{A})$ satisfying $\beta = \gamma \circ \alpha \circ \gamma$. If for a given state ω, for every $\alpha, \beta \in P_\omega$ the corresponding γ satisfies $\omega \circ \gamma = \omega$, then there exists also the isomorphic mapping of type (5.2) and the property of irreducibility depends only on the representation itself.

Let ω be an α-positive state on $\mathscr{A}$. For a fixed $\alpha \in P_\omega$, we define the set

$$E_\alpha^\omega = \{\tilde{\omega}\colon\ \tilde{\omega} \text{ is } \alpha\text{-positive}\}.$$

We say that the state ω is *α-extremal* if ω is an extremal point of the set E_α^ω (and in this case we write $\omega \in \partial_e E_\alpha^\omega$).

Proposition 5.1: $\omega \in \partial_e E_\alpha^\omega$ iff $(\pi_\omega)'_{\omega,\alpha} = \{\lambda\,1 : \lambda \in \mathbb{C}\}$.

Proof: Suppose that $\omega \notin \partial_e E_\alpha^\omega$. There exist $\omega_1, \omega_2 \in E_\alpha^\omega$ such that $\omega = \lambda\,\omega_1 + (1-\lambda)\omega_2$ and $\omega_1 \neq \omega_2$. Let us define

$$b_\alpha(X_A^\omega, X_B^\omega) = \lambda\omega_1(\alpha(A^*)B). \tag{5.4}$$

Since

$$0 \leqslant b_\alpha(X_A^\omega, X_B^\omega) = \lambda\omega_1(\alpha(A^*)A) < \omega(\alpha(A^*)A) = \|X_A^\omega\|_\alpha^2$$

there exists $\hat{B} \in B(\mathscr{H}_{\omega,\alpha})$, $\hat{B} < 1$, such that

$$b_\alpha(X_A^\omega, X_B^\omega) = (X_A^\omega, \hat{B}X_B^\omega)_\alpha.$$

It is easy to check that $\hat{B} \in (\pi_\omega)'_{\omega,\alpha}$, so $(\pi_\omega)'_{\omega,\alpha}$ is not trivial. Suppose now that $\hat{B} \in (\pi_\omega)'_{\omega,\alpha}$ and $\hat{B} \neq_\mu 1$. Take $0 < \hat{B} < 1$, i.e., $0 < (X, \hat{B}X)_\alpha < (X, X)_\alpha$. Since $(\Omega, \hat{B}\Omega)_\alpha > 0$ we can define two states

$$\omega_1(A) = \|\hat{B}^{1/2}\Omega\|_\alpha^{-2}(\Omega, \hat{B}\pi_\omega(A)\Omega)_\alpha,$$
$$\omega_2(A) = \|(1-\hat{B})^{1/2}\Omega\|_\alpha^{-2}(\Omega, (1-\hat{B})\pi_\omega(A)\Omega)_\alpha.$$

Thus we have $\omega_1,\ \omega_2 \in E_\alpha^\omega$ and $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ $[\lambda = (\Omega, \hat{B}\Omega)_\alpha]$.

B. Reducing subspaces and self-adjoint J^*-representations

Now we consider another characterization of irreducibility of the given representation, i.e., nonexistence of nontrivial subrepresentations. For a J^*-representation $(\pi, D(\pi), \{I_\pi(\alpha)\colon\ \alpha \in j(\pi)\})$ we introduce the notion of an *α-reducing subspace*, i.e., a subspace $D_\alpha \subset D(\pi)$ such that

(A) $\pi(\mathscr{A})\,D_\alpha \subset D_\alpha$,

(B) $I_\pi(\alpha)\,D_\alpha \subset D_\alpha$.

For any α-reducing subspace D_α, $(\pi \restriction D_\alpha, D_\alpha, \{I_\pi(\alpha)\})$ is also a J^*-representation of $\mathscr{A}$ and moreover, $\hat{D}_\alpha = \overline{D_\alpha}^{\|\cdot\|_\alpha}$ is an orthocomplemented subspace of the Krein space $\mathscr{H}_{\pi,\alpha}$, i.e.,

$$\mathscr{H}_{\pi,\alpha} = \hat{D}_\alpha \oplus \hat{D}_\alpha^\perp$$

(not every closed subspace of the Krein space is orthocomplemented). In this context it is natural to call a J^*-representation α-irreducible if it has no nontrivial α-reducing subspaces. But in the general case there is no connection between this definition of α-irreducibility and the previous one, because the set $(\pi)'_{\omega,\alpha}$ is not even an algebra. In this subsection we define, following Ref. 3, the class of J^*-representations for which the set $(\pi)'_{\omega,\alpha}$ is the von Neumann algebra of operators in $\mathscr{H}_{\pi,\alpha}$. Let

$$D(\pi^*) = \bigcap_{A \in \mathscr{A}} D(\pi(A)^*), \tag{5.5}$$

$$\pi^*(A)\,X = \pi(A^*)^*X, \quad X \in D(\pi^*). \tag{5.6}$$

Proposition 5.2: For a fixed $\alpha \in j(\pi)$, $(\pi^*, D(\pi^*))$ has the following properties: (A) $(\pi^*, D(\pi^*))$ is the representation of $\mathscr{A}$; and (B) $\pi^*(\alpha(A))X = I_\pi(\alpha)\pi^*(A)I_\pi(\alpha)\,X$, $X \in D(\pi^*)$.

Proof: (A) One can repeat the corresponding proof from Ref. 3 having in mind the characterization of the set $D(\pi(A)^*)$ (Lemma 2.2).

(B) Let $X \in D(\pi^*)$, $Y \in D(\pi)$. Since

$$|\langle I_\pi(\alpha)\,X, \pi(A)Y\rangle_\alpha| = |\langle X, \pi(\alpha(A))I_\pi(\alpha)\,Y\rangle_\alpha| \leqslant k\,\|I_\pi(\alpha)\,Y\|_\alpha = k\,\|Y\|_\alpha$$
$$[I_\pi(\alpha)\,Y \in D(\pi)],$$

$I_\pi(\alpha)\,X \in D(\pi^*)$ and $I_\pi(\alpha)\colon D(\pi^*) \to D(\pi^*)$. For every $X \in D(\pi^*)$ and $Y \in D(\pi)$, we have

$$\langle X, I_\pi(\alpha)\pi(A)I_\pi(\alpha)\,Y\rangle_\alpha = \langle I_\pi(\alpha)\pi(A^*)I_\pi(\alpha)\,X, Y\rangle_\alpha,$$

thus

$$(I_\pi(\alpha)\pi(A)I_\pi(\alpha))^*X = I_\pi(\alpha)\pi(A)^*I_\pi(\alpha)X, \quad X \in D(\pi^*),$$

and

$$\pi^*(\alpha(A))X = \pi(\alpha(A^*))X = (I_\pi(\alpha)\pi(A^*)I_\pi(\alpha))^*X$$
$$= I_\pi(\alpha)\pi(A^*)^*I_\pi(\alpha)X = I_\pi(\alpha)\pi^*(A)I_\pi(\alpha)X.$$

One can show the following proposition by a method similar to that in Ref. 3.

Proposition 5.3: For every $\hat{B} \in (\pi)'_{\omega,\alpha}$, we have

$$\hat{B}D(\pi) \subset D(\pi^*), \quad \hat{B}\pi(A)X = \pi^*(A)\hat{B}X, \quad X \in D(\pi).$$

At this point it is natural to introduce the following notion: a J^*-representation $(\pi, D(\pi), \{I_\pi(\alpha)\colon\ \alpha \in j(\pi)\})$ is *$*$-self-adjoint in the Krein space $K_{\pi,\alpha}$* if for $(\pi^*, D(\pi^*))$ we have $D(\pi^*) = D(\pi)$ and $\pi^* = \pi$.

Corollary 5.1: [12] For the $*$-self-adjoint J^*-representation in the Krein space $\mathscr{H}_{\pi,\alpha}$ the set $(\pi)'_{\omega,\alpha}$ is the von Neumann algebra of operators in $\mathscr{H}_{\pi,\alpha}$.

For the formulation of the next proposition, we have to introduce the following notion: $D_\alpha \subset D(\pi)$ is a $*$-self-adjoint α-reducing subspace if J^*-representation $(\pi \restriction D_\alpha, D_\alpha, \{I_\pi(\alpha)\})$ is $*$-self-adjoint in the Krein space $\hat{D}_\alpha$.

Proposition 5.4: For a $*$-self-adjoint J^*-representation of $\mathscr{A}$ there is a one-to-one correspondence between projection (in the sense of Krein space) in $(\pi)'_{\omega,\alpha}$ and $*$-self-adjoint α-reducing subspaces.

Proof: Suppose that $\hat{E} \in (\pi)'_{\omega,\alpha}$ and $\hat{E}^2 = \hat{E}$, $\hat{E}^* = \hat{E}$. Let us define $D_\alpha = \hat{E}D(\pi)$. Since $\hat{E}\colon D(\pi) \to D(\pi)$, $D_\alpha \subset D(\pi)$. On the other hand,

$$\pi(A)D_\alpha = \pi(A)\hat{E}D(\pi) = \hat{E}\pi(A)D(\pi) \subset D_\alpha,$$
$$I_\pi(\alpha)D_\alpha = I_\pi(\alpha)\hat{E}D(\pi) = \hat{E}I_\pi(\alpha)D(\pi) \subset D_\alpha.$$

So D_α is an α-reducing subspace. To show that D_α is a $*$-self-adjoint α-reducing subspace, one can repeat the corresponding proof from Ref. 3. Suppose now that D_α is a $*$-self-ad-

joint α-reducing subspace for the $*$-self-adjoint representation $(\pi, D(\pi), \{I_\pi(\alpha): \alpha \in j(\pi)\})$. Let $\hat{E}$ be a projector (in the sense of Hilbert space) on the closure of D_α in $\mathscr{H}_{\pi,\alpha}$. Hence $\hat{E}D(\pi) \supset D_\alpha$. Now we show that $\hat{E}D(\pi) \subset D_\alpha$. Let $X \in \hat{E}D(\pi)$, $X = \hat{E}\tilde{X}$ with $\tilde{X} \in D(\pi)$. For every $Y \in D_\alpha$, we have

$$\begin{aligned}
&\langle X, \pi(A)Y\rangle_\alpha \\
&\quad = \langle \hat{E}\tilde{X}, \pi(A)Y\rangle_\alpha = (\hat{E}\tilde{X}, I_\pi(\alpha)\pi(A)Y)_\alpha \\
&\quad = (\hat{E}\tilde{X}, \pi(\alpha(A))I_\pi(\alpha)Y)_\alpha = (\tilde{X}, \hat{E}\pi(\alpha(A))I_\pi(\alpha)Y)_\alpha \\
&\quad = (\tilde{X}, \pi(\alpha(A))I_\pi(\alpha)Y)_\alpha = \langle \tilde{X}, \pi(A)Y\rangle_\alpha.
\end{aligned}$$

Since $\tilde{X} \in D(\pi) = D(\pi^*)$, for every $Y \in D(\pi)$,

$$|\langle \tilde{X}, \pi(A)Y\rangle_\alpha| \leqslant k\|Y\|_\alpha.$$

Thus

$$|\langle X, \pi(A)Y\rangle_\alpha| = |\langle \tilde{X}, \pi(A)Y\rangle_\alpha| \leqslant k\|Y\|_\alpha,$$

for every $Y \in D_\alpha$, so $X \in D((\pi(A) \restriction D_\alpha)^*)$. But $\pi \restriction D_\alpha$ is $*$-self-adjoint, so $X \in D(\pi \restriction D_\alpha) = D_\alpha$.

Now let $X, Y \in D(\pi)$, since

$$(I_\pi(\alpha)X, \hat{E}Y)_\alpha = (X, \hat{E}I_\pi(\alpha)\hat{E}Y)_\alpha$$

and

$$\begin{aligned}
(\hat{E}X, I_\pi(\alpha)Y)_\alpha &= (I_\pi(\alpha)\hat{E}X, Y)_\alpha \\
&= (\hat{E}I_\pi(\alpha)\hat{E}X, Y)_\alpha = (X, \hat{E}I_\pi(\alpha)\hat{E}Y)_\alpha,
\end{aligned}$$

we have

$$(I_\pi(\alpha)X, \hat{E}Y)_\alpha = (\hat{E}X, I_\pi(\alpha)Y)_\alpha.$$

On the other hand, for every $A \in \mathscr{A}$ and $X, Y \in D(\pi)$, we have

$$(\pi(\alpha(A^*))X, \hat{E}Y)_\alpha = (X, \hat{E}\pi(A)EY)_\alpha$$

and

$$\begin{aligned}
(\hat{E}X, \pi(A)Y)_\alpha &= (\pi(\alpha(A^*))\hat{E}X, Y)_\alpha \\
&= (\hat{E}\pi(\alpha(A^*))\hat{E}X, Y)_\alpha = (X, \hat{E}\pi(A)\hat{E}Y)_\alpha.
\end{aligned}$$

So we also have

$$(X, \hat{E}\pi(A)Y)_\alpha = (\pi(\alpha(A^*))X, \hat{E}Y)_\alpha.$$

From these two equalities, it follows that $\hat{E}^* = \hat{E}$ and $\hat{E} \in (\pi)'_{w,\alpha}$.

Corollary 5.2: For $*$-self-adjoint J^*-representations in the Krein space, α-irreducibility is equivalent to the nonexistence of nontrivial $*$-self-adjoint subrepresentation.

VI. INTEGRAL DECOMPOSITION OF J^*-REPRESENTATIONS

In this section we consider the problem of decomposition of a J^*-representation of some topological $*$-algebra into α-irreducible parts. As in the standard case we should decompose π with respect to a maximal Abelian algebra in the weak commutant $(\pi)'_{w,\alpha}$. But since operators $\pi(A)$, $A \in \mathscr{A}$, are unbounded, the weak commutant is, in general, not an algebra and we have to extend the operators $\pi(A)$, $A \in \mathscr{A}$, in such a way that the weak commutant will coincide with the strong one. To do this we can apply the extension theory from Ref. 4.

Let $(\pi, D(\pi), \{I_\pi(\alpha): \alpha \in j(\pi)\})$ be a J^*-representation and $\alpha \in j(\pi)$ be fixed. Then $(\{\pi(A): A \in \mathscr{A}\}, I_\pi(\alpha): D(\pi))$ is the operator family in the Hilbert space $\mathscr{H}_{\pi,\alpha}$ (we assume that $\mathscr{H}_{\pi,\alpha}$ is separable). Let us define the strong commutant $(\pi)'_{s,\alpha}$ as

$$\begin{aligned}
(\pi)'_{s,\alpha} = \{\hat{B} \in B(\mathscr{H}_{\pi,\alpha}): \hat{B}D(\pi) \subset D(\pi) \text{ and} \\
\hat{B}\pi(A)X = \pi(A)\hat{B}X,\ \hat{B}I_\pi(\alpha)X = I_\pi(\alpha)\hat{B}X\}.
\end{aligned} \tag{6.1}$$

Now we can formulate the following proposition.

Proposition 6.1 [13]: For the operator family $(\{\pi(A): A \in \mathscr{A}\}, I_\pi(\alpha); D(\pi))$ there exists a so-called maximal regular induced extension in the separable Hilbert space $\tilde{\mathscr{H}}_{\pi,\alpha}$: $(\{\tilde{\pi}(A);\ A \in \mathscr{A}\}, \tilde{I}_\pi(\alpha), \tilde{N}, \tilde{D}(\pi))$ such that

$$(\tilde{\pi})'_{w,\alpha} \cap \tilde{N}' = (\tilde{\pi})'_{s,\alpha} \cap \tilde{N}' = \tilde{N}, \tag{6.2}$$

where $\tilde{N}$ is a commutative algebra of operators in $\tilde{\mathscr{H}}_{\pi,\alpha}$.

From the above proposition follows that $\{\tilde{N}, \tilde{\mathscr{H}}_{\pi,\alpha}\}$ is the commutative von Neumann algebra of operators in $\tilde{\mathscr{H}}_{\pi,\alpha}$. There exists the measure space (Λ, μ) such that[14]

$$\{\tilde{N}, \tilde{\mathscr{H}}_{\pi,\alpha}\} = \int_\Lambda^\oplus \{\tilde{N}_\lambda, \tilde{\mathscr{H}}_{\pi,\alpha;\lambda}\}\, d\mu(\lambda). \tag{6.3}$$

Equation (6.3) means that $\tilde{\mathscr{H}}_{\pi,\alpha}$ is the direct integral of Hilbert spaces $\{\tilde{\mathscr{H}}_{\pi,\alpha;\lambda}: \lambda \in \Lambda\}$ and $\tilde{N}$ contains diagonal operators with respect to the decomposition

$$\tilde{\mathscr{H}}_{\pi,\alpha} = \int_\Lambda^\oplus \tilde{\mathscr{H}}_{\pi,\alpha;\lambda}\, d\mu(\lambda). \tag{6.4}$$

Proposition 6.2 [15]: Suppose that $D(\pi)$ is a separable nuclear vector space and $\{\pi(A): A \in \mathscr{A}\}$ is a separable topological space. Suppose also that (1) the imbedding $D(\pi) \to \mathscr{H}_{\pi,\alpha}$ is continuous; (2) the mapping $(\pi(A), X) \mapsto \pi(A)X$ is separately continuous on $\pi(\mathscr{A}) \times D(\pi) \to D(\pi)$; and (3) the mapping $I_\pi(\alpha)$: $D(\pi) \to D(\pi)$ is continuous. Let $(\{\tilde{\pi}(A): A \in \mathscr{A}\}, \tilde{I}_\pi(\alpha), \tilde{N}, \tilde{D}(\pi))$ be the maximal regular extension and

$$\{\tilde{N}, \tilde{\mathscr{H}}_{\pi,\alpha}\} = \int_\Lambda^\oplus \{\tilde{N}_\lambda, \tilde{\mathscr{H}}_{\pi,\alpha;\lambda}\}\, d\mu(\lambda)$$

be the corresponding decomposition of $\{\tilde{N}, \tilde{\mathscr{H}}_{\pi,\alpha}\}$. Then for every $\lambda \in \Lambda$ there is a linear mapping E_λ: $D(\pi) \to \tilde{\mathscr{H}}_{\pi,\alpha;\lambda}$ such that we have the following.

(A) $D_\lambda = E_\lambda D(\pi)$ is a nuclear space, continuously imbedded in $\tilde{\mathscr{H}}_{\pi,\alpha;\lambda}$ and dense in $\tilde{\mathscr{H}}_{\pi,\alpha;\lambda}$ for μ-almost all $\lambda \in \Lambda$.

(B) For all $X \in D(\pi)$,

$$X = \int_\Lambda^\oplus E_\lambda X\, d\mu(\lambda).$$

(C) $\pi_\lambda(A)E_\lambda X := E_\lambda(\pi(A)X)$ defines for μ-almost all λ the linear operator such that $\pi_\lambda(A)D_\lambda \subset D_\lambda$.

(D) $I_\lambda(\alpha)E_\lambda X := E_\lambda(I_\pi(\alpha)X)$ defines for μ-almost all λ the linear operator such that $I_\lambda(\alpha)^2 = \mathbf{1}_\lambda$ and

$$(I_\lambda(\alpha)E_\lambda X, E_\lambda Y)_{\alpha;\lambda} = (E_\lambda X, I_\lambda(\alpha)E_\lambda Y)_{\alpha;\lambda}.$$

(E) The mapping $\pi(A) \to \pi_\lambda(A)$ preserves all algebraic relations.

(F) $\pi_\lambda(\alpha(A))E_\lambda X = I_\lambda(\alpha)\pi_\lambda(A)I_\lambda(\alpha)E_\lambda X$ for μ-almost all λ.

(G) $(\pi_\lambda)'_{w,\alpha} = \{\rho\, \mathbf{1}_\lambda: \rho \in \mathbf{C}\}$ for μ-almost all λ.

For the application of this result to our problem, we need some topology on the algebra $\mathscr{A}$. If we assume that $\mathscr{A}$

is a separable, nuclear topological algebra and π is strongly continuous and α-cyclic (with α-cyclic vector Ω_π), then we can define the nuclear topology on $D(\pi) = \pi(\mathscr{A})\Omega_\pi$ as the quotient topology of $\mathscr{A}$ modulo the kernel of the continuous map

$$\Phi_\pi\colon\ \mathscr{A} \to \pi(\mathscr{A})\Omega_\pi \subset \mathscr{K}_{\pi,\alpha}.$$

If we put also the quotient topology of $\mathscr{A}/\ker\pi$ on $\pi(\mathscr{A})$ we obtain the following results: (A) $D(\pi)$ is a separable nuclear vector space; (B) $\pi(\mathscr{A})$ is a separable topological space; and (C) the mapping $\pi(\mathscr{A}) \times D(\pi) \ni (\pi(A), X) \mapsto \pi(A)X$ is separately continuous. Since (by assumption) the $*$-automorphism α is continuous on $\mathscr{A}$ we have also that (D) the mapping $I_\pi(\alpha)\colon\ D(\pi) \to D(\pi)$ is continuous.

Corollary 6.1: Let $\mathscr{A}$ be a separable nuclear $*$-algebra and $(\pi, D(\pi), \{I_\pi(\alpha)\})$ be a strongly continuous α-cyclic J^*-representation of $\mathscr{A}$. Then there exists a separable Hilbert space $\tilde{\mathscr{K}}_{\pi,\alpha}$ containing $\mathscr{K}_{\pi,\alpha}$ as a closed subspace, a direct integral decomposition

$$\tilde{\mathscr{K}}_{\pi,\alpha} = \int_\Lambda^\oplus \tilde{\mathscr{K}}_{\pi,\alpha;\lambda}\, d\mu(\lambda),$$

and strongly continuous representations (in the sense of Hilbert space) $\{(\pi_\lambda, D_\lambda)\colon \lambda \in \Lambda\}$ such that (A) for every $X \in D(\pi)$,

$$\pi(A)X = \int_\Lambda^\oplus \pi_\lambda(A)X_\lambda\, d\mu(\lambda);$$

(B) $\pi_\lambda(\alpha(A))X_\lambda = I_\lambda(\alpha)\pi_\lambda(A)I_\lambda(\alpha)X_\lambda$ for μ-almost all λ, where

$$I_\pi(\alpha) = \int_\Lambda^\oplus I_\lambda(\alpha)\, d\mu(\lambda);$$

and (C) $(\pi_\lambda)'_{w,\alpha} = \{\rho\, \mathbb{1}_\lambda\colon \rho \in \mathbb{C}\}$ for μ-almost all λ.

Remark: For μ-almost all $\lambda \in \Lambda$, $(\pi_\lambda, D_\lambda, \{I_\lambda(\alpha)\})$ is a J^*-representation of $\mathscr{A}$ since (A) $(D_\lambda, \langle\,,\,\rangle_\lambda)$ is an indefinite inner product space with respect to $\langle\,,\,\rangle_\lambda := (\cdot, I_\lambda(\alpha)\cdot)_{\alpha;\lambda}$;

(B)
$$\begin{aligned}\langle \pi_\lambda(A)X_\lambda, Y_\lambda\rangle_\lambda &= (\pi_\lambda(A)X_\lambda, I_\lambda(\alpha)Y_\lambda)_{\alpha;\lambda}\\ &= (X_\lambda, \pi_\lambda(\alpha(A^*))I_\lambda(\alpha)Y_\lambda)_{\alpha;\lambda}\\ &= (X_\lambda, I_\lambda(\alpha)\pi_\lambda(A^*)Y_\lambda)_{\alpha;\lambda}\\ &= \langle X_\lambda, \pi_\lambda(A^*)Y_\lambda\rangle_\lambda;\end{aligned}$$

and

(C) $I_\lambda(\alpha)^2 = \mathbb{1}_\lambda$; $\langle I_\lambda(\alpha)X_\lambda, Y_\lambda\rangle_\lambda = \langle X_\lambda, I_\lambda(\alpha)Y_\lambda\rangle_\lambda$.

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A metric space construction for the boundary of space-time

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A distance function between points in space-time is defined and used to consider the manifold as a topological metric space. The properties of the distance function are investigated: conditions under which the metric and manifold topologies agree, the relationship with the causal structure of the space-time and with the maximum lifetime function of Wald and Yip, and in terms of the space of causal curves. The space-time is then completed as a topological metric space; the resultant boundary is compared with the causal boundary and is also calculated for some pertinent examples.

I. INTRODUCTION

The singularity theorems of Penrose and Hawking demonstrate that in many cases solutions of Einstein's equation must be singular (Hawking and Ellis,[1] hereinafter HE, Chap. 8). The theorems do not say much about the form this singular behavior will take, however, because the manifolds which represent space-time in general relativity do not include the singularities. The approach to studying the singular behavior thus has been to attach a boundary to the space-time manifold, i.e., to define a new topological space in which the space-time is an open, dense subspace. One then interprets the points of the boundary as "singular points."[2] To describe the singular behavior precisely Einstein's equation must now be solved near the singularity. Here "near" is defined by the procedure used to attach the boundary to space-time.

Several boundary constructions have been given (HE,[1] Chaps. 6 and 8; Beem and Ehrlich,[3] hereinafter BE, Chap. 5), but all suffer from some drawback. The b-boundary construction[4] has been shown to have unphysical topological properties[5] as has, recently, a wide class of constructions, including the g boundary,[6] by Geroch, Liang, and Wald.[7] Moreover, in general it is difficult or impossible to extend the causal and differentiable structure of the space-time to the boundary. Clearly this is crucial to solving the equations near the singularity. Belinskii, Khalatnikov, and Lifshitz[8] did this using a method of successive approximations in Einstein's equations, assuming certain coordinate conditions. The validity of these coordinate conditions has been examined by Barrow and Tipler[9] and more recently by Wald and Yip[10] in the special case of "simultaneous synchronous coordinates" (Gaussian normal coordinates in which the singularity takes place everywhere at $t = 0$), although the most general version[8] of the work of Belinskii, Khalatnikov, and Lifshitz does not use simultaneous synchronous coordinates.

This paper suggests a new approach through which solutions to some of these problems may be found. The manifold is made into a topological metric space by the introduction of a distance function, where the distance between two points is a measure of the difference between the chronological pasts and futures of the points. The metric space is then completed and the additional points form the boundary of this construction. Although the metric defined here is not differentiable it may be usable to obtain bounds for derivatives in some approximation procedure. And by its very nature, of course, it provides a precise definition of "near" a singularity. Moreover, being closer in spirit to the causal boundary construction of Geroch, Kronheimer, and Penrose,[2] it is more "global" than the constructions considered by Geroch, Liang, and Wald[7] and avoids the difficulties in the example they present.

In Sec. II we define the distance function D and show that it is a metric. In Sec. III we investigate some properties of the metric, concentrating on its continuity, since when D is continuous, the metric and manifold topologies agree. We consider necessary and sufficient conditions for continuity, relating properties of D to the causal structure of the space-time, to conditions on the maximum lifetime function of Wald and Yip,[10] and in terms of the space of causal curves on M, given the usual C^0 topology.

We construct the D boundary in Sec. IV and consider several examples. Then, in order to compare the D boundary to the related causal boundary, we define a causal structure on the completed metric space. This enables us to show that the part of the D boundary which has either a past or a future is homeomorphic to the part of the causal boundary which is generated by uniformly continuous curves, thus generalizing some of the observations made in the discussion of the examples. Finally in the conclusion, Sec. V, we summarize and suggest further directions to be investigated.

II. PRELIMINARIES

Let (M,g) be a space-time, i.e., a paracompact connected C^∞ Hausdorff manifold with a Lorentz metric g of signature $(-,+,+,+)$ and a time orientation. Denote the proper length of a future directed causal curve $\gamma: F \to M$ (F an interval of $\mathbb{R}$) by $L(\gamma)$. (The notation is as in HE[1] unless otherwise indicated.) The height of any subset $U \subset M$ is defined to be

$$d(U) \equiv \sup L(\gamma),$$

where γ ranges over all future directed causal curves contained in U.

Consider the collection of past sets in M, alternatively $\{U \subset M : U = I^-(U)\}$. We define the distance between two past sets to be

$$D(U,V) \equiv d(U \triangle V),$$

where

$$U \triangle V \equiv (U - V) \cup (V - U)$$

is the symmetric difference of U and V.

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Proposition 2.1: D is a topological metric on the collection of past sets in M.

Proof: D must satisfy three conditions.

(i) $D(U,V) \geqslant 0$ and $D(U,V) = 0 \Leftrightarrow U = V$. That D is non-negative is immediate since $L(\gamma)$ is. If $U = V$ then $U \triangle V = \varnothing$ so $D(U,V) = 0$. Conversely, suppose $D(U,V) = 0$ but $U \neq V$. Then there is a $p \in U - V$, say. Since U,V are past sets, $I^+(p) \cap (U - V) \neq \varnothing$ so there is a $q \in U - V$ such that $q \in I^+(p)$. Connecting p and q by a timelike curve forces $D(U,V) > 0$, a contradiction.

(ii) $D(U,V) = D(V,U)$. Trivial since the symmetric difference is symmetric.

(iii) $D(U,V) \leqslant D(U,W) + D(W,V)$ (triangle inequality). First observe that for $A,B \subset M$, $d(A \cup B) \leqslant d(A) + d(B)$. To see this consider the image of a causal curve $\gamma \subset A \cup B$. Let $\gamma_A = \gamma \cap A, \gamma_B = \gamma \cap B$. Then $L(\gamma_A) \leqslant d(A), L(\gamma_B) \leqslant d(B)$, so

$$L(\gamma) \leqslant L(\gamma_A) + L(\gamma_B) \leqslant d(A) + d(B).$$

Since this holds for all $\gamma \subset A \cup B$ the result follows. Now,

$$U \triangle V \subset (U \triangle W) \cup (W \triangle V),$$

since any point in $U \triangle V$ is in exactly one of U and V and is thus in exactly one of U and W or exactly one of W and V. So applying this result gives

$$\begin{aligned} D(U,V) &= d(U \triangle V) \\ &\leqslant d(U \triangle W) + d(W \triangle V) \\ &= D(U,W) + D(W,V). \end{aligned}$$

Property (iii), the triangle inequality, is really the key property. The triangle inequality is often the hardest property to satisfy when one attempts to define a topological metric. The fact that it emerges neatly here out of the causal structure of space-time is some reason to take D seriously.

Now we use D to define a topological metric on M. Let

$$D^-(p,q) \equiv D(I^-(p), I^-(q)), \quad p,q \in M.$$

Proposition 2.2: Provided (M,g) is distinguishing, D^- is a topological metric on M.

Proof: Since $I^-(p)$ and $I^-(q)$ are past sets, the proof of Proposition 2.1 carries over line by line except for the second statement in (i). But (M,g) is distinguishing means that for all $p,q \in M$, if $I^+(p) = I^+(q)$ or $I^-(p) = I^-(q)$, then $q = p$. Thus $D^-(p,q) = 0 \Leftrightarrow p = q$.

Replacing past by future throughout the preceding discussion gives a dually defined metric D^+. (For most of the definitions and results which follow, only one of the past–future dyad will be stated explicitly; the dual is to be assumed.) Then, abusing the notation slightly, we define

$$D(p,q) \equiv D^+(p,q) + D^-(p,q), \quad p,q \in M,$$

and observe that D is a metric on M since D^+ and D^- are. The pair (M,D) is now a topological metric space so we will be able to complete it and thus effectively to attach a boundary to M. Before doing so, however, we investigate some of the properties of (M,D).

III. PROPERTIES

Although D is a metric on M, $D(p,q)$ need not be finite. For example, Minkowski space $D(p,q)$ is infinite for all $p \neq q \in M$, since there are timelike curves of arbitrarily long length in $I^-(p) \triangle I^-(q)$. To avoid situations like this we restrict our attention to space-times of finite timelike diameter (BE,[3] p. 329), that is, those with finite length for all timelike curves. This includes, e.g., the closed Friedmann universe, the region $0 < r < 2m$ in the maximally extended Schwarzschild solution, and any globally hyperbolic space-time which is the future development of a Cauchy surface on which the maximum lifetime function of Wald and Yip[10] is finite.

Since $D(p,q)$ depends on the length of curves in

$$p \triangle q \equiv (I^-(p) \triangle I^-(q)) \cup (I^+(p) \triangle I^+(q)),$$

even restricting D to be finite does not prevent properties of the space-time far from p and q being reflected in the behavior of D near p and q. In particular, consider the continuity of D. Two-dimensional "step Minkowski space" gives an example where D is neither upper nor lower semicontinuous. In Fig. 1,

$$D(p,q) \leqslant \limsup D(p,q_n),$$

$$D(q,r) \geqslant \liminf D(q_n,r).$$

We will investigate conditions on (M,g) under which D is continuous for the following reason. Define $\mathscr{D}$ to be the metric topology, i.e., the topology generated by the open balls of D:

$$B_\epsilon(p) \equiv \{q \in M : D_p(q) < \epsilon\},$$

where $D_p(q) \equiv D(p,q)$. We have then the following theorem.

Theorem 3.1: D is continuous $\Leftrightarrow$ $\mathscr{D}$ agrees with $\mathscr{M}$, where $\mathscr{M}$ is the manifold topology.

The importance of this property will become apparent when we attach a boundary to M using this construction. Before giving the proof we prove a lemma.

Lemma 3.2: D is continuous $\Leftrightarrow$ D^+ and D^- are continuous.

Proof: ($\Leftarrow$) Trivial.

($\Rightarrow$) D is continuous means, since M is paracompact, that $p_n \to p$, $q_n \to q \Rightarrow D(p_n,q_n) \to D(p,q)$. Thus $p_n \to p \Rightarrow D_p(p_n) \to 0$. Moreover, the converse holds as well: if $p_n \to p \Rightarrow D_p(p_n) \to 0$ and $q_n \to q \Rightarrow D_q(q_n) \to 0$, the triangle inequality gives

$$D(p_n,q_n) \leqslant D(p,p_n) + D(p,q) + D(q_n,q),$$

$$D(p,q) \leqslant D(p,p_n) + D(p_n,q_n) + D(q_n,q),$$

so $D(p_n,q_n) \to D(p,q)$.

Thus D is continuous $\Leftrightarrow$ D_p is continuous for all $p \in M$. But $p_n \to p$ implies

$$D_p(p_n) = D_p^+(p_n) + D_p^-(p_n) \to 0.$$

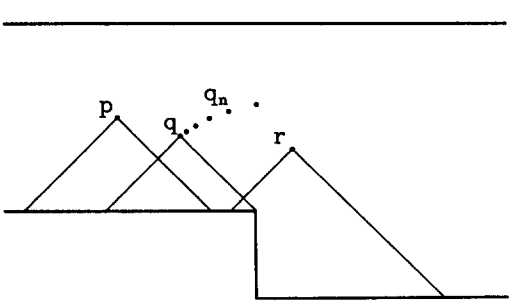

FIG. 1. The metric D is not semicontinuous in "step Minkowski space."

Then, since D^+ and D^- are non-negative, both $D_p^+(p_n)$ and $D_p^-(p_n)$ must go to zero as $p_n \to p$. Since D^+ and D^- satisfy the triangle inequality, the argument in the preceeding paragraph shows that each of D^+ and D^- is continuous.

Proof (of 3.1): ($\Rightarrow$) Consider $B_\epsilon(p) \in \mathscr{D}$. We have $B_\epsilon(p) \equiv D_p^{-1}([0,\epsilon)) \in \mathscr{M}$ since D is continuous; therefore D_p is continuous and $[0,\epsilon)$ is open in $[0,\infty)$.

Now consider any open set $O \in \mathscr{M}$. For all $p \in O$ there is a neighborhood $U(p) \in \mathscr{M}$ such that $\overline{U}$ is compact and $U \subset O$, since M is paracompact. Let $\partial U = \overline{U} - U$. Now $\partial U = \overline{U} \cap \overline{U}^C$, so ∂U is closed. Then, since $\partial U \subset \overline{U}$ which is compact, ∂U is also compact. The continuous image of a compact set is compact, so $D_p^{\pm}(\partial U)$ are compact and, being contained in $\mathscr{R}$, which is Hausdorff, are closed. Let $\epsilon^{\pm} = \inf D_p^{\pm}(\partial U)$. Since $p \notin \partial U$, and since $D^{\pm}$ are both metrics, $\epsilon^{\pm} > 0$.

Claim: Let $\delta = \frac{1}{2}(\epsilon^+ + \epsilon^-)$. Then $B_\delta(p) \subset U$.

Proof: We consider $r \in M - U$ in the four possible regions and find, in each case, a $q \in \partial U$ such that $D^-(p,r) \geqslant D^-(p,q) \geqslant \epsilon^-$.

(i) If $I^-(r) \cap I^-(p) = \varnothing$, then $I^-(p) \subset p \bigtriangleup^- r$, where

$$p \bigtriangleup^- r \equiv I^-(p) \bigtriangleup I^-(r),$$

so any $q \in I^-(p) \cap \partial U$ works.

(ii) If $I^-(r) \cap \partial U \cap I^-(p) = \varnothing$ but $I^-(r) \cap I^-(p) \neq \varnothing$, then p is contained in the common future of $I^-(r) \cap I^-(p)$, which is defined as $\{s : s \in I^+(t) \forall t \in I^-(r) \cap I^-(p)\}$, so there is a $q \in \overline{\partial U \cap I^-(p)}$ which is also. But then $p \bigtriangleup^- q \subset r \bigtriangleup^- p$.

(iii) If $r \in I^+(p) - U$, then there is a $q \in \partial U \cap I^-(r)$ such that $p \bigtriangleup^- q = I^-(q) - I^-(p) \subset I^-(r) - I^-(p) = r \bigtriangleup^- p$.

(iv) All other $r \in M - U$ must have $I^-(r) \cap \partial U \neq \varnothing$. Let $q \in \overline{I^-(r) \cap \partial U}$. Then $p \bigtriangleup^- q \subset p \bigtriangleup^- r$.

The dual argument shows that $D^+(p,r) \geqslant \epsilon^+$ for all $r \in M - U$ so $D(p,r) \geqslant \epsilon^- + \epsilon^+$. Thus $B_\delta(p) \subset U$. Therefore $O \in \mathscr{D}$.

($\Leftarrow$) Suppose D is not continuous. Then there is a $p \in M$ and an $\epsilon > 0$ such that for all neighborhoods $U(p)$, there is a $q \in U$ such that $D(p,q) > \epsilon$. Consider the set $B_{\epsilon/2}(p) \in \mathscr{D}$. Then there is no neighborhood $U(p) \in \mathscr{M}$ such that $U \subset B_{\epsilon/2}(p)$. Thus $B_{\epsilon/2}(p) \notin \mathscr{M}$. Hence the topologies do not agree, which is a contradiction. This concludes the proof of Theorem 3.1.

We have seen in Fig. 1 that D is not continuous for "step Minkowski space." In fact, this illustrates a necessary condition for the continuity of D.

Proposition 3.3: D is continuous $\Rightarrow M$ is causally continuous.[11]

Proof: Suppose M is not causally continuous. Then there is a $p \in M$ such that either I^- or I^+ is not outer continuous at p. Without loss of generality, let I^- be not outer continuous. Then (BE,[3] HE,[1] and Hawking and Sachs[11]) there is a compact set $K \subset M - \overline{I^-(p)}$ such that for all neighborhoods $U(p) \in \mathscr{M}$ there is a $q \in U(p)$ such that $K \cap \overline{I^-(q)} \neq \varnothing$.

Consider the set $\{I^+(r) : r \in M - \overline{I^-(p)}\}$. This is an open cover of K so there is a finite open subcover, say $\{I^+(r_i) : 1 \leqslant i \leqslant n\}$. Let $s \in K \cap \overline{I^-(q)}$, where $q \in U(p)$ is such that $K \cap \overline{I^-(q)} \neq \varnothing$. Since $s \in K$, $s \in I^+(r_i)$ for some i. Since $s \in \overline{I^-(q)}$, there is a sequence $s_n \to s$, $s_n \in I^-(q)$; and $I^+(r_i)$ is open, so there is a neighborhood $V(s) \subset I^+(r_i)$. Choose $s_n \in V$ (there must be one since $s_n \to s$). Then there is a future directed timelike curve from r_i to q which contains s_n, so $r_i \in I^-(q)$. Thus $I^-(r_i) \subset I^-(q)$.

Let $\epsilon = \min d(I^-(r_i))$, $1 \leqslant i \leqslant n$. Then $\{q : D(p,q) < \epsilon\} \in \mathscr{D}$ contains no open set of $\mathscr{M}$, but is not empty (it contains p), and so is not open in $\mathscr{M}$. By Theorem 3.1, since the topologies do not agree, D is not continuous.

A simple example shows that causal continuity is the strongest of the usual causal conditions (BE[3] and Ref. 11) which is necessary for the continuity of D. Let M be Minkowski space with t restricted to some open interval $\mathscr{R}$ (to guarantee finite timelike dimeter). If a single point is removed, M is no longer causally simple (the weakest causality condition stronger than causal continuity) since there exists a $p \in M$ such that $J^+(p)$ is not closed in $\mathscr{M}$. Nevertheless it is clear that D is unaffected by the removal of a single point.

However, D reflects more than the causal structure of M. Since D depends on lengths of curves in M, conformal changes in the metric can affect continuity. In their discussion of the existence of simultaneous synchronous coordinates, Wald and Yip[10] define a maximum lifetime function $f : M \to \mathscr{R}$. In our notation $f(p) = d(J^+(p))$, but since null portions of causal curves have zero length, $f(p) = d(I^+(p))$. This is clearly a measure of the effect of the metric on lengths of future directed causal curves through p, so we expect relationships between properties of D and properties of f. The next few results illuminate the connection between the continuity of D and various conditions on f.

Figure 2 is an example of Wald and Yip in which f is not continuous. A conformal factor $\Omega(t,x) = 1 + h(\theta)/r$, where $r = (t^2 + x^2)^{1/2}$ and $\tan\theta = -t/x$, multiplies the Minkowski metric in two dimensions. The function $h(\theta)$ is smooth, non-negative, vanishes outside the wedge, and rises to a maximum of 1 on an open θ interval inside the wedge. They show that there is an $\epsilon > 0$ such that $f(p) > \epsilon$ for points p which have access to the wedge, i.e., $I^+(p)$ intersects the $r < \delta$ portion of the wedge, for some $\delta > 0$. Thus, f is discontinuous along the null segment shown, terminating at q such that $f(q) = \epsilon$. Moreover, D is clearly discontinuous along the entire null cone. This example illustrates, therefore, that causal continuity is not a sufficient condition for the continuity of D, and motivates the following proposition.

Proposition 3.4: D is continuous $\Rightarrow f$ is continuous.

Proof: Suppose f is not continuous. Then there is a $p \in M$ and an $\epsilon > 0$ such that for all neighborhoods $U(p) \in \mathscr{M}$, there is a $q \in U$ such that $|f(q) - f(p)| > \epsilon$. Without loss of generality, we may assume that $f(q) > f(p)$. Then there exists a

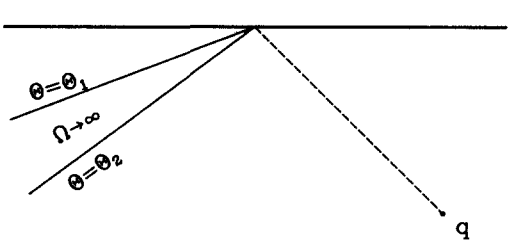

FIG. 2. The maximum lifetime function f is discontinuous along the dotted null segment.

future directed causal curve γ from q such that $L(\gamma) - f(p) > \frac{1}{2}\epsilon$. Choose $r \in \gamma$ such that $L(\gamma;q,r) \geqslant L(\gamma) - \frac{1}{4}\epsilon$. Then $D^+(r,p) \leqslant f(p)$ and $D^+(r,q) \geqslant L(\gamma) - \frac{1}{4}\epsilon$ so

$$D^+(r,q) - D^+(r,p) \geqslant L(\gamma) - \tfrac{1}{4}\epsilon - f(p) > \tfrac{1}{4}\epsilon.$$

Thus D^+ is not continuous and therefore, by Lemma 3.2, D is not continuous.

It is clear, however, that even continuity of f is not sufficient to guarantee the continuity of D. In the example of Fig. 2, consider removing the null segment along which f is discontinuous. Since D is discontinuous on the entire null cone this provides a counterexample to the converse of Proposition 3.4. The following theorem shows that one of the other conditions of Wald and Yip on f is sufficient, though not necessary, for the continuity of D.

Theorem 3.5: Provided (M,g) is strongly causal, $f \to 0$ along every future inextendable causal curve (and the dual of this condition) $\Rightarrow D$ is continuous.

Proof: Suppose D is not continuous. Then by Lemma 3.2 there is a $p \in M$ and a $\delta > 0$ such that for all neighborhoods $U(p) \in \mathscr{M}$, there is a $q \in U$ such that $D^+(p,q) > \delta$. Choose a sequence of such q_n which converges to p in $\mathscr{M}$. For any $\epsilon > 0$, there is, for each q_n, a future inextendable causal curve $\gamma_n \subset p\bigtriangleup^+ q_n$ such that

$$L(\gamma_n) > D^+(p,q_n) - \epsilon > \delta - \epsilon.$$

Since this holds for any $\epsilon > 0$, there are $\gamma_n \subset p \bigtriangleup^+ q_n$ such that $L(\gamma_n) \geqslant \delta$. Now p is an accumulation point of $\{\gamma_n\}$ so, by Proposition 2.18 of BE,[3] there is a causal limit curve γ of $\{\gamma_n\}$ such that $p \in \gamma$ and γ is future inextendable.

Note that $\gamma \cap J^+(p)$ must be null, i.e., $\gamma \cap J^+(p)$ is contained in $J^+(p) - I^+(p)$, since, if γ were to intersect $I^+(p)$ at a point r, we could find a neighborhood $V(r) \subset I^+(p)$ and a point $s \in \gamma \cap I^+(p) \cap I^-(r)$ such that $s \notin V$. Then $I^-(s)$ would be a neighborhood of p so for $q_n \in I^-(s)$, $\gamma_n \cap V = \varnothing$, hence r cannot lie on γ if γ is a limit curve of $\{\gamma_n\}$. But $\gamma \subset J^+(p)$, since γ is causal and $p \in \gamma$. Thus γ is null and $L(\gamma) = 0$.

Now consider a sequence of points $\{r_m\} \subset \gamma$ such that $r_{m+1} \in I^+(r_m)$ and $\{r_m\}$ is not convergent. Such a sequence exists because γ is future inextendable. Since γ is a limit curve of $\{\gamma_n\}$, for each r_m we can find a sequence of points $\{s_{n,m}\} \subset \gamma_n$ such that $s_{n,m} \to r_m$. By construction, the segment of γ from p to r_m, denoted by $\gamma; p \to r_m$, is a limit curve of the sequence of segments of γ_n terminating at $s_{n,m}$, denoted $\{\gamma_n; \to s_{n,m}\}$. By Proposition 2.21 of BE,[3] since M is strongly causal, there is a subsequence of $\{\gamma_n; \to s_{n,m}\}$ which converges to $\gamma; p \to r_m$ in the C^0 topology on curves. For convenience we also denote this subsequence by $\{\gamma_n; \to s_{n,m}\}$. Since the length functional is upper semicontinuous with respect to the C^0 topology on curves (Penrose,[12] p. 54),

$$L(\gamma; p \to r_m) \geqslant \limsup_n L(\gamma_n; \to s_{n,m})$$

$$\Rightarrow 0 = \limsup_{n,m} L(\gamma_n; \to s_{n,m}).$$

Thus

$$L(\gamma_n) = L(\gamma_n; \to s_{n,m}) + L(\gamma_n; s_{n,m} \to) \geqslant \delta$$

$$\Rightarrow L(\gamma_n; s_{n,m} \to) \geqslant \delta - L(\gamma_n; s_{n,m})$$

$$\Rightarrow \liminf_{n,m} L(\gamma_n; s_{n,m} \to)$$

$$\geqslant \liminf_{n,m} [\delta - L(\gamma_n; \to s_{n,m})]$$

$$\geqslant \delta - \limsup_{n,m} L(\gamma_n; \to s_{n,m})$$

$$= \delta.$$

Now $I^-(\gamma)$ is a terminal indecomposable past set (TIP) [see Sec. IV for a review of TIP's and terminal indecomposable future sets (TIF's)], so there is a future inextendable timelike curve λ such that $I^-(\gamma) = I^-(\lambda)$ (Ref. 2).

Claim: $f \nrightarrow 0$ along λ.

Proof: Let $t \in \lambda$. Then $t \in I^-(\gamma)$ so there is an M such that $m > M \Rightarrow t \in I^-(r_m)$. Therefore, $r_m \in I^+(t)$ for all $m > M$. Since $I^+(t)$ is open, there is a neighborhood of r_m contained in $I^+(t)$ so there is an N such that $n > N, m > M \Rightarrow s_{n,m} \in I^+(t)$. But

$$f(t) \geqslant \sup_{m>M,\, n>N} f(s_{n,m})$$

$$\geqslant \liminf_{m,n} L(\gamma_n; s_{n,m} \to)$$

$$= \delta.$$

The dual argument is the same so the theorem follows from Lemma 3.2.

Using Proposition 3.4 we also have the following incidental, but immediate, corollary.

Corollary 3.6: If (M,g) is strongly causal and $f \to 0$ along every future inextendable causal curve (and the dual condition holds) then f is continuous.

Having explored in some detail the relationship between the continuity of D and the various conditions which can be placed on the maximum lifetime function of Wald and Yip, we now examine the continuity of D from another point of view.

The usual C^0 topology on the space of causal curves (Ref. 12, p.49) can be modified to give a C^0 topology on the space of future (or past) inextendable causal curves. Let M be strongly causal and let $\mathscr{C}$ denote the set of all future inextendable causal curves in M. Define $\mathscr{C}_R(P,Q) = \{\gamma : \gamma$ is a future inextendable causal curve in R from a point of P into, but not out of, $Q\}$. The C^0 topology on $\mathscr{C}$ is defined by taking as the base the sets with $P \in \mathscr{M}$, $Q = I^+(p)$ for $p \in I^-(\gamma)$, where γ is a future inextendable causal curve from a point of P, and $R \in \mathscr{M}$ such that $P \subset R$ and $Q \subset R$. That this is indeed a topology on $\mathscr{C}$ follows immediately: $\gamma \in \mathscr{C}_R(P,Q)$ and $\gamma \in \mathscr{C}_{R'}(P',Q') \Rightarrow \gamma \in \mathscr{C}_{R''}(P'',Q'')$, where $R'' = R \cap R'$, $P'' = P \cap P''$, and $Q'' = Q \cap Q'$.

The proper length of future inextendable causal curves is a functional $L: \mathscr{C} \to \mathscr{R}$. Using this we can formulate the following proposition.

Proposition 3.7: D^+ is continuous at $p \in M \Leftrightarrow L$ is continuous across the null cone of p.

Proof: ($\Leftarrow$) Suppose D^+ is not continuous at p. Then for any neighborhood $U(p) \in \mathscr{M}$, there is a $q \in U$ such that $D^+(p,q) > \epsilon$. But then there can be no nonempty C^0 neighborhood of the null cone at p in which all the future inextendable causal curves have length less than ϵ, a contradiction.

($\Rightarrow$) We must show that for any $\epsilon > 0$ there is a C^0 neighborhood of the null cone in which all curves have length less than ϵ. Since D^+ is continuous at p, $B^+_{\epsilon/2} \in \mathscr{M}$, so let $P = B^+_{\epsilon/2}(p)$. Let $R = I^+(P) - \overline{\uparrow P}$ Here $\uparrow P \equiv I^+(\{q: q \in I^+(r) \text{ for all } r \in P\})$ is the chronological common future[11] of P. Then all causal curves in R have length less than ϵ because the segment lying outside $I^+(p)$, starting at q, say, has length less than $\frac{1}{2}\epsilon$, as does the segment lying inside $I^+(p)$ since it lies outside $I^+(r)$ for some $r \in P$. Finally, let Q be the union of all $I^+(q)$, where $q \in I^+(P)$ such that $I^+(q) \cap \overline{\uparrow P} = \varnothing$ and $I^+(q) \subset R$. Then $\mathscr{C}_R(P,Q)$ is a C^0 neighborhood of the null cone at p in which all future inextendable causal curves have length less than ϵ.

Applying Lemma 3.2 we conclude that D is continuous if and only if the length functional on both past and future inextendable causal curves is continuous across the light cone.

IV. BOUNDARY

We now return to the question of attaching a boundary to M. Since (M, D) is a metric space there is an isometric embedding of (M, D) into a complete metric space.[13] Moreover, there is such an embedding under which the image of M is dense[14]; here we denote the complete metric space by $(\overline{M}, \overline{D})$, the completion of (M, D) and write $\overline{M} = M \cup \partial_D M$ where $\partial_D M$ will be termed the D boundary of M. We note immediately that $(\overline{M},\overline{D})$ is Hausdorff since it is a metric space.

In $(\overline{M}, \overline{D})$ all Cauchy sequences converge; thus points in $\overline{M}$ can be identified with equivalence classes of Cauchy sequences of points in M. Then the D boundary of M consists of those equivalence classes containing Cauchy sequences which do not converge in (M, D). Consider some examples.

Example 1: The simplest example is a strip of Minkowski space. That is, let $M =$ Minkowski space with $0 < t < 1$. In this case we can compute D explicitly. In fact, for $p,q \in M$,

$$D^-(p,q) = \begin{cases} A, & d \geqslant a, \\ [A^2 - (a-d)^2]^{1/2}, & d \leqslant a, \end{cases}$$

$$D^+(p,q) = \begin{cases} A', & d \geqslant a', \\ [A'^2 - (a'-d)^2]^{1/2}, & d \leqslant a', \end{cases}$$

where $A = \max(t_p,t_q)$, $a = \min(t_p,t_q)$, $A' = \max(1-t_p, 1-t_q)$, $a' = \min(1-t_p, 1-t_q)$, and $d = |\mathbf{x}_p - \mathbf{x}_q|$. Then $D = D^+ + D^-$. To determine the D boundary of M we must find the equivalence classes of Cauchy sequences which do not converge in M. It is clear that the points $\{p_n\}$ of any such Cauchy sequence will have t coordinates approaching 0 or 1 and that d for p_n, p_m with $n,m > N$ will approach 0 as $N \to \infty$. Hence equivalence classes of Cauchy sequences will be determined by the limit of their t coordinates (either 0 or 1) and some value of $\mathbf{x}$. Thus $\partial_D M$ consists of two pieces isomorphic to $\mathscr{R}^3$. This is exactly what we expect since D is continuous, so Theorem 3.1 tells us that $\mathscr{D}$ agrees with $\mathscr{M}$; hence the space-time can be extended to all of Minkowski space and will then include points with these coordinates as the boundary of the open set M.

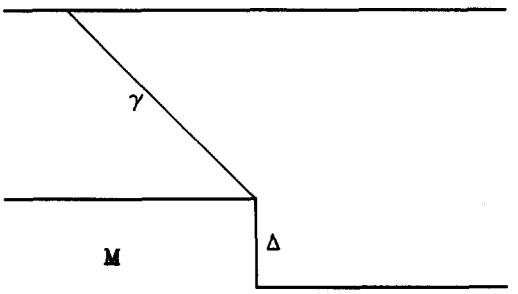

FIG. 3. Example 2: M is step Minkowski space with step height Δ.

Having written down D explicitly, we can also check differentiability. Take, for example, $p = (t_0, \mathbf{0})$ and consider a point q approaching p along the t axis from below. Then if $q = (t_0 - \epsilon, \mathbf{0})$,

$$D_p^-(t) \equiv D_p^-(q) = [t_0^2 - (t_0 - \epsilon)^2]^{1/2} = [2\epsilon t_0 - \epsilon^2]^{1/2}$$

$$\Rightarrow \frac{dD_p^-(t)}{dt} = \lim_{\epsilon \to 0} \frac{[2\epsilon t_0 - \epsilon^2]^{1/2}}{\epsilon},$$

which is infinite. In fact, this nondifferentiability will manifest itself at all points even in this simplest of examples. Thus (M, D) is only a C^0 manifold.

Example 2: We have already considered two-dimensional "step Minkowski space" in Sec. III. As in Example 1 we can compute D explicitly for this manifold M. In Sec. III we observed that D is not continuous across the shadow of the step, the part of the light cone labelled γ in Fig. 3. Thus we know that $\mathscr{D}$ will not agree with $\mathscr{M}$ and the D boundary will therefore not be the boundary of M considered as an open set embedded in full two-dimensional Minkowski space. In fact, it is easy to see that the future D boundary will be in two pieces: one to the left of γ in Fig. 3, and one to the right, each constructed just as in Example 1, but with a discontinuity at γ since across γ, D jumps by the height Δ of the step; see Fig. 4. Moreover, sequences of points which converge to a point of γ in M only do so in (M, D) if they do not approach from the right, since a sequence which approaches from the right, although Cauchy, will have distance Δ from its limit point (in M) on γ. Thus we will identify such sequences as points of $\partial_D M$. Finally, again treating the past D boundary as two pieces, to the left and right of γ, it is clear that each is just the boundary of the open set embedded in full two-dimensional Minkowski space. Thus we see that the structure of the past singularity causes $(\overline{M}, \overline{D})$ to consist of two components a distance Δ apart, as shown in Fig. 4.

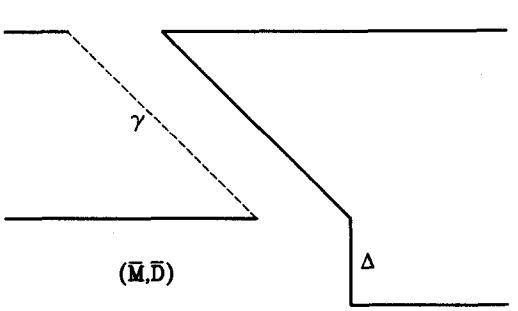

FIG. 4. Example 2: The completed manifold with boundary $(\overline{M}, \overline{D})$ has two components.

Example 3: We now consider an example where we cannot write D explicitly. The closed Friedmann universe has Robertson–Walker metric

$$ds^2 = S^2(\tau)[-d\tau^2 + d\chi^2 + f^2(\chi)(d\theta^2 + \sin^2\theta\, d\phi^2)],$$

where $f(\chi) = \sin(\chi)$ and $S(\tau)$ is proportional to $1 - \cos\tau$ in a matter dominated era and to $\sin\tau$ in a radiation dominated era. In this metric, radial geodesics satisfy

$$\chi'(\tau) = (1 + \epsilon^2 S^2)^{-1/2},$$

where ϵ is an arbitrary constant which is zero for null geodesics and infinite for the geodesics which are the world lines for fundamental particles. Thus the length of a geodesic γ is

$$\begin{aligned} L(\gamma) &= \int S(\tau)(\chi'^2 - 1)^{1/2}\, d\tau \\ &= \int S(\tau)\,[(1 + \epsilon^2 S^2)^{-1} - 1]^{1/2}\, d\tau \\ &= \int \epsilon S^2 [1 + \epsilon^2 S^2]^{-1/2}\, d\tau. \end{aligned}$$

Now, a sequence of points $\{q_n\}$ which converges to a point p of M will have converging null cones, and geodesics lying in $p \triangle q_n$ will therefore approach the null cone of p. But

$$L(\gamma) \sim \int \epsilon S^2 \left(1 - \frac{1}{2}\epsilon^2 S^2\right) d\tau = O(\epsilon), \quad \epsilon \to 0,$$

so $\{q_n\}$ is a Cauchy sequence in (M, D) which converges to p. Thus $\mathscr{D}$ agrees with $\mathscr{M}$. Moreover, any sequence of points whose pasts or futures converge to a TIP or TIF will be a Cauchy sequence in (M, D), and hence a point in $\partial_D M$ by the same argument, so the D boundary and the causal boundary agree in this space, each consisting of two pieces isomorphic to S^3. This motivates the review of the causal boundary construction and the results relating the two boundaries which follow later in this section.

Example 4: This is the example for which Geroch, Liang, and Wald[7] show that all geodesically continuous boundary constructions in which every incomplete geodesic of the original space-time terminates at a boundary point give non-T_1 (and hence non-Hausdorff) behavior. We know, *a priori*, that this cannot occur for our metric space construction, but let us examine exactly why the D boundary works for this example.

Take a strip of two-dimensional Minkowski space and choose three points p, s, and r as in Fig. 5, where r lies on the future light cone of s. Let $\{\gamma_i\}$ be a sequence of smooth timelike curves which converge in the $C^0(p,r)$ topology to γ followed by λ. Each λ_i is a geodesic except for a short section of acceleration near s. These short sections can be covered by nonintersecting open sets, and Geroch, Liang, and Wald show that a conformal factor Ω can be chosen such that Ω makes each γ_i a timelike geodesic, $\Omega = 1$ on each γ_i and $\Omega = 1$ outside the open sets. Thus Ω can be chosen to be smooth everywhere but s so we excise s from the manifold M. Now, since the lengths of the geodesics γ_i approach the length of γ, in any geodesically continuous boundary construction the sequence $\{r\}$ will converge to the boundary point at s. (For more detail see Ref. 7.)

What happens near s if we define D on this space-time? Although this is a singularity which blue-shifts nearby geodesics, any sequence of points which converges to s in the original Minkowski space will still be a Cauchy sequence in (M, D). Thus the D boundary contains a point which we can identify with s. Moreover, $D(r, s)$ is then clearly positive so the non-T_1 behavior of a geodesically continuous boundary construction has disappeared. This is consistent with the fact that the D boundary construction is not geodesically continuous in all cases. For example, in the "step Minkowski space" considered in Example 2, the boundary is clearly not geodesically continuous across γ. In general this is a reflection of the global character of D discussed in Sec. III.

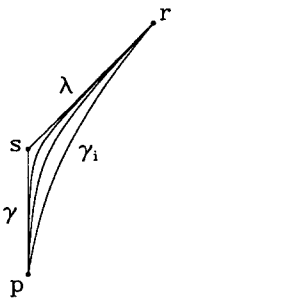

FIG. 5. Example 4: The D boundary is Hausdorff.

What relation does the D boundary construction have to other boundary constructions? To answer this question we begin by extending the causal structure of M to $\overline{M}$.

Let $F = [a,b) \subset \mathscr{R}$. Consider a causal curve $\gamma: F \to M$. Then $p \in \partial_D M$ is a future boundary point (FBP) of γ at $c \in F$, if for all neighborhoods $U(p) \in \overline{\mathscr{D}}$ there is a $t_0 \in F$ such that $\gamma(t) \in U$ for all $t \in F$ with $t_0 \leqslant t < c$. If $c = b$ and γ is future inextendable, p is a future boundary endpoint (FBE) of γ. Here $\overline{\mathscr{D}}$ is the metric topology on $(\overline{M}, \overline{D})$. The past boundary point (PBP) and endpoint (PBE) are defined dually.

Lemma 4.1: A FBP at c is unique if it exists.

Proof: Suppose not. Then there are $p \neq q$ such that q and p are FBP's of a curve γ at c. Since $(\overline{M}, \overline{D})$ is Hausdorff there are neighborhoods $U(p)$, $V(q) \in \overline{\mathscr{D}}$ such that $U \cap V = \varnothing$, a contradiction.

In particular, the FBE of a curve is unique if it exists. With this result an extension of γ into $(\overline{M}, \overline{D})$ is well defined: Let $\overline{\gamma}: \overline{F} \to (\overline{M}, \overline{D})$ be given by $\overline{\gamma}(t) = \gamma(t)$ for all $t \in F$, $\overline{\gamma}(b) = p$ if p is the FBE of γ.

Lemma 4.2: If $\mathscr{M} = \mathscr{D}$, $\overline{\gamma}$ is continuous.

Proof: Since $\mathscr{M} = \mathscr{D}$, $\gamma: F \to (M, D)$ is continuous. Hence, by definition, $\overline{\gamma}$ is continuous on F. Consider a sequence $\{x_n\} \subset F$ with $x_n \to b$. Then for all $t_0 \in F$ there is an N such that $n > N \Rightarrow x_n > t_0$. Since p is the FBE of γ, for all $\epsilon > 0$ there is a $t_0 \in F$ such that $\gamma(t) \in B_\epsilon(p)$ if $t_0 < t < b$. Thus there is an N such that $n > N > \gamma(x_n) \in B_\epsilon(p)$. Therefore $\gamma(x_n) \to p$, so $\overline{\gamma}$ is continuous.

Lemma 4.3: Provided $\mathscr{M} = \mathscr{D}$, $\gamma: F \to (M, D)$ has a FBE $\Leftrightarrow$ γ is uniformly continuous.

Proof: ($\Leftarrow$) Since γ is uniformly continuous there is a unique uniformly continuous extension $\overline{\gamma}: \overline{F} \to \overline{M}$. Then $\overline{\gamma}(b)$ is the FBE of γ.

($\Rightarrow$) If γ has a FBE then $\bar{\gamma}$ is continuous (by Lemma 4.2), and hence uniformly continuous since $\overline{F}$ is compact, so γ is uniformly continuous also.

Now we can define the chronology on $\overline{M}$. For $p,q \in \overline{M}$, define p to be to the chronological past of q (and q to be to the chronological future of p) if there is a timelike curve γ such that $p \in \gamma$, or p is a PBP of γ and $q \in \gamma$, or q is FBP of γ. This clearly reduces to the chronology on M if so restricted, so we continue to write $p \in I^-(q)$ and $q \in I^+(p)$.

We observe first that for $p \in \partial_D M$, $I^-(p) \cap M$ is open in $\mathscr{M}$ by the usual argument (see Ref. 12, p. 13). Moreover, we have the following lemma.

Lemma 4.4: For $p \in \overline{M}$, $I^+(p)$ is open in $\overline{\mathscr{D}}$.

Proof: Consider $q \in I^+(p)$. Since $q \in I^+(p)$ there is a timelike curve γ either through p and q or with boundary points at p and/or q. Suppose $I^+(p)$ is not open at q. Then for every neighborhood $U(q) \in \overline{\mathscr{D}}$, U intersects the complement of $I^+(p)$. Thus we can choose a Cauchy sequence $\{r_n\} \subset M$ such that $r_n \to q$, i.e., $\overline{D}(r_n,q) \to 0$, and $I^-(r_n) \cap I^+(p) = \varnothing$ for all n. But then $\gamma \subset r_n \bigtriangleup q$ so $\bar{D}(r_n,q) \geqslant L(\gamma) > 0$, a contradiction.

With this lemma we can relate the chronological pasts and futures of points on the D boundary to the TIP's and TIF's of the Geroch, Kronheimer, and Penrose causal completion.[2] Recall that an indecomposable past set (IP) is a nonempty past set which cannot be written as the union of two proper subsets which are also nonempty past sets. A terminal IP (TIP) is an IP which cannot be written as $I^-(p)$ for any $p \in M$. Indecomposable future sets (IF's) and TIF's are defined dually. Alternatively, IP's are the past of timelike curves while IF's are their futures. Applying the same argument used to prove Lemma 4.4 we obtain a corollary.

Corollary 4.5: IP's and IF's are open in $\overline{\mathscr{D}}$.

We will use this result shortly, but the next step is the following proposition.

Proposition 4.6: Let $p \in \partial_D M$. Then if $I^-(p) \neq \varnothing$, $I^-(p) \cap M$ is an IP.

Proof: For the purposes of this proof we will use I^- to denote I^- restricted to M. Since $I^-(p)$ is nonempty, p is a FBP of some curve $\gamma: F \to M$. Consider the IP in M generated by γ, $I^-(\gamma)$. Suppose $I^-(\gamma) \neq I^-(p)$. Then either (i) $\exists r \in I^-(\gamma) - I^-(p)$, which is impossible since, if $r \in I^-(\gamma)$, then $r \in I^-(p)$, or (ii) $\exists r \in I^-(p) - I^-(\gamma)$, which is also impossible since $p \in I^+(r)$. So by Lemma 4.4 and the fact that p is a FBP in $I^-(p)$ of γ, $\gamma \cap I^-(r) \neq \varnothing$ and hence $r \in I^-(\gamma)$.

Note that $I^-(p) \cap M$ is a TIP $\Leftrightarrow p$ is a FBE, i.e., the curve γ which generates $I^-(p) \cap M$ is future inextendable.

Thus to compare the D boundary to the causal boundary, we define a mapping $i:(\overline{M}, \overline{D}) \to \overline{M}_c$ given by the entries $i(p)$ in the following table:

	$I^+(p) \neq \varnothing$	$I^+(p) = \varnothing$
$I^-(p) \neq \varnothing$	$[I^+(p)] = [I^-(p)]$	$[I^-(p)]$
$I^-(p) = \varnothing$	$[I^+(p)]$	$\varnothing$

Here $[I^+(p)]$ denotes the equivalence class of IP's and IF's identified with $I^+(p) \cap M$ under the causal completion procedure. To verify that this mapping is well defined we must check that the identification $[I^+(p)] = [I^-(p)]$ is really made in $\overline{M}_c$.

First we briefly review the construction of $\overline{M}_c$. (For a thorough account see Ref. 2.) If M is required to be strongly causal, then $\hat{M}$ is the set of all IP's, $\check{M}$ is the set of all IF's, and $M^\#$ is the disjoint union $\hat{M} \cup \check{M}$ with the identification of $I^-(p) \in \hat{M}$ and $I^+(p) \in \check{M}$ for all $p \in M$. If $P \in \hat{M}$ or $P \in \check{M}$, the corresponding element of $M^\#$ is denoted by $P^\#$.

The topology on $M^\#$ is the coarsest in which the sets

$$A^{\text{int}} = \{P^\# : P \in \hat{M} \text{ and } P \cap A \neq \varnothing\},$$

$$A^{\text{ext}} = \{P^\# : P \in \hat{M} \text{ and } \forall S \subset M, P = I^-(S) \Rightarrow I^+(S) \not\subset A\},$$

and their duals B^{int} and B^{ext} are open, for $A \in \check{M}$ and $B \in \hat{M}$. Finally, $\overline{M}_c$ is $M^\#/\sim$, where the equivalence relation $\sim$ makes the fewest identifications necessary to obtain a Hausdorff space. We denote the associated topology by $\overline{\mathscr{C}}$.

Since M is isometrically embedded in $\overline{M}$ and since $I^+(p)$ and $I^-(p)$ are identified in $M^\#$ for $p \in M$, the mapping $i:\overline{M} \to \overline{M}_c$ is well defined for $p \in M$. For $p \in \partial_D M$ consider $I^-(p) \cap M \neq \varnothing$ as an IP. Then $I^-(p) \cap M$ has neighborhoods in $M^\#$ of the form $A_1^{\text{int}} \cap \cdots \cap A_m^{\text{int}} \cap A_1^{\text{ext}} \cap \cdots \cap A_n^{\text{ext}}$. Since A^{int} and A^{ext} are sets of IP's they are, considered as subsets of $\overline{M}$, open in $\overline{\mathscr{D}}$ by Corollary 4.5. Thus every neighborhood of $I^-(p) \cap M$ (considered as an IP) is open in $\overline{\mathscr{D}}$ and hence intersects $I^+(p) \cap M$ (considered as an IF), so since $\overline{M}_c$ is Hausdorff, the two must be identified.

This shows that $i: \overline{M} \to \overline{M}_c$ is well defined and, moreover, continuous. Is this map open as well? That is, for $U \in \overline{\mathscr{D}}$ is there a $V \in \overline{\mathscr{C}}$ such that $i(U) = V$? For a strongly causal space M, $\overline{\mathscr{C}}$ restricted to M agrees with $\mathscr{M}$ (Ref. 7). Since i identifies $p \in M$ in $\overline{M}$ and $\overline{M}_c$, i is open on M if and only if the image of every open set in $\mathscr{D}$ is open in $\mathscr{M}$, i.e., $\mathscr{D}$ agrees with $\mathscr{M}$. (We already know that the preimage of every open set in $\overline{\mathscr{C}}$ is open in $\overline{\mathscr{D}}$.) Thus by Theorem 3.1 i is open on M if and only if D is continuous.

Now consider an open set $U \in \overline{\mathscr{D}}$ which contains points of $\partial_D M$ and suppose $i(U)$ is not open in $\overline{\mathscr{C}}$. That is, suppose there is some point $p \in \partial_D M$ such that every open set in $\overline{\mathscr{C}}$ containing $i(p)$ contains points which are not in $i(U)$. These points are equivalence classes of TIP's and TIF's which either correspond to points in $\partial_D M$ which are not in U, or correspond to no point of $\partial_D M$ [which means, by Lemma 4.3, that they are generated by curves which are not uniformly continuous maps of F into (M, D)]. In either case this means that there must be causal curves of length greater than some ϵ arbitrarily near and outside the null cone of p. But then each null curve in the null cone of p is also a null curve through points of M, and hence, by Proposition 3.7, D is not continuous. We have just proved the first of the following propositions.

Proposition 4.7: For a strongly causal space-time M, $i:(\overline{M}, \overline{D}) \to \overline{M}_c$ is open $\Leftrightarrow D$ is continuous.

Proposition 4.8: If i is an open map, it is also one to one.

Proof: Suppose not. Then there are two points $p \neq q$ in $\overline{M}$ such that $i(p) = i(q)$. Since $p \neq q$ and $(\overline{M}, \overline{D})$ is Hausdorff there are neighborhoods $U(p)$, $V(q) \in \overline{\mathscr{D}}$ such that $U \cap V = \varnothing$. Consider $i(U)$ and $i(V)$. Since i is open, these images are open; hence, since they both contain $i(p) = i(q)$ they intersect in an open set $W \in \overline{\mathscr{C}}$. Since M is dense in $\overline{M}_c$, and $\overline{\mathscr{C}}$ restricted to M agrees with $\mathscr{M}$, $W \cap M$ is open in $\mathscr{M}$. But $i^{-1}(W)$ contains

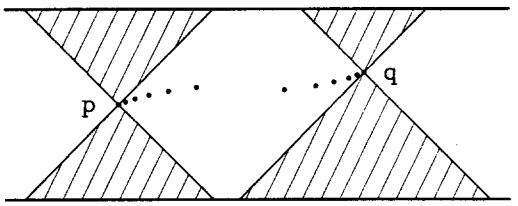

FIG. 6. Example 5: Strip Minkowski space with $\overline{I^{\pm}(p)}$ and $\overline{I^{\pm}(q)}$ removed. Cauchy sequences approaching p and q are identified.

points of M which must then be in both U and V, a contradiction.

We can now combine Lemma 4.3, Proposition 4.7, and Proposition 4.8 in the following theorem which summarizes the relationship between the D boundary and the causal boundary.

Theorem 4.9: The part of $\partial_D M$ which has either a past or a future is homeomorphic to the part of $\partial_C M$ which is generated by uniformly continuous curves. That is, $\{p \in \partial_D M$: $I^+(p) \neq \emptyset$ or $I^-(p) \neq \emptyset\} \approx \{P \in \partial_C M$: $P = [I^+(\gamma)]$ or $P = [I^-(\gamma)]$ where γ: $F \to (M, D)$ is uniformly continuous$\}$.

R. Geroch (private communication via R. Wald and D. Eardley) has suggested the following example in which there is a part of $\partial_D M$ with no past or future.

Example 5: Consider a strip of Minkowski space-time again, as in Example 1; consider two spacelike separated points p and q in the strip. Remove the closures of their pasts and futures; see Fig. 6. Then we have the curious phenomenon that Cauchy sequences approaching p and q are identified in the construction of $\partial_D M$. Roughly speaking, p and q map to a single point in $\partial_D M$. This phenomenon is generic to the case where the part of $\partial_D M$ with no past or future is nonempty, and illustrates the fact that it always consists of exactly one point in this case. This boundary point is always missing in M_c because no TIP's or TIF's belong to it.

V. CONCLUSION

We have seen that defining a metric space topology on a spacetime, and then completing the metric space to obtain the D boundary provides a new procedure for constructing the "singular points" of a spacetime manifold. The new construction is different from, but related to several older constructions. In particular, it is closely related to the causal boundary, and conditions under which the two are the same have been obtained.

The new construction is different from the causal boundary, though, in that it provides a metric topology on the boundary. Also, the D boundary is by its nature more global than the g boundary and thus avoids the particular problem of the unphysical topology in the example of Geroch, Liang, and Wald. The detailed relation between the D boundary and this as well as other boundary constructions could be explored in future work. Moreover, the global and metric nature of the new construction suggests that it may be possible to use it to obtain bounds on solutions of Einstein's equation, despite the fact that, since D in general is not differentiable, it does not provide adequate coordinates in which to solve the equations exactly.

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Dimensional reduction of invariant linear connections and tensor fields on multidimensional space-time

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Let the compact Lie group G act smoothly on the C^∞ manifold S with a single orbit type G/H, where H is a closed subgroup of G, and let $N(H)/H$ be a Lie group [$N(H)$ denotes the normalizer of H in G]. Assuming a given connection in the fiber bundle $S \to M$, where $M = S/G$ is the orbit space (to be identified with the physical space-time) and $N(H)/H$ is the structure (gauge) group, the G-invariant tensor fields and linear connections on S are analyzed. A kind of "dimensional reduction" for these objects is established: every field corresponds uniquely to a field on M, and the linear connection defines uniquely a set of fields and a linear connection on M.

I. INTRODUCTION

Field theories defined on a multidimensional space-time became part of a proliferated conception for a unified description of the fundamental interactions. Moreover, there is a different physical content in the dynamical structure of a multidimensional field theory for models based on the so-called "spontaneous compactification," Kaluza–Klein schemes, or dimensional reduction (see, e.g., Ref. 1).

In the present work we suppose that the description of gravity and Yang–Mills interactions in four-dimensional space-time results from an appropriately chosen dynamic of tensor and spinor fields defined on a manifold S with dimension greater than 4. We assume that S is equipped with the smooth action of a compact Lie group G such that its orbits have a single type G/H, where H is a closed subgroup of G. This allows for S to be fibered over the orbit space S/G with a typical fiber diffeomorphic to G/H; the four-dimensional space-time is then identified with the manifold $M = S/G$.

The picture of a field theory on a multidimensional universe with the properties of S has been proposed by Coquereaux and Jadczyk.[2] They have described the G-invariant metrics on S and the G-invariant connections in a principal fiber bundle $P \to S$, whose structure group is a *compact* Lie group (see Refs. 3 and 4) and made applications to model building. An approach similar to that in Refs. 3 and 4 has been developed in Ref. 5.

At a preliminary stage before studying a possible dynamics over S we describe in this paper the G-invariant tensor fields (an example is a metric on S) and the G-invariant linear connections on S: these objects are, in some sense, most naturally related to the manifold S and will be considered as basic ingredients in a dynamical scheme. (In a forthcoming work we shall extend this consideration by the inclusion of spinor fields.) We shall suppose that a G-invariant Yang–Mills connection is given in the fiber bundle $S \to M$ whose structure (gauge) group is the group $N(H)/H$, where $N(H)$ is the normalizer of H in G. This assumption together with the property of G invariance leads to a kind of "dimensional reduction" of both the tensor fields and the linear connection on S: every field corresponds uniquely to a field on the orbit space $M = S/G$, and the linear connection defines uniquely a set of fields and a linear connection on M.

The material in this paper is organized in the following way. In Sec. II we introduce some of our notations and review the basic properties of a G space S with a single type of orbits. In Sec. III we consider the structure of the bundle of linear frames $F(S)$ over S with regard to the naturally induced action of the group G. We show that in the presence of a Yang–Mills connection in the bundle $S \to M$, $F(S)$ admits a structure of a fiber bundle with base M and typical fiber—a homogeneous space of the group $\mathrm{GL}(\dim S, \mathbf{R}) \times G$. Section IV is devoted to the description of the G-invariant fields over S with values in fiber bundles associated to $F(S)$. The examples of G-invariant vector and tensor fields are considered. In the final section we describe the so-called G-invariant pseudotensorial fields on S (cf. Ref. 6. Chap. 2, §5), and, in more detail, arbitrary linear connection on S. It is the property of $F(S)$ to admit a fibering over M which allows the G-invariant fields and the linear connection on S to be uniquely determined by a set of fields and a linear connection on M, i.e., to be *dimensionally reduced* (cf. Ref. 7).

Throughout the paper all manifolds and mappings are supposed from class C^∞. A principal fiber bundle with total space P, base space Q, structure group N, and projection p: $P \to Q$ will be denoted by $P(Q,N,p)$ or $P(Q,N)$. For a fiber bundle E associated to $P(Q,N)$ by some action of the group N on the typical fiber F we shall use the notation $E = (P \times F)/N$. Occasionally we shall write an element from E in the form $[u,f]$, $u \in P$, $f \in F$, where $[\,,\,]$ denotes the equivalence class defined in $P \times F$ with respect to the action of the group N. For the vector spaces $A_1,\ldots,A_n$ and B we denote by $L(A_1,\ldots,A_n;B)$ the space of linear maps of $A_1 \times \cdots \times A_n$ into B.

II. STRUCTURE OF THE FIBER BUNDLES S_0 AND S

Let G be a compact Lie group and H a closed subgroup of G. Then the homogeneous space G/H is reductive, i.e., the Lie algebra $\mathfrak{G}$ of the G admits a decomposition (as a vector space)

$$\mathfrak{G} = \mathfrak{H} \oplus \mathfrak{M}, \tag{2.1}$$

where $\mathfrak{H}$ is the Lie algebra of H and the subspace $\mathfrak{M}$ is $\mathrm{Ad}(H)$ invariant: $\mathrm{Ad}(H)\mathfrak{M} \subseteq \mathfrak{M}$.

We suppose that the natural action of G on G/H,

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$gH \mapsto g'gH$, is effective. If it is not the case, i.e., the normal subgroup

$$G_0 = \{ g_0 \in G: g_0 gH = gH, \forall g \in G \} \subset H$$

is nontrivial, one forms the quotient groups $G' = G/G_0$, $H' = H/G_0$, and then G' has an effective action on G'/H'.

Let $N(H)$ be the normalizer of H in G,

$$N(H) = \{ n \in G: nhn^{-1} \in H, \forall h \in H \}.$$

Then $\mathfrak{G} = \mathfrak{N} \oplus \mathfrak{L}$ is a direct sum decomposition, where $\mathfrak{N}$ is the Lie algebra of $N(H)$ and the subspace $\mathfrak{L}$ is $\mathrm{Ad}(N(H))$ invariant.

We also require that the factor group $K = N(H)/H$ be a Lie group. The Lie algebra $\mathfrak{N}$ of $N(H)$ then admits a direct sum decomposition

$$\mathfrak{N} = \mathfrak{H} \oplus \mathfrak{K}, \tag{2.2}$$

where $\mathfrak{K}$ is a subalgebra of $\mathfrak{N}$ isomorphic to the Lie algebra of K. It follows from (2.1) that (cf. Ref. 2)

$$\mathfrak{G} = \underbrace{\mathfrak{H} \oplus \overbrace{\mathfrak{K}}^{\mathfrak{M}}}_{\mathfrak{N}} \oplus \mathfrak{L}. \tag{2.3}$$

Note that the adjoint action of the algebra $\mathfrak{N}$ leaves the vector space $\mathfrak{L}$ invariant.

In $\mathfrak{G}$ we fix a basis $\{e_r\}$ $(r = 1,...,\dim \mathfrak{G})$ adapted to the decomposition (2.3) and consisting of

$$\begin{aligned} &\{e_{\bar{r}}\}(\bar{r} = 1,...,\dim \mathfrak{H}) \quad \text{basis for } \mathfrak{H}, \\ &\{e_t\}(t = 1,...,q = \dim \mathfrak{K}) \quad \text{basis for } \mathfrak{K}, \\ &\{e_{\bar{t}}\}(\bar{t} = 1,...,l = \dim \mathfrak{L}) \quad \text{basis for } \mathfrak{L}. \end{aligned} \tag{2.4}$$

The set $\{e_i\} = \{e_t\} \cup \{e_{\bar{t}}\}$ $(i = 1,...,m = \dim \mathfrak{M})$ is a basis for $\mathfrak{M}$.

Having fixed the basis $\{e_i\}$ we identify $\mathfrak{M}$ with $\mathbb{R}^m$, $\mathfrak{K}$ with $\mathbb{R}^q$, and $\mathfrak{L}$ with $\mathbb{R}^l$, respectively, where $\mathbb{R}^m = \mathbb{R}^q \oplus \mathbb{R}^l$. Consequently, the corresponding invertible linear maps, $\mathfrak{M} \to \mathfrak{M}$, $\mathfrak{K} \to \mathfrak{K}$, and $\mathfrak{L} \to \mathfrak{L}$, are identified with the groups $\mathrm{GL}(m,\mathbb{R})$, $\mathrm{GL}(q,\mathbb{R})$, and $\mathrm{GL}(l,\mathbb{R})$, respectively. In particular, since the adjoint action of $N(H)$ on $\mathfrak{G}$ leaves $\mathfrak{M}$ invariant, it follows that the homomorphism $n \mapsto \mathrm{Ad}\, n|\mathfrak{M}$ of $N(H)$ into the space of linear maps $\mathfrak{M} \to \mathfrak{M}$ induces a homomorphism

$$\lambda: N(H) \to \mathrm{GL}(m,\mathbb{R}) \tag{2.5}$$

[for $n \in N(H)$, $\lambda(n)$ is the matrix of the linear map $\mathrm{Ad}\, n: \mathfrak{M} \to \mathfrak{M}$ in the basis $\{e_i\}$]. We write $\lambda(N(H))$ or simply $\lambda(N)$ for the image of $N(H)$ under the homomorphism λ and use the notation

$$\Lambda(K) = \lambda(N)/\lambda(H), \tag{2.6}$$

for the factor group with elements $\Lambda(k) \equiv \lambda(n)\lambda(H)$, $k = nH \in K$.

In a similar way, the Ad action of K on $\mathfrak{K}$ induces a homomorphism

$$\lambda': K \to \mathrm{GL}(q,\mathbb{R}), \tag{2.7}$$

where $\lambda'(K)$ is the matrix of the linear map $\mathrm{Ad}\, k: \mathfrak{K} \to \mathfrak{K}$, $k \in K$, in the basis $\{e_t\}$. We note that $\lambda(N)|\mathbb{R}^q = \lambda'(K)$. Denoting $\lambda(N)|\mathbb{R}^l$ by $\lambda'(N)$ we have

$$\begin{aligned} &\lambda(n) = (\lambda'(n), \lambda'(k)) \in \mathrm{GL}(l,\mathbb{R}) \times \mathrm{GL}(q,\mathbb{R}), \\ &\quad \text{for every } n \in N(H), \quad \text{with } k = nH. \end{aligned} \tag{2.8}$$

Let S be a smooth manifold equipped with a smooth left action of G, such that all G orbits have the same type G/H. According to a well-known result (Ref. 8, Chap. 2, Theorem 5.8 and Chap. 6, §2) the manifold S admits a structure of a fiber bundle $\pi: S \to S/G$ with typical fiber G/H and structure group $K = N(H)/H$, i.e.,

$$S = (G/H \times S_0)/K. \tag{2.9}$$

Here S_0 is the submanifold of S consisting of the H-invariant points and the free left action of K on S_0 is induced by the action of $N(H)$ on S. Thus if $\pi_0 = \pi|S_0$, we have a principal K bundle $\pi_0: S_0 \to S_0/K$, and $S_0/K = S/G$. The action of the structure group K on the typical fiber G/H is identified with the right action of the automorphism group of the homogeneous space G/H (see Ref. 8, Chap. 1)

$$k: gH \mapsto gnH, \quad \text{for } k = nH. \tag{2.10}$$

In order to simplify the notations, we shall write

$$ns_0 = ks_0 \quad (\forall s_0 \in S_0) \quad \text{and} \quad gnH = gHk \tag{2.11}$$

if $k = nH$. The action of K on $G/H \times S_0$,

$$(gH, s_0) \mapsto (gHk^{-1}, ks_0),$$

generates an equivalence relation in $G/H \times S_0$: $(gH,s_0) \sim (g'H,s_0')$ iff $g'H = gHk$ and $s_0' = k^{-1}s_0$ for some $k \in K$. Factorizing with respect to $\sim$, we obtain $S = (G/H \times S_0)/K$, where the equivalence class $[gH,s_0]$ determined by the pair (gH,s_0) equals $s = gs_0$.

Let $\{W_\alpha\}_{\alpha \in I}$ be an open covering of the smooth manifold $M = S/G$ with coordinate neighborhoods. Then $S_0|W_\alpha$ and, consequently, $S|W_\alpha$, are trivial for every α:

$$\pi_0^{-1}(W_\alpha) \simeq W_\alpha \times K \quad \text{and} \quad \pi^{-1}(W_\alpha) \simeq W_\alpha \times G/H.$$

Let $\sigma_\alpha: W_\alpha \to \pi_0^{-1}(W_\alpha)$, $\alpha \in I$, be a family of local sections of the bundle $S_0(M,K,\pi_0)$ and let $k_{\alpha\beta}: W_\alpha \cap W_\beta \to K$ denote the corresponding transition functions

$$\sigma_\alpha(x) = k_{\alpha\beta}(x)\sigma_\beta(x), \quad x \in W_\alpha \cap W_\beta. \tag{2.12}$$

We introduce local trivializations $\bar{\sigma}_\alpha$: $W_\alpha \times G/H \to S$, which correspond to σ_α:

$$\bar{\sigma}_\alpha(x, gH) = g \cdot \sigma_\alpha(x) = [gH, \sigma_\alpha(x)], \quad x \in W_\alpha. \tag{2.13}$$

For every $x \in W_\alpha$ the G orbit $\pi^{-1}(x) \subset S$ is identified with G/H in the standard manner: if $s \in \pi^{-1}(x)$, then

$$s = g\sigma_\alpha(x), \tag{2.14}$$

for some $g \in G$, and from (2.13) the correspondence with G/H is established by the diffeomorphism

$$s \in \pi^{-1}(x) \mapsto \mathrm{pr}_2(\bar{\sigma}_\alpha^{-1}(s)) \in G/H.$$

Consider now G/H as a base of the principal H bundle $G(G/H,H)$ with the natural projection $g \mapsto gH$, $g \in G$. Since G is locally trivial over G/H, there exists a set of local sections $g_a: U_a \to G$ where $\{U_a\}_{a \in J}$ is an open covering of G/H. The corresponding transition functions h_{ab}: $U_a \cap U_b \to H$ satisfy

$$g_b(gH) = g_a(gH)h_{ab}(gH), \quad \text{for} \quad gH \in U_a \cap U_b. \tag{2.15}$$

Using the open covering $\{U_a\}$ of G/H, we define a family of open sets in S by

$$V_{\alpha a} = \{ s \in \pi^{-1}(W_\alpha): \mathrm{pr}_2 \circ \bar{\sigma}_\alpha^{-1}(s) \in U_a \}, \quad \alpha \in I, \quad a \in J. \tag{2.16}$$

Then

$$\pi^{-1}(W_\alpha) = \bigcup_{a \in J} V_{\alpha a}.$$

If $s \in V_{\alpha a}$, we can use the local sections $g_a : U_a \to G$ to rewrite (2.14) in the form

$$s = g_{\alpha a}(s)\sigma_\alpha(\pi(s)), \tag{2.17}$$

where

$$g_{\alpha a}(s) = g_a(\mathrm{pr}_2 \circ \bar{\sigma}_\alpha^{-1}(s)). \tag{2.18}$$

Suppose that $s \in V_{\alpha a} \cap V_{\beta b}$. Then $x = \pi(s) \in W_\alpha \cap W_\beta$ and $s = g_{\alpha a}(s)\sigma_\alpha(x) = g_{\beta b}(s)\sigma_\beta(x)$. From here

$$\sigma_\alpha(x) = g_{\alpha a}(s)^{-1} g_{\beta b}(s)\sigma_\beta(x)$$

and we obtain a smooth mapping

$$n_{\alpha a, \beta b} : V_{\alpha a} \cap V_{\beta b} \to N(H) \tag{2.19}$$

defined by

$$n_{\alpha a, \beta b}(s) = g_{\alpha a}(s)^{-1} g_{\beta b}(s). \tag{2.20}$$

It follows from (2.12) that it satisfies

$$n_{\alpha a, \beta b}(s)H = k_{\alpha\beta}(\pi(s)), \quad s \in V_{\alpha a} \cap V_{\beta b}. \tag{2.21}$$

We equip the product space $G \times S_0$ with a right action of $N(H)$:

$$(g, s_0) \mapsto (gn, n^{-1}s_0), \quad n \in N(H). \tag{2.22}$$

Lemma 2.1: With respect to the action (2.22), $G \times S_0$ is the total space of a principal $N(H)$-fiber bundle over S with projection p: $G \times S_0 \to S$ given by $p(g, s_0) = gs_0$.

Proof: It is clear that $p^{-1}(s)$ is diffeomorphic to $N(H)$ for every $s \in S$. A family of local sections can be defined in the following way: with the open covering $\{V_{\alpha a}\}_{\alpha \in I,\ a \in J}$ of S we associate the local mappings

$$q_{\alpha a} : V_{\alpha a} \to G \times S_0 \tag{2.23}$$

defined by

$$q_{\alpha a}(s) = [\, g_{\alpha a}(s), \sigma_\alpha(\pi(s))\,] \tag{2.24}$$

[cf. Eqs. (2.17) and (2.18)]. One derives that the corresponding transition functions are $n_{\alpha a, \beta b} : V_{\alpha a} \cap V_{\beta b} \to N(H)$ given by (2.20).

Remark 2.1: The above result is a simple generalization of the statement that for every Lie group G and every closed subgroup H of G the natural projection $g \mapsto gH$ is the projection in the principal H bundle $G \to G/H$. The simplest case of generalization appears when S is just one orbit of G and S_0 is diffeomorphic to K, i.e., $M = S/G$ reduces to one point only. Thus every orbit S of a Lie group G can be considered as a base of a principal fiber bundle with total space $G \times S_0$, with S_0 being the set of H-invariant points and the projection p: $G \times S_0 \to S$ is given by $p(g, s_0) = gs_0$. The choice of an H-invariant point $s_0 \in S_0$ reduces S_0 to s_0 and identifies the orbit with G/H.

III. THE BUNDLE OF LINEAR FRAMES OVER S

The bundle of linear frames over S is a principal fiber bundle Π: $F(S) \to S$ with typical fiber $\mathrm{GL}(p)$, $p = m + d$, $m = \dim G/H$, $d = \dim M$ [we use the notation $\mathrm{GL}(n)$ instead of $\mathrm{GL}(n, \mathbb{R})$ and $\mathfrak{gl}(n)$ instead of $\mathfrak{gl}(n, \mathbb{R})$ for the corresponding Lie algebra]. For every $r \in F(S)$ the right action of the element $a \in \mathrm{GL}(p)$ is denoted by

$$r \mapsto R_a r \equiv r \cdot a. \tag{3.1}$$

The action of the group G on S induces a natural action on the bundle of linear frames over S which we denote by

$$r \mapsto L_g r \equiv g \cdot r, \quad r \in F(S), \quad g \in G. \tag{3.2}$$

This allows us to define a left action of the group $\tilde{G} = G \times \mathrm{GL}(p)$ on $F(S)$ by

$$r \mapsto \tilde{g} \cdot r = L_g R_{a^{-1}} r, \quad \text{for} \quad \tilde{g} = (g, a) \in \tilde{G}. \tag{3.3}$$

Given a fixed connection τ in the bundle $S(M, G/H)$, induced by a connection τ_0 in the principal fiber bundle $S_0(M, K)$, the tangent space at every $s \in S$ can be uniquely split into a vertical part V_s and a horizontal part H_s,

$$T_s(S) = V_s \oplus H_s,$$

with H_s possessing the following property.

Lemma 3.1: If $s_0 \in S_0$ and $s = gs_0$ for some $g \in G$, then

$$H_s = g \cdot H_{s_0}.$$

Proof: Following the standard construction of horizontal spaces at the points of an associated fiber bundle (see, e.g., Ref. 6, Chap. 2, §7), we find that every horizontal curve in S through $s = gs_0$ is of the form $\bar{\gamma}_t = g \cdot \gamma_t$, where γ_t is a horizontal curve in S_0 through s_0.

In the following we shall assume that a connection is fixed once and forever in the fiber bundle $S(M, G/H)$.

A. The bundle of vertical frames over S

We call a vertical frame at the point $s \in S$ every basis $r^v = (X_1, \ldots, X_m)$ in the vertical tangent space V_s, $X_i \in V_s$ $(i = 1, \ldots, m)$. The set $F^v(S)$ of the vertical frames has a structure of a principal fiber bundle with base S and typical fiber $\mathrm{GL}(m)$.

In the following we shall use the same notations as in (3.1) and (3.2) for the right action of $\mathrm{GL}(m)$ and for the induced natural action of G on $F^v(S)$, respectively:

$$r^v \mapsto R_a r^v, \quad a \in \mathrm{GL}(m), \tag{3.4a}$$

$$r^v \mapsto L_g r^v, \quad g \in G, \quad r^v \in F^v(S) \tag{3.4b}$$

[see also Sec. II for the identification of $\mathrm{GL}(m)$ with the invertible linear maps $\mathfrak{M} \to \mathfrak{M}$].

Lemma 3.2: The restriction $F^v(S)|S_0$ of $F^v(s)$ to the points of S_0 is a trivial fiber bundle.

Proof: Let $\{e_i\}$ $(i = 1, \ldots, m)$ be the fixed basis from (2.5) in $\mathfrak{M}$. The fundamental vector fields

$$\epsilon_i(s_0) = \frac{d}{dt} \exp(te_i) \cdot s_0|_{t=0}, \quad s_0 \in S_0, \tag{3.5}$$

define a vertical frame

$$\eta^v(s_0) = \{\epsilon_1(s_0), \ldots, \epsilon_m(s_0)\} \in F^v(S)|S_0, \tag{3.6}$$

at every $s_0 \in S_0$ and we obtain a global section

$$\eta^v : S_0 \to F^v(S)|S_0.$$

Lemma 2.1 states that $G \times S_0$ is the total space of a principal $N(H)$ bundle with base S. One easily verifies the following connection with the vertical frame bundle.

Proposition 3.3: There exists a fiber bundle homomorphism j of the principal bundle $G \times S_0 \to S$ into the principal bundle $F^v(S) \to S$,

$$j': G \times S_0 \to F^v(S), \quad j'': N(H) \to \mathrm{GL}(m), \tag{3.7}$$

defined by

$$j'(g,s_0) = L_g \eta^v(s_0), \quad (g,s_0) \in G \times S_0,$$

and

$$j''(n) = \lambda(n), \quad n \in N(H)$$

[see (2.5) for the subgroup $\lambda(N) \subset \mathrm{GL}(m)$].

Remark 3.1: The content of this proposition means that the image of $G \times S_0$ under j is a subbundle of $F^v(S)$ and, therefore, the structure group $\mathrm{GL}(m)$ of the latter admits a reduction to $\lambda(N)$.

This statement contains a generalization of the particular case when $S = G/H$, and, instead of $G \times S_0$ we have only G. Then the bundle of vertical frames coincides with the bundle of linear frames over G/H and the latter can be reduced to a subbundle with structure group $\lambda(H)$ (see, e.g., Ref. 6, Chap. 10, §2).

It follows from the definitions of η^v and of λ: $N(H) \to \mathrm{GL}(m)$ that for $h \in H \subset N(H)$ we have

$$L_h \eta^v(s_0) = R_{\lambda(h)} \eta^v(s_0), \quad \forall h \in H, \quad s_0 \in S_0, \tag{3.8}$$

so we derive that for all points $\eta^v(s_0)$ one has the same representations $\lambda: H \to \mathrm{GL}(m)$ of the isotropy group (cf. Ref. 6, Chap. 10, §1).

We define a left action of the group $\tilde{G}^v = G \times \mathrm{GL}(m)$ on $F^v(S)$ by

$$r^v \mapsto \tilde{g} \cdot r^v = L_g R_{a^{-1}} r, \quad \text{for} \quad \tilde{g} = (g,a) \in \tilde{G}^v. \tag{3.9}$$

Every point $\eta^v(s_0)$, $s_0 \in S_0$, is left invariant under the action of the subgroup $\tilde{H}^v$ of $\tilde{G}^v$, defined by

$$\tilde{H}^v = \{(h,\lambda(h)) \in \tilde{G}^v : h \in H\}, \tag{3.10}$$

as follows from (3.8) and (3.9). Next, it is easily seen that with respect to the left action of the group $\tilde{G}^v$ on the manifold $F^v(S)$ the isotropy groups of all points are conjugated to $\tilde{H}^v$. Therefore, the $\tilde{G}^v$ orbits in $F^v(S)$ have the same orbit type $\tilde{G}^v/\tilde{H}^v$.

Let $\tilde{N}^v$ be the subgroup of $\tilde{G}^v$ defined by

$$\tilde{N}^v = \{(n,\lambda(n)) \in \tilde{G}^v : n \in N(H)\}. \tag{3.11}$$

Here $\tilde{H}^v$ is a normal subgroup of $\tilde{N}^v$ and the factor group $\tilde{K}^v = \tilde{N}^v/\tilde{H}^v$ is isomorphic to $K = N(H)/H$ due to the mapping

$$i: \tilde{k} = (n,\lambda(n))H^v \in \tilde{K}^v \mapsto k = nH \in K, \quad n \in N(H). \tag{3.12}$$

The action of $\tilde{N}^v$ restricted to $\eta^v(S_0)$ gives a free action of $\tilde{K}^v$:

$$\tilde{k} \cdot \eta^v(s_0) = \tilde{n} \cdot \eta^v(s_0) = L_n R_{\lambda(n^{-1})} \eta^v(s_0), \quad \forall s_0 \in S_0, \tag{3.13}$$

for $\tilde{k} = \tilde{n}\tilde{H}^v$, where $\tilde{n} = (n,\lambda(n))$, $n \in N(H)$. From (3.5) and (3.6) we obtain

$$\tilde{k} \cdot \eta^v(s_0) = \eta^v(ks_0), \quad \text{with } k = i(\tilde{k}). \tag{3.14}$$

Lemma 3.4: The map $\eta^v: S_0 \to F^v(S)|S_0$ defined by (3.6) endows $\eta^v(S_0)$ with a structure of a principal $\tilde{K}^v$ bundle with base M.

Proof: A set of local sections $\{\eta^v_\alpha\}_{\alpha \in I}$ for the natural projection $\eta^v(S_0) \to M$ is determined by means of the local sections $\sigma_\alpha: W_\alpha \to S_0$ of $S_0(M,K)$, where the $\{W_\alpha\}_{\alpha \in I}$ form an open covering of M, namely

$$\eta^v_\alpha(x) = \eta^v(\sigma_\alpha(x)), \quad x \in W_\alpha.$$

For $x \in W_\alpha \cap W_\beta$ we have, from (2.12),

$$\eta^v_\alpha(x) = \eta^v(k_{\alpha\beta}(x)\sigma_\beta(x)) = \tilde{k}_{\alpha\beta}(x)\eta^v_\beta(x).$$

B. The bundle of horizontal frames over S

We call a horizontal frame at the point $s \in S$ every basis $r^h = (X_1,...,X_d)$ in the horizontal tangent space H_s, $X_i \in H_s$ $(i = 1,...,d)$. The set $F^h(S)$ of horizontal frames is a principal fiber bundle with base S and typical fiber $\mathrm{GL}(d)$. Similarly, the set $F^h(S_0)$ of horizontal frames over S_0 is a principal $\mathrm{GL}(d)$ bundle with base S_0.

Remark 3.2: The vectors X_i $(i = 1,...,d)$, which form a horizontal frame $r^h(s_0)$ at $s_0 \in S_0$, are horizontal lifts of d vectors $Y_i = \pi(X_i)$ tangent to $x = \pi(s_0) \in M$. We shall say that $r^h(s_0)$ is the horizontal lift to s_0 of the linear frame $r(x) = (Y_1,...,Y_d)$ at the point $x = \pi(s_0)$ and we will write

$$r^h(s_0) = \mathrm{hor}\, r(x)|_{s_0}. \tag{3.15}$$

For the right action of $\mathrm{GL}(d)$ on $F^h(S)$ and for the induced natural action of G on $F^h(S)$, we shall use the same notations as in (3.1) and (3.2), respectively:

$$r^h \mapsto R_a r^h, \quad a \in \mathrm{GL}(d), \tag{3.16a}$$

$$r^h \mapsto L_g r^h, \quad g \in G, \quad r^h \in F^h(S). \tag{3.16b}$$

We define a left action of the group $\tilde{G}^h = G \times \mathrm{GL}(d)$ on $F^h(S)$ by

$$r^h \mapsto \tilde{g} \cdot r^h = L_g R_{a^{-1}} r^h, \quad \text{for} \quad \tilde{g} = (g,a) \in \tilde{G}. \tag{3.17}$$

The points from $F^h(S_0)$ are left invariant by the subgroup $\tilde{H}^h = H \times \mathrm{id}_{\mathrm{GL}(d)} \approx H$ of $\tilde{G}^h$. The restriction of $\tilde{G}^h$ to $F^h(S_0)$ is $\tilde{N}^h = N(H) \times \mathrm{GL}(d)$ and provides a free action of the group $\tilde{K}^h = \tilde{N}^h/\tilde{H}^h \approx K \times \mathrm{GL}(d)$:

$$\tilde{k}: \quad r^h(s_0) \mapsto \tilde{k} \cdot r^h(s_0) = \tilde{n} \cdot r^h(s_0) = L_n R_{a^{-1}} r^h(s_0), \tag{3.18a}$$

for $\tilde{k} = \tilde{n}\tilde{H}^h$, $\tilde{n} = (n,a) \in \tilde{N}^h$. Since the left action $r^h(s_0) \mapsto L_n r^h(s_0)$ of $N(H)$ on $F^h(S_0)$ is identical to the transformations $r^h(s_0) \mapsto L_k r^h(s_0)$ induced from the action of K on S_0, we can write (3.18a) in the form

$$r^h(s_0) \mapsto \tilde{k} \cdot r^h(s_0) = L_k R_{a^{-1}} r^h(s_0), \tag{3.18b}$$

for $\tilde{k} = (n,a)\tilde{H}^h$ and $k = nH$. We also note that in terms of the notation (3.15), the frame $r^h(s_0) = \mathrm{hor}\, r(\pi(s_0))|_{s_0}$, transformed by $\tilde{k} = (n,a)\tilde{H}^h$, becomes

$$\tilde{k} \cdot (\mathrm{hor}\, r(x)|_{s_0}) = R_{a^{-1}}(\mathrm{hor}\, r(x)|_{ks_0}), \quad x = \pi(s_0). \tag{3.19}$$

Lemma 3.5: The manifold $F^h(S_0)$ admits a structure of a principal fiber bundle over M with typical fiber $\tilde{K}^h$. The restriction $F^h(S)|S_0$ coincides with $F^h(S_0)$.

Proof: Let $\{W_\alpha\}_{\alpha \in I}$ be an open covering of M by coordinate neighborhoods and let $\{x^\mu\}$ $(\mu = 1,...,d)$ be a set of coordinate functions on some W_α; we choose a family of local sections $\sigma_\alpha: W_\alpha \to S_0$ *of* $S_0(M,K)$. The horizontal lifts $\mathrm{hor}(\partial/\partial x^\mu)$ $(\mu = 1,...,d)$ at the points $\sigma_\alpha(x) \in S_0$ of the tangent vectors $\partial/\partial x^\mu \in T_x(M)$ define a horizontal frame at every $\sigma_\alpha(x)$:

$$\eta^h_\alpha(x) = \left(\mathrm{hor}\left(\frac{\partial}{\partial x^1}\right),...,\mathrm{hor}\left(\frac{\partial}{\partial x^d}\right)\right) \tag{3.20}$$

and we get a smooth mapping

$$\eta_\alpha^h: W_\alpha \to F^h(S_0).$$

If the $\{x^{\mu'}\}$ are coordinate functions in $W_{\alpha'}$ and $x \in W_\alpha \cap W_{\alpha'}$, we have $\sigma_{\alpha'}(x) = k_{\alpha'\alpha}(x)\sigma_\alpha(x)$ with $k_{\alpha'\alpha}: W_{\alpha'} \cap W_\alpha \to K$ and so

$$\eta_\alpha^h(x) = L_{k_{\alpha\alpha'}(x)} R_{a_{\alpha\alpha'}^{-1}(x)} \eta_{\alpha'}^h(x), \tag{3.21}$$

where

$$a_{\alpha\alpha'}(x) = \left(\frac{\partial x^\mu}{\partial x^{\mu'}}\right) \in \mathrm{GL}(d). \tag{3.22}$$

C. Reduction of the linear frame bundle $F(S)$

Let us denote by $F(m,d)$ the subset of linear frames on S which at every $s \in S$ are of type $(X_1,\ldots,X_m,X_{m+1},\ldots,X_{m+d})$, with $(X_1,\ldots,X_m)$ forming a vertical frame and $(X_{m+1},\ldots,X_{m+d})$ forming a horizontal frame at s. In other words, considered as a linear isomorphism $\mathbf{R}^{m+d} \to T_s(S)$, a frame r at s belongs to $F(m,d)$ if an only if it maps $\mathbf{R}^m$ onto V_s and $\mathbf{R}^d$ onto H_s. The manifold $F(m,d)$ is a subbundle of the principal fiber bundle $F(S)$ with base S and typical fiber the subgroup $\mathrm{GL}(m)\times\mathrm{GL}(d)$ of $\mathrm{GL}(p)$.

Convention: For sake of brevity and to avoid ambiguity we shall identify $P'\times \mathrm{id}_{\mathrm{GL}(d)}$ with P' and $\mathrm{id}_{\mathrm{GL}(m)}\times P''$ with P'', where $P' \subseteq \mathrm{GL}(m)$, $P'' \subseteq \mathrm{GL}(d)$; e.g., every element $(\lambda(n),\mathrm{id}_{\mathrm{GL}(d)}) \in \mathrm{GL}(p)$ $[n \in N(H)]$ is identified with $\lambda(n) \in \mathrm{GL}(m)$.

We define a bundle homomorphism f^v: $F(m,d) \to F^v(S)$ by

$$f^v(r) = (X_1,\ldots,X_m), \quad \text{for} \quad r = (X_1,\ldots,X_{m+d}) \in F(m,d), \tag{3.23}$$

corresponding to the natural group homomorphism $\mathrm{GL}(m)\times\mathrm{GL}(d) \to \mathrm{GL}(m)$. Clearly, $F^v(S)$ is isomorphic to $F(m,d)/\mathrm{GL}(d)$.

Analogously, corresponding to the natural group homomorphism $\mathrm{GL}(m)\times\mathrm{GL}(d) \to \mathrm{GL}(d)$, there is a bundle homomorphism f^h: $F(m,d) \to F^h(S)$ defined by

$$f^h(r) = (X_{m+1},\ldots,X_{m+d}) \quad \text{for} \quad r = (X_1,\ldots,X_{m+d}) \in F(m,d). \tag{3.24}$$

Therefore, the bundle $F^h(S)$ is isomorphic to $F(m,d)/\mathrm{GL}(m)$.

For every frame $r \in F(m,d)$ at the point s, we shall write for simplicity

$$r = (r^v, r^h), \tag{3.25}$$

where r^v and r^h are a vertical and a horizontal frame at s, respectively. Denoting by $F^v(S)\underset{S}{\times}F^h(S)$ the fibered product over S (see, e.g., Ref. 6, Chap. 2, §6) of the bundles $F^v(S)$ and $F^h(S)$ we immediately check the first part of the following proposition.

Proposition 3.6: (a) The map

$$f: F(m,d) \to F^v(S) \underset{S}{\times} F^h(S), \tag{3.26}$$

defined by

$$f(r) = (f^v(r), f^h(r)), \tag{3.27}$$

where f^v and f^h are given by (3.23) and (3.24), respectively, is a fiber bundle isomorphism.

(b) The structure group $\mathrm{GL}(p), p = m + d$, of the principal fiber bundle $F(S)$ admits a reduction to the subgroup $\lambda(N)\times\mathrm{GL}(d)$.

Proof of part (b): Follows from remark 3.1 and the fact that $F(m,d) \to S$ is a reduced subbundle of $F(S)$ with structure group $\mathrm{GL}(m)\times\mathrm{GL}(d)$.

Proposition 3.7: The structure group $\mathrm{GL}(p)$ of the principal fiber bundle $F(S)|S_0$ admits a reduction to the subgroup $\mathrm{GL}(d)$. The total space of the reduced subbundle is

$$F_0 = \{(\eta^v(s_0), r^h(s_0)) \in F(S)|S_0: \; s_0 \in S_0, \quad r^h(s_0) \in F^h(S_0)\}.$$

Proof: Follows from Lemma 3.2 and from Proposition 3.6(a).

Every point $r(s_0) = (\eta^v(s_0), r^h(s_0)) \in F_0$ is invariant under the action of the subgroup $\tilde{H}$ of $\tilde{G}$ defined by

$$\tilde{H} = \{(h, \lambda(h)) \in \tilde{G}: h \in H\}. \tag{3.28}$$

The restriction of $\tilde{G}$ to F_0 reads

$$\tilde{N} = \{(n, \lambda(n)a) \in \tilde{G}: n \in N(H), a \in \mathrm{GL}(d)\} \tag{3.29}$$

and provides a free action of the group $\tilde{K} = \tilde{N}/\tilde{H}$ on F_0:

$$\tilde{k}: r(s_0) \mapsto \tilde{k}\cdot r(s_0) = \tilde{n}\cdot r(s_0) = L_n R_{\lambda(n^{-1})a^{-1}} r(s_0), \tag{3.30}$$

for $\tilde{k} = \tilde{n}\tilde{H}, \tilde{n} = (n, \lambda(n)a) \in \tilde{N}$. Note the group isomorphism $\tilde{K} \simeq K \times \mathrm{GL}(d)$ given by

$$(n, \lambda(n)a)\tilde{H} \in \tilde{K} \mapsto (nH, a) \in K \times \mathrm{GL}(d). \tag{3.31}$$

Proposition 3.8: The manifold

$$F_0 = \{(\eta^v(s_0), r^h(s_0)) \in (F^v(S)|S_0) \underset{S_0}{\times} F^h(S_0): s_0 \in S_0\} \tag{3.32}$$

has a structure of a principal fiber bundle over M with typical fiber $\tilde{K}$, $\hat{\pi}: F_0 \to M$.

Proof: From (3.30), (3.13), and (3.18),

$$\tilde{k}\cdot(\eta^v(s_0), r^h(s_0)) = (\tilde{k}^v\cdot\eta^v(s_0), \tilde{k}^h\cdot r^h(s_0)), \quad \forall \tilde{k} \in \tilde{K},$$

where $\tilde{k}^v \in \tilde{K}^v$ and $\tilde{k}^h \in \tilde{K}^h$ are uniquely determined by the element $\tilde{k}$. Then the statement follows from Lemmas 3.4 and 3.5.

Using (3.15) we can write every element from F_0 in the form

$$r(s_0) = (\eta^v(s_0), \mathrm{hor}\, r(x)|_{s_0}), \quad s_0 \in S_0, \tag{3.33}$$

for some linear frame $r(x)$ at the point $x = \pi(s_0) \in M$. Now we note that factorizing F_0 with respect to the action of K [cf. (3.31)] one gets the isomorphism of fiber bundles

$$F_0/K \simeq F(M, \mathrm{GL}(d)), \tag{3.34}$$

where $F(M,\mathrm{GL}(d))$ denotes the bundle of linear frames over M. In (3.34) the K orbit passing through $r(s_0) \in F_0$ is identified with the frame $r(\pi(s_0))$ at the point $\pi(s_0) \in M$ following (3.33). In an analogous way the factorization of F_0 with respect to the action of $\mathrm{GL}(d)$ gives the bundle isomorphism

$$F_0/\mathrm{GL}(d) \simeq S_0(M,K), \tag{3.35}$$

namely the orbit of $\mathrm{GL}(d)$ passing through $r(s_0) \in F_0$ is identified with s_0.

With respect to the $\tilde{G}$ action on $F(S)$ the isotropy groups of all points are conjugated to $\tilde{H}$. Therefore, the $\tilde{G}$ orbits in $F(S)$ have the same orbit type $\tilde{G}/\tilde{H}$.

Proposition 3.9: The manifold $F(S)$ has a structure of a fiber bundle over M with typical fiber $\tilde{G}/\tilde{H}$ associated to the principal fiber bundle $F_0(M,\tilde{K})$.

Proof: We have a right action of $\tilde{K}$ on $\tilde{G}/\tilde{H}$ given by

$$\tilde{k}\colon (g,b)\tilde{H} \mapsto (g,b)\tilde{H}\cdot\tilde{k} = (gn,ba\lambda(n))\tilde{H},$$

for $\tilde{k} = \tilde{n}\tilde{H}$, $\tilde{n} = (n,\lambda(n)a)$, with $a \in \mathrm{GL}(d)$, $n \in N(H)$, $g \in G$, and $b \in \mathrm{GL}(p)$. It gives rise to an equivalence relation $\sim$ in $\tilde{G}/\tilde{H}\times F_0$:

$$(\tilde{g}\tilde{H},r(s_0)) \sim (\tilde{g}'\tilde{H},r'(s_0')) \quad \text{iff } \tilde{g}'\tilde{H} = \tilde{g}\tilde{H}\cdot\tilde{k},\ r'(s_0') = \tilde{k}\cdot r(s_0),$$

for some $\tilde{k} \in \tilde{K}$. Factorizing with respect to $\sim$, we obtain

$$F(s) = (\tilde{G}/\tilde{H}\times F_0)/\tilde{K},$$

where the equivalence class $[\tilde{g}\tilde{H},r(s_0)]$, determined by the pair $(\tilde{g}\tilde{H},r(s_0)) \in \tilde{G}/\tilde{H}\times F_0$, is the linear frame

$$r = \tilde{g}\cdot r(s_0) = L_g R_{a^{-1}} r(s_0), \quad \tilde{g} = (g,a) \in \tilde{G}, \tag{3.36}$$

at the point $s = gs_0$.

Remark 3.3: In an analogous way one can show that $F^v(S)$ and $F^h(S)$ admit a fiber bundle structure with a typical fiber $\tilde{G}^v/\tilde{H}^v$ and $G/H\times\mathrm{GL}(d)$, respectively:

$$F^v(S) = (\tilde{G}^v/\tilde{H}^v\times\eta^v(S_0))/\tilde{K}^v,$$
$$F^h(S) = ((G/H\times\mathrm{GL}(d))\times F^h(S_0))/\tilde{K}^h.$$

Remark 3.4: We can interpret the last two propositions in the following way. We obtain that the principal fiber bundle $F(S)$ over S with structure group $\mathrm{GL}(p)$, where S is a fiber bundle with base M, structure group K, equipped with a connection τ, becomes completely determined (via the $\tilde{G}$ action) by its submanifold $F_0 \subset F(S)$, which itself has a structure of a principal bundle over M. In that sense we can say that the principal $\mathrm{GL}(p)$ bundle $F(S) \to S$ is dimensionally reduced to the principal bundle $F_0 \to M$ with a structure group $\tilde{K} \approx K\times\mathrm{GL}(d)$, $\mathrm{GL}(d) \subset \mathrm{GL}(p)$.

IV. *G*-INVARIANT FIELDS ON *S*

Let the group G act as a group of automorphisms on the fiber bundle $p\colon Q \to B$:

$$u \mapsto g\cdot u, \quad p(u) \mapsto g\cdot p(u), \quad \forall u \in Q, \quad g \in G \tag{4.1}$$

(we use the same notation for the action of G on Q and the induced G action on B). By means of the action (4.1) every cross section $\varphi\colon B \to Q$ is mapped into the cross section $\theta_g\varphi\colon B \to Q$, where

$$\theta_g\varphi(u) = g\cdot\varphi(g^{-1}\cdot u), \tag{4.2}$$

so that the diagram

$$\begin{array}{ccc} Q & \xrightarrow{g} & Q \\ {\scriptstyle\varphi}\uparrow & & \uparrow{\scriptstyle\theta_g\varphi} \\ B & \xrightarrow{g} & B \end{array} \tag{4.3}$$

is commutative. We say that a cross section φ of Q, i.e., a Q-valued field φ on B, is G *invariant* if

$$\theta_g\varphi = \varphi, \quad \forall g \in G, \tag{4.4a}$$

or, equivalently, if

$$\varphi(g\cdot u) = g\cdot\varphi(u). \tag{4.4b}$$

In what follows we shall describe the G-invariant sections of the fiber bundles associated to the bundle of linear frames $F(S)$ over the manifold S.

Let $\mathscr{F}$ be a manifold equipped with a left action ρ of the group $\mathrm{GL}(p)$:

$$f \mapsto \rho(a)f, \quad f \in \mathscr{F}, \quad a \in \mathrm{GL}(p). \tag{4.5}$$

Let $E = F(S)\times\mathscr{F}/\mathrm{GL}(p)$ be the fiber bundle associated to $F(S)$ by the representation ρ of $\mathrm{GL}(p)$ in $\mathscr{F}$. There is a left G action on E induced from the action of G on $F(S)$: writing every element from the fiber E_s over $s \in S$ as the equivalence class $[r(s),f]$, where $(r(s),f) \in F(S)\times\mathscr{F}$ and $r(s)$ denotes a linear frame at s, we have

$$g\colon [r(s),f] \in E_s \mapsto g\cdot[r(s),f] = [L_g r(s),f] \in E_{gs}, \quad \forall g \in G.$$

Let $\varphi\colon S \to E$ be a G-invariant field on S. In terms of the $\mathrm{GL}(p)$-equivariant map $\tilde{\varphi}\colon F(S) \to \mathscr{F}$, which corresponds to the field φ by the formula

$$\varphi(s) = [r(s),\tilde{\varphi}(r(s))],$$
$$\tilde{\varphi}(R_a r(s)) = \rho(a^{-1})\tilde{\varphi}(r(s)), \quad a \in \mathrm{GL}(p),$$

the property (4.4b) translates into

$$\tilde{\varphi}(L_g r(s)) = \tilde{\varphi}(r(s)), \quad g \in G.$$

Considering (4.5) as a representation of the group $\tilde{G} = G\times\mathrm{GL}(p)$ given by

$$\rho(g,a) = \rho(a), \quad g \in G, \quad a \in \mathrm{GL}(p),$$

we see that the G-invariant field $\varphi\colon S \to E$ is equivalently described by the map

$$\tilde{\varphi}\colon F(S) \to \mathscr{F}$$

with the transformation property

$$\tilde{\varphi}(g\cdot r(s)) = \rho(a)\tilde{\varphi}(r(s)), \quad \tilde{g} = (g,a) \in \tilde{G}.$$

Then it follows from Proposition 3.9 [see Eq. (3.36)] that the map $\tilde{\varphi}$ is completely determined by its restriction $\tilde{\varphi}|F_0$. The latter has to satisfy $\tilde{\varphi}(r(s_0)) = \rho(\lambda(h))\tilde{\varphi}(r(s_0))$ for every $h \in H$ and

$$\tilde{\varphi}(\tilde{k}\cdot r(s_0)) = \rho(\lambda(n)a)\tilde{\varphi}(r(s_0)), \quad \forall\tilde{k} = (n,\lambda(n)a)\tilde{H} \in \tilde{K}.$$

Thus, denoting the subspace of $\lambda(H)$-invariant points from $\mathscr{F}$ by $\mathscr{F}_0$,

$$\mathscr{F}_0 = \{ f \in \mathscr{F}\colon \rho(\lambda(h))f = f,\ \forall h \in H \},$$

we obtain a $\tilde{K}$-equivariant map $\tilde{\varphi}|F_0\colon F_0 \to \mathscr{F}_0$. Here the representation of $\tilde{K}$ in $\mathscr{F}_0$ is given by

$$\tilde{k} \equiv (n,\lambda(n)a)\tilde{H} \mapsto \rho(\lambda(n)a). \tag{4.6}$$

The $\tilde{K}$-equivariant map $\tilde{\varphi}|F_0$ determines uniquely a cross seciton $\hat{\varphi}$ of the fiber bundle $(F_0\times\mathscr{F}_0)/\tilde{K}$ over M associated to $F_0(M,\tilde{K})$ via the representation (4.6) of $\tilde{K}$ in $\mathscr{F}_0$. Here $\hat{\varphi}$ is defined by the formula

$$\hat{\varphi}(\pi(s_0)) = [r(s_0),\tilde{\varphi}(r(s_0))]', \quad r(s_0) \in F_0,$$

where the equivalence class $[\ ,\ ]'$ is taken with respect to the action of the group $\tilde{K}$ in $F_0\times\mathcal{F}_0$. From here we obtain the following proposition.

Proposition 4.1: Given a connection in the principal fiber bundle $S_0(M,K)$, the G-invariant fields on S,

$$\varphi: S\to E=(F(S)\times\mathcal{F})/\mathrm{GL}(p),\quad \varphi(s)=[r(s),\tilde{\varphi}(r(s))],$$

are in one-to-one correspondence with the fields $\hat{\varphi}$: $M\to E_0=(F_0\times\mathcal{F}_0)/\tilde{K}$ on M defined by

$$\hat{\varphi}(\pi(s_0))=[r(s_0),\tilde{\varphi}(r(s_0))]'.$$

We say that the G-invariant fields φ on S admit *dimensional reduction* to the fields $\hat{\varphi}$ on M, constructed according to Proposition 4.1 (cf. Remark 3.4). We call $\hat{\varphi}$ a *dimensionally reduced field*, corresponding to the G-invariant field φ.

Examples: (a) G-invariant vector fields on S: In this case we have a section

$$\varphi: S\to T(S)=(F(S)\times\mathbb{R}^p)/\mathrm{GL}(p),\quad \varphi(gs)=g\cdot\varphi(s)$$

[$\mathcal{F}=\mathbb{R}^p$ and $\rho(a)=a$, $a\in\mathrm{GL}(p)$]. According to Proposition 4.1 the G-invariant vector field φ is determined by a field $\hat{\varphi}$: $M\to T_0=(F_0\times(\mathbb{R}^q\oplus\mathbb{R}^d))/\tilde{K}$ on M. We can split the corresponding $\tilde{K}$-equivariant map $\tilde{\varphi}|F_0$: $F_0\to\mathbb{R}^q\oplus\mathbb{R}^d$ to a sum of two mappings since

$$\tilde{\varphi}(r(s_0))=\mathrm{pr}_{\mathbb{R}^q}\circ\tilde{\varphi}(r(s_0))+\mathrm{pr}_{\mathbb{R}^d}\circ\tilde{\varphi}(r(s_0)),$$
$$\forall r(s_0)\in F_0. \tag{4.7}$$

The first mapping, $\mathrm{pr}_{\mathbb{R}^q}\circ\tilde{\varphi}|F_0$, is invariant with respect to the action of the subgroup $\mathrm{GL}(d)$ of $\tilde{K}$ and due to the bundle isomorphism (3.35): $F_0/\mathrm{GL}(d)\simeq S_0$, it determines a K-equivariant map $\tilde{\varphi}^v$: $S_0\to\mathbb{R}^q$ by

$$\tilde{\varphi}^v(s_0)=\mathrm{pr}_{\mathbb{R}^q}\circ\tilde{\varphi}(r(s_0)).$$

Identifying $\mathbb{R}^q$ and the subspace $\mathfrak{R}\subset\mathfrak{G}$ (see the beginning of Sec. II) we obtain a cross section φ^v of the vector bundle $(S_0\times\mathfrak{R})/K$ associated to $S_0(M,K)$ by the Ad action of K on its Lie algebra. Then φ^v is given by the formula

$$\varphi^v(\pi(s_0))=[s_0,\tilde{\varphi}^v(s_0)].$$

The second map in (4.7), $\mathrm{pr}_{\mathbb{R}^d}\circ\tilde{\varphi}|F_0$, is invariant with respect to the action of the subgroup K of $\tilde{K}$, and the bundle isomorphism (3.34): $F_0/K\simeq F(M)$ leads to a $\mathrm{GL}(d)$-equivariant map $\tilde{\varphi}^h$: $F(M)\to\mathbb{R}^d$ by

$$\tilde{\varphi}^h(r(x))=\mathrm{pr}_{\mathbb{R}^d}\circ\tilde{\varphi}(r(s_0))\quad[x=\pi(s_0)],$$

where $r(s_0)=(\eta^v(s_0),\mathrm{hor}\,r(x)|_{s_0})$, [see (3.33)]. The map $\tilde{\varphi}^h$ determines a unique cross section φ^h of the vector bundle $E=(F(M)\times\mathbb{R}^d)/\mathrm{GL}(d)$ isomorphic to $T(M)$ [since E is associated to $F(M)$ by the natural action of $\mathrm{GL}(d)$ on $\mathbb{R}^d$]. We have, for each $x\in M$,

$$\varphi^h(x)=[r(x),\tilde{\varphi}^h(r(x))].$$

Thus one finds that the G-invariant vector fields on S are in one-to-one correspondence with the pairs of fields (φ^v,φ^h), where φ^v is a cross section φ^v: $M\to(S_0\times\mathfrak{R})/K$ and φ^h: $M\to T(M)$ is a vector field on M.

(b) Vector-valued tensor fields on S: Let $T^\mu_\nu(S)$ denote the bundle of μ times covariant and ν times contravariant tensors over S. If V is a vector space, the tensor product $E^\mu_\nu=T^\mu_\nu(S)\otimes V$ is a vector bundle over S with typical fiber $\mathcal{F}=L((\mathbb{R}^p)^\mu,(\mathbb{R}^p)^\nu;V)$. The space $\mathcal{F}$ is endowed with the induced representation of $\mathrm{GL}(p)$,

$$\rho(a): l\mapsto l\circ((a^{-1})^\mu\otimes({}^ta)^\nu),\quad \forall a\in\mathrm{GL}(p),\quad l\in\mathcal{F} \tag{4.8}$$

(${}^ta$ is the transposed matrix of a), i.e.,

$$(\rho(a)l)(\xi_1,\dots,\xi_\mu;\eta_1,\dots,\eta_\nu)$$
$$=l(a^{-1}\cdot\xi_1,\dots,a^{-1}\cdot\xi_\mu;{}^ta\cdot\eta_1,\dots,{}^ta\cdot\eta_\nu),$$

where $(\xi_1,\dots,\xi_\mu)\equiv\xi\in(\mathbb{R}^p)^\mu$, $(\eta_1,\dots,\eta_\nu)\equiv\eta\in(\mathbb{R}^p)^\nu$. We can consider E^μ_ν as the fiber bundle

$$E=(F(S)\times\mathcal{F})/\mathrm{GL}(p) \tag{4.9}$$

associated to $F(S)$ by the action (4.8) of $\mathrm{GL}(p)$.

We say that a cross section φ: $M\to E^\mu_\nu$, φ: $s\mapsto L(T^\mu_{\nu,s};V)$, is a *G-invariant tensor field* on S of type $(\mu,\nu;V)$ if

$$\varphi_{gs}(g\cdot\bar{\xi}_1,\dots,g\cdot\bar{\xi}_\mu;(g^{-1})^*\cdot\bar{\eta}_1,\dots,(g^{-1})^*\cdot\bar{\eta}_\nu)$$
$$=\varphi_s(\bar{\xi}_1,\dots,\bar{\xi}_\mu;\bar{\eta}_1,\dots,\bar{\eta}_\nu), \tag{4.10a}$$
$$(\bar{\xi}_1,\dots,\bar{\xi}_\mu;\bar{\eta}_1,\dots,\bar{\eta}_\nu)\equiv(\bar{\xi};\bar{\eta})\in T^\mu_{\nu,s},\quad g\in G,\quad s\in S,$$

or in a compact notation,

$$\varphi_{gs}=\varphi_s\circ g^{-1}. \tag{4.10b}$$

Writing the elements from E^μ_ν as equivalence classes of the $\mathrm{GL}(p)$ action in $F(S)\times\mathcal{F}$, we have

$$\varphi_s=[r(s),\tilde{\varphi}_{r(s)}],\quad s\in S,$$

where $r(s)\in F(S)_s$ is a frame at the point s and $\tilde{\varphi}$ is a mapping $F(S)\to\mathcal{F}$, which obeys

$$\tilde{\varphi}_{R_a r(s)}=\rho(a^{-1})\tilde{\varphi}_{r(s)}, \tag{4.11}$$

and, from (4.10),

$$\tilde{\varphi}_{g\cdot r(s)}=\tilde{\varphi}_{r(s)}. \tag{4.12}$$

If $(\xi;\eta)\in(\mathbb{R}^p)^\mu\times(\mathbb{R}^p)^\nu$ are the coordinates of the element $(\bar{\xi};\bar{\eta})\in T^\mu_{\nu,s}$ in the frame $r(s)$, i.e.,

$$(\bar{\xi};\bar{\eta})=[r(s),(\xi;\eta)],$$

we have

$$\varphi_s(\bar{\xi};\bar{\eta})=\tilde{\varphi}_{r(s)}(\xi;\eta)\in V. \tag{4.13}$$

According to Proposition 4.1, the field φ admits dimensional reduction. The dimensionally reduced field is a cross section of the fiber bundle $E^\mu_{\nu,0}=(F_0\times\mathcal{F}_0)/\tilde{K}$, where $\mathcal{F}_0$ is the subspace of $L((\mathbb{R}^p)^\mu,(\mathbb{R}^p)^\nu;V)$ consisting of the $\lambda(H)$-invariant points, i.e., $l\in\mathcal{F}_0$ iff

$$l\circ((\lambda(h^{-1}))^\mu\otimes({}^t\lambda(h))^\nu)=l,\quad\forall h\in H.$$

(c) G-invariant metrics on S: For a description see Refs. 2 and 4.

V. G-INVARIANT PSEUDOTENSORIAL FIELDS AND LINEAR CONNECTIONS ON S

A. Pseudotensorial fields

Let V be a vector space and ρ a linear representation of $\mathrm{GL}(p)$ in V: $v\mapsto\rho(a)v$, $\forall v\in V$, $a\in\mathrm{GL}(p)$. We write $T^\nu(F(S))$ for the direct product

$$T(F(S))\times\cdots\times T(F(S))\quad(\nu\text{ factors}).$$

Denote by V^ν the tensor product fiber bundle $V^\nu=T^\nu(F(S))^*\otimes V$; its fiber over every $r\in F(S)$ is

$$V_r^\nu = (T_r^\nu)^* \otimes V = L(T_r^\nu; V).$$

We say that a cross section φ of the fiber bundle V^ν,

$$\varphi: r \mapsto \varphi_r \in L(T_r^\nu; V),$$

satisfying

$$\varphi_{R_a r}(\xi_1,\ldots,\xi_\nu) = \rho(a^{-1})\varphi_r(R_{a^{-1}}\xi_1,\ldots,R_{a^{-1}}\xi_\nu), \tag{5.1}$$

for every $a \in \mathrm{GL}(p)$, $(\xi_1,\ldots,\xi_\nu) \in T^\nu_{R_a r}$, in other terms, a *pseudotensorial field* of type $(\nu, \rho; V)$ on S (cf. Ref. 6, Chap. 2, §5) is G-invariant if

$$\varphi_{L_g r}(L_g\xi_1,\ldots,L_g\xi_\nu) = \varphi_r(\xi_1,\ldots,\xi_\nu), \quad \forall g \in G. \tag{5.2}$$

In terms of the group $\tilde{G} = G \times \mathrm{GL}(p)$ denoting the induced representation of $\tilde{G}$ in V^ν by $\tilde{\rho}$,

$$\tilde{\rho}(\tilde{g})l = \rho(a) \circ l \circ (R_a L_{g^{-1}})^\nu, \tag{5.3}$$

for every $l \in V^\nu$ and $\tilde{g} = (g,a) \in \tilde{G}$, we write Eqs. (5.1) and (5.2) in a unified form:

$$\varphi_{\tilde{g}\cdot r} = \tilde{\rho}(\tilde{g})\varphi_r. \tag{5.4}$$

The last formula means that every G-invariant pseudotensorial field $\varphi: F(S) \to V^\nu$ of type $(\nu, \rho; V)$ on S is a $\tilde{G}$-invariant tensor field of type $(\nu; V)$ on $F(S)$ with the $\tilde{G}$ action on V^ν given by the representation $\tilde{\rho}$.

It follows from Proposition 3.9 that φ is determined by the restriction $\varphi|F_0$, which takes values in the subbundle V_0^ν of V^ν with total space consisting of the $\tilde{\rho}(\tilde{H})$-invariant points, i.e., those for which [see (3.28)]

$$\tilde{\rho}(\tilde{h})\varphi_{r(s_0)} = \varphi_{r(s_0)}, \quad \forall \tilde{h} \in \tilde{H}. \tag{5.5}$$

The subbundle V_0^ν of V^ν is a fiber bundle over F_0 whose fiber over each $r(s_0) \in F_0$ consists of the $\tilde{H}$-invariant linear maps from $T^\nu_{r(s_0)}(F(S))$ into V, i.e.,

$$V^\nu_{0,r(s_0)} = \{ l \in V^\nu_{r(s_0)}: \rho(\lambda(h)) \circ l \circ (R_{\lambda(h)} L_{h^{-1}})^\nu = l, \ \forall h \in H \}.$$

Let us denote by $\tilde{\rho}(\tilde{K})$ the natural representation of $\tilde{K}$ in V_0^ν obtained from the restriction of $\tilde{\rho}(\tilde{N})$ to V_0^ν [see (3.29) for the definition of the subgroup $\tilde{N}$]:

$$\tilde{\rho}(\tilde{k})l = \rho(\lambda(n)a) \circ l \circ (R_{\lambda(n)} L_{n^{-1}})^\nu, \tag{5.6}$$

for every $l \in V_0^\nu$, $\tilde{k} = (n, \lambda(n)a)\tilde{H}$. Then as a consequence of (5.4), we obtain that $\varphi|F_0$ is a $\tilde{K}$-invariant field with values in the fiber bundle $V_0^\nu \to F_0$:

$$\varphi|F_0: F_0 \to V_0^\nu, \quad \varphi_{\tilde{k}\cdot r(s_0)} = \tilde{\rho}(\tilde{k})\varphi_{r(s_0)},$$

or in full notation

$$\varphi_{(n,\lambda(n)a)r(s_0)}(\xi_1,\ldots,\xi_\nu) = \rho(\lambda(n)a)\varphi_{r(s_0)}(R_{\lambda(n)a}L_{n^{-1}}\xi_1,\ldots,R_{\lambda(n)a}L_{n^{-1}}\xi_\nu). \tag{5.7}$$

Summarizing, we find the following proposition.

Proposition 5.1: Given a connection in the principal fiber bundle $S_0(M,K)$, the G-invariant pseudotensorial fields of type $(\nu, \rho; V)$ on S are in one-to-one correspondence with the $\tilde{K}$-invariant fields on F_0 with values in the subbundle $V_0^\nu \to F_0$ of V^ν.

Remark 5.1: Although F_0 is a principal $\tilde{K}$ bundle over M, we note that a $\tilde{K}$-invariant field on F_0, in general, does not define a field on M (cf. Sec. V B).

B. G-invariant linear connection on S

A G-invariant linear connection on S is distinguished by the property (see, e.g., Ref. 6, Chap. 2, §6) that under the action of every $g \in G$ the horizontal subspaces satisfy

$$L_g H_r = H_{L_g r}, \quad \forall r \in F(S),$$

or, equivalently, the corresponding connection form obeys

$$L_g^* \omega = \omega. \tag{5.8}$$

Due to the equivariance property with respect to the action of the structure group $\mathrm{GL}(p)$,

$$R_a^* \omega = \mathrm{Ad}(a^{-1}) \cdot \omega, \quad \forall a \in \mathrm{GL}(p), \tag{5.9}$$

and the G invariance, the connection form ω is a G-invariant pseudotensorial field of type $(1, \mathrm{Ad}; \mathfrak{gl}(p))$ on S (in the notations of Sec. V A). Putting this in other terms, ω is a G-invariant tensor field of type $(1; \mathfrak{gl}(p))$ on $F(S)$:

$$\omega: F(S) \to T(F(S))^* \otimes \mathfrak{gl}(p),$$

$$\omega_{\tilde{g}\cdot r(s_0)}(\xi) \equiv \omega_{(g,a)\cdot r(s_0)}(\xi) = \mathrm{Ad}\, a \cdot \omega_{r(s_0)}(R_a L_{g^{-1}}\xi),$$

for every $r(s_0) \in F_0$, $\xi \in T_{\tilde{g}r(s_0)}(F(S))$, and $\tilde{g} = (g,a) \in \tilde{G}$. The representation of G in $T(F(S))^* \otimes \mathfrak{gl}(p)$ is given by

$$\rho(\tilde{g})l = \mathrm{Ad}\, a \cdot l \circ (R_a L_{g^{-1}}), \tag{5.10}$$

for each $l \in T(F(S))^* \otimes \mathfrak{gl}(p)$, $\tilde{g} = (g,a) \in \tilde{G}$.

Following our previous discussion, ω is completely determined by the restriction $\omega|F_0$, which takes values in the subbundle $\mathscr{E}$ of $T(F(S))^* \otimes \mathfrak{gl}(p)$ consisting of the $\tilde{\rho}(\tilde{H})$-invariant points

$$\mathscr{E} = \{ l \in L(T_{r(s_0)}(F(S)); \mathfrak{gl}(p)): \tilde{\rho}(\tilde{h})l = l, \quad \forall \tilde{h} \in \tilde{H}, \quad r(s_0) \in F_0 \}.$$

For $\omega|F_0: F_0 \to \mathscr{E}$, we have

$$\omega_{r(s_0)} = \tilde{\rho}(\tilde{h})\omega_{r(s_0)} \equiv \mathrm{Ad}(\lambda(h))\omega_{r(s_0)} \circ R_{\lambda(h)} L_{h^{-1}}, \tag{5.11}$$

for every $\tilde{h} = (h, \lambda(h)) \in \tilde{H}$. In this particular case the representation (5.6) of the group $\tilde{K}$ in $\mathscr{E}$ reads

$$\tilde{\rho}(\tilde{k})l = \mathrm{Ad}(\lambda(n)a)l \circ (R_{\lambda(n)a} L_{n^{-1}}), \quad \forall l \in \mathscr{E}, \tag{5.12}$$

$\tilde{k} = (n, \lambda(n)a)\tilde{H} \in \tilde{K}$. With respect to the $\tilde{K}$ action in $\mathscr{E}$ realized by (5.12) the mapping $\omega|F_0: F_0 \to \mathscr{E}$ is a $\tilde{K}$-equivariant field on F_0:

$$\omega_{\tilde{k}\cdot r(s_0)}(\xi) = \mathrm{Ad}(\lambda(n)a)\omega_{r(s_0)}(R_{\lambda(n)a} L_{n^{-1}}\xi), \tag{5.13}$$

for each $\xi \in T_{\tilde{k}r(s_0)}F(S))$.

Since, for every vertical fundamental vector field $\tilde{A}$ generated by some $A \in \mathfrak{gl}(p)$, we have

$$\omega(\tilde{A}) = A, \tag{5.14}$$

it is sufficient to specify the values of ω only for the natural lifts to the points from F_0 (see, e.g., Ref. 6, Chap. 6, §2) of the vector fields defined on neighborhoods $U \subset S$ of the points $s_0 \in S_0$. Every such vector field $\tilde{\xi}$ is uniquely decomposed into the sum

$$\tilde{\xi} = \overline{X} + \overline{Y} + \overline{Z}, \tag{5.15}$$

where $\overline{X}$ is the horizontal lift with respect to the connection τ (see the beginning of Sec. III) of a vector field X on $\pi(U) \subset M$, $\overline{Y}$ is a vector field generated by some $Y \in \mathfrak{K} \subset \mathfrak{G}$, and $\overline{Z}$ is a vector field generated by some $Z \in \mathfrak{L} \subset \mathfrak{G}$ [recall that $T^v_{s_0}(S) \approx \mathfrak{M} = \mathfrak{K} \oplus \mathfrak{L}$].

Due to the linear property, it follows from (5.15) that the natural lift $\tilde{\xi}$ of the local vector field $\bar{\xi} = \bar{X} + \bar{Y} + \bar{Z}$ decomposes uniquely into the sum

$$\tilde{\xi} = \tilde{X} + \tilde{Y} + \tilde{Z} \tag{5.16}$$

of the natural lifts of the vector fields $\bar{X}$, $\bar{Y}$, and $\bar{Z}$, respectively. Thus for the study of ω, it is sufficient to specify the values appearing in the right-hand side of the equality

$$\omega_{r(s_0)}(\tilde{X} + \tilde{Y} + \tilde{Z}) = \omega_{r(s_0)}(\tilde{X}) + \omega_{r(s_0)}(\tilde{Y}) + \omega_{r(s_0)}(\tilde{Z}), \tag{5.17}$$

$\forall r(s_0) \in F_0$. In (5.17) and below we shall keep the following notations: X for a vector field in a neighborhood of $\hat{\pi}(r(s_0)) \in M$, Y for the elements from $\mathfrak{K}$, and Z for the elements from $\mathfrak{L}$. We recall that $\mathfrak{M} = \mathfrak{K} \oplus \mathfrak{L}$ is identified with $\mathbb{R}^m$, and $\mathfrak{K}$ and $\mathfrak{L}$ with $\mathbb{R}^q$ and $\mathbb{R}^l$, respectively; these identifications will be used in what follows.

For the vector fields $\tilde{X}$, $\tilde{Y}$, and $\tilde{Z}$ we have

$$\tilde{X}_{\tilde{k} \cdot r(s_0)} = L_n R_{\lambda(n^{-1})a^{-1}} \tilde{X}_{r(s_0)}, \tag{5.18}$$

$$\tilde{Y}_{\tilde{k} \cdot r(s_0)} = L_n R_{\lambda(n^{-1})a^{-1}} \widetilde{(\lambda(n^{-1})Y)}_{r(s_0)}, \tag{5.19}$$

$$\tilde{Z}_{\tilde{k} \cdot r(s_0)} = L_n R_{\lambda(n^{-1})a^{-1}} \widetilde{(\lambda(n^{-1})Z)}_{r(s_0)}, \tag{5.20}$$

$\forall r(s_0) \in F_0$, $\tilde{k} = (n, \lambda(n)a)\tilde{H} \in \tilde{K}$. So it is clear from (5.11) that the restriction of $\omega|F_0$ to the vector fields of the type $\tilde{X} + \tilde{Y}$ takes values in the commutant $\mathfrak{Z}_H$ of $\lambda(H)$ in $\mathfrak{GI}(p)$,

$$\mathfrak{Z}_H = \{ f \in \mathfrak{GI}(p) : \mathrm{Ad}(\lambda(h))f = f, \forall h \in H \}, \tag{5.21}$$

or

$$\omega_{r(s_0)}(\tilde{X}) \in \mathfrak{Z}_H, \quad \omega_{r(s_0)}(\tilde{Y}) \in \mathfrak{Z}_H, \quad \text{for every} \quad r(s_0) \in F_0. \tag{5.22}$$

Further, using the properties of $\mathfrak{L}$, it is an algebraic exercise to show that

$$\mathrm{pr}_{\mathfrak{Z}_H} \omega_{r(s_0)}(\tilde{Z}) = 0, \quad \forall r(s_0) \in F_0, \tag{5.23}$$

for every vector field of the type $\tilde{Z}$.

For our further analysis it is convenient to introduce the direct sum decomposition of $\mathbb{R}^p$ of the form

$$\mathbb{R}^p \to \begin{pmatrix} \mathbb{R}^l \\ \mathbb{R}^q \\ \mathbb{R}^d \end{pmatrix}.$$

Correspondingly, we have the following block-matrix forms for the matrices from $\lambda(H)$ and $\lambda(N) \times \mathrm{GL}(d)$:

$$\lambda(h) \in \lambda(H) \to \begin{pmatrix} \lambda(h) & & \\ & \mathrm{id}_{\mathrm{GL}(q)} & \\ & & \mathrm{id}_{\mathrm{GL}(d)} \end{pmatrix}, \tag{5.24a}$$

$$\lambda(n)a \in \lambda(N) \times \mathrm{GL}(d) \to \begin{pmatrix} \lambda'(n) & & \\ & \lambda'(k) & \\ & & a \end{pmatrix}, \tag{5.24b}$$

where $k = nH \in K$ and we have used the notation from Eq. (2.8). We shall also use the direct sum decomposition of the Lie algebra $\mathfrak{GI}(p)$ of the type

$$\mathfrak{GI}(p) = \begin{pmatrix} \mathfrak{GI}(l) & A'' & B'' \\ A' & \mathfrak{GI}(q) & C'' \\ B' & C' & \mathfrak{GI}(d) \end{pmatrix}. \tag{5.25}$$

Now the commutant $\mathfrak{Z}_H$ of $\lambda(H)$ in $\mathfrak{GI}(p)$ has the form

$$\mathfrak{Z}_H = \begin{pmatrix} C_H & & \\ & \mathfrak{GI}(q+d) & \end{pmatrix} = \begin{pmatrix} C_H & & \\ & \mathfrak{GI}(q) & C'' \\ & C' & \mathfrak{GI}(d) \end{pmatrix}, \tag{5.26}$$

where C_H is the commutant of $\lambda(H)$ in $\mathfrak{GI}(l)$.

We introduce an $\mathrm{Ad}(\lambda(N))$-invariant complement J of C_H in $\mathfrak{GI}(l)$ with respect to some $\mathrm{Ad}(\lambda(N))$-invariant metric in $\mathfrak{GI}(l)$:

$$\mathfrak{GI}(l) = C_H \oplus J. \tag{5.27}$$

Then for the $\mathrm{Ad}(\lambda(N))$-invariant complement I of $\mathfrak{Z}_H$ in $\mathfrak{GI}(p)$, we have

$$I = J \oplus A' \oplus A'' \oplus B' \oplus B''. \tag{5.28}$$

Denote by $L_0(\mathfrak{L};I)$ the subspace of $L(\mathfrak{L};I)$ consisting of the linear maps l with the property

$$\mathrm{Ad}(\lambda(h)) \cdot l \circ \lambda(h^{-1}) = l, \quad \forall h \in H. \tag{5.29}$$

From (5.11) and (5.23) we see that $\omega|F_0$, restricted to the natural lifts $\tilde{Z}$ of the vertical vector fields $\bar{Z}$ generated by elements Z from $\mathfrak{L}$ ($\simeq \mathbb{R}^l$), defines a mapping $\tilde{\nu}$: $F_0 \to L_0(\mathbb{R}^l;I)$ by the formula

$$\tilde{\nu}_{r(s_0)}(Z) = \omega_{r(s_0)}(\tilde{Z}), \quad \forall r(s_0) \in F_0. \tag{5.30}$$

The mapping $\tilde{\nu}$ is $\tilde{K}$ equivariant with respect to the representation of $\tilde{K}$ in $L_0(\mathbb{R}^l;I)$ given by

$$\rho(\tilde{k}) : l \mapsto \mathrm{Ad}(\lambda(n)a) \cdot l \circ \lambda(n^{-1}), \tag{5.31}$$

$\forall l \in L_0(\mathbb{R}^l;I)$, $\tilde{k} = (n, \lambda(n)a)\tilde{H} \in \tilde{K}$. Indeed $\tilde{\nu}$ satisfies

$$\tilde{\nu}_{\tilde{k} \cdot r(s_0)}(Z) = \mathrm{Ad}\,\lambda(n)a) \cdot \tilde{\nu}_{r(s_0)}(\lambda(n^{-1})Z), \tag{5.32}$$

(a) The representation of the subgroup $\mathrm{GL}(d) \subset \tilde{K}$ in the subspace $L_0(\mathbb{R}^l;J \oplus A' \oplus A'')$ of $L_0(\mathbb{R}^l;I)$ is trivial. Therefore the projection $\mathrm{pr}_{J \oplus A' \oplus A''} \circ \tilde{\nu}$, which is a $\tilde{K}$-equivariant map $F_0 \to L(\mathbb{R}^l;J \oplus A' \oplus A'')$, is constant on every $\mathrm{GL}(d)$ orbit in F_0. Now by virtue of the bundle isomorphism (3.35), $F_0/\mathrm{GL}(d) \simeq S_0(M,K)$, $\tilde{\nu}$ induces a K-equivariant map $\tilde{\nu}^J$: $S_0(M,K) \to L_0(\mathbb{R}^l;J \oplus A' \oplus A'')$ by

$$\tilde{\nu}^J(s_0) = \mathrm{pr}_{J \oplus A' \oplus A''} \circ \tilde{\nu}_{r(s_0)}, \quad \forall r(s_0) \in \Pi^{-1}(s_0) \cap F_0, \tag{5.33}$$

with

$$\tilde{\nu}^J(ks_0) = \rho(k)\tilde{\nu}^J(s_0) = \mathrm{Ad}(\lambda(n)) \cdot \tilde{\nu}^J(s_0) \circ \lambda(n^{-1}),$$

$k = nH$ [see (5.31)]. The K-equivariant map $\tilde{\nu}^J$ defines a cross section ν^J of the vector bundle $E_1 = (S_0 \times L_0(\mathbb{R}^l;J \oplus A' \oplus A''))/K$ with base M associated to $S_0(M,K)$ by the restriction of the representation ρ to the group K and to $J \oplus A' \oplus A''$:

$$\nu^J : M \to E_1, \quad \nu^J(\pi(s_0)) = [s_0, \tilde{\nu}^J(s_0)], \tag{5.34}$$

where $[,]$ denotes the equivalence class in $S_0 \times L_0(\mathbb{R}^l;J \oplus A' \oplus A'')$ with respect to the action of K. The field ν^J over M is given locally by mappings ν^J_α: $W_\alpha \to L_0(\mathbb{R}^l;J \oplus A' \oplus A'')$ satisfying $\nu^J_\alpha(x) = \rho(k_{\alpha\beta}(x)) \times \nu^J_\beta(x)$ for $x \in W_\alpha \cap W_\beta$, where $k_{\alpha\beta}$: $W_\alpha \cap W_\beta \to K$ are the transition functions for $S_0(M,K)$ corresponding to the open covering $\{W_\alpha\}$ of M.

(b) The projection $\mathrm{pr}_{B'\oplus B''}\circ\tilde{\nu}: F_0\to L_0(\mathbb{R}^l;B'\oplus B'')$ is a K-equivalent map of the principal bundle $F_0(M,\tilde{K})$ into a subspace of $L_0(\mathbb{R}^l;I)$. So it defines a cross section ν^B of the vector bundle $E_2=(F_0\times L_0(\mathbb{R}^l;B'\oplus B''))/\tilde{K}$ over M associated to $F_0(M,\tilde{K})$ by the restriction of the representation (5.31) to $L_0(\mathbb{R}^l;B'\oplus B'')$:

$$\nu^B: M\to E_2,\quad \nu^B(\pi(s_0))=[r(s_0),\mathrm{pr}_{B'\oplus B''}\circ\tilde{\nu}_{r(s_0)}], \tag{5.35}$$

where $r(s_0)\in\Pi^{-1}(s)\cap F_0$ and $[\,,\,]$ denotes the relevant equivalence class. The field ν^B over M is given locally by mappings ν^B_α: $W_\alpha\to L_0(\mathbb{R}^l,B'\oplus B'')$ satisfying $\nu^B_\alpha(x)=\rho(\tilde{k}_{\alpha\beta}(x))\times\nu^B_\beta(x)$, for $x\in W_\alpha\cap W_\beta$, where $\tilde{k}_{\alpha\beta}: W_\alpha\cap W_\beta\to\tilde{K}$ are the transition functions for $F_0(M,\tilde{K})$.

(c) Summarizing, we find that the restriction of $\omega|F_0$ to vector fields of the type $\tilde{Z}$ is completely determined by the pair (ν^l,ν^B) of fields (5.34) and (5.35) defined on M.

According to (5.22) the restriction of $\omega|F_0$ to the natural lifts $\tilde{Y}$ of the vertical fields of the type $\overline{Y}$ generated by elements Y from $\mathfrak{K}(\mathbb{R}^q)$ defines a mapping $\tilde{\varkappa}: F_0\to L(\mathbb{R}^q;\mathfrak{Z}_H)$ by the formula

$$\tilde{\varkappa}_{r(s_0)}(Y)=\omega_{r(s_0)}(\tilde{Y}),\quad \forall Y\in\mathfrak{K}. \tag{5.36}$$

The mapping $\tilde{\varkappa}$ is $\tilde{K}$-equivariant with respect to the representation ρ' of $\tilde{K}$ in $(\mathbb{R}^q;\mathfrak{Z}_H)$ given by

$$\rho'(\tilde{k}):\quad l\mapsto \mathrm{Ad}(\lambda(n)a)\cdot l\circ\lambda'(k^{-1}), \tag{5.37}$$

$\forall l\in L(\mathbb{R}^q;\mathfrak{Z}_H)$, $\tilde{k}=(n,\lambda(n)a)\tilde{H}\in\tilde{K}$ [we use the notation from (2.8)]. Indeed, it satisfies

$$\tilde{\varkappa}_{\tilde{k}\cdot r(s_0)}(Y)=\mathrm{Ad}(\lambda(n)a)\cdot\tilde{\varkappa}_{r(s_0)}(\lambda'(k^{-1})Y),$$

due to (5.13) and (5.19).

Taking into account (5.24)–(5.26), we split the space $L(\mathbb{R}^q;\mathfrak{Z}_H)$ into a direct sum of the following $\tilde{K}$-invariant subspaces $L(\mathbb{R}^q;\mathfrak{Z}_H)=L(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q))\oplus L(\mathbb{R}^q,\mathfrak{GI}(d))\oplus L(\mathbb{R}^q;C)$, where $C=C'\oplus C''$. Then $\tilde{\varkappa}$ decomposes into a sum of $\tilde{K}$-equivariant mappings from F_0 into the corresponding subspaces of $L(\mathbb{R}^q;\mathfrak{Z}_H)$:

$$\tilde{\varkappa}_{r(s_0)}(Y)=\mathrm{pr}_{C_H\oplus\mathfrak{GI}(q)}(\tilde{\varkappa}_{r(s_0)}(Y))+\mathrm{pr}_{\mathfrak{GI}(d)}(\tilde{\varkappa}_{r(s_0)}(Y))+\mathrm{pr}_C(\tilde{\varkappa}_{r(s_0)}(Y)), \tag{5.38}$$

for every $r(s_0)\in F_0$, $Y\in\mathfrak{K}$. [Of course, the $\tilde{K}$-equivariance is with respect to the relevant restriction of the representation (5.37).] We proceed to analyze the different projections appearing in (5.38).

(a) The first term in the decomposition (5.38) is the map

$$\mathrm{pr}_{C_H\oplus\mathfrak{GI}(q)}\circ\tilde{\varkappa}: F_0\to L(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q)), \tag{5.39}$$

which is constant on every $\mathrm{Gl}(d)$ orbit in F_0 since this group acts trivially on $L(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q))$. Applying the bundle isomorphism $F_0/\mathrm{Gl}(d)\simeq S_0(M,K)$, we obtain that the mapping (5.39) induces a mapping $\tilde{\varkappa}^q: S_0\to(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q))$ by the formula

$$\tilde{\varkappa}^q_{s_0}=\mathrm{pr}_{C_H\oplus\mathfrak{GI}(q)}\circ\tilde{\varkappa}_{r(s_0)},\quad r(s_0)\in\Pi^{-1}(s_0)\cap F_0. \tag{5.40}$$

The mapping $\tilde{\varkappa}^q$ is K equivariant with respect to the representation ρ' of the group K in $L(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q))$, which follows from (5.37):

$$\rho'(k)l=\mathrm{Ad}(\lambda(n))\cdot l\circ\lambda'(k^{-1}),$$

$$k=nH,\quad l\in L(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q)). \tag{5.41}$$

In fact, we have, for every $Y\in\mathbb{R}^q(\simeq\mathfrak{K})$,

$$\tilde{\varkappa}^q_{ks_0}(Y)=\mathrm{Ad}(\lambda(n))\cdot\tilde{\varkappa}^q_{s_0}(\lambda(k^{-1})Y).$$

Therefore, it defines a cross section $\varkappa^q$ of the vector bundle $E_3=(S_0\times L(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q)))/K$ with base M associated to $S_0(M,K)$ by the representation (5.41):

$$\varkappa^q:\quad M\to E_3,\quad \varkappa^q(\pi(s_0))=[s_0,\tilde{\varkappa}^q_{s_0}]. \tag{5.42}$$

The field $\varkappa^q$ is given locally by mappings $W_\alpha\to L(\mathbb{R}^q;C_H\oplus\mathfrak{GI}(q))$: for $x\in W_\alpha\cap W_\beta$ they are related by the transition functions $\rho'(k_{\alpha\beta}(x))$.

(b) The mapping

$$\mathrm{pr}_{\mathfrak{GI}(d)}\circ\tilde{\varkappa}:\quad F_0\to L(\mathbb{R}^q;\mathfrak{GI}(d))$$

defines

$$\tilde{\varkappa}^d: F_0\to L(\mathbb{R}^q;\mathfrak{GI}(d)),\qquad \tilde{\varkappa}^d_{r(s_0)}=\mathrm{pr}_{\mathfrak{GI}(d)}\circ\tilde{\varkappa}_{r(s_0)}. \tag{5.43}$$

The map $\tilde{\varkappa}^d$ is equivariant with respect to the representation of $\tilde{K}$ in $L(\mathbb{R}^q;\mathfrak{GI}(d))$ induced from (5.37):

$$\rho'(\tilde{k})l=\mathrm{Ad}\,a\cdot l\circ\lambda'(k^{-1}),\quad \forall\tilde{k}=(k,a)\in\tilde{K}. \tag{5.44}$$

Indeed, $\tilde{\varkappa}^d$ satisfies

$$\tilde{\varkappa}^d_{kr(s_0)}(Y)=\mathrm{Ad}(a^{-1})\cdot\tilde{\varkappa}^d_{r(s_0)}(\lambda'(k^{-1})Y),$$

for every $Y\in\mathbb{R}^q$. Thus $\tilde{\varkappa}^d$ determines a cross section $\varkappa^d$ of the vector bundle $E_4=(F_0\times L(\mathbb{R}^q;\mathfrak{GI}(d)))/\tilde{K}$ with base M associated to F_0 by representation (5.44) of $\tilde{K}$:

$$\varkappa^d:\quad M\to E_4,\quad \varkappa^d(\pi(s_0))=[r(s_0),\tilde{\varkappa}^d_{r(s_0)}]. \tag{5.45}$$

The field $\varkappa^d$ over M is given locally by mappings $W_\alpha\to L(\mathbb{R}^q;\mathfrak{GI}(d))$ with transition functions $\rho'(\tilde{k}_{\alpha\beta}(x))$.

(c) Finally, the mapping

$$\mathrm{pr}_C\circ\tilde{\varkappa}:\quad F_0\to L(\mathbb{R}^q;C),\quad C=C'\oplus C'',$$

defines a cross section $\varkappa^c:\quad M\to E_5=(F_0\times L(\mathbb{R}^q;C))/\tilde{K}$ of the vector bundle E_5 with base M associated to F_0 by the representation ρ' of $\tilde{K}$ [see (5.37)] restricted to $L(\mathbb{R}^q;C)$:

$$\varkappa^c(\pi(s_0))=[r(s_0),\mathrm{pr}_C\circ\tilde{\varkappa}_{r(s_0)}]. \tag{5.46}$$

The field $\varkappa^c$ on M is given locally by maps $W_\alpha\to L(\mathbb{R}^q;C)$ with transition functions $\rho'(\tilde{k}_{\alpha\beta}(x))$ for $x\in W_\alpha\cap W_\beta$.

(d) A summary of the results obtained in this subsection shows that the restriction of $\omega|F_0$ to the vector fields of the type $\tilde{Y}$ is uniquely described by the set $(\varkappa^q,\varkappa^d,\varkappa^c)$ of fields on M given by (5.42) (5.45), and (5.46), respectively.

At the end we have to consider the values of $\omega|F_0$ for the vector fields $\tilde{X}$, each of which projects into a local vector field X defined in some open set $U\subset M$ [see (5.16) and (5.22)]. We note that every vector field of the type $\tilde{X}$ defined on a neighborhood in $F(S)|S_0$ is a local vector field on F_0. Then the restriction of $\omega|F_0$ to the vector fields $\tilde{X}$ defines a $\mathfrak{Z}_H$-valued and $\tilde{K}$-equivariant one-form $\tilde{\mu}$ on $T(F_0)$ in the following way. We write each local vector field $\tilde{V}$ on F_0 as the sum

$$\tilde{V}=\tilde{X}+\tilde{Y}'+\tilde{A},\quad \tilde{Y}'=\tilde{Y}-\lambda'(Y), \tag{5.47}$$

where the (local) vector fields $\tilde{X}$, $\tilde{Y}$, are defined as earlier in this section [cf. (5.16)] and $\tilde{A}$, $\lambda'(A)$, are fundamental vector fields generated by the elements $A\in\mathfrak{GI}(d)$, $\lambda'(Y)\in\mathfrak{GI}(q)$.

Then we define a one-form $\tilde{\mu}$ on F_0 by the formulas

$$\tilde{\mu}_{r(s_0)}(\tilde{X}) = \omega_{r(s_0)}(\tilde{X}), \tag{5.48}$$

$$\tilde{\mu}_{r(s_0)}(\tilde{Y}') = 0, \tag{5.49}$$

$$\tilde{\mu}_{r(s_0)}(\tilde{A}) = A, \tag{5.50}$$

$\forall r(s_0) \in F_0$, $s_0 \in S_0$. The splitting of $\tilde{\mu}(\tilde{V})$ in accordance with (5.26),

$$\tilde{\mu}(\tilde{V}) = \mathrm{pr}_{C_H \oplus \mathfrak{GI}(q)}(\tilde{\mu}(\tilde{V})) + \mathrm{pr}_{\mathfrak{GI}(d)}(\tilde{\mu}(\tilde{V})) + \mathrm{pr}_{C' \oplus C''}(\tilde{\mu}(\tilde{V})), \tag{5.51}$$

gives rise to a set of fields and a linear connection on M. They are determined in the following way.

(a) The mapping

$$\mathrm{pr}_{C_H \oplus \mathfrak{GI}(q)} \circ \tilde{\mu}: \quad F_0 \to T(F_0)^* \otimes (C_H \oplus \mathfrak{GI}(q))$$

is a $\tilde{K}$-equivariant one-form on the principal fiber bundle $F_0(M,\tilde{K})$, which is horizontal due to (5.49) and (5.50). Since this mapping is constant on every $\mathrm{GL}(d)$ orbit in F_0, the bundle isomorphism $F_0/\mathrm{GL}(d) \simeq S_0$ allows one to determine a horizontal [by virtue of (5.49)] one-form $\bar{\mu}$ on the principal fiber bundle $S_0(M,K)$ with values in $C_H \oplus \mathfrak{GI}(q)$ by

$$\bar{\mu}_{s_0}(\overline{X}) = \mathrm{pr}_{C_H \oplus \mathfrak{GI}(q)}(\tilde{\mu}_{r(s_0)}(\tilde{X})), \tag{5.52}$$

$$\bar{\mu}_{s_0}(\overline{Y}) = 0, \tag{5.53}$$

where $\overline{X}$, $\tilde{X}$ and $\overline{Y}$ are defined as in (5.15) and (5.16). Owing to the K equivariance,

$$\bar{\mu}_{ks_0} = \mathrm{Ad}(\lambda(n)) \cdot \bar{\mu}_{s_0}, \quad \forall k = nH \in K,$$

the horizontal form $\bar{\mu}$ determines a unique one-form μ' on M by the formula

$$\mu'_x(X) = [s_0, \bar{\mu}_{s_0}(\overline{X})], \quad s_0 \in \pi^{-1}(x), \tag{5.54}$$

where X is the local vector field on M whose horizontal lift to S_0 is $\overline{X}$ and $[\,,\,]$ denotes the equivalence class determined in $S_0 \times (C_H \oplus \mathfrak{GI}(q))$ with respect to the action of the group K [K is acting on $C_H \oplus \mathfrak{GI}(q)$ by $\mathrm{Ad}(\lambda(N))/\mathrm{Ad}(\lambda(H))$. So we obtain that μ' is a cross section of the fiber bundle

$$T(M)^* \otimes [(S_0 \times (C_H \oplus \mathfrak{GI}(q)))/K].$$

(b) For the projection

$$\tilde{\mu}^d = \mathrm{pr}_{\mathfrak{GI}(d)} \circ \tilde{\mu},$$

using the $\tilde{K}$ equivariance, we find from (5.13) and (5.18) that

$$\tilde{\mu}^d_{\tilde{k} \cdot r(s_0)} = \mathrm{Ad}\, a \cdot \tilde{\mu}^d_{r(s_0)}, \quad \forall r(s_0) \in F_0, \quad \tilde{k} = (n, \lambda(n)a)\tilde{H} \in \tilde{K}, \tag{5.55}$$

since $\lambda(n)$ commutes with $\mathfrak{GI}(d)$. Taking into account the property (5.55) and the bundle isomorphism $F_0/K \simeq F(M)$, we obtain a $\mathfrak{GI}(d)$-valued one-form μ^d on $F(M)$ of type Ad: for every linear frame $r(x)$ at the point $x \in M$ we set

$$\mu^d_{r(x)}(A') = \tilde{\mu}_{r(s_0)}(\tilde{A}) = A, \tag{5.56}$$

where $r(s_0) = (\eta^v(s_0), \mathrm{hor}\, r(x)|_{s_0})$, $s_0 \in \pi^{-1}(x)$ [see (3.33)] and A' is the fundamental vector field on $F(M)$ generated by the element $A \in \mathfrak{GI}(d)$ [cf. (5.50)]; further, for the natural lift X' to $F(M)$ of the local vector field X on M we put

$$\mu^d_{r(x)}(X') = \bar{\mu}_{r(s_0)}(\tilde{X}), \tag{5.57}$$

where $\tilde{X}$ is the natural lift of $\overline{X}$ to $F_0 \subset F(S)$ [see (5.15) and (5.16)]. From the above we deduce that the one-form μ^d is a linear connection form on M.

(c) The projection

$$\tilde{\mu}^c = \mathrm{pr}_C \circ \tilde{\mu}, \quad C = C' \oplus C'',$$

is a $\tilde{K}$-equivariant horizontal one-form on the principal bundle $F_0(M,\tilde{K})$. It induces a one-form μ^c on M with values in the vector bundle $(S_0 \times C)/K$ associated to $S_0(M,K)$ by the action $\mathrm{Ad}(\lambda(N))/\mathrm{Ad}(\lambda(H))$ of K on C. Here μ^c is defined by [see Eq. (5.47)]

$$\mu^c_x(X) = [s_0, \tilde{\mu}^c_{r(s_0)}(\tilde{X} + \tilde{Y}' + \tilde{A})]', \quad s_0 \in \pi^{-1}(x), \tag{5.58}$$

i.e., μ^c is a cross section: $M \to T(M)^* \otimes ((S_0 \times C)/K)$. In (5.58) $[\,,\,]'$ denotes the elements of $(S_0 \times C)/K$.

The full description of any G-invariant linear connection on S is contained in the following proposition.

Proposition 5.2: Given a connection in the principal fiber bundle $S_0(M,K)$, the G-invariant linear connections on S are in one-to-one correspondence with the set $(\mu^d, \nu^J, \nu^B, \varkappa^q, \varkappa^d, \mu', \mu^c)$, where μ^d is a linear connection on M; ν^J, ν^B, $\varkappa^q$, $\varkappa^d$, and $\varkappa^c$ are fields over M defined by (5.34), (5.35), (5.42), (5.45), and (5.46), respectively, and μ', μ^c are one-forms on M with values in vector bundles over M and defined by (5.54) and (5.58).

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Geometrical properties of the algebraic spinors for $R^{3,1}$

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The different geometrical properties of Majorana, "even," Dirac, and Chevalley spinors in the Clifford algebra approach are investigated.

I. INTRODUCTION

Recently there has been increased interest in different kinds of spinors that can be related to a given model of space-time. It appears that the different physical theories are based on a different kind of spinor representation, which determines the basic properties of a physical description of interactions. For example, some kinds of spinors admit a mass term but some of them do not, this depends on the possibility of the construction of "Lorentz" invariants bilinear in the spinor fields. Also, supersymmetry theories impose a strong restriction on the possible properties of spinors, etc.

The main purpose of our investigation is to give the full classification of all the spinor representations of any space-time, to show their consequences on the physical theories based on them, and to explain their geometrical significance as well as constraints and obstructions related with any concrete spinor bundle over a space-time manifold $\mathcal{M}$. In this paper we shall consider only the case of a four-dimensional space-time of signature (3,1). In Ref. 1 we are considering the general case of n-dimensional pseudo-Riemannian manifolds. Although the four-dimensional case is thought to be known completely, we hope that we are able to give some additional new facts, which have never been introduced before.

II. MAJORANA SPINORS ζ_ϵ

Let us consider the Minkowski vector space-time $R^{3,1}$ together with a set of unit vectors $\{e_1,e_2,e_3,e_4\}$, which form an orthogonal basis ϵ for $R^{3,1}$,

$$e_1^2 = e_2^2 = e_3^2 = -e_4^2 = 1. \tag{2.1}$$

Its universal Clifford algebra $R_{3,1}$ has a matrix representation given by an algebra of 4×4 real matrices $R(4)$ (see Ref. 2). The underlying vector space for the faithful representation of the Clifford algebra $R_{3,1}$ is given by its minimal left (or right) ideal[3]

$$\zeta = R_{3,1} f \quad (\text{or } \tilde{\zeta} = f R_{3,1}). \tag{2.2}$$

Here f is a primitive idempotent $f^2 = f$ of $R_{3,1}$. It can be seen that ζ is a four-dimensional real vector space, which we shall call the Majorana spinor space for $R^{3,1}$. Let us take, for example, an idempotent f of the form

$$f_\epsilon = \tfrac{1}{2}(1 + e_1)\tfrac{1}{2}(1 + e_3e_4). \tag{2.3}$$

It allows us to build the concrete left minimal ideal ζ_ϵ. The basis $\{s_1,s_2,s_3,s_4\}$ of ζ_ϵ can be taken as follows:

$$s_1 = f_\epsilon = e_1 f_\epsilon, \quad s_3 = e_3 f_\epsilon = e_4 f_\epsilon,$$
$$s_2 = e_2 f_\epsilon, \quad s_4 = e_3 e_2 f_\epsilon. \tag{2.4}$$

The real algebra isomorphism

$$\tau\colon R_{3,1} \to \mathrm{End}_R\, \zeta_\epsilon, \quad u \to \tau(u), \quad \forall\, u \in R_{3,1}, \tag{2.5}$$

is defined by relation

$$\tau(u)\psi = u\psi, \quad \forall\, \psi \in \zeta_\epsilon, \tag{2.5'}$$

and is determined by $\tau(e_\mu)$. We shall denote $\tau(e_\mu)$ by γ_μ. Hence to construct the matrix representation of $R_{3,1}$ it is enough to fix a matrix form of γ_μ's. We can choose them in such a way that the elements of s_k will be given by matrices

$$s_k = \overset{\downarrow}{k}\overset{\uparrow}{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}. \tag{2.6}$$

For this we should take

$$\gamma_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$
$$\gamma_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$
$$\gamma_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$
$$\gamma_4 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{2.7}$$

Using the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.8}$$

we have for (2.7)

$$\gamma_1 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix},$$
$$\gamma_3 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}. \tag{2.7'}$$

Thus our spinor space ζ_ϵ contains the matrices of the form

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$$\zeta_\epsilon = \left\{ \begin{pmatrix} \psi_1 & 0 & 0 & 0 \\ \psi_2 & 0 & 0 & 0 \\ \psi_3 & 0 & 0 & 0 \\ \psi_4 & 0 & 0 & 0 \end{pmatrix}; \quad \psi_i \in \mathbb{R} \right\}. \tag{2.9}$$

In the general theory of the Clifford algebras one constructs a subring F of any minimal left ideal $\zeta = R_{s,t} f$ as a division ring with a unity given by

$$F = f R_{s,t} f. \tag{2.10}$$

In our case we obtain

$$F_\epsilon = f_\epsilon R_{3,1} f_\epsilon = \left\{ \begin{pmatrix} \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \quad \lambda \in R \right\}. \tag{2.11}$$

Now, the scalar products on the spinor space ζ are defined as the maps $\zeta \times \zeta \to F$. Namely, the identity I and the reflection $-I$ on the Minkowski space-time $R^{3,1}$ induce anti-involutions of the Clifford algebra $R_{3,1}$. They are usually denoted by β_+ and β_-, respectively. The scalar products

$$(\cdot,\cdot)_\pm : \zeta_\epsilon \times \zeta_\epsilon \to F_\epsilon \tag{2.12}$$

will be defined according to the following formulas:

$$(\psi,\varphi)_\pm = \omega_\pm \beta_\pm(\psi)\varphi, \quad \forall\, \varphi,\psi \in \zeta_\epsilon. \tag{2.13}$$

The above definition uses some elements $\omega_\pm \in R_{3,1}$. Thus to make it clear we have to make precise which elements $\omega_\pm$ are taken. The $\omega_\pm$ should have the property

$$\omega_\pm \beta_\pm(f_\epsilon)\omega_\pm^{-1} = f_\epsilon. \tag{2.14}$$

Then $\omega_\pm \beta_\pm(u f_\epsilon)u' f_\epsilon = f_\epsilon \omega_\pm \beta_\pm(u)u' f_\epsilon \in F_\epsilon$ (here $u f_\epsilon = \psi$ and $u' f_\epsilon = \varphi$ for appropriate $u,u' \in R_{3,1}$). Let us consider the product $(\cdot,\cdot)_+$. We have

$$\beta_+(\varphi) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\varphi_4 & \varphi_3 & -\varphi_2 & \varphi_1 \end{pmatrix}. \tag{2.15}$$

Thus ω_+ would transform the fourth row into the first one. For example, as ω_+ we can take the product $\gamma_3\gamma_2$, i.e.,

$$\omega_+ = e_3 e_2. \tag{2.16}$$

Now

$$\omega_+^{-1}\beta_+(\varphi)\psi = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \in F_\epsilon, \tag{2.17}$$

with

$$a = \varphi_1\psi_4 + \varphi_3\psi_2 - \varphi_2\psi_3 - \varphi_4\psi_2. \tag{2.18}$$

Similarly, for β_- we have

$$\beta_-(\varphi) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\varphi_3 & -\varphi_4 & \varphi_1 & \varphi_2 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \tag{2.19}$$

hence ω_- can be taken as

$$\omega_- = e_3 = \omega_-^{-1} \tag{2.20}$$

and

$$(\varphi,\psi)_- = \omega_-^{-1}\beta_-(\varphi)\psi = \begin{pmatrix} b & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \in F_\epsilon, \tag{2.21}$$

with

$$b = \varphi_1\psi_3 + \varphi_2\psi_4 - \varphi_3\psi_1 - \varphi_1\psi_2. \tag{2.22}$$

Let G_+ and G_- be Lie groups that preserve the scalar products $(\,,\,)_+$ and $(\,,\,)_-$, respectively. From (2.17) and (2.21) we see that both these groups are isomorphic to Sp(4,R). It is easy to see that the $G_\pm$ are realized as subsets of invertible elements of $R_{3,1}$ given by the following properties:

$$G_\pm = \{ s \in R_{3,1} :\ \beta_\pm(s)s = 1 \}. \tag{2.23}$$

The Lie algebras $\mathcal{g}_\pm$ corresponding to them are determined by

$$\mathcal{g}_\pm = \{ b \in R_{3,1} \mid \beta_\pm(b) + b = 0 \}. \tag{2.24}$$

Thus we see that

$$\mathcal{g}_+ \cong R^2_{3,1} \oplus R^3_{3,1}, \quad \mathcal{g}_- \simeq R^2_{3,1} \oplus R^1_{3,1} \tag{2.25}$$

(here $R^k_{3,1}$ is the subspace of $R_{3,1}$ formed by k vectors space). It is easy to see that, for example, the scalar product $(\,,\,)_+$ can be written as

$$(\varphi,\psi)_+ = \varphi^T J \psi, \tag{2.26}$$

where

$$J = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad J^2 = -\mathbf{1}. \tag{2.27}$$

In this way we see that if we determine the scalar product $(\,,\,)_+$ on ζ_ϵ then we also determine the almost complex structure on ζ_ϵ described by the matrix J. Thus, the four-dimensional real spinor space ζ_ϵ can be treated as a two-complex dimensional space.

Because

$$(\varphi_1,\varphi_2,\varphi_3,\varphi_4) \overset{J}{\longmapsto} (-\varphi_4,\varphi_3,-\varphi_2,\varphi_1), \tag{2.28}$$

this complex vector space can be spanned by elements

$$\rho_1 = s_1 + i s_4, \quad \rho_2 = s_3 + i s_2. \tag{2.29}$$

Of course spin $\mathrm{Spin}_+(3,1) \cong \mathrm{SL}(2,\mathbb{C})$ preserves the scalar products, hence SL(2,C) is also the symmetry group of two-dimensional space $\{\rho_1,\rho_2\}$.

We have built our concrete spinor space ζ_ϵ starting from some fixed orthonormal base $\epsilon = (e_1,e_2,e_3,e_4)$ as well as from the fixed primitive idempotent f_ϵ. Obviously we could fix another orthonormal base ϵ' and take $f_{\epsilon'}$, which has the same form as f_ϵ, or change its form.

Let $f'_{\epsilon'}$ denote the general form of the primitive idempotent, which, in base ϵ', can be written as

$$f'_{\epsilon'} = \tfrac{1}{4}(1 + e'_{s_1})(1 + e'_{s_2}), \tag{2.30}$$

where the s_1,s_2 are appropriate multi-indexes. It determines a concrete minimal left ideal $\zeta_{\epsilon'}(f')$.

Now we can choose such a matrix representation of the universal Clifford algebra $R_{3,1}$ such that $\zeta_{\epsilon'}(f') = R_{3,1} f'_{\epsilon'}$ will be given by matrices of the form

$$\begin{pmatrix} x_1 & 0 & 0 & 0 \\ x_2 & 0 & 0 & 0 \\ x_3 & 0 & 0 & 0 \\ x_4 & 0 & 0 & 0 \end{pmatrix}, \quad x_i \in \mathbb{R}. \tag{2.31}$$

Hence all properties will be the same as for $\zeta_\epsilon(f)$.

Now let us define some isomorphism $\chi: \zeta_\epsilon \otimes \zeta_\epsilon \to R_{3,1}$ by the following formulas:

$$\chi(\psi \otimes \psi') = \psi\omega_+ \beta_+(\psi'), \quad \forall\, \psi,\psi' \in \zeta_\epsilon, \tag{2.32}$$

where ω_+ is an element of $R_{3,1}$ given by (2.13) and (2.14). To show this isomorphism let us recall that our Clifford algebra $R_{3,1}$ is the simple sum of four left minimal ideals

$$R_{3,1} = \overset{4}{\underset{i/1}{\oplus}} \zeta^i, \tag{2.33}$$

where the f^i are pairwise annihilating primitive idempotents $f^i f^j = 0$, for $i \neq j$, $\Sigma f^i = 1$, and $\zeta^i = R_{3,1} f^i$. Let us denote our primitive idempotent $f_\epsilon = \frac{1}{4}(1 + e_1)(1 + e_{34})$ by f^1 and

$$\begin{aligned} f^2 &:= \tfrac{1}{4}(1 + e_1)(1 - e_{34}) = \beta_+(f^1), \\ f^3 &:= \tfrac{1}{4}(1 - e_1)(1 + e_{34}) = \alpha(f^1), \\ f^4 &:= \tfrac{1}{4}(1 - e_1)(1 - e_{34}) = \beta_-(f^1). \end{aligned} \tag{2.34}$$

We shall introduce the following notation for the basis elements of ζ_ϵ:

$$\begin{aligned} s_1 &= f_\epsilon := u_1 f^1, \quad s_3 = e_3 f_\epsilon = u_3 f^1, \\ s_2 &= e_2 f_\epsilon := u_2 f^1, \quad s_4 = e_3 e_2 f_\epsilon = u_4 f^1. \end{aligned} \tag{2.35}$$

Because the u_i are not uniquely determined we fix

$$(u_1,u_2,u_3,u_4) = (1,e_2,e_3,e_3e_2). \tag{2.36}$$

We can check that

$$\begin{aligned} &f^1 u_4 = u_4 f^2, \quad f^2 u_3 = u_3 f^3, \\ &f^2 u_2 = u_2 f^4, \quad \beta_+(\omega_+) = \omega_+^{-1} = -u_4. \end{aligned} \tag{2.37}$$

Hence we obtain

$$\begin{aligned} &\chi(s_1 \otimes s_1) = u_4 f^2, \quad \chi(s_1 \otimes s_2) = u_3 f^4, \\ &\chi(s_2 \otimes s_1) = -u_3 f^2, \quad \chi(s_2 \otimes s_2) = -u_4 f^4, \\ &\chi(s_3 \otimes s_1) = u_2 f^2, \quad \chi(s_3 \otimes s_2) = f^4, \\ &\chi(s_4 \otimes s_1) = -f^2, \quad \chi(s_4 \otimes s_2) = -u_2 f^4, \end{aligned} \tag{2.38}$$

and

$$\begin{aligned} &\chi(s_1 \otimes s_3) = -u_2 f^3, \quad \chi(s_1 \otimes s_4) = f^1, \\ &\chi(s_2 \otimes s_3) = -f^3, \quad \chi(s_2 \otimes s_4) = u_2 f^1, \\ &\chi(s_3 \otimes s_3) = -u_4 f^3, \quad \chi(s_3 \otimes s_4) = u_3 f^1, \\ &\chi(s_4 \otimes s_3) = -u_3 f^3, \quad \chi(s_4 \otimes s_4) = u_4 f^1. \end{aligned} \tag{2.38'}$$

The above relations show us that the image of elements $s_i \otimes s_1$ lies in ζ^2 and spans it. Similarly the $\chi(s_i \otimes s_2)$ span ζ^4 and so on.

Let us find the elements of $\zeta_\epsilon \otimes \zeta_\epsilon = \zeta^1 \otimes \zeta^1$ that pass onto basis elements of $R^{3,1} \hookrightarrow R_{3,1}$. We have

$$\begin{aligned} e_1 &= f^1 + f^2 - f^3 - f^4 \\ &= \chi[(s_1 \otimes s_4 - s_4 \otimes s_1) + (s_2 \otimes s_3 - s_3 \otimes s_2)], \\ e_2 &= u_2(f^1 + f^2 + f^3 + f^4) \\ &= \chi[(s_2 \otimes s_4 - s_4 \otimes s_2) + (s_1 \otimes s_3 - s_3 \otimes s_1)], \\ e_3 &= u_3(f^1 + f^2 + f^3 + f^4) \\ &= \chi[(s_3 \otimes s_4 - s_4 \otimes s_3) + (s_1 \otimes s_2 - s_2 \otimes s_1)], \\ e_4 &= u_3(f^1 - f^2 + f^3 - f^4) \\ &= \chi[(s_3 \otimes s_4 - s_4 \otimes s_3) + (s_2 \otimes s_1 - s_1 \otimes s_2)]. \end{aligned} \tag{2.39}$$

When we introduce the map $\varphi = \chi \circ \mathscr{A}$, where

$$\mathscr{A}(\psi \otimes \psi') = \psi \otimes \psi' - \psi' \otimes \psi, \tag{2.40}$$

we obtain

$$\begin{aligned} e_1 &= \varphi(s_1 \otimes s_4 + s_2 \otimes s_3), \\ e_2 &= \varphi(s_2 \otimes s_4 + s_1 \otimes s_3), \\ e_3 &= \varphi(s_3 \otimes s_4 + s_1 \otimes s_2), \\ e_4 &= \varphi(s_3 \otimes s_4 + s_2 \otimes s_1). \end{aligned} \tag{2.41}$$

III. EVEN SPINOR SPACE

In the previous section we mentioned that the universal Clifford algebra $R_{3,1}$ has its faithful matrix representation given by the algebra of 4×4 real matrices. Hence we can identify $R_{3,1}$ with the algebra of the linear endomorphism of some real four-dimensional vector space. As we have seen, this space can be given by any minimal left ideal of the Clifford algebra itself. Moreover, any such ideal is also among others the underlying space of the vector representation of the Spin(3,1) group. However, this group is contained in the even subalgebra $R^{(0)}_{3,1}$ of $R_{3,1}$. This suggests that we should be interested in the matrix representation of the even subalgebra $R^{(0)}_{3,1}$ as well as in its minimal left ideals $\Sigma_{\epsilon'}(f')$. As usual, to fix any minimal left ideal, it is enough to choose some primitive idempotent. The idempotent

$$f^{(0)}_\epsilon = \tfrac{1}{2}(1 + e_3 e_4) \tag{3.1}$$

of the Clifford algebra $R_{3,1}$ is a primitive in the even subalgebra. Thus

$$\Sigma_\epsilon(f) = R^{(0)}_{3,1} f^{(0)}_\epsilon. \tag{3.2}$$

Let us define the linear map

$$R^{3,1} \leftarrow R^{3,0} \to R^{(0)}_{3,1} \tag{3.3}$$

by the correspondence

$$:e_i \to e'_i = e_i e_4, \quad i = 1,2,3. \tag{3.4}$$

Because of $e'^2_i = e^2_i$ and the set $\{e'_i\}$ generates the whole even subalgebra $R^{(0)}_{3,1}$ of $R_{3,1}$, hence we have

$$R^{(0)}_{3,1} \cong R_{3,0} \cong \mathbb{C}(2). \tag{3.5}$$

Indeed, the product $e_J = e^1_1 e^1_2 e^1_3$, which commutes with all elements of $R^{(0)}_{3,1}$ and the square of which is equal -1, can be identified with a pure imaginary unit i'. It implies

$$i'e'_1 = e'_2 e'_3, \quad i'e'_2 = e'_3 e'_1, \quad i'e'_3 = e'_1 e'_2. \tag{3.6}$$

As a real vector space, Σ is a four-dimensional one and can be spanned by elements

$$(\rho_1,\rho_2,\rho_3,\rho_4) = (f^{(0)}_\epsilon, e'_1 f^{(0)}_\epsilon, e'_2 f^{(0)}_\epsilon, e'_1 e'_2 f^{(0)}_\epsilon). \tag{3.7}$$

We can find its matrix representation using the correspondence (2.7). In this base we have

$$\gamma_1' = -\begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \quad \gamma_2' = -\begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix},$$
$$\gamma_3' = -\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.8}$$

whereas

$$\gamma_1'\gamma_2'\gamma_3' \overset{\text{of}}{=} \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \overset{df}{=} J'. \tag{3.9}$$

Using (3.6) we see that $\rho_3 = i'\rho_2$ and $\rho_4 = i'\rho_1$. Hence the spinor module $\Sigma_\epsilon(f)$ has the naturally defined structure of a complex vector space spanned by $\{\rho_1, \rho_2\}$. It is obvious that the groups $G_\pm$ cannot be the symmetry groups of the spinor module $\Sigma_\epsilon(f)$ [see (2.25)] and that only their common subgroup isomorphic to SL(2,C) will survive. Thus we can introduce in $\Sigma_\epsilon(f)$ only the scalar product determined by the skew metric tensor

$$\epsilon^{AB} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Now let us return to the map (3.4). It allows us to define the vector isomorphism between the left minimal ideals of the $R_{3,1}^{(0)}$ algebra and the left minimal ideals $\zeta^{3,0}$ of the whole Clifford algebra $R_{3,0} \hookrightarrow R_{3,1}$. However, it can be seen that the complex character of the $\zeta^{3,0}$ ideal corresponds to the matrix

$$\hat{J} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \tag{3.10}$$

belonging to the algebra R (4). Because $\hat{J} \neq J'$ they define two inequivalent complex structures on the space $\zeta_\epsilon(f)$. It implies that when we pass [by (3.5)] to the left minimal ideal of $R_{3,0} \hookrightarrow R_{3,1}$, then the SL(2,$C$) symmetry of $\Sigma_\epsilon(f)$ is broken to SU(2). We can see this immediately when we recall that the group Sl(2,C) can be treated as the complexification of the SU(2) group. In other words, the Lie algebra sl(2,C) is spanned by the set $\{\sigma_i, i'\sigma_i\}$ with i' related to the matrix J' (3.9), whereas the complex structure of $\zeta^{3,0} \hookrightarrow R_{3,0} \hookrightarrow R_{3,1}$ is related to another pure imaginary unit $\hat{i}$ determined by $\hat{J}$.

The nonequivalent character of $e_1e_2e_3$ and $e_1'e_2'e_3'$ playing the role of pure imaginary units in $R_{3,0}$ and $R_{3,1}^{(0)}$ algebras, respectively, can be seen also when we consider the map β_+. Namely we have

$$\beta_+(e_1e_2e_3) = -e_1e_2e_3, \tag{3.11}$$

whereas

$$\beta_+(e_1'e_2'e_3') = e_1'e_2'e_3'. \tag{3.12}$$

Similarly as in the previous section we can define the isomorphism

$$\chi: \Sigma_\epsilon \otimes \Sigma_\epsilon \to R_{3,1}^{(0)}, \tag{3.13}$$

given by

$$\chi(\psi' \otimes \psi) = \psi'\omega_+\beta_+(\psi), \quad \forall\, \psi,\psi' \in \Sigma_\epsilon, \tag{3.14}$$

with

$$\omega_+ = e_1'.$$

IV. DIRAC SPINORS Ψ_ϵ

Although we have constructed two different "spinor spaces" $\zeta_\epsilon(f)$ and $\Sigma_\epsilon(f)$ for the Minkowski space-time $R^{3,1}$, it is not enough from the physical point of view. Namely to describe the electron in relativistic quantum mechanics we have to use the function ψ from $R^{3,1}$ to four-dimensional complex vector space $\Psi^{3,1} \equiv \Psi$, usually called the Dirac spinor space. This space is reducible with respect to the SL(2,C) group, and decomposes onto two two-complex dimensional Weyl spinor subspaces. The simplest way to obtain such a space is to pass to the complexification $R_{3,1}^{\mathbb{C}}$ of the Clifford algebra $R_{3,1}$ and to (related to this) complexification of the spinor spaces.

However, we shall define the Dirac spinors for $R^{3,1}$ as elements of the left minimal ideal of the universal Clifford algebra $R_{4,1}$. In other words, we shall treat $R^{3,1}$ spanned by $\{e_1,e_2,e_3,e_4\}$ as a subspace of $R^{4,1}$ spanned by $\{e_0,e_1,e_2,e_3,e_4\}$. The additional element e_0, $e_0^2 = +1$ allows us to introduce an imaginary unit i and, as a matter of fact, leads to the Clifford algebra isomorphic to the complexified $R_{3,1}^{\mathbb{C}} \cong \mathbb{C}(4)$. Nevertheless the properties of such an introduced Dirac space Ψ are different than the complexification of Majorana spinors. Let (e_0,e_1,e_2,e_3,e_4) be the canonical basis of $R^{4,1}$ obtained by adding the orthogonal complement e_0 to the basis ϵ of $R^{3,1} \hookrightarrow R^{4,1}$ fixed by (2.1). It is obvious that f_ϵ given by (2.3) is also a primitive idempotent of $R_{4,1}$. However, in this case the division ring $F = f_\epsilon R_{4,1} f_\epsilon$ can be identified with the complex field $\mathbb{C}$ with $e_J = e_0e_1e_2e_3e_4$ playing the role of the pure imaginary unit i. The Dirac space Ψ will be, by definition, the space

$$\Psi = \Psi_\epsilon(f) = R_{4,1} f_\epsilon, \tag{4.1}$$

with a basis

$$(s_1,s_2,s_3,s_4) = (f_\epsilon, e_2f_\epsilon, e_3f_\epsilon, e_3e_2f_\epsilon). \tag{4.2}$$

Again, as in Sec. II, we can take the matrix representation of $R_{4,1}$ in which the s_i are given by the matrices (2.6). It is easy to see that e_0 acts on the elements s_i in such a way that it has to be represented by a matrix $\gamma_0 = \tau(e_0)$ of the form

$$\gamma_0 = \begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix} \tag{4.3}$$

(we have used $i = e_0e_1e_2e_3e_4$). Thus

$$\Psi_\epsilon(f) = \left\{ \begin{pmatrix} \psi_1 & 0 & 0 & 0 \\ \psi_2 & 0 & 0 & 0 \\ \psi_3 & 0 & 0 & 0 \\ \psi_4 & 0 & 0 & 0 \end{pmatrix}; \psi_i \in \mathbb{C} \right\} \tag{4.1'}$$

and

$$F = \left\{ \begin{pmatrix} \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \lambda \in \mathbb{C} \right\}. \tag{4.4}$$

The difference between $\zeta_\epsilon^{\mathbb{C}}(f)$ and $\Psi_\epsilon(f)$ will appear when we start to introduce scalar products on these spaces induced

by the anti-involutions β_+ and β_-, respectively. For $(\psi,\varphi)_+ \in F$, $\psi,\varphi \in \Psi_\epsilon(f)$, we have $\beta_+(i) = i$. Hence we should obtain the same results as for the complexification $\zeta_\epsilon^{\mathbb{C}}(f)$ of $\zeta_\epsilon(f)$. Indeed

$$(\psi,\varphi)_+ = \omega_+ \beta_+(\psi)\varphi \cong \psi_1\varphi_4 + \psi_3\varphi_2 - \psi_2\varphi_3 - \psi_4\varphi_2, \tag{4.5}$$

with $\omega_+ = e_3e_2$. This means that the group G_+ of the automorphisms of $\Psi_\epsilon(f)$, which preserve the scalar product $(\,,\,)_+$, is isomorphic to Sp(4,C).

Now let us consider the product $(\,,\,)_-$. We can check that

$$\beta_-(\psi) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\psi_3^* & -\psi_4^* & \psi_1^* & \psi_2^* \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{4.6}$$

Thus we see that the group G_- is isomorphic to $U(2,2)$, i.e., it is completely different as obtained for complexified space $\zeta_\epsilon^{\mathbb{C}}(f)$. This fact has the following explanation. Namely, for the $R_{3,1}^{\mathbb{C}}$ algebra we have

$$\beta_+(i) = \beta_-(i) = i, \tag{4.7}$$

whereas for the $R_{4,1}$ algebra

$$\beta_+(i) = -\beta_-(i) = i, \quad i \Leftrightarrow e_0e_1e_2e_3e_4. \tag{4.8}$$

Hence $\zeta_\epsilon^{\mathbb{C}}(f)$ can be equipped with Sp(4,C), SO(4,C), and their subgroups as the possible symmetry groups, whereas the Dirac space $\Psi_\epsilon(f)$ has additionally the $U(2,2)$ symmetry. Thus, when we take the spinor function $\psi: R^{3,1} \to \Psi_\epsilon(f)$, this spinor function can undergo some $U(2,2)$ transformations.

Using the canonical embedding $(e_1,e_2,e_3,e_4) \hookrightarrow (e_0,e_1,e_2,e_3,e_4)$, we can construct the projection operators of $R_{4,1}$. These are built from the element e_0 and have the matrix representation

$$W_\pm = \tfrac{1}{2}(1 \pm \gamma_0). \tag{4.9}$$

By means of these operators (Weyl operators) we can decompose the Dirac space $\Psi = \Psi_\epsilon(f)$ onto its proper subspaces $\Psi_\pm$:

$$W_+\Psi_i = \Psi_+ = \left\{ \begin{pmatrix} \psi_1 - i\psi_2 & 0 & 0 & 0 \\ i\psi_1 + \psi_2 & 0 & 0 & 0 \\ \psi_3 + i\psi_4 & 0 & 0 & 0 \\ -i\psi_3 + \psi_4 & 0 & 0 & 0 \end{pmatrix} \right\} \tag{4.10}$$

and

$$W_-\Psi_i = \Psi_- = \left\{ \begin{pmatrix} \psi_1 + i\psi_2 & 0 & 0 & 0 \\ -i\psi_1 + \psi_2 & 0 & 0 & 0 \\ \psi_3 - i\psi_4 & 0 & 0 & 0 \\ i\psi_3 + \psi_4 & 0 & 0 & 0 \end{pmatrix} \right\}. \tag{4.11}$$

From (4.10) and (4.11) we see that any element $\psi_\pm \in \Psi_\pm$ can be written

$$\psi_+ = \begin{pmatrix} \chi_1 & 0 & 0 & 0 \\ i\chi_1 & 0 & 0 & 0 \\ \xi_1 & 0 & 0 & 0 \\ i\xi_1 & 0 & 0 & 0 \end{pmatrix}, \quad \psi_- = \begin{pmatrix} \chi_2 & 0 & 0 & 0 \\ -i\chi_2 & 0 & 0 & 0 \\ \xi_2 & 0 & 0 & 0 \\ i\xi_2 & 0 & 0 & 0 \end{pmatrix}. \tag{4.12}$$

Equivalently, employing the basis (s_1,s_2,s_3,s_4) of Ψ, we obtain

$$W_+s_1 = \rho_1, \quad W_+s_3 = \sigma_1,$$
$$W_+s_2 = -i\rho_1, \quad W_+s_4 = i\sigma_1, \tag{4.13}$$

i.e., ρ_1 and σ_1 span the subspace Ψ_+. We obtain a similar result for W_- and Ψ_-. In the physical literature the subspaces Ψ_+ and Ψ_- of the Dirac space Ψ are called the Weyl spinor spaces. Because

$$e_0 = -e_{01234}e_{1234} \cong -ie_{1234}, \tag{4.14}$$

we see that we can construct appropriate Weyl operators $\tilde{W}_\pm$ in $\zeta_\epsilon^{\mathbb{C}}(f)$ with $\gamma_0 = -i\gamma_1\gamma_2\gamma_3\gamma_4$. Similarly as above we obtain the decomposition of $\zeta_\epsilon^{\mathbb{C}}(f)$ onto the proper subspaces of $\tilde{W}_\pm$. However for the Dirac space $\Psi \equiv \Psi_\epsilon(f)$ we obtain some new surprising pictures. It appears that the Weyl subspaces $\Psi_\pm \subset \Psi$ are the totally isotropic subspaces of the Dirac space with respect to the scalar product $(\,,\,)_-$:

$$(\psi_+,\varphi_+)_- = 0, \quad \forall\, \psi_+,\varphi_+ \in \Psi_+,$$
$$(\psi_-,\varphi_-)_- = 0, \quad \forall\, \psi_-,\varphi_- \in \Psi_-. \tag{4.15}$$

By definition the construction of our concrete Dirac spinor space $\Psi_\epsilon(f)$ for the Minkowski space-time $R^{3,1}$ is based on the fixed decomposition of the vector space $R^{4,1}$ onto $R^{3,1}$ spanned by $\{e_1,e_2,e_3,e_4\}$ and $R^{1,0}$ spanned by e_0. In other words, another concrete Dirac space $\Psi_{\epsilon'}(f')$ is obtained when we choose the primitive idempotent f' of $R_{3,1}$ using another orthonormal basis (e_1',e_2',e_3',e_4') or $R^{3,1}$. Hence we can identify the set of concrete Dirac spinor spaces as the family of minimal left ideals of $R_{4,1}$ determined by all primitive idempotents of $R_{3,1} \hookrightarrow R_{4,1}$. Thus we see that we can treat any concrete Dirac spinor space $\Psi_\epsilon(f)$ as a complexification of the appropriate Majorana spinor space $\zeta_\epsilon^{\mathbb{C}}(f)$. All differences between them came from the different behavior of the appropriate pure imaginary units under the maps $\beta_\pm$. So the Weyl operators $W_\pm$ will be exactly the same for all concrete Dirac spaces and, as a matter of fact, they will have a rigid nature. Hence, the natural question will appear: which subgroups $\hat{G}_+$, $\hat{G}_-$ of G_+ and G_-, respectively, obtained after the action of the Weyl operators, will survive on Ψ_+ and Ψ_-? Again, because the Clifford algebra $R_{4,1}$ is simple, the groups $G_\pm$ are realized by the set of elements of $R_{4,1}$ that satisfy conditions (2.23) and (2.24). Thus

$$\hat{G}_-(\Psi_+) = \{s \in W_+R_{4,1};\ \beta_-(s)s = 1\}, \tag{4.16}$$

and similarly

$$\hat{G}_-(\Psi_-) = \{s \in W_-R_{4,1};\ \beta_-(s)s = 1\}. \tag{4.17}$$

But we see immediately that the conditions

$$\beta_-(\tfrac{1}{4}(1+\gamma_0)s)(1+\gamma_0)s = 1 \tag{4.18}$$

and

$$\beta_-(\tfrac{1}{4}(1-\gamma_0)s)(1-\gamma_0)s = 1 \tag{4.19}$$

cannot be fulfilled. It means that the scalar product $(\,,\,)_-$ does not induce any proper symmetry on the Weyl subspaces Ψ_+ and Ψ_-. It is a consequence of the fact that the $\Psi_\pm$ are totally isotropic with respect to the $(\,,\,)_-$ product. To see $\hat{G}_+(\Psi_\pm)$, it is better to consider the Lie algebra approach. Namely, for Ψ_+ the condition

$$\beta_+(\tfrac{1}{2}(1+\gamma_0)b + \tfrac{1}{2}(1+\gamma_0)b) = 0 \tag{4.20}$$

gives

$$\beta_+(b)+b=-(\beta_+(b)\gamma_0+\gamma_0 b), \tag{4.21}$$

which can be satisfied by the spin (3,1) subalgebra of $\mathcal{G}_+$. We obtain the same result for $\hat{G}_+(\Psi_-)$. Thus the decomposition of the Dirac space $\Psi_\epsilon(f)$ onto two Weyl subspaces can be viewed as a decomposition onto two totally isotropic subspaces with respect to SU(2,2) symmetry [related to the $(\,,\,)_-$ product], each of which inherits SL(2,C) symmetry [related to the $(\,,\,)_+$ product]. Because $\beta_+(e_0e_1e_2e_3e_4)=e_0e_1e_2e_3e_4$, we have that the map

$$\chi:\Psi_\epsilon(f)\otimes\Psi_\epsilon(f)\to R_{4,1} \tag{4.22}$$

is given by (2.38)–(2.41) completed by relations

$$\chi(is_k\otimes s_\gamma)=\chi(s_k\otimes is_\gamma)=i\chi(s_k\otimes s_\gamma) \tag{4.23}$$

and

$$\begin{aligned} e_0&=e_0(f^1+f^2+f^3+f^4)\\ &=i\chi(s_2\otimes s_4-s_4\otimes s_2+s_1\otimes s_3-s_3\otimes s_1)\\ &=i\varphi(s_2\otimes s_4+s_1\otimes s_3). \end{aligned} \tag{4.24}$$

V. CHEVALLEY–CRUMEYROLLE SPINOR SPACE V_ϵ

We have already shown that the complexification $R^{\mathbb{C}}_{3,1}$ of the real Clifford algebra $R_{3,1}$ is isomorphic to the real Clifford algebra $R_{4,1}$ and that they both have matrix representation given by $\mathbb{C}(4)$. Because the complexification $R^{\mathbb{C}}_{3,1}$ of $R_{3,1}$ can be identified with the Clifford algebra for the complexified Minkowski space-time we shall consider spinor spaces as consequences of passing from

$$R^{3,1}\rightsquigarrow(R^{3,1})^{\mathbb{C}}\cong\mathbb{C}^4 \tag{5.1}$$

instead of embedding

$$R^{3,1}\hookrightarrow R^{4,1} \tag{5.2}$$

as in Sec. IV. Employing the complexification (5.1) we can introduce an isotropic basis of $\mathbb{C}^4$ (see Ref. 3)

$$\begin{aligned} &x_1=\tfrac{1}{2}(e_1+ie_2),\quad y_1=\tfrac{1}{2}(e_1-ie_2),\\ &x_2=\tfrac{1}{2}(e_3+e_4),\quad y_2=\tfrac{1}{2}(e_3-e_4), \end{aligned} \tag{5.3}$$

with (e_1,e_2,e_3,e_4) given by (2.1).

Let us take the minimal left ideal V_ϵ of $R^{\mathbb{C}}_{3,1}$ of the form

$$V_\epsilon=R^{\mathbb{C}}_{3,1}y_1y_2. \tag{5.4}$$

Let us denote the isotropic bivector y_1y_2 by v, the maximal isotropic subspace determined by $\{y_1,y_2\}$ by N and its transverse, spanned by $\{x_1,x_2\}$, by P. If we choose the base (v_1,v_2,v_3,v_4) of V_ϵ as

$$\begin{aligned} &v_1=e_1e_3v=x_1x_2v,\quad v_3=e_1v=x_1v,\\ &v_2=v,\quad v_4=e_3v=x_2v, \end{aligned} \tag{5.5}$$

then the space of Chevalley–Crumeyrolle spinors V_ϵ can be identified with the vector space of the exterior algebra $\wedge P$.

Using the matrix representation (2.7) of the generators e_1,e_2,e_3,e_4 we have

$$v_1=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&-1&i\\0&0&-i&-1\end{pmatrix},$$

$$v_2=\begin{pmatrix}0&0&1&-i\\0&0&-i&-1\\0&0&0&0\\0&0&0&0\end{pmatrix},$$

$$v_3=\begin{pmatrix}0&0&1&-i\\0&0&i&1\\0&0&0&0\\0&0&0&0\end{pmatrix},$$

$$v_4=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&-1&i\\0&0&-i&-1\end{pmatrix}. \tag{5.6}$$

Let us write elements v_k of V_ϵ as

$$v_k=\mathscr{A}_k+i\mathscr{B}_k, \tag{5.7}$$

with $\mathscr{A}_k,\mathscr{B}_k$ real 4×4 matrices given by (5.6). Because the matrices $\mathscr{B}_k$ cannot be obtained by any linear combination of $\mathscr{A}_k$ matrices, hence v_k cannot be expressed by any complex combination of any basis (s'_1,s'_2,s'_3,s'_4) of the Dirac space $\Psi_{\epsilon'}(f')$. Hence using isomorphism of algebras $R^{\mathbb{C}}_{3,1}\cong R_{4,1}$ induced by correspondence

$$i\leftrightarrow e_0e_1e_2e_3e_4, \tag{5.8}$$

we see that the space of Chevalley–Crumeyrolle spinors V_ϵ can not be identified with any Dirac spinor space $\Psi_{\epsilon'}(f')$. This can be seen immediately when we write $v=y_1y_2$ as

$$v=e_1e_3\tfrac{1}{2}(1-ie_1e_2)\tfrac{1}{2}(1-e_3e_4)=e_1e_3\tilde{f}_\epsilon. \tag{5.9}$$

Since to any primitive idempotent $\tilde{f}$ of $R^{\mathbb{C}}_{3,1}$ corresponds, by (5.8), a primitive idempotent $\hat{f}$ of $R_{4,1}$, we have

$$R^{\mathbb{C}}_{3,1}\ni\tilde{f}_\epsilon\rightsquigarrow\hat{f}_\epsilon\in R_{4,1}, \tag{5.10}$$

according with

$$\hat{f}_\epsilon=\tfrac{1}{4}(1+e_{034})(1-e_{34}). \tag{5.11}$$

Thus we have

$$V_\epsilon=R^{\mathbb{C}}_{3,1}\tilde{f}_\epsilon=R^{\mathbb{C}}_{3,1}v\Leftrightarrow\hat{V}_\epsilon=R_{4,1}\hat{f}_\epsilon \tag{5.12}$$

as vector spaces. Nevertheless it is obvious that $\hat{V}_\epsilon$ cannot be given as any Dirac spinor space $\Psi_{\epsilon'}(f')$. The basis elements $v_i\in V_\epsilon$ can be written as

$$\begin{aligned} &v_1=-f,\quad v_3=e_3f,\\ &v_2=e_1e_3f,\quad v_4=-e_1f, \end{aligned} \tag{5.13}$$

where $f\equiv\tilde{f}_\epsilon$ for shortness. Thus we have

$$v_i=u_iv,\quad\text{with}\quad(u_1,u_2,u_3,u_4)=(x_1x_2,1,x_1,x_2), \tag{5.14}$$

as well as

$$v_i=\tilde{u}_if,\quad\text{with}\quad(\tilde{u}_1,\tilde{u}_2,\tilde{u}_3,\tilde{u}_4)=(-1,e_1,e_3,e_3,-e_1). \tag{5.15}$$

So any element $\psi\in V_\epsilon$ can be written as

$$\psi=\psi_iu_iv=\psi_iu_ie_1e_3f=\psi_i\tilde{u}_if. \tag{5.16}$$

Now let us consider the map $\chi: V_\epsilon \otimes V_\epsilon \to R^{\mathbb{C}}_{3,1}$. As usual,

$$\chi(\psi \otimes \psi') = \psi\omega_+ \beta_+(\psi'), \tag{5.17}$$

with ω_+ determined by f and given, for example, by $\omega_+ = e_1 e_3 = \tilde{u}_2$. Now

$$\begin{aligned}\chi(v_i \otimes v_k) &= \tilde{u}_i f \omega_+ \beta_+(f)\beta_+(\tilde{u}_k)\\ &= \tilde{u}_i f \omega_+ \beta_+(\tilde{u}_k)\\ &= -\tilde{u}_i \omega_+ v \omega_+ \beta_+(\tilde{u}_k)\\ &= u_i v \beta_+(u_k).\end{aligned}$$

This implies immediately that the map χ can be considered as

$$\tilde{\chi}(u \otimes u') = uv\beta_+(u'), \tag{5.18}$$

where $u = \psi_i u_i$, $u' = \psi_i' u_i \in \wedge P$ are uniquely determined by elements $\psi, \psi' \in V_\epsilon$. Thus we have obtained that (5.17) is equivalent to Chevalley's isomorphism of the form (5.18).

VI. CONCLUSIONS

We have defined the different concrete spinor spaces ζ_ϵ, Σ_ϵ, Ψ_ϵ, and V_ϵ for the Minkowski space-time $R^{3,1}$ by the left minimal ideals of appropriate Clifford algebras. We have seen that when we are interested only in the real Clifford algebras then automatically our Majorana spinor space ζ_ϵ is equipped with two inequivariant almost complex structures J and J', respectively. We can check that their product gives another almost complex structure J'',

$$JJ' = J'', \tag{6.1}$$

and that

$$JJ' + J'J = 0. \tag{6.2}$$

In other words we obtain the quaternion algebra Q on the vector space ζ_ϵ. It is given by an algebra of linear transformations $\{J, J', J''\}$ of ζ_ϵ isomorphic to the algebra of real quaternions and whose unit element is the identity transformation of ζ_ϵ. So we may view ζ_ϵ as a quaternionic vector space over Q.

Now let us consider the space-time manifold $\mathcal{M}$. It is known[4] that the spinor structure in the sense of Milnor–Lichnerowicz does exist if we can construct a global field of orthonormal tetrads on $\mathcal{M}$. But this gives us the possibility of construction of any concrete algebraic spinor bundles $\mathcal{S}\mathcal{M}$, $\Sigma\mathcal{M}$, $\Psi\mathcal{M}$, and $V\mathcal{M}$. These bundles are determined by global fields of primitive idempotents, which, with respect to a fixed global field of tetrads $\Sigma(x)$, have the form (2.3), (3.2), or (5.9), respectively. We have seen that one of the differences between Dirac and Chevalley–Crumeyrolle spinor spaces lies in the fact that they are not related to $\Gamma(3,1)$ equivalent primitive idempotents (2.3) and (5.9), respectively. [$\Gamma(3,1)$ is the Clifford group of the quadratic form $(+\ +\ +\ -)$.] The second difference is that the imaginary units of the corresponding division rings (4.2) and complexified (2.11) have different properties with respect to anti-involutions $\beta_\pm$. This implies that the Weyl decomposition of the Dirac space is related to the Penrose correspondence between the totally isotropic two-subspaces of twistor space and points of Minkowski vector space.[5]

Let us consider, for example, the subspace Ψ_+. It contains the Dirac spinors ψ, which, in the base (4.4), have the components

$$(\psi_1,\psi_2,\psi_3,\psi_4) = (a_1, ia_1, a_2, -ia_2), \quad a_1 a_2 \in \mathbb{C}. \tag{6.3}$$

Making an appropriate linear transformation of the basis elements (4.4), after which ψ and φ have components $\psi = \{\chi_i\}$, $\varphi = \{\rho_i\}$, $i = 1, \ldots, 4$, we obtain

$$(\psi,\varphi)_- = \chi_1^*\rho_3 + \chi_3^*\rho_1 + \chi_2^*\rho_4 + \chi_4^*\rho_2. \tag{6.4}$$

This formula suggests the interpretation of these new components as the Penrose components $(\omega^A, \pi_{A'})$ of any twistor Z_α,[5] i.e.,

$$(\chi_1,\chi_2,\chi_3,\chi_4) = (\omega_0, \omega^1, \pi_{0'}, \pi_{1'}).$$

We see that although the Dirac spinor space Ψ_ϵ can be equipped with the SU(2,2) symmetry, the decomposition of Ψ_ϵ onto the Weyl subspaces is different than the decomposition onto the Penrose ω and π subspaces. By Penrose correspondence we have that with any totally isotropic two-subspace of Ψ_ϵ we can relate a point of the real Minkowski space, the components of which can be given as

$$x^\mu \equiv x^{AA'} = (\mu_B, \pi^{B'})^{-1}(\omega^A \mu^{A'} - \lambda^A \pi^{A'}),$$

where $\psi = (\omega^A, \pi_{A'})$, $\varphi = (\lambda^A, \mu_{A'})$ are any elements of Ψ_+. The simple calculation shows that the subspace Ψ_+ is related to the point $x^\mu = (0,0,-1,0) \in R^{3,1}$ [in the base (2.1)].

Making some SU(2,2) transformation s of our concrete Dirac spinor space Ψ_ϵ we obtain another decomposition related to the projector $\frac{1}{2}(1 + s\gamma_0 s^{-1})$

$$\Psi_\epsilon = s\Psi_+ \oplus s\Psi_- := \Psi^s_+ \oplus \Psi^s_-.$$

In the case of the Chevalley–Crumeyrolle spinors we have also the natural possibility of the decomposition of V_ϵ onto the half-spinor spaces. Because $V_\epsilon \cong \wedge P$, the natural decomposition of the exterior algebra $\wedge P$ onto even and odd parts implies the decomposition V_ϵ onto subspaces V_e and V_o spanned by

$$V_e = \{x_1 x_2 v, v\}, \quad V_o = \{x_1 v, x_2 v\},$$

respectively. Making use of the correspondence (5.9) we can build the Weyl operators $\tilde{W}_\pm$ also for Chevalley's spinor space

$$\tilde{W}_\pm = \tfrac{1}{2}(1 \mp i\gamma_1\gamma_2\gamma_3\gamma_4).$$

It appears that $V_+ = V_o$ and $V_- = V_e$ but now neither V_+ nor V_- are totally isotropic subspaces of V_ϵ. Besides, we have also the difference between the geometrical properties of elements of $V_\pm$ and $\Psi_\pm$. Namely, any half-spinor $\psi \in V_+$ determines a maximal totally isotropic subspace of $(R^{3,1})^{\mathbb{C}} \cong \mathbb{C}^4$, which crosses the real slice $R^{3,1}$ of $\mathbb{C}^4$ along a light line given by $\chi(\psi \otimes \psi^*)$. On the other side, any Weyl spinor $\psi \in \Psi^s_+$, $\psi = (\omega^A, \pi_{A'})$ determines a light line in $R^{3,1}$ passing by the point a'_μ corresponding to Ψ^s_+ and given by $\pi \otimes \pi^*$.

Now let us consider the space-time manifold $\mathcal{M}$. We have two ways to introduce the Dirac spinor spaces $\Psi(x)$ in a smooth way. We can extend the structure group of the principal bundle of the orthonormal tetras to the $SO_+(4,1)$ group. Then we can take the associated vector bundle with the fiber equal to R^5. This bundle may be seen as a Whitney

sum of the tangent bundle $T\mathscr{M}$ and a linear bundle $L\mathscr{M}$. Now using the global field of primitive idempotents, which determines the Majorana bundle $\mathscr{S}\mathscr{M}$, we can repeat the construction of Sec. IV point by point. Let us notice that any decomposition of the spinor bundle $\Psi\mathscr{M}$ onto Weyl subbundles determines uniquely the same vector field tangent to the manifold $\mathscr{M}$. The second possibility of introducing the Dirac spinor bundle into the theory is to pass to some five-dimensional manifold E of signature (4,1) such that the observable four-dimensional space-time manifold is suitably regularly embedded into E. This case is considered in the next paper.

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On the generation of equivalent Hamiltonians

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A new approach to the equivalence problem (in phase space) is presented. Given a Hamiltonian describing a system of particles with two degrees of freedom (and the corresponding Hamilton–Jacobi equation), it is shown how to find the most general family of Hamiltonian functions that generates a new Hamilton–Jacobi equation with the following (and essential) characteristic, here defined as equivalence: Every new solution is also a solution of the original Hamilton–Jacobi equation and vice versa.

I. INTRODUCTION

The usual approaches to the mechanical equivalence problem are based on Lagrangian formulation.[1–3] The problem in phase space is an open one. The purpose of this note is to present a technique for solving this problem by using the Hamiltonian formulation. In order to achieve this aim we shall assume that the Hamilton–Jacobi equation describes a mechanical system and use the following theorem.[4]

Theorem: Suppose we have the pair of first-order partial differential equations

$$f(x,y,z,z_x,z_y)=0 \tag{1}$$

and

$$g(x,y,z,z_x,z_y)=0, \tag{2}$$

where (a) x and y are independent variables; (b) z is the dependent variable; and (c) $z_x=\partial z/\partial x$ and $z_y=\partial z/\partial y$. Suppose further that the Jacobian $J=\partial(f,g)/\partial(z_x,z_y)$ is different from zero. The condition that the pair of equations [(1) and (2)] should be compatible is

$$[f,g]\equiv\frac{\partial(f,g)}{\partial(x,z_x)}+\frac{\partial(f,g)}{\partial(z,z_x)}z_x+\frac{\partial(f,g)}{\partial(y,z_y)}+\frac{\partial(f,g)}{\partial(z,z_y)}z_y=0. \tag{3}$$

II. EQUIVALENT HAMILTONIANS

Suppose two Hamiltonians $H(q_1,q_2,p_1,p_2)$ and $\bar{H}(q_1,q_2,p_1,p_2)$ yield, respectively, the following Hamilton–Jacobi equations:

$$f\equiv H\left(q_1,q_2,\frac{\partial S}{\partial q_1},\frac{\partial S}{\partial q_2}\right)-\alpha=0 \tag{4}$$

and

$$g\equiv \bar{H}\left(q_1,q_2,\frac{\partial S}{\partial q_1},\frac{\partial S}{\partial q_2}\right)-\beta=0 \tag{5}$$

(α and β being constants of motion).

By the use of the above theorem, f and g will be equivalent whenever

$$J=\frac{\partial(f,g)}{\partial(p_1,p_2)}\neq 0 \quad \text{and} \quad [f,g]=0.$$

The last condition implies $[H,\bar{H}]=0$. This is the basic equation and, since H and $\bar{H}$ do not depend explicitly on S, it may be written as

$$\frac{\partial H}{\partial q_1}\frac{\partial \bar{H}}{\partial p_1}-\frac{\partial H}{\partial p_1}\frac{\partial \bar{H}}{\partial q_1}+\frac{\partial H}{\partial q_2}\frac{\partial \bar{H}}{\partial p_2}-\frac{\partial H}{\partial p_2}\frac{\partial \bar{H}}{\partial q_2}=0, \tag{6}$$

which may be considered an equation for $\bar{H}$ (in fact a first-order partial differential equation). Its solution[5] is the arbitrary function G so that

$$\bar{H}(q_1,q_2,p_1,p_2)=G(u_1,u_2,u_3), \tag{7}$$

where $u_i(q_1,q_2,p_1,p_2)=c_i$ (c_i being constants) are independent solutions of the subsidiary equations

$$-\frac{dq_1}{\partial H/\partial p_1}=-\frac{dq_2}{\partial H/\partial p_2}=\frac{dp_1}{\partial H/\partial q_1}=\frac{dp_2}{\partial H/\partial q_2}. \tag{8}$$

As a consequence, Eqs. (4) and (5) have the same solutions, provided $\bar{H}$ is given by Eq. (7).

Definition: H and $\bar{H}$ are equivalent if and only if Eq. (4) and (5) have the same solutions.

Moreover, if there is another function $\bar{H}'$ equivalent to H, it belongs to the family defined by $\bar{H}$ since this is the general solution of the compatibility condition implied by Eq. (6). It is important to remark that Eq. (6) is a linear one and so it has no singular (envelope) solution.

Finally, it is also worthwhile to mention that the technique may be generalized to a higher-dimensional phase space.

III. APPLICATION

To clarify the procedure above, consider an isotropic and bidimensional harmonic oscillator described by the Hamiltonian

$$H=p_1p_2+q_1q_2, \tag{9}$$

where the q_i are the generalized coordinates and the p_i the generalized momenta.

Equation (6) now reads

$$q_2\frac{\partial \bar{H}}{\partial p_1}-p_2\frac{\partial \bar{H}}{\partial q_1}+q_1\frac{\partial \bar{H}}{\partial p_2}-p_1\frac{\partial \bar{H}}{\partial q_2}=0. \tag{10}$$

This is a first-order linear partial differential equation, with a subsidiary system given by

$$-\frac{dq_1}{p_2}=-\frac{dq_2}{p_1}=\frac{dp_1}{q_2}=\frac{dp_2}{q_1}=\frac{d\bar{H}}{0}.$$

Its independent solutions are

$$u_1=q_1^2+p_2^2=c_1,$$

$$u_2=q_2^2+p_1^2=c_2,$$

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$$u_3 = q_1 q_2 + p_1 p_2 = c_3.$$

Therefore Eq. (10) has the general solution

$$\bar{H} = G(q_1^2 + p_2^2,\ q_2^2 + p_1^2,\ q_1 q_2 + p_1 p_2), \tag{11}$$

where G is an arbitrary function.

The function given by Eq. (11) represents a family of Hamiltonian functions equivalent to H.

As a final comment, we mention the configuration space counterpart of the above equivalence.

The Lagrangian corresponding to the harmonic oscillator described by Eq. (9) is

$$L = \dot{q}_1 \dot{q}_2 - q_1 q_2.$$

This Lagrangian is equivalent[3] to

$$\bar{L}' = \tfrac{1}{2}(\dot{q}_1^2 + \dot{q}_2^2) - \tfrac{1}{2}(q_1^2 + q_2^2),$$

which corresponds to the Hamiltonian

$$\bar{H}' = \tfrac{1}{2}(p_1^2 + p_2^2) + \tfrac{1}{2}(q_1^2 + q_2^2).$$

It is easy to see that $\bar{H}'$ is a member of our (broader) family of Hamiltonians $\bar{H}$ given by Eq. (11).

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Comment on an aspect of a paper by G. Thompson

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G. Thompson [J. Math. Phys. **25**, 3474 (1984)], by way of example of a general method, examined the existence of integrals of the form $I=(yp_x-xp_y)^3+A(x,y)p_x+B(x,y)p_y$, for the Hamiltonian $H=\frac{1}{2}(p_x^2+p_y^2)+V(x,y)$. The treatment was not complete. A complete solution is given here as well as indications for further development to integrals of higher order in the momenta.

I. INTRODUCTION

Thompson[1] investigated the existence of first integrals, which are polynomial in the momenta, and applied the results to a variety of Hamiltonian systems. The Hamiltonian was the standard particle one of classical mechanics,

$$H=\tfrac{1}{2}p_ip_i+V(q_i)\,, \tag{1.1}$$

for an autonomous system. (The summation convention is adopted.) Thompson showed that, if one were seeking first integrals in involution with H and polynomial in the momenta, it was necessary and sufficient to consider only first integrals which were odd or even in the momenta. Thus one would posit either

$$I_{\text{even}}=f(\mathbf{q})+f_{ij}(\mathbf{q})p^ip^j+f_{ijkl}(\mathbf{q})p^ip^jp^kp^l+\cdots\,, \tag{1.2}$$

or

$$I_{\text{odd}}=f_i(\mathbf{q})p^i+f_{ijk}(\mathbf{q})p^ip^jp^k+\cdots\,, \tag{1.3}$$

as the structure for the first integral and determine the f's and V from the Liouville equation

$$\dot{I}=[I,H]_{PB}=0\,. \tag{1.4}$$

It is appreciated that there are limitations on Thompson's method as it treats only autonomous systems and time-independent first integrals. However, there is considerable interest in autonomous systems[2] and, in seeking integrals in involution with H, progress is made in identifying those systems which are integrable. From the examples discussed by Thompson, it is evident that the calculation of first integrals of higher degree than quadratic in the momenta is feasible. This is the benefit gained by his restriction to autonomous systems. Even in the case of one-dimensional nonautonomous systems, an integral of greater degree than quadratic in the momentum has not been possible when stated as a general problem. The reason is that the potential has to be determined from a nonlinear integral equation.[3,4] It is surmised that the situation would be no better for systems of more than one degree of freedom. Indeed, the complexities of the calculation of quadratic first integrals for systems of two[5] and three[6] degrees of freedom for time-dependent systems are most daunting.

In this paper[1] Thompson discussed seven examples. For the first six, explicit and interesting results were obtained. In the seventh example, specialized to the determination of a first integral of the form

$$I=(yp_x-xp_y)^3+A(x,y)p_x+B(x,y)p_y\,, \tag{1.5}$$

for the Hamiltonian

$$H=\tfrac{1}{2}(p_x^2+p_y^2)+V(x,y)\,, \tag{1.6}$$

Thompson was unable to give an explicit result. Briefly stated, forms for the first integral and the structure of the potential were given in terms of two functions which were the solutions of a pair of coupled ordinary differential equations. It is the purpose of this short note to determine the explicit forms of the functions A, B, and V in (1.5) and (1.6). Further, the case of the quartic analog of (1.5) is treated and a conjecture made for the structure of first integrals of higher degree in the momenta of the type (1.5).

II. THE CUBIC INTEGRAL AND CORRESPONDING POTENTIAL

When (1.5) and (1.6) are substituted into the Liouville equation (1.4), the left-hand side is a polynomial in third-order and first-order terms in the momenta. Equating the coefficients of independent terms to zero we obtain, after some rearrangement,

$$\frac{\partial A}{\partial x}=3y^2\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)V\,, \tag{2.1}$$

$$\frac{\partial A}{\partial y}+\frac{\partial B}{\partial x}=-6xy\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)V\,, \tag{2.2}$$

$$\frac{\partial B}{\partial y}=3x^2\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)V\,, \tag{2.3}$$

$$A\frac{\partial V}{\partial x}+B\frac{\partial V}{\partial y}=0\,. \tag{2.4}$$

For the moment we write

$$U=\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)V \tag{2.5}$$

to simplify the right-hand sides of (2.1)–(2.3). For these equations to be integrable, the following condition must be satisfied:

$$\frac{\partial^2}{\partial y^2}\left(\frac{\partial A}{\partial x}\right)-\frac{\partial^2}{\partial x\partial y}\left(\frac{\partial A}{\partial y}+\frac{\partial B}{\partial x}\right)+\frac{\partial^2}{\partial x^2}\left(\frac{\partial B}{\partial y}\right)=0\,. \tag{2.6}$$

This implies that

$$\frac{\partial^2}{\partial y^2}(y^2U)+\frac{\partial^2}{\partial x\partial y}(2xyU)+\frac{\partial^2}{\partial x^2}(x^2U)=0\,. \tag{2.7}$$

We may rearrange (2.7) to obtain

$$\left\{\left(x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}\right)^2+5\left(x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}\right)+6\right\}U=0\,, \tag{2.8}$$

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so that V is a solution of

$$\left(x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+2\right)\left(x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+3\right)\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)V=0\,. \tag{2.9}$$

Noting that the operators $x(\partial/\partial x)+y(\partial/\partial y)$ and $y(\partial/\partial x)-x(\partial/\partial y)$ commute, we introduce new variables η and ζ by the definitions

$$\frac{\partial}{\partial\eta}=x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y},\quad \frac{\partial}{\partial\zeta}=y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}, \tag{2.10}$$

so that (2.9) becomes

$$\left(\frac{\partial}{\partial\eta}+2\right)\left(\frac{\partial}{\partial\eta}+3\right)\frac{\partial}{\partial\zeta}V=0\,, \tag{2.11}$$

which has the solution

$$V(\eta,\zeta)=K(\eta)\zeta^{-2}+L(\eta)\zeta^{-3}+M(\zeta)\,. \tag{2.12}$$

Given the form of V, it is appropriate to introduce the canonical transformation

$$\begin{aligned}&\eta=\arctan(x/y)\,, &&p_\eta=yp_x-xp_y\,,\\ &\zeta=\tfrac{1}{2}\log(x^2+y^2)\,, &&p_\zeta=xp_x+yp_y\,.\end{aligned} \tag{2.13}$$

In terms of the new variables, we are studying the problem of the existence of a first integral of the form

$$I=p_\eta^3+A(\eta,\zeta)p_\eta+B(\eta,\zeta)p_\zeta\,, \tag{2.14}$$

for the Hamiltonian

$$H=\tfrac{1}{2}e^{-2\zeta}(p_\eta^2+p_\zeta^2)+V(\eta,\zeta)\,, \tag{2.15}$$

where

$$V(\eta,\zeta)=K(\eta)\zeta^{-2}+L(\eta)\zeta^{-3}+M(\zeta)\,. \tag{2.16}$$

Rather than transforming equations (2.1)–(2.4) to the new variables, it is more appropriate to recalculate $[I,H]_{PB}$ in the new variables, and so obtain a new set of equations. They are

$$\frac{\partial B}{\partial\zeta}+B=0\,, \tag{2.17}$$

$$\frac{\partial A}{\partial\zeta}+\frac{\partial B}{\partial\eta}=0\,, \tag{2.18}$$

$$\left(\frac{\partial A}{\partial\eta}+B\right)e^{-2\zeta}-3K'\zeta^{-2}-3L'\zeta^{-3}=0\,, \tag{2.19}$$

$$-A(K'\zeta^{-2}+L'\zeta^{-3})+B(2K\zeta^{-3}+3L\zeta^{-4}-M')=0\,, \tag{2.20}$$

where $'$ denotes differentiation with respect to the argument of the function. From (2.17) and (2.18) we obtain

$$B=b(\eta)e^{-\zeta}\,, \tag{2.21}$$

$$A=a(\eta)+b'(\eta)e^{-\zeta}\,. \tag{2.22}$$

Then, from (2.19) we see that

$$\begin{aligned}&K'=0, &&K=\alpha\,,\\ &L'=0, &&L=\beta,\\ &a'=0, &&a=\gamma,\\ &b''+b=0, &&b=\mu\sin\eta+\nu\cos\eta\,,\end{aligned} \tag{2.23}$$

where α, β, γ, μ, and ν are constants. Equation (2.20) becomes

$$(\mu\sin\eta+\nu\cos\eta)e^{-\zeta}(2a\zeta^{-3}+3\beta\zeta^{-4}-M')=0\,,$$

from which it is evident that either $\mu=0=\nu$ or $M=-\alpha\zeta^{-2}-\beta\zeta^{-3}$ to within an ignorable constant.

Case (i): $\mu=0=\nu$, i.e., $B=0$,

$$I=p_\eta^3+\gamma p_\eta\,, \tag{2.24}$$

$$H=\tfrac{1}{2}e^{-2\zeta}(p_\eta^2+p_\zeta^2)+\alpha\zeta^{-2}-\beta\zeta^{-3}+M(\zeta)\,, \tag{2.25a}$$

$$=\tfrac{1}{2}e^{-2\zeta}(p_\eta^2+p_\zeta^2)+M(\zeta)\,. \tag{2.25b}$$

We note that the potential is just of the form $V(r)$, where r is the radial variable, and that the first integral is not truly cubic, but rather is a cubic function of a first integral linear in the momenta, the conserved angular momentum.

Case (ii): $M=-\alpha\zeta^{-2}-\beta\zeta^{-3}$,

$$I=p_\eta^3+\gamma p_\eta+\mu(\cos\eta p_\eta+\sin\eta p_\zeta)e^{-\zeta}+\nu(-\sin\eta p_\eta+\cos\eta p_\zeta)e^{-\zeta}\,, \tag{2.26}$$

$$H=\tfrac{1}{2}e^{-2\zeta}(p_\eta^2+p_\zeta^2)\,. \tag{2.27}$$

Here I is not a true cubic first integral since p_η is itself a first integral. The integrals associated with the constants μ and ν are just the conserved momenta, p_x and p_y, of the free particle which has the Hamiltonian (2.27).

In contrast to the conclusion drawn by Thompson, there does not exist a nontrivial first integral of the structure (1.5) for the Hamiltonian (1.6).

III. THE QUARTIC FIRST INTEGRAL AND CORRESPONDING POTENTIAL

It is of interest to see for what potentials $V(x,y)$ there exists a first integral of the general type of (1.5) which is quartic in the momenta, i.e.,

$$I=(yp_x-xp_y)^4+A(x,y)p_x^2+B(x,y)p_xp_y+C(x,y)p_y^2=D(x,y)\,. \tag{3.1}$$

The analysis is very similar to that in Sec. II and we merely highlight the results. The integrability condition on the analogs to (2.1)–(2.3) leads to the potential having the form

$$V(\eta,\zeta)=K(\eta)\zeta^{-2}+L(\eta)\zeta^{-3}+M(\eta)\zeta^{-4}+N(\zeta)\,, \tag{3.2}$$

where η and ζ are the coordinates defined in (2.13). If we rewrite (3.1) as

$$I=p_\eta^4+A(\eta,\zeta)p_\eta^2+B(\eta,\zeta)p_\eta p_\zeta+C(\eta,\zeta)p_\zeta^2+D(\eta,\zeta)\,, \tag{3.3}$$

and apply the condition $[I,H]_{PB}=0$ with H (2.5) and V (3.3), we find, after following the analysis of Sec. II, that

$$\begin{aligned}&K=k,\quad L=l,\quad M=m\,,\\ &A=\alpha+(\beta\cos\zeta-\gamma\sin\eta)e^{-\zeta}+(\delta-\mu\sin2\eta-\nu\cos2\eta)e^{-2\zeta}\,,\\ &B=(\beta\sin\eta+\alpha\cos\eta)e^{-\zeta}+2(\mu\cos2\eta-\nu\sin2\eta)e^{-2\zeta}\,,\\ &C=(\delta+\mu\sin2\eta+\nu\cos2\eta)e^{-2\zeta}\,,\end{aligned} \tag{3.4}$$

where the lowercase letters (apart from η and ζ) are all constants.

The function $D(\eta,\zeta)$ is determined by the two differential relations

$$\frac{\partial D}{\partial \eta} + Be^{2\zeta}(2k\zeta^{-3} + 3l\zeta^{-4} + 4m\zeta^{-5} - N') = 0, \tag{3.5}$$

$$\frac{\partial D}{\partial \zeta} + 2Ce^{2\zeta}(2k\zeta^{-3} + 3l\zeta^{-4} + 4m\zeta^{-5} - N') = 0. \tag{3.6}$$

Writing the term in parentheses in (3.5) and (3.6) as $X(\zeta)$, the integrability condition for D is

$$(\beta \sin\eta + \gamma\cos\eta)e^{\zeta}(X + X') + 2(\mu\cos 2\eta - \nu \sin 2\eta)(X' - 2X) = 0. \tag{3.7}$$

We distinguish four cases.

Case (i): $\beta = 0 = \gamma, \mu, \nu \neq 0$. Equation (3.7) becomes

$$X' - 2X = 0, \quad X = Re^{2\zeta}, \tag{3.8}$$

whence

$$N = -\tfrac{1}{2}Re^{2\zeta} - k\zeta^{-2} - l\zeta^{-3} - m\zeta^{-4}, \tag{3.9}$$

and the Hamiltonian is

$$H = \tfrac{1}{2}e^{-2\zeta}(p_\eta^2 + p_\zeta^2) - \tfrac{1}{2}Re^{2\zeta}, \tag{3.10}$$

which we identify as a Hamiltonian of oscillator type. The first integral (3.3) is not a true quartic, as p_η is itself a first integral. [This is immediately evident from (3.10).]

Case (ii): $\beta, \gamma \neq 0, \mu = 0 = \nu$. Equation (3.7) becomes

$$X' + X = 0, \quad X = Re^{-\zeta}, \tag{3.11}$$

whence

$$N = \tfrac{1}{2}Re^{-\zeta} - k\zeta^{-2} - l\zeta^{-3} - m\zeta^{-4}, \tag{3.12}$$

and the Hamiltonian is

$$H = \tfrac{1}{2}e^{-2\zeta}(p_\eta^2 + p_\zeta^2) + \tfrac{1}{2}Re^{-\zeta}, \tag{3.13}$$

which we identify as a Hamiltonian of Kepler type. Again the first integral (3.3) is not a true quartic, as p_η is itself a first integral.

Case (iii): $\beta = 0 = \gamma = \mu = \nu, \delta \neq 0$. Equation (3.5) and (3.6) become

$$\frac{\partial D}{\partial \eta} = 0,$$

$$\frac{\partial D}{\partial \zeta} = 2\delta(2k\zeta^{-3} + 3l\zeta^{-4} + 4m\zeta^{-5} - N'),$$

so that

$$N(\zeta) = -(1/2\delta)D(\zeta) - k\zeta^{-2} - l\zeta^{-3} - m\zeta^{-4}, \tag{3.14}$$

and the Hamiltonian is

$$H = \tfrac{1}{2}e^{-2\zeta}(p_\eta^2 + p_\zeta^2) - (1/2\delta)D(\zeta), \tag{3.15}$$

which is just the Hamiltonian of a particle moving in a general radial potential. The first integral is, again, not a true quartic.

Case (iv): $\beta, \gamma, \mu, \nu, \delta \neq 0$. The integrability condition (3.7) separates into two equations for X,

$$X' - 2X = 0, \tag{3.16}$$

$$X' + X = 0, \tag{3.17}$$

from which it is evident that $X = 0$, and the Hamiltonian is that of a free particle,

$$H = \tfrac{1}{2}e^{-2\zeta}(p_\eta^2 + p_\zeta^2). \tag{3.18}$$

Again, the first integral is not a true quartic.

We do not bother to write down the various first integrals associated wth the different cases as they are very well known.

IV. DISCUSSION

We have looked at the nature of the cubic and quartic first integrals of the form

$$I = (yp_x - xp_y)^3 + A(x,y)p_x + B(x,y)p_y, \tag{4.1}$$

$$I = (yp_x - xp_y)^4 + A(x,y)p_x^2 + B(x,y)p_xp_y + C(x,y)p_y^2 + D(x,y), \tag{4.2}$$

for the Hamiltonian

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + V(x,y), \tag{4.3}$$

following the prescription of Thompson. Our results for (4.1) do not agree with this, which were, as we noted above, incomplete. It turned out that (4.1) was not a true cubic, nor (4.2) a true quartic. Furthermore, the existence of time-independent first integrals, apart from the energy ($= H$) and the angular momentum, was limited to the free particle in the case of (4.1) and the oscillator, Kepler problem, and free particle in the case of (4.2).

The clue to the successful analysis of both the cubic and quartic cases was the recognition of the commuting differential operators

$$\frac{\partial}{\partial \eta} = y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}, \quad \frac{\partial}{\partial \zeta} = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}, \tag{4.4}$$

which enabled the general form of the permissible potential to be identified readily. Recasting the problems in terms of the corresponding canonical coordinates considerably simplified the subsequent analysis.

It is evident that, if one were to treat the problem for which

$$I = (yp_x - xp_y)^n + A(x,y)p_x^{n-2} + \cdots \tag{4.5}$$

was the postulated structure of the first integral, the general form of the potential would be

$$V(\eta,\zeta) = \sum_{i=0}^{n-2} K_i(\eta)\zeta^{-2-i} + M(\zeta). \tag{4.6}$$

The analysis could then be undertaken in similar fashion to that in Sec. II. We would expect an increase in the complexity of the analysis in terms of possible cases. However, whether new Hamiltonians with first integrals other than the energy and angular momentum would eventuate is an open question.

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The Lorentz group and the Thomas precession. II. Exact results for the product of two boosts

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The product of two Lorentz boosts in different directions is equal to the product of a pure boost and a spatial rotation. To second order, the resulting boost is simply the sum of the individual boosts, and the rotation is responsible for the Thomas precession. Here the resulting boost and the rotation correction are calculated exactly. The calculation of higher-order corrections to the sum of two finite Lorentz boosts is not usually done, and here previous exact results are critically compared. The complete expression is, to the best of the author's knowledge, a new result.

I. INTRODUCTION

The Thomas precession arises as a spatial rotation correction to the product of two consecutive Lorentz boosts in different directions.[1-7] This rotational effect is physically important because it is easily measurable in the laboratory. Mathematically, the correction arises because the result of a product of two Lorentz boosts is not itself a Lorentz boost, but contains a spatial rotation correction term. Even though this is obvious from the commutation relations of the Lorentz Lie algebra (the commutator of two boosts is a rotation), it is not always referred to explicitly.

Most calculations of the rotation correction to the product of two boosts are done to second order only. In a previous paper,[7] which is the predecessor of this paper, we determine what happens at the next order of approximation. The mathematical techniques used are formulas akin to the Baker–Campbell–Hausdorff formula, which correct the product of noncommuting exponentials in the Clifford algebra. There are an infinite number of correction terms to the product of two exponentials. The result of paper I (Ref. 7) is that the third-order correction is a correction to the Lorentz boost, and not a correction to the spatial rotation.

In this paper, we employ more general mathematical techniques for evaluating exact products of exponentials, following the spirit of Ref. 8. We are thereby able to obtain the exact net Lorentz boost as well as the exact spatial rotation correction.

Among related work on the Thomas precession, we mention Hestenes[9] and Han, Kim, and Son.[10] The separate results of these authors are critically compared with our results in the text. The net Lorentz boost is calculated and related to the standard result for the addition of nonparallel velocities.

II. THE DIFFERENTIAL FORM REALIZATION OF THE LORENTZ GROUP

The mathematical framework upon which all our results are based is the Clifford algebra of differential forms of Kähler and the author.[11-17] Article I (Ref. 7) includes enough of a review for the reader to follow the present paper. For more details, see Refs. 14–16. The key in the construction is to use the basis differential forms $\sigma^\mu = dx^\mu$ of Lorentz–Minkowski space-time ($\sigma^1 = dx$, $\sigma^2 = dy$, $\sigma^3 = dz$, $\sigma^4 = dt$) with metric diag($-1, -1, -1, +1$) to realize antisymmetric tensor fields. Elements of the algebra are real-coefficient differential forms called "tensor types."

The product in the algebra is the associative and invertible vee product of differential forms $\vee$. The vee product combines the totally antisymmetric exterior (Grassmann) product $\wedge$ with the metric inner product by using the permutation group. Sample formulas for the vee product of tensor types are provided for reference in Tables I and II. Some of the multiplication rules are familiar from the rules for multiplying linear combinations of Dirac gamma matrices, which give a specific matrix representation of the Clifford algebra in Lorentz–Minkowski space-time (see, however, Ref. 18).

The volume elements are used to define the duality in both three and four dimensions. For example, vee multiplication by the volume element $\eta = \sigma^1 \wedge \sigma^2 \wedge \sigma^3$ in three-dimensional space gives the space dual ${}^*_3 A$ of a spatial tensor type A. Similarly, vee multiplication by the volume element $\omega = \sigma^1 \wedge \sigma^2 \wedge \sigma^3 \wedge \sigma^4$ in space-time gives the space-time dual ${}^*_4 B$ of any tensor type B.

The reason for choosing to work with the Clifford algebra is that tensor types in the space $M^{1,3}$ have an intrinsic group of inner automorphisms, which is locally isomorphic to SO(1,3), the Lorentz group. Hence, working in the Clifford algebra automatically guarantees intrinsic Lorentz covariance. The theorem responsible for this covariance de-

TABLE I. Vee products of vector types in Minkowski space-time.

$$\mathbf{a} = a^i \sigma^i, \quad (\mathbf{a}\cdot\mathbf{b}) = a^i b^i, \quad |\mathbf{a}| = \sqrt{a^i a^i},$$

$$\mathbf{a}\vee\mathbf{b} = -(\mathbf{a}\cdot\mathbf{b}) - \eta\vee(\mathbf{a}\times\mathbf{b}),$$

$${}^*_3\mathbf{a} = -\eta\vee\mathbf{a}, \quad \mathbf{a}\vee\sigma^4 = -\sigma^4\vee\mathbf{a}, \quad \eta\vee\mathbf{a} = \mathbf{a}\vee\eta, \quad \omega\vee\mathbf{a} = -\mathbf{a}\vee\omega,$$

$$\begin{cases} \eta\vee\sigma^4 = \omega = -\sigma^4\vee\eta, \\ \omega\vee\sigma^4 = \eta = -\sigma^4\vee\omega, \\ \eta\vee\omega = \sigma^4 = -\omega\vee\eta, \\ \eta\vee\eta = 1, \quad \omega\vee\omega = -1, \end{cases}$$

$$\eta\vee\sigma^i = \sigma^i\vee\eta, \quad i = 1,2,3,$$

$$\omega\vee\sigma^\mu = -\sigma^\mu\vee\omega, \quad \mu = 1,2,3,4.$$

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TABLE II. Exponentials of tensor types in Minkowski space-time.

$$\exp(\mathbf{a}\wedge\sigma^4)=\cosh|\mathbf{a}|+[(\mathbf{a}\wedge\sigma^4)/|\mathbf{a}|]\sinh|\mathbf{a}|\,,$$
$$\exp({}^*_3\,\boldsymbol{\theta})=\cos|\boldsymbol{\theta}|+({}^*_3\,\boldsymbol{\theta}/|\boldsymbol{\theta}|)\sin|\boldsymbol{\theta}|$$
$$=\cos|\boldsymbol{\theta}|-[(\eta\vee\boldsymbol{\theta})/|\boldsymbol{\theta}|]\sin|\boldsymbol{\theta}|\,.$$

fines the "twisted Clifford group," and is well known (Theorem 3 of Ref. 7).

We give the differential form realization of the Lorentz Lie algebra using the basis two-forms in space-time. Define the Lorentz boost generators K^i and the spatial rotation generators L^i as follows[7]:

$$L^i=\tfrac{1}{2}\,{}^*_3\sigma^i=\omega\vee K^i={}^*_4\,K^i\,,\quad i=1,2,3\,,$$
$$K^i=\tfrac{1}{2}\,\sigma^i\wedge\sigma^4=-\tfrac{1}{2}\,\omega\vee L^i=-\tfrac{1}{2}\,{}^*L^i\,. \tag{1}$$

The two sets of generators in the full Lorentz group are duals of each other. The commutation relations of SO(1,3) are realized by the basis (1) in the vee product

$$[L^i,L^j]=\epsilon^{ijk}L^k\,,$$
$$[L^i,K^j]=\epsilon^{ijk}K^k\,, \tag{2}$$
$$[K^i,K^j]=-\epsilon^{ijk}L^k\,.$$

The origin of the Thomas precession correction is a consequence of the third commutator in (2): the product of two distinct boosts generates a spatial rotation.

The exponential mapping takes the local Lie algebra into the corresponding Lie group.[19,20] The elements of the Lorentz group are therefore exponentials of linear combinations of the Lorentz basis (1). We label a combination of the six basis two-forms as a tensor type two J:

$$J=\tfrac{1}{2}\,J^{\mu\nu}\sigma^\mu\wedge\sigma^\nu\,. \tag{3}$$

This tensor type two may be decomposed via the space-time decomposition[14–16] in the same way that an electromagnetic field is decomposed into electric and magnetic vectors. We label two space vectors $\boldsymbol{\theta}$ and $\mathbf{b}$ as the spatial and space-time components of the tensor type (3)

$$J=\mathbf{b}\wedge\sigma^4-{}^*_3\boldsymbol{\theta}=\mathbf{b}\vee\sigma^4+\eta\vee\boldsymbol{\theta};$$
$$b^i=J^{i4}\,,\quad \theta^i=-\tfrac{1}{2}\,\epsilon^{ijk}J^{jk}\,. \tag{4}$$

The space-time decomposition identifies the three boost components b^i, $i=1,2,3$, and the three spatial rotation components θ^i of the Lorentz group. We have the identification

$$J=2b^iK^i-2\theta^iL^i\,. \tag{5}$$

The elements of the Lorentz group are the exponentials of the tensor type two J. It is instructive to consider boosts and rotations separately for the moment. The pure boosts are defined by the relative frame velocity $\mathbf{V}$ and the following equations (carets denote unit vectors):

$$\mathbb{L}(\mathbf{b})=\exp(-\tfrac{1}{2}\,\mathbf{b}\wedge\sigma^4)=\exp(-b^iK^i)$$
$$=\cosh\tfrac{1}{2}|\mathbf{b}|-\hat{\mathbf{b}}\wedge\sigma^4\sinh\tfrac{1}{2}|\mathbf{b}|\,, \tag{6a}$$
$$\hat{\mathbf{b}}=\hat{\mathbf{V}}\,,\quad \tanh|\mathbf{b}|=|\mathbf{V}|\,,\quad \gamma=(1-|\mathbf{V}|^2)^{-1/2}=\cosh|\mathbf{b}|\,. \tag{6b}$$

In the Clifford algebra, the Lorentz boost operator $\mathbb{L}$ is a combination of a scalar and a space-time tensor type two, demonstrating that the exponential mapping is not type-preserving. Similarly, the spatial rotation operator is defined in terms of the rotation vector $\boldsymbol{\theta}$ as follows:

$$\mathbb{R}(\boldsymbol{\theta})=\exp(\tfrac{1}{2}\,{}^*_3\boldsymbol{\theta})=\exp(\theta^iL^i)$$
$$=\cos\tfrac{1}{2}|\boldsymbol{\theta}|-\eta\vee\hat{\boldsymbol{\theta}}\sin\tfrac{1}{2}|\boldsymbol{\theta}|\,. \tag{7}$$

A tensor type A (or a combination of distinct tensor types) is transformed by the inner automorphisms as

$$A'=\mathbb{L}(\mathbf{b})\vee A\vee\mathbb{L}(-\mathbf{b})\,, \tag{8a}$$
$$A''=\mathbb{R}(\boldsymbol{\theta})\vee A\vee\mathbb{R}(-\boldsymbol{\theta})\,. \tag{8b}$$

Using the forms for the exponentials, Eqs. (8a) and (8b) may be separately evaluated to give the general expressions for a Lorentz boost, and a three-dimensional conical rotation, respectively. An advantage over conventional treatments is the complete generality of the type A in (8) (in the usual treatments, A is a vector). In the Clifford algebra the same general equation (8) performs the inner automorphisms regardless of the rank of the field A (see Ref. 7).

The most general element of the transformation group is the exponential of J (3,4,5) which combines both a boost $\mathbf{b}$ and a rotation $\boldsymbol{\theta}$.

III. THE PRODUCT OF TWO CONSECUTIVE BOOSTS

The following statement is correct to second order: "The end result of two consecutive Lorentz boosts in different directions is a boost by the sum of the two individual boosts, accompanied by a spatial rotation correction."

The infinitesimal transformations of first order do not include even the first rotation correction, which is of second order. We show here that when one includes all the higher-order corrections, they contribute to both the total boost as well as to the rotation correction. The infinitesimal treatments give the following approximation for the product of two boosts defined by the boost vectors $\mathbf{a}$ and $\mathbf{b}$.

First order:

$$\mathbb{L}(\mathbf{b})\vee\mathbb{L}(\mathbf{a})\approx\mathbb{L}(\mathbf{a}+\mathbf{b})\,. \tag{9}$$

The next-order approximation is the spatial rotation correction, which is responsible for the Thomas precession.[3,5,7]

Second order:

$$\mathbb{L}(\mathbf{b})\vee\mathbb{L}(\mathbf{a})\approx\mathbb{R}(\boldsymbol{\theta})\vee\mathbb{L}(\mathbf{a}+\mathbf{b})\,,\quad \boldsymbol{\theta}\approx\tfrac{1}{2}\mathbf{a}\times\mathbf{b}\,. \tag{10}$$

In paper I (Ref. 7) we compute the next-order correction, which turns out to be a correction to the boost, and not to the rotation.

Third Order:

$$\mathbb{L}(\mathbf{b})\vee\mathbb{L}(\mathbf{a})=\mathbb{R}(\boldsymbol{\theta})\vee\mathbb{L}(\mathbf{d})\,, \tag{11a}$$
$$\boldsymbol{\theta}\approx\tfrac{1}{2}\,\mathbf{a}\times\mathbf{b}\,, \tag{11b}$$
$$\mathbf{d}\approx\left[1-\tfrac{1}{6}|\mathbf{a}|^2-\tfrac{1}{3}(\mathbf{a}\cdot\mathbf{b})\right]\mathbf{b}+\left[1+\tfrac{1}{3}|\mathbf{b}|^2+\tfrac{1}{6}(\mathbf{a}\cdot\mathbf{b})\right]\mathbf{a}\,. \tag{11c}$$

Note, in particular, the lack of symmetry between the two consecutive boost vectors $\mathbf{a}$ and $\mathbf{b}$ in the correction $\mathbf{d}$ (11c). It is the object of this paper to obtain exact values for the rotation correction $\boldsymbol{\theta}$ and for the net boost vector $\mathbf{d}$.

IV. CALCULATION OF THE EXACT ROTATION CORRECTION

We wish to solve the exponential separation (11a) exactly. It is worthwhile noting why this is practicable in the framework of the Clifford algebra of differential forms. The separation follows after performing a space-time decomposition of the product of exponentials as in (4). This is transparent when using the differential form basis, but is extremely difficult to achieve within an explicit matrix representation such as the Dirac gamma matrices.[17]

Using the vee product rules, expand the left-hand side of (11a):

$$\begin{aligned}&\mathbf{L}(\mathbf{b})\vee\mathbf{L}(\mathbf{a})\\&\quad=\exp(-\tfrac{1}{2}\,\mathbf{b}\vee\sigma^4)\vee\exp(-\tfrac{1}{2}\,\mathbf{a}\vee\sigma^4)\\&\quad=\cosh\tfrac{1}{2}|\mathbf{a}|\cosh\tfrac{1}{2}|\mathbf{b}|+(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}})\sinh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|\\&\qquad-(\hat{\mathbf{a}}\sinh\tfrac{1}{2}|\mathbf{a}|\cosh\tfrac{1}{2}|\mathbf{b}|+\hat{\mathbf{b}}\cosh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|)\vee\sigma^4\\&\qquad-\eta\vee(\hat{\mathbf{a}}\times\hat{\mathbf{b}})\sinh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|\,.\end{aligned}\tag{12}$$

Similarly, the right-hand side of (11a) is

$$\begin{aligned}&\mathbf{R}(\boldsymbol{\theta})\vee\mathbf{L}(\mathbf{d})\\&\quad=\exp(-\tfrac{1}{2}\,\eta\vee\boldsymbol{\theta})\vee\exp(-\tfrac{1}{2}\,\mathbf{d}\vee\sigma^4)\\&\quad=\cos\tfrac{1}{2}|\boldsymbol{\theta}|\cosh\tfrac{1}{2}|\mathbf{d}|-\omega(\hat{\boldsymbol{\theta}}\cdot\hat{\mathbf{d}})\sin\tfrac{1}{2}|\boldsymbol{\theta}|\sinh\tfrac{1}{2}|\mathbf{d}|\\&\qquad-[\hat{\mathbf{d}}\cos\tfrac{1}{2}|\boldsymbol{\theta}|\sinh\tfrac{1}{2}|\mathbf{d}|\\&\qquad+(\hat{\boldsymbol{\theta}}\times\hat{\mathbf{d}})\sin\tfrac{1}{2}|\boldsymbol{\theta}|\sinh\tfrac{1}{2}|\mathbf{d}|]\vee\sigma^4\\&\qquad-\eta\vee\hat{\boldsymbol{\theta}}\sin\tfrac{1}{2}|\boldsymbol{\theta}|\cosh\tfrac{1}{2}|\mathbf{d}|\,.\end{aligned}\tag{13}$$

Equating the scalar, vector, type two, and type four tensor types in (12) and (13) gives a set of equations that can be solved uniquely to give $\boldsymbol{\theta}$ and $\mathbf{d}$ in terms of $\mathbf{a}$ and $\mathbf{b}$. An immediate result is the orthogonality of the rotation correction vector $\boldsymbol{\theta}$ to the net Lorentz boost $\mathbf{d}$. This follows since there is no tensor type four (scalar times ω, the four-volume element) in (12), hence the tensor type four term in (13) containing $\hat{\boldsymbol{\theta}}\cdot\hat{\mathbf{d}}$ must vanish identically.

Comparing the spatial tensor type two in (12) and (13) (a space vector times the space volume element η) shows that $\boldsymbol{\theta}$ is along $\mathbf{a}\times\mathbf{b}$. From vector algebra, the direction of $\mathbf{d}$ is a linear combination of the directions of $\mathbf{a}$ and $\mathbf{b}$. This is a result and not an assumption in our treatment. We have

$$\begin{aligned}&\hat{\boldsymbol{\theta}}\cdot\hat{\mathbf{d}}=0\,,\quad\hat{\boldsymbol{\theta}}=(\mathbf{a}\times\mathbf{b})/|\mathbf{a}\times\mathbf{b}|\\&\Rightarrow\hat{\mathbf{d}}=\alpha\hat{\mathbf{a}}+\beta\hat{\mathbf{b}}\,.\end{aligned}\tag{14}$$

Later, in Sec. V, we solve for the length of $\mathbf{d}$ and the scalar functions α and β in order to reconstruct the boost vector $\mathbf{d}=|\mathbf{d}|\,\hat{\mathbf{d}}$. At this point we wish to calculate the total angle of the rotation correction. Equating the scalar types and the spatial tensor type twos in (12) and (13) gives two equations

$$\begin{aligned}&\cosh\tfrac{1}{2}|\mathbf{a}|\cosh\tfrac{1}{2}|\mathbf{b}|+(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}})\sinh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|\\&\quad=\cos\tfrac{1}{2}|\boldsymbol{\theta}|\cosh\tfrac{1}{2}|\mathbf{d}|\,,\end{aligned}\tag{15a}$$

$$(\hat{\mathbf{a}}\times\hat{\mathbf{b}})\sinh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|=\hat{\boldsymbol{\theta}}\sin\tfrac{1}{2}|\boldsymbol{\theta}|\cosh\tfrac{1}{2}|\mathbf{d}|\,.\tag{15b}$$

It is convenient to define an angle ξ between the individual boost vectors $\mathbf{a}$ and $\mathbf{b}$ by

$$(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}})=\cos\xi\,,\quad|\hat{\mathbf{a}}\times\hat{\mathbf{b}}|=\sin\xi\,.\tag{16}$$

Since $\boldsymbol{\theta}$ is parallel to $\mathbf{a}\times\mathbf{b}$, we obtain a scalar relation from (15b) as follows:

$$\begin{aligned}&\hat{\mathbf{a}}\times\hat{\mathbf{b}}=\hat{\boldsymbol{\theta}}\sin\xi\Rightarrow\sin\xi\sinh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|\\&\qquad=\sin\tfrac{1}{2}|\boldsymbol{\theta}|\cosh\tfrac{1}{2}|\mathbf{d}|\,.\end{aligned}\tag{17}$$

Dividing (17) by (15a) and using (16) gives an expression for $\tan\frac{1}{2}|\boldsymbol{\theta}|$, which we label as Φ. The total correction angle then follows from (14).

$$\Phi=\tan\tfrac{1}{2}|\boldsymbol{\theta}|=\sin\xi/(\coth\tfrac{1}{2}|\mathbf{a}|\coth\tfrac{1}{2}|\mathbf{b}|+\cos\xi)\tag{18a}$$

$$\Rightarrow\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}|\boldsymbol{\theta}|=2(\hat{\mathbf{a}}\times\hat{\mathbf{b}}/\sin\xi)\arctan\Phi\,.\tag{18b}$$

This result is generally not referred to in the literature, even though it is given in Ref. 4 [an expression equivalent to (18a) appears in problem 13, p. 336], and in Ref. 9 [Eq. (18.29)].

Han, Kim, and Son[10] obtain a similar, though entirely distinct, expression for the total rotation correction. We recall that result from Ref. 10 [Eq. (11)], where the special case $|\mathbf{a}|=|\mathbf{b}|$ is calculated (note that their angle between boost vectors is $\pi-\xi$):

$$\theta_{\mathrm{HKS}}=2\arcsin\left[\sin\xi/(\coth^2\tfrac{1}{2}|\mathbf{a}|+\cos\xi)\right]\,.\tag{19}$$

This expression is to be compared to our expression (18). Either expression for $\boldsymbol{\theta}$ reduces to zero when $\mathbf{a}$ is parallel to $\mathbf{b}$. Also, it is easy to expand for a small angle ξ between $\mathbf{a}$ and $\mathbf{b}$ to obtain the first-order term $\boldsymbol{\theta}\approx\frac{1}{2}\,\mathbf{a}\times\mathbf{b}$ from (18), and the same expression with $|\mathbf{a}|=|\mathbf{b}|$ from (19). The case which distinguishes between (18) and (19) is the orthogonal case where $(\mathbf{a}\cdot\mathbf{b})=0$. We can then compare our expression (18) for $|\mathbf{a}|=\mathbf{b}|$ with (19) in the limit as $|\mathbf{a}|$ becomes infinite. One has, for $\xi=\pi/2$,

$$\theta=2\arctan(\tanh\tfrac{1}{2}|\mathbf{a}|\tanh\tfrac{1}{2}|\mathbf{b}|)\,,\tag{20a}$$

$$\theta_{\mathrm{HKS}}=2\arcsin(\tanh^2\tfrac{1}{2}|\mathbf{a}|)\,,\quad|\mathbf{a}|=|\mathbf{b}|\,.\tag{20b}$$

When we examine the special case $|\mathbf{a}|=|\mathbf{b}|$ in the limit as $|\mathbf{a}|$ becomes very large, we find that the corresponding expressions differ by a factor of 2:

$$\lim_{|\mathbf{a}|\to\infty}\theta=\pi/2\,,\tag{21a}$$

$$\lim_{|\mathbf{a}|\to\infty}\theta_{\mathrm{HKS}}=\pi\,.\tag{21b}$$

From the physical picture of a boost by equal vectors at an angle $\pi/2$ to each other, one would intuitively expect the rotation correction to approach $\pi/2$ and not π.

V. THE EXACT BOOST CORRECTION

In this section we calculate an exact expression for the net boost $\mathbf{d}$ which is the result of two consecutive boosts $\mathbf{a}$ and $\mathbf{b}$. We solve (17) for $\cosh\frac{1}{2}|\mathbf{d}|$ and then square the result to obtain $\cosh|\mathbf{d}|$ [substitute $\sin\frac{1}{2}|\boldsymbol{\theta}|$ from Eq. (18a)]. With the Lorentz factors defined by (6b), one obtains

$$\cosh|\mathbf{d}|=\cosh|\mathbf{a}|\cosh|\mathbf{b}|+\cos\xi\sinh|\mathbf{a}|\sinh|\mathbf{b}|\tag{22a}$$

$$\Rightarrow\gamma_d=\gamma_a\gamma_b(1+(\mathbf{V}_a\cdot\mathbf{V}_b))\,.\tag{22b}$$

This is a standard result.[1,4,6,9] The magnitude of the relative frame velocity $\mathbf{V}_d$ is easily obtained by converting Eq. (22) to $\tanh|\mathbf{d}|=|\mathbf{V}_d|$:

$$|\mathbf{V}_d|=(|\mathbf{V}_a+\mathbf{V}_b|^2-|\mathbf{V}_a\times\mathbf{V}_b|^2)^{1/2}/[1+(\mathbf{V}_a\cdot\mathbf{V}_b)]\,.\tag{23}$$

This is also a standard result [Ref. 6, Eq. (11.32) or Ref. 4, problem 7, p. 335].

One may obtain the length of the net boost vector $|\mathbf{d}|$ from (22) as

$$|\mathbf{d}| = 2\,\mathrm{arcsinh}[\tfrac{1}{2}(\cos^2\tfrac{1}{2}\xi\,\cosh(|\mathbf{a}|+|\mathbf{b}|) + \sin^2\tfrac{1}{2}\xi\,\cosh(|\mathbf{a}|-|\mathbf{b}|)-1)]^{1/2}\,. \tag{24}$$

We compare this result with the corresponding result in Ref. 10, which gives the length of the net boost vector in the special case $|\mathbf{a}| = |\mathbf{b}|$ [Ref. 10, Eq. (10) (note that their angle is $\pi - \xi$)]:

$$|\mathbf{d}| = 2\,\mathrm{arcsinh}[\cos(\xi/2)\sinh|\mathbf{a}|]\,,\quad |\mathbf{a}| = |\mathbf{b}|\,. \tag{25}$$

This agrees exactly with expression (24) for $|\mathbf{a}| = |\mathbf{b}|$.

When we directly calculate the direction of the net boost vector, we obtain a result that is entirely distinct from that obtainable by the standard methods. We proceed to calculate the direction of the net boost vector by solving Eq. (11a) for the net boost and expanding. Comparing the (vector) $\vee\sigma^4$ terms gives

$$\begin{aligned}&\mathbf{R}^{-1}(\boldsymbol{\theta})\vee\mathbf{L}(\mathbf{b})\vee\mathbf{L}(\mathbf{a}) = \mathbf{L}(\mathbf{d})\\ &\Rightarrow\hat{\mathbf{b}}\begin{bmatrix}-\sin\tfrac{1}{2}|\boldsymbol{\theta}|(\csc\xi\sinh\tfrac{1}{2}|\mathbf{a}|\cosh\tfrac{1}{2}|\mathbf{b}| + \cot\xi\cosh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|)\\ +\cos\tfrac{1}{2}|\boldsymbol{\theta}|\cosh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|\end{bmatrix}\\ &\quad+\hat{\mathbf{a}}\begin{bmatrix}+\sin\tfrac{1}{2}|\boldsymbol{\theta}|(\cot\xi\sinh\tfrac{1}{2}|\mathbf{a}|\cosh\tfrac{1}{2}|\mathbf{b}| + \csc\xi\cosh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|)\\ +\cos\tfrac{1}{2}|\boldsymbol{\theta}|\sinh\tfrac{1}{2}|\mathbf{a}|\cosh\tfrac{1}{2}|\mathbf{b}|\end{bmatrix}\\ &\quad=\hat{\mathbf{d}}\sinh\tfrac{1}{2}|\mathbf{d}|\,.\end{aligned} \tag{26}$$

It is convenient to define two variables x and y as follows:

$$\begin{aligned}x &= \sinh\tfrac{1}{2}|\mathbf{a}|\cosh\tfrac{1}{2}|\mathbf{b}|\\ &= \tfrac{1}{2}(\cosh|\mathbf{a}|\,\cosh|\mathbf{b}| + \cosh|\mathbf{a}| - \cosh|\mathbf{b}| - 1)^{1/2}\\ &= \tfrac{1}{2}(\gamma_a\gamma_b + \gamma_a - \gamma_b - 1)^{1/2}\,,\end{aligned} \tag{27a}$$

$$\begin{aligned}y &= \cosh\tfrac{1}{2}|\mathbf{a}|\sinh\tfrac{1}{2}|\mathbf{b}|\\ &= \tfrac{1}{2}(\cosh|\mathbf{a}|\,\cosh|\mathbf{b}| - \cosh|\mathbf{a}| + \cosh|\mathbf{b}| - 1)^{1/2}\\ &= \tfrac{1}{2}(\gamma_a\gamma_b - \gamma_a + \gamma_b - 1)^{1/2}\,.\end{aligned} \tag{27b}$$

These variables satisfy the identities

$$\begin{aligned}&x^2 + y^2 = \tfrac{1}{2}(\cosh|\mathbf{a}|\cosh|\mathbf{b}| - 1) = \tfrac{1}{2}(\gamma_a\gamma_b - 1)\,,\\ &xy = \tfrac{1}{4}\sinh|\mathbf{a}|\sinh|\mathbf{b}| = \tfrac{1}{4}\gamma_a\gamma_b|\mathbf{V}_a|\,|\mathbf{V}_b|\,.\end{aligned} \tag{28}$$

We have already determined that the net boost vector $\mathbf{d}$ may be decomposed as (14):

$$\hat{\mathbf{d}} = \alpha\hat{\mathbf{a}} + \beta\hat{\mathbf{b}} \tag{29a}$$

$$\Rightarrow\alpha^2 + \beta^2 + 2\alpha\beta\cos\xi = 1\,. \tag{29b}$$

Using x and y in (26) enables us to write the net boost vector in the decomposition (29a) exactly, since the coefficients are

$$\begin{aligned}\alpha &= \frac{x\cos\tfrac{1}{2}|\boldsymbol{\theta}| + \sin\tfrac{1}{2}|\boldsymbol{\theta}|(x\cot\xi + y\csc\xi)}{\sinh\tfrac{1}{2}|\mathbf{d}|}\,,\\ \beta &= \frac{y\cos\tfrac{1}{2}|\boldsymbol{\theta}| - \sin\tfrac{1}{2}|\boldsymbol{\theta}|(x\csc\xi + y\cot\xi)}{\sinh\tfrac{1}{2}|\mathbf{d}|}\,.\end{aligned} \tag{30}$$

In order to simplify the expressions for the α and β coefficients (30) we use the combination Φ (18a), and also $\cosh|\mathbf{d}|$ (22), which is equal to γ_d. We rewrite Φ in terms of the frame velocities,

$$\Phi = \frac{\gamma_a\gamma_b|\mathbf{V}_a\times\mathbf{V}_b|}{1+\gamma_a+\gamma_b+\gamma_d} = \tan\tfrac{1}{2}|\boldsymbol{\theta}| \tag{31a}$$

$$\Rightarrow\begin{cases}\sin\tfrac{1}{2}|\boldsymbol{\theta}| = \Phi(1+\Phi^2)^{-1/2}\,,\\ \cos\tfrac{1}{2}|\boldsymbol{\theta}| = (1+\Phi^2)^{-1/2}\,,\end{cases} \tag{31b}$$

$$\gamma_d = \cosh|\mathbf{d}| = \gamma_a\gamma_b(1 + (\mathbf{V}_a\cdot\mathbf{V}_b)) \tag{31c}$$

$$\Rightarrow\sinh\tfrac{1}{2}|\mathbf{d}| = (\tfrac{1}{2}(\gamma_d - 1))^{1/2}\,. \tag{31d}$$

We finally have the following expressions for the α and β coefficients:

$$\begin{aligned}\alpha &= \frac{x + \Phi(x\cot\xi + y\csc\xi)}{[\tfrac{1}{2}(1+\Phi^2)(\gamma_d - 1)]^{1/2}}\,,\\ \beta &= \frac{y - \Phi(x\csc\xi + y\cot\xi)}{[\tfrac{1}{2}(1+\Phi^2)(\gamma_d - 1)]^{1/2}}\,.\end{aligned} \tag{32}$$

Here, ξ is the angle between the two boost vectors $\mathbf{a}$ and $\mathbf{b}$; x and y are given by (27); and Φ and γ_d are given in (31). The α and β coefficients can thereby be written in terms of $\mathbf{V}_a$ and $\mathbf{V}_b$.

Equations (29a) and (32) give the direction for the net boost vector $\mathbf{d}$, which is the result of two successive boosts by $\mathbf{a}$ and $\mathbf{b}$. The magnitude of $\mathbf{d}$ is given by Eq. (24). It is easy to verify the identity (29b) directly from (32) using (28), thus demonstrating the consistency of our derivation.

We examine some special cases for the net boost direction. First, for $\mathbf{b} = 0$, we have $\Phi = 0$, $\gamma_d = \gamma_a$, $x = (\tfrac{1}{2}(\gamma_a - 1))^{1/2}$, and $y = 0$, which implies that $\alpha = 1$, $\beta = 0$, hence $\hat{\mathbf{d}} = \hat{\mathbf{a}}$ as expected.

Second, the parallel case becomes the usual velocity addition law, since there is no rotation correction. One has the result $(\alpha+\beta)^2 = 1\Rightarrow(\alpha+\beta) = 1\Rightarrow\hat{\mathbf{d}} = \hat{\mathbf{a}}$, from identity (29b). With $\mathbf{V}_a$ parallel to $\mathbf{V}_b$, Eq. (23) is the velocity addition law.

We now address the reasons why the direction of the net boost vector $\mathbf{d}$ is different from that obtained by the standard methods. The standard result is [Ref. 1, Eq. (2.55'), or Ref. 6, Eq. (11.31)]

$$\begin{aligned}\mathbf{V}_{\text{standard}} &= \frac{\mathbf{V}_a + (1/\gamma_a)\mathbf{V}_b + (1 - 1/\gamma_a)(\mathbf{V}_b\cdot\mathbf{V}_a)\mathbf{V}_a}{1 + (\mathbf{V}_a\cdot\mathbf{V}_b)}\\ &= \frac{\mathbf{V}_a + \mathbf{V}_b + (1-1/\gamma_a)(\mathbf{V}_b\times\hat{\mathbf{V}}_a)\times\hat{\mathbf{V}}_a}{1 + (\mathbf{V}_a\cdot\mathbf{V}_b)}\,.\end{aligned} \tag{33}$$

[Note that the corresponding expression in Ref. 9, Eq. (18.27) has a sign mistake.] The standard expression for the net velocity vector $\mathbf{V}_s$ (33) can be written in the form (29a) with the following coefficients, using (23):

$$\alpha_s = \frac{|\mathbf{V}_a| + |\mathbf{V}_b|(1 - 1/\gamma_a)\cos\xi}{[|\mathbf{V}_a + \mathbf{V}_b|^2 - |\mathbf{V}_a \times \mathbf{V}_b|^2]^{1/2}}, \tag{34a}$$

$$\beta_s = \frac{|\mathbf{V}_b|/\gamma_a}{[|\mathbf{V}_a + \mathbf{V}_b|^2 - |\mathbf{V}_a \times \mathbf{V}_b|^2]^{1/2}}. \tag{34b}$$

The α and β coefficients derived via the usual method (34) are entirely distinct from those obtained in this paper (32). This is true even though they both separately satisfy identity (29b). The reason for this discrepancy is that the usual derivation fails to take into account the finite rotation correction to the product of two boosts.

The magnitude of the net boost vector $\mathbf{d}$ is not in question; that is given by both methods as (23) or (24). Nevertheless, the correct direction of the net boost vector, which is the result of two arbitrary boosts, poses a problem. The two methods give entirely distinct expressions, which agree only in the parallel case. We feel that one definitely needs to take into account the finite rotation correction, which rotates the net boost towards the direction of the second boost.

Since the magnitude of the net velocity vector is the same whether obtained by the usual method or in the derivation of this paper, the relationship is some spatial rotation. Denote the rotation parameter by ϕ. It follows from (29a) that this rotation is in the plane defined by the individual boosts $\mathbf{a}$ and $\mathbf{b}$. To analyze this rotation, define a boost vector $\mathbf{s}$, which corresponds to the standard net velocity $\mathbf{V}_s$ (33). Both $\mathbf{s}$ and $\mathbf{d}$ and, correspondingly, $\mathbf{V}_s$ and $\mathbf{V}_d$, have the same magnitude:

$$\begin{aligned} &\hat{\mathbf{s}} = \alpha_s \hat{\mathbf{a}} + \beta_s \hat{\mathbf{b}} = \hat{\mathbf{V}}_s, \\ &|\mathbf{s}| = |\mathbf{d}|, \quad |\mathbf{V}_s| = |\mathbf{V}_d| = \tanh|\mathbf{s}| = \tanh|\mathbf{d}|, \\ &\gamma_s = \gamma_d. \end{aligned} \tag{35}$$

As noted above, there is a spatial rotation which transforms $\mathbf{s}$ into $\mathbf{d}$, or, equivalently, $\mathbf{V}_s$ into $\mathbf{V}_d$:

$$\begin{aligned} &\mathbf{V}_d = \mathbb{R}(\boldsymbol{\phi}) \vee \mathbf{V}_s \vee \mathbb{R}^{-1}(\boldsymbol{\phi}), \quad \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{\theta}} = \hat{\mathbf{a}} \times \hat{\mathbf{b}} \csc\xi \\ &\Rightarrow \mathbf{d} = \mathbb{R}(\boldsymbol{\phi}) \vee \mathbf{s} \vee \mathbb{R}^{-1}(\boldsymbol{\phi}) \\ &\Rightarrow \alpha\hat{\mathbf{a}} + \beta\hat{\mathbf{b}} = \mathbb{R}(\boldsymbol{\phi}) \vee (\alpha_s \hat{\mathbf{a}} + \beta_s \hat{\mathbf{b}}) \vee \mathbb{R}^{-1}(\boldsymbol{\phi}). \end{aligned} \tag{36}$$

Perform the spatial rotation using (8b) or the formula for a conical rotation of a vector[4,7] to obtain the following relations for the α and β coefficients:

$$\begin{aligned} &\alpha = \alpha_s \cos|\boldsymbol{\phi}| - \sin|\boldsymbol{\phi}|(\alpha_s \cot\xi + \beta_s \csc\xi), \\ &\beta = \beta_s \cos|\boldsymbol{\phi}| + \sin|\boldsymbol{\phi}|(\alpha_s \csc\xi + \beta_s \cot\xi). \end{aligned} \tag{37}$$

Comparing (37) with (32) allows us to solve for $\tan|\boldsymbol{\phi}|$, which turns out to equal the combination Φ[(18a), (31a)]:

$$\tan|\boldsymbol{\phi}| = -\Phi \Rightarrow \boldsymbol{\phi} = -\boldsymbol{\theta}/2. \tag{38}$$

The net boost vector $\mathbf{V}_d$ is therefore obtained from the standard net boost vector $\mathbf{V}_s$ by rotating through one-half the rotation correction angle $\boldsymbol{\theta}$. With this result, we can write the net effect of two consecutive Lorentz boosts as follows [remember that $\mathbb{R}^{-1}(\boldsymbol{\theta}) = \mathbb{R}(-\boldsymbol{\theta})$]:

$$\begin{aligned} \mathbb{L}(\mathbf{b}) \vee \mathbb{L}(\mathbf{a}) &= \mathbb{R}(\boldsymbol{\theta}) \vee \mathbb{L}(\mathbf{d}) \\ &= \mathbb{R}(\boldsymbol{\theta}) \vee \mathbb{L}[\mathbb{R}(-\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbf{s} \vee \mathbb{R}(\tfrac{1}{2}\boldsymbol{\theta})]. \end{aligned} \tag{39}$$

Now apply theorem (5.1) or Ref. 19 and use Lemma (3.4) from Ref. 7 to write (39) in terms of the boost vector $\mathbf{s}$:

$$\begin{aligned} \mathbb{L}(\mathbf{b}) \vee \mathbb{L}(\mathbf{a}) &= \mathbb{R}(\boldsymbol{\theta}) \vee \mathbb{R}(-\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbb{L}(\mathbf{s}) \vee \mathbb{R}(\tfrac{1}{2}\boldsymbol{\theta}) \\ &= \mathbb{R}(\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbb{L}(\mathbf{s}) \vee \mathbb{R}(\tfrac{1}{2}\boldsymbol{\theta}). \end{aligned} \tag{40}$$

This is our final result. Equations (39) and (40) express the decomposition of two consecutive Lorentz boosts into a net boost and a spatial rotation. To the best of our knowledge, this exact decomposition does not appear elsewhere in the literature. We discuss the physical consequences of this result in the following section.

VI. SUMMARY AND DISCUSSION

In this section we review the usual arguments concerning the composition of two boosts and relate them to the results of the previous sections. The standard net velocity $\mathbf{V}_s$ is obtained by Lorentz transforming the velocity vector $\mathbf{V}_b$ back into the frame of $\mathbf{a}$. Use the four-velocities u_b and u_s to perform the transformation in the usual manner:

$$\begin{aligned} &u_b = \gamma_b(\mathbf{V}_b + \sigma^4), \quad u_s = \gamma_s(\mathbf{V}_s + \sigma^4), \\ &u_s = \mathbb{L}^{-1}(\mathbf{a}) \vee u_b \vee \mathbb{L}(\mathbf{a}) \\ &\Rightarrow \begin{cases} \gamma_s = \gamma_a\gamma_b(1 + (\mathbf{V}_a \cdot \mathbf{V}_b)), \\ \mathbf{V}_s = \dfrac{\mathbf{V}_a + (1/\gamma_a)\mathbf{V}_b + (1 - 1/\gamma_a)(\mathbf{V}_b \cdot \hat{\mathbf{V}}_a)\hat{\mathbf{V}}_a}{1 + (\mathbf{V}_a \cdot \mathbf{V}_b)}. \end{cases} \end{aligned} \tag{41}$$

If we are boosting a tensor type A first from the rest frame to the $\mathbf{a}$ frame, and then from the $\mathbf{a}$ frame to the $\mathbf{b}$ frame, it is tempting to assume that this is equivalent to a direct boost from rest to the $\mathbf{s}$ frame, where $\mathbf{s}$ is the boost corresponding to the combination of the two frame velocities (41). Even though some authors caution that the transformation of a velocity is not the same as the composition of boosts, this point is not always emphasized. It is, therefore, very easy to be led to the false conclusion that $\mathbb{L}(\mathbf{b}) \vee \mathbb{L}(\mathbf{a})$ is equal to $\mathbb{L}(\mathbf{s})$. The actual result of combining $\mathbb{L}(\mathbf{a})$ and $\mathbb{L}(\mathbf{b})$ involves the rotation correction in an intrinsic manner. In the above sections, we have shown that the following decompositions are unique:

$$\mathbb{L}(\mathbf{b}) \vee \mathbb{L}(\mathbf{a}) = \mathbb{R}(\boldsymbol{\theta}) \vee \mathbb{L}(\mathbf{d}) = \mathbb{R}(\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbb{L}(\mathbf{s}) \vee \mathbb{R}(\tfrac{1}{2}\boldsymbol{\theta}), \tag{42a}$$

$$\boldsymbol{\theta} = [(\mathbf{V}_a \times \mathbf{V}_b)/|\mathbf{V}_a \times \mathbf{V}_b|]\, 2 \arctan\Phi, \tag{42b}$$

$$\begin{aligned} \Phi &= \frac{\gamma_a\gamma_b|\mathbf{V}_a \times \mathbf{V}_b|}{1 + \gamma_a + \gamma_b + \gamma_a\gamma_b(1 + (\mathbf{V}_a \cdot \mathbf{V}_b))} \\ &= \frac{\gamma_a\gamma_b|\mathbf{V}_a \times \mathbf{V}_b|}{1 + \gamma_a + \gamma_b + \gamma_s}, \end{aligned} \tag{42c}$$

where $\mathbf{s}$ is given by (35) and (41), $\mathbf{d}$ by (23), (24), (29a), and (32), and $|\mathbf{V}_s| = |\mathbf{V}_d|$ by (23).

We wish to see what a general tensor type A looks like after it has been boosted first by $\mathbf{a}$, and then by $\mathbf{b}$. Or, rather, what the result of the two successive boosts A' looks like in

the original laboratory frame. We have the relations

$$A' = \mathbb{L}(\mathbf{b}) \vee \mathbb{L}(\mathbf{a}) \vee A \vee \mathbb{L}^{-1}(\mathbf{a}) \vee \mathbb{L}^{-1}(\mathbf{b}), \tag{43a}$$

$$A = \mathbb{L}^{-1}(\mathbf{a}) \vee \mathbb{L}^{-1}(\mathbf{b}) \vee A' \vee \mathbb{L}(\mathbf{b}) \vee \mathbb{L}(\mathbf{a}). \tag{43b}$$

Using the result (42a) with $\mathbb{L}^{-1}(\mathbf{a}) = \mathbb{L}(-\mathbf{a})$ in (43) gives a transformation as our final result for the decomposition of the product of two boosts:

$$A' = \mathbf{R}(\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbb{L}(\mathbf{s}) \vee \mathbf{R}(\tfrac{1}{2}\boldsymbol{\theta}) \vee A \vee \mathbf{R}(-\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbb{L}^{-1}(\mathbf{s}) \vee \mathbf{R}(-\tfrac{1}{2}\boldsymbol{\theta}), \tag{44a}$$

$$A = \mathbf{R}^{-1}(\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbb{L}(-\mathbf{s}) \vee \mathbf{R}^{-1}(\tfrac{1}{2}\boldsymbol{\theta}) \vee A' \vee \mathbf{R}(\tfrac{1}{2}\boldsymbol{\theta}) \vee \mathbb{L}^{-1}(-\mathbf{s}) \vee \mathbf{R}(\tfrac{1}{2}\boldsymbol{\theta}). \tag{44b}$$

The physical picture is the following. The net effect of two consecutive nonparallel boosts is equivalent to rotating around $\mathbf{a}\times\mathbf{b}$ by one-half the correction angle (42b) then boosting by the standard combination of velocities (41), and then rotating once more by one-half the correction angle in the same sense. The total net rotation is through the entire correction angle. Alternatively, one can perform a boost accompanied by a single rotation in one step, but in that case, one cannot use the standard velocity combination (41), but must use the boost vector $\mathbf{d}$ and the velocity $\mathbf{V}_d$ derived in the preceding section.

There is considerable confusion as to the precise description of the combination of two boosts. To the best of our knowledge, the literature does not explicitly resolve this problem, but, as shown above, the result follows directly from the Lorentz group. This analysis suggests that it is misleading to speak of "addition" of nonparallel velocities, since one cannot "add" nonparallel velocities without generating a spatial rotation as well.

VII. CONCLUSION

In this paper we have discussed two components of the product of nonparallel Lorentz boosts. First, we calculated the exact spatial rotation correction to the product of two boosts. This effect is responsible for the well-known Thomas precession in the infinitesimal case. The finite result is not widely known, even though it is given in Refs. 4 and 9.

Second, the net Lorentz boost, which results from two consecutive boosts, was calculated exactly. The magnitude of the net boost vector is a standard result. The direction of the net boost vector is, however, a problem. We obtained a result that differs entirely from that obtainable by the standard methods. The direction of the net boost vector, or equivalently, the net frame velocity, is the usual result rotated through one-half the finite correction angle calculated previously. The reason for this discrepancy is that the usual method cannot account for the finite rotation correction to the product of two boosts.

Note added in proof: The exact finite rotation angle [Eq. (18)] is also derived in Ref. 21, Eqs. (13) and (28). Professor Ben-Menahem calls this the "Wigner angle."

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Forces and the existence of stresses in invariant continuum mechanics

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In an invariant formulation of pth-grade continuum mechanics, forces are defined as elements of the cotangent bundle of the Banach manifold of C^p embeddings of the body in space. It is shown that forces can be represented by measures which generalize the stresses of continuum mechanics. The mathematical representation procedure makes the restriction of forces to subbodies possible. The local properties of the stress measures are examined. For the case where stresses are given in terms of smooth densities, it is shown that the structure of forces agrees with the form of forces one assumes in the traditional formulation, and the equilibrium differential equations are obtained.

I. INTRODUCTION

It is well known that the laws of continuum mechanics, the mechanics of deformable bodies, cannot be deduced from the laws of mechanics of material points and rigid bodies. Additional assumptions are introduced and new notions such as internal forces, external forces, stresses, and the equilibrium equation emerge.

The geometric framework in which the classical theory of continuum mechanics is developed is the three-dimensional Euclidean space. The following paragraphs review the basic structure of the theory.

The first basic assumption made in continuum mechanics regarding the nature of forces is that the total force acting on a body B is of the form

$$f = \int_B b\, dv + \int_{\partial B} t\, da, \tag{1}$$

where b is a continuous vector field, called the body force, defined in the body, and t is a continuous vector field, called the surface force, defined on the boundary of the body. The basic problem of continuum mechanics is encountered when we try to restrict a given force on B to a subbody. Considering a subbody P of the body B, the total force f_P acting on it should also be given in terms of a body force and a surface force as in Eq. (1). In general, the fields b and t associated with the subbody P are different from those given on B. In particular, physical experience shows that even if P is disjoint from the boundary of B, a surface force acts on the boundary of P. This newly emerged surface force is traditionally termed internal force or traction as it may be interpreted as the force that is applied on P by its complement in the body. Thus, the values of b and t at a point $X \in P$ will depend in general on the subbody P under consideration and we write

$$b = b(X,P), \quad t = t(X,P).$$

The next assumption, called Cauchy's postulate, deals with the dependence of b and t on P. It states that b does not depend on P so that $b = b(X)$, and that the surface force depends on P only through the unit vector n perpendicular to the boundary of P at X, i.e., $t = t(X,n)$. Clearly, this last hypothesis does not provide all the necessary information needed in order to determine t.

Assuming that the total force on each subbody of the body B vanishes, it is possible to prove the following results.

There exists a tensor field σ in the body such that

$$t(X,n) = \sigma(X)(n(X)). \tag{2}$$

The tensor field σ is the stress field, and it has to satisfy the differential equation

$$\operatorname{div}\sigma + b = 0 \quad \text{in } B. \tag{3}$$

If we assume in addition that the total moment on each subbody of B vanishes, we find that σ is symmetric.

From Eqs. (1) and (2) it is clear that if σ is given, one can associate a unique body force field and a unique surface force field with each subbody. However, the differential equation (3), known as the equlibrium equation, and the boundary condition (2) cannot determine the stress uniquely for given b and t on B. This lack of uniqueness in the determination of the stress field means that the force on a body cannot be restricted to subbodies in a unique fashion. In order to determine the stress field, constitutive relations are introduced. The constitutive relations, obtained by physical experiments, relate the stress with the configuration of the body and supply all the necessary information so that the stress can be determined uniquely. Clearly, using Eq. (2), σ can be determined uniquely if t is given for every subbody P of B.

Modern attempts to axiomatize the theory of forces and stresses can be found in Gurtin and Williams,[1] Gurtin and Martins,[2] and Truesdell.[3] The authors postulate a system of axioms describing the properties of forces in general. In addition, they assume equilibrium and they assume that external forces are composed of body forces that are absolutely continuous with respect to the volume measure, and surface forces that are absolutely continuous with respect to the surface area of the body. With these assumptions the authors prove that forces are given in the form of Eq. (1) and that Cauchy's postulate holds. Marsden and Hughes[4] have generalized the theory to Riemannian manifolds using an invariance principle for an assumed form of a balance of energy where they assume the transformation rules for the various variables including b and t.

During the 1960's, in an attempt to formulate theories that would account for interactions that are more complicated than those afforded by the classical theory, the theories of couple stresses and the theories of materials of grade $p > 1$

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were developed. A historical account of the subject together with a review of the various approaches can be found in Truesdell and Noll[5] (pp. 389–401). For a variety of applications one can consult Mindlin[6] and references cited therein. Unlike Cauchy's theory, the theories of materials of grade p are based on energy principles in which the potential energy density is assumed to depend on derivatives of order p of the deformation.

In this paper we propose a theory of forces and stresses based on the principle that forces should be defined as elements of the cotangent bundle T^*Q of and appropriate configuration manifold Q. Specifically, we show that pth-order continuum mechanics corresponds to the case where the configuration space is the set of all p-times differentiable embeddings of the body in space equipped with the C^p topology. It turns out that in this case forces can be represented by measures on the pth jet bundle over the body where the representing measures generalize the stresses. For example, it follows that in first-order continuum mechanics and the case of three-dimensional Euclidean geometry [where the first jet bundle can be identified with $B \times R^3 \oplus L(R^3, R^3)$] any force can be represented in the form

$$f(u) = \int_B u^i \, d\mu_i + \int_B u^i_{,j} \, d\mu^j{}_i ,$$

where μ_i, and $\mu^j{}_i$ are the components of a measure over B valued in $R^3 \oplus L(R^3, R^3)$. The first three components vanish if a Euclidean symmetry requirement is imposed and the $\mu^j{}_i$ correspond to the stress. If these measures are differentiable with respect to the volume measure, their densities are the components of the stress field. In the more general case where a connection is specified on the space manifold, any force can be represented in the form

$$f(u) = \sum_{k=0}^{p} \int_B \nabla^k u \, d\sigma_k,$$

where ∇^k is the k th covariant derivative and the $\{\sigma_k\}$ are the representing measures.

The resulting structure has the following features.

(a) The theory applies in the general geometry of differentiable manifolds.

(b) The definition of a force extends the definition given in the case of finite-dimensional classical mechanics by Arnold[7] and Tulczyjew[8] to the infinite-dimensional case. Thus, it clarifies the point of departure of continuum mechanics from analytical mechanics.

(c) Some assumptions made in the classical construction, such as the form (1) of the forces on bodies, are obtained mathematically as results of the definition of forces.

(d) The theory links the properties of forces and stresses with the axiom of impenetrability.

(e) The theory allows stresses which are as irregular as measures, while the classical theory deals with continuous stresses only.

(f) The theories of materials of grade p are generalized to differentiable manifolds. The suggested formulation is free of any energy considerations and the relation between the theory of materials of grade one and materials of a higher grade is clear and simple. The grade of a material is a consequence of the choice of a topology on the set of configurations.

(g) A generalized form of the equilibrium equation is obtained as a result of the mathematical procedure, and the origin of the nonuniqueness in the relation between stresses and forces is explained.

(h) A simple constitutive theory is suggested in which body self-determinism and continuity imply jet locality.

II. THE BASIC STRUCTURE

Definition 2.1: A *body* is a compact differentiable manifold with corners. A typical body will be denoted by B and its dimension will be denoted by m.

Definition 2.2: The *physical space* is a differentiable manifold S without a boundary.

Definition 2.3: A *configuration of class p* is a C^p embedding of a body B in the physical space for $p \geqslant 1$.

The requirement that a configuration of a body into space is an embedding is a result of two traditional principles: the principle of impenetrability stating that one portion of the matter never penetrates within another, and the principle of permanence of matter stating that no region of positive finite volume is deformed into one of zero or infinite volume (cf. Truesdell and Toupin,[9] pp. 234–244).

For a fixed body B and a given p, the *configuration space* Q is the set of all configurations of class p of the body in space.

We recall[10–13] that the set $C^p(B,S)$ of C^p mappings of B into S can be given the structure of a Banach manifold. For any $\kappa \in C^p(B,S)$, the tangent space $TC^p(B,S)_\kappa$ can be identified with $C^p(\kappa^*\tau_S)$, the Banachable space of C^p sections of the pullback of the tangent bundle τ_S by κ. The Banach space topology of $C^p(\kappa^*\tau_S)$ is given as follows. Let $v: K \to R^n$ be a C^p mapping defined on a compact set K. We use the notation

$$\|v\|_p = \max_j \sup_{x \in K} \{|D^j v(x)|\}, \quad 0 \leqslant j \leqslant p.$$

Clearly, $\| \ \|_p$ is a norm for the space of all such C^p mappings.

Now, let $B_1,\ldots,B_r$ be a covering of B by compact submanifolds of the same dimension as B such that each B_i is contained in the domain of a vector bundle chart ψ_i of $\kappa^*\tau_S$. Then for $u \in C^p(\kappa^*\tau_S)$ define

$$\|u\| = \max_i \|\underline{u}_i\|, \quad i = 1,\ldots,r,$$

where $\underline{u}_i$ is the local representative of u in the chart ψ_i. Again, $\| \ \|$ is a norm on $C^p(\kappa^*\tau_S)$ and any other norm induced by another covering will induce an equivalent topology on $C^p(\kappa^*\tau_S)$.

The tangent space $TC^p(B,S)_\kappa$ can also be identified with the vector space of vector fields along κ, i.e., $\{u \in C^p(B,TS); \ \tau_S \circ u = \kappa\}$.

In addition, we recall that since $p \geqslant 1$, the set of C^p embeddings is an open subset[14] of $C^p(B,S)$. Hence, Q is a Banach manifold and we have

$$TQ_\kappa \cong C^p(\kappa^*\tau_S) \cong \{u \in C^p(B,TS);\quad \tau_S \circ u = \kappa\}.$$

An element of TQ is a *virtual displacement*, a term motivated by the second interpretation we gave of TQ_κ.

Definition 2.4: A *force* (*of grade* p) is an element of the cotangent bundle T^*Q.

Let $f \in T^*Q_\kappa$ and $u \in TQ_\kappa$ for some configuration κ. The evaluation $f(u)$ is traditionally called the *virtual work* performed by the force f on the virtual displacment u.

The basic structure, as defined in this section, has been given for the finite-dimensional configuration space by Arnold[7] and Tulczyjew.[8] In the infinite-dimensional case considered here, the specification of the class of admissible configurations and the topology chosen will determine the nature of forces. It is our aim to study the consequences of these choices and to show that the basic properties of forces and stresses in continuum mechanics can be obtained naturally in the suggested framework.

III. THE REPRESENTATION OF FORCES BY STRESSES AND THE PRINCIPLE OF VIRTUAL WORK

Given $\kappa \in Q$, the identification of TQ_κ with $C^p(\kappa^*\tau_S)$ allows us to identify the forces in T^*Q_κ with section distributions in $C^p(\kappa^*\tau_S)^*$. Thus, the problem of restriction of forces from a given body to its subbodies means mathematically that we have to study the restrictions of C^p section distributions.

Consider the jet extension mapping

$$j_p:\quad C^p(\kappa^*\tau_S) \to C^0(J^p(\kappa^*\tau_S)).$$

We note that j_p is linear, injective and if we use natural charts on both $\kappa^*\tau_S$ and $J^p(\kappa^*\tau_S)$ and norms induced on $C^p(\kappa^*\tau_S)$ and $C^0(J^p(\kappa^*\tau_S))$ by these charts, we observe that j_p is also norm preserving. It follows that every force in $C^p(\kappa^*\tau_S)^*$ is of the form $j_p^*(\sigma)$ for some $\sigma \in C^0(J^p(\kappa^*\tau_S))^*$, where

$$j_p^*:\quad C^0(J^p(\kappa^*\tau_S))^* \to C^p(\kappa^*\tau_S)^*$$

is the adjoint of the jet extension mapping. The elements of $C^0(J^p(\kappa^*\tau_S))^*$ are called *stresses*. Hence, if $f = j_p^*(\sigma)$, we have $f(u) = \sigma(j_p(u))$ for every virtual displacement u and we say that the stress σ represents the force f. This is a generalization of the principle of virtual work in continuum mechanics which states that the virtual work performed by the force on a virtual displacment is equal to the virtual work performed by the stress on the derivative of the virtual displacement.

IV. LOCAL PROPERTIES OF STRESSES

By their definition, forces are special types of section distributions or currents (Choquet-Bruhat *et al.*[15] pp. 400–406, DeRham,[16] Schwartz[17]) and stresses that belong to a simpler class of distributions (measures) represent them. In this section we consider the local properties of stresses.

Let $B_1,\ldots,B_r$ be compact submanifolds of B of the same dimension as B whose interiors cover B and let $\phi_1,\ldots,\phi_r$ be a C^∞ partition of unity such that supp $\phi_i \subset$ interior B_i. It can be shown that if π is a vector bundle over B, then

$$\tilde{C}^0(\pi) = \Big\{(w_1,\ldots,w_r) \in \overset{r}{\underset{i=1}{\oplus}} C^0(\pi|B_i);\quad w_i|B_i \cap B_j = w_j|B_i \cap B_j\Big\}$$

is isomorphic to $C^0(\pi)$. The isomorphism is given by $w \mapsto (w|B_1,\ldots,w|B_r)$ and its inverse given by $(w_1,\ldots w_r) \mapsto \Sigma_i \tilde{w}_i$, where $\tilde{w}_i \in C^0(\pi)$ is given by $\tilde{w}_i|B_i = \phi_i w_i$ and $\tilde{w}_i = 0$ outside B_i (for a complete proof see Palais,[10] pp. 10 and 11).

Given vector bundle charts

$$\Psi_i: \pi|B_i \to K \times R^N,\quad K \subset R^m$$

(assuming that B is m-dimensional and that the fiber of π is N-dimensional) and denoting by ψ_i the first component of Ψ_i, $C^0(\pi|B_i)$ can be identified with $C^0(\psi_i(B_i))^N$, the space of N-tuples of continuous real valued functions on $\psi_i(B_i)$ for each i. Thus, $C^0(\pi)$ is isomorphic with[10]

$$\Big\{(\underset{\sim}{w}_1,\ldots,\underset{\sim}{w}_r) \in \overset{r}{\underset{i=1}{\oplus}} C^0(\psi_i(B_i))^N;\quad \Psi_i^{-1} \circ \underset{\sim}{w}_i \circ \psi_i = \Psi_j^{-1} \circ \underset{\sim}{w}_j \circ \psi_j \text{ on } B_i \cap B_j\Big\}$$

via $w \mapsto (\underset{\sim}{w}_1,\ldots,\underset{\sim}{w}_r)$, where $\underset{\sim}{w}_i = \Psi_i \circ w|B_i \circ \psi_i^{-1}$, and the inverse is given by $w = \Sigma_i \tilde{w}_i$, where $\tilde{w}_i \in C^0(\pi)$ are given by $\tilde{w}_i|B_i = \phi_i(\Psi_i^{-1} \circ \underset{\sim}{w}_i \circ \psi_i)$ and $\tilde{w}_i = 0$ outside B_i.

We conclude, therefore, that given a partition of unity, a vector bundle atlas, and $\mu \in C^0(\pi)^*$, there exists a collection $\{\underset{\sim}{\mu}_i\}$, $i = 1,\ldots,r$, $\underset{\sim}{\mu}_i \in C^0(\psi_i(B_i))^{N*}$, such that

$$\mu(w) = \sum_{i=1}^{r} \underset{\sim}{\mu}_i(\Psi_i \circ w|B_i \circ \psi_i^{-1}).$$

Identifying $C^0(\psi_i(B_i))^{N*}$ with $C^0(\psi_i(B_i))^{*N}$ and observing that $C^0(\psi_i(B_i))^*$ is the space of Radon measures on $\psi_i(B_i)$, we conclude that each $\underset{\sim}{\mu}_i$ is a collection of N measures on $\psi_i(B_i)$.

Let $\{U_\alpha, \Psi_\alpha, \psi_\alpha\}$ be a vector bundle atlas of π, and let $C_c^0(\psi_\alpha(U_\alpha))$ denote the Banach space of continuous functions with compact support in $\psi_\alpha(U_\alpha)$ equipped with the usual topology so that $C_c^0(\psi_\alpha(U_\alpha))^*$ is the space of Radon measures on $\psi_\alpha(U_\alpha)$. Assume that for each α there is a given $\underset{\sim}{\mu}_\alpha \in C_c^0(\psi_\alpha(U_\alpha))^{*N}$, such that for each pair of indices, $\underset{\sim}{\mu}_\alpha(\Psi_\alpha \circ w \circ \psi_\alpha^{-1}) = \underset{\sim}{\mu}_\beta(\Psi_\beta \circ w \circ \psi_\beta^{-1})$, for each $w \in C^0(\pi)$ whose support is contained in $U_\alpha \cap U_\beta$. We now define $\mu \in C^0(\pi)^*$ by

$$\mu(w) = \sum_i \underset{\sim}{\mu}_i(\Psi_i \circ \phi_i w \circ \psi_i^{-1}),\quad w \in C^0(\pi),$$

where $\{\phi_i\}$ is a finite partition of unity such that supp $\phi_i \subset U_\alpha$. It can be shown that μ is independent of the partition of unity so that any collection of local measures that satisfies the transformation rule define an element of $C^0(\pi)^*$.

Having reviewed the local properties of elements of $C^0(\pi)^*$, we extend them to a wider class of sections, the integrable sections. We say that a function $\underset{\sim}{u}_i:\ \psi_i(U_i) \to R^N$ is integrable with respect to the collection of measures $\{\underset{\sim}{\mu}_{ik}\}$, $k = 1,\ldots,N$, if each component is integrable with respect to all the $\underset{\sim}{\mu}_{ik}$, i.e., if

$$\|\underset{\sim}{u}_i\|_{L^1} = \sup_{j,k} \int_{\psi_i(U_i)} |\underset{\sim}{u}_{ij}|\, d\,|\underset{\sim}{\mu}_{ik}| < \infty.$$

It can be shown that for a section u of π with support in $U_i \cap U_j$ and measures $\underset{\sim}{\mu}_i$ and $\underset{\sim}{\mu}_j$ on $\psi_i(U_i)$ and $\psi_j(U_j)$, respectively, satisfying the compatibility condition given above, $\Psi_i \circ u \circ \psi_i^{-1}$ is $\underset{\sim}{\mu}_i$ integrable if and only if $\Psi_j \circ u \circ \psi_j^{-1}$ is $\underset{\sim}{\mu}_j$ integrable. Thus, we say that a section of π is integrable with respect to $\mu \in C^0(\pi)^*$ if its local representatives are integrable with respect to the local representatives of $\underset{\sim}{\mu}_i$ of μ.

Let χ_T be the characteristic function of a subset T of B. If $T \cap U_i$ is $\underset{\sim}{\mu}_i$ measurable, $\chi_{T\cap U_i}$ is integrable with respect to each of the $\underset{\sim}{\mu}_{ik}$, $k = 1,...,N$, and we can restrict $\underset{\sim}{\mu}_i$ to $T \cap U_i$ by $\underset{\sim}{\mu}_i | T \cap U_i = \chi_{T\cap U_i} \underset{\sim}{\mu}_i$. In case the family $\{\underset{\sim}{\mu}_i\}$ satisfies the compatibility condition on the intersections of domains of charts so that it contains local representatives of some $\mu \in C^0(\pi)^*$, the same holds for the collection $\{\underset{\sim}{\mu}_i | T \cap U_i\}$ which will represent $\mu | T = \chi_T \mu$, the restriction of μ to T. In particular, if P is a subbody of B, i.e., a compact m-dimensional submanifold of B, μ can be restricted to P.

Applying the foregoing results to the case where π is the vector bundle $J^p(\kappa^*(\tau_S))$, we conclude that a stress is represented locally by a collection of N Radon measures that transform according to the rule given above, where N is the dimension of the fiber of $J^p(\kappa^*(\tau_S))$. Conversely, any such collection of measures satisfying the transformation rule represents a stress.

We denote the evaluation of the stress measure $\sigma \in C^0(J^p(\kappa^*\tau_S))^*$ on a section w by $\int_B w\, d\sigma$, and for a subbody P, we denote the evaluation of $\sigma | P$ on a section u of $J^p((\kappa|P)^*(\tau_S))$ by $\int_P u\, d\sigma$.

V. THE CASE OF A CONNECTION

We now assume that connections are specified both on the vector bundle τ_S: $TS \to S$ and the vector bundle τ_B: $TB \to B$. The connection on τ_S induces a connection on $\kappa^*\tau_B$ and we recall that given a connection on both τ_B and $\kappa^*\tau_B$ we have an induced connection on the vector bundle of p-multilinear mappings $L^p(\tau_B, \kappa^*\tau_S)$: $L^p(TB, \kappa^*TS) \to B$, such that we have covariant derivatives

$$\nabla^i u \in C^{p-i}(L^i(\tau_B, \kappa^*\tau_S)), \quad 0 \leqslant i \leqslant p,$$

for $u \in C^p(\kappa^*\tau_S)$ (see Eliasson[11] for details).

Consider the mapping

$$\underset{\sim}{\nabla}^p : C^p(\kappa^*\tau_S) \to C^0\Big(\bigoplus_{i=0}^{p} L^i(\tau_B, \kappa^*\tau_S)\Big)$$

given by

$$u \mapsto (u, \nabla u, ..., \nabla^p u).$$

Again, this is a linear continuous injection with a closed image, and since

$$C^0\Big(\bigoplus_{i=0}^{p} L^i(\tau_B, \kappa^*\tau_S)\Big)^* = \Big(\bigoplus_{i=0}^{p} C^0(L^i(\tau_B, \kappa^*\tau_S))\Big)^* = \bigoplus_{i=0}^{p} C^0(L^i(\tau_B, \kappa^*\tau_S))^*,$$

we have a representation of forces by collections of tensor measures $(\sigma_0, \sigma_1, ..., \sigma_p)$, $\sigma_i \in C^0(L^i(\tau_B, \kappa^*\tau_S))^*$, in the form

$$f(u) = \sum_{i=0}^{p} \int_B \nabla^i u\, d\sigma_i.$$

Thus, in case connections are specified on τ_B and τ_S, forces can be represented by tensor valued measures. We note that the case $p = 1$ corresponds to classical continuum mechanics, where σ_1 is the tensor measure which corresponds to the stress tensor. In this case we do not need the connection on τ_B, as it is not required for the first covariant derivative.

VI. THE RELATION TO PREVIOUS WORKS

In this section we review some ideas suggested in previous works,[18–20] and relate them to the formulation given here.

In Refs. 19 and 20 it was suggested that vector bundles over B and S can serve as mathematical models for the local properties of both body and space so that the vector space attached to each point represents mathematically the neighborhood of this point. A local configuration was defined as a vector bundle morphism between the two vector bundles. The local configuration space, local virtual displacements, and local forces were defined for this new model, termed the *local model*, in analogy with the previous set of definitions which will be referred to henceforth as the *global model*. The local configuration space is the Banach manifold of all local configurations, local virtual displacements are elements of the tangent bundle, and local forces are elements of the cotangent bundle of the local configuration space. It was shown that local forces generalize the stresses of continuum mechanics, and the principle of virtual work was obtained as a result of a requirement for compatibility between these two models. The particular case where τ_B and τ_S represented the body and space in the local model was studied. In this case the local configuration space is the collection of vector bundle morphisms $\tau_B \to \tau_S$ which can be identified with the collection of sections of the jet bundle $\pi^1: J^1(B, S) \to B$.

Using the language of jet bundles and the properties of manifolds of sections of jet bundles,[10] the following obvious generalization can be made. A *local configuration of order p* is a continuous section of $\pi^p: J^p(B, S) \to B$. The *local configuration space* is the manifold of sections $C^0(\pi^p)$. A *local virtual displacement* is an element of the tangent bundle $TC^0(\pi^p)$, and a *local force* σ is an element of the cotangent bundle $T^*C^0(\pi^p)$.

Since both the global model and the local model represent the same physical phenomenon they are related by *compatibility conditions* in the following way.

Consider the jet extension mapping

$$j_p: \quad C^p(\pi^0) \to C^0(\pi^p).$$

We say that *a local configuration* $\chi \in C^0(\pi^p)$ *is compatible with a global configuration* $\kappa \in C^p(\pi^0)$ if $\chi = j_p(\kappa)$. *A local virtual displacement* $w \in TC^0(\pi^p)$ *is compatible with a global virtual displacement* $u \in TC^p(\pi^0)$ if $w = T(j_p)(u)$. We say that *a global force* $f \in T^*C^p(\pi^0)$ *is compatible with the local force* $\sigma \in T^*C^0(\pi^p)|_{\text{image } j_p}$ if $f = T^*(j_p)(\sigma)$. These definitions can be summarized by saying that the two models are related by the jet functor J^P.

The relation between the formulation given in this section and the rest of this paper is established in the following proposition.

Proposition 6.1: (i) For any global configuration, κ, $T^*C^0(\pi^p)_{j_p(\kappa)}$, the space of local forces at the local configuration compatible with κ, can be identified with the space of stresses representing forces at κ.

(ii) A global force f is compatible with a local force σ if and only if the stress that can be identified with σ by (i) represents f.

Proof: The proof of the proposition becomes obvious once the following results of Palais[10] on sections of jet bundles are used.

(a) Given $\kappa \in C^p(\pi^0)$, there is a natural isomorphism

$$TC^0(\pi^p)_{j_p(\kappa)} \cong C^0(J^p(\kappa^* \tau_S)).$$

(b) For $\kappa \in C^p(\pi^0)$, the tangent to the jet extension mapping

$$T(j_p)_\kappa : TC^p(\pi^0)_\kappa \to TC^0(\pi^p)_{j_p(\kappa)}$$

is given by $u \mapsto j_p(u)$, where $u \in C^p(\kappa^* \tau_S) \cong TC^p(\pi^0)_\kappa$ and the identification of (i) is used.

The assertions follow immediately.

VII. FORCE SYSTEMS

The representation of forces by stress measures provides an answer to the basic problem of restriction of forces to subbodies. Given a stress measure σ, a unique force f_P is induced on every subbody P by

$$f_P(u) = \int_P j_p(u)\, d\sigma, \quad u \in C^p((\kappa|P)^* \tau_S),$$

or in other words, the force on P is represented by the restriction of the stress measure to P.

We will use the term *force system* for a set function assigning a force $f_P \in C^p((\kappa|P)^* \tau_S)^*$ to every subbody P of B. We will say that a force system is *consistent* if there exists a stress representation σ such that the force given on any subbody P is represented by the restriction of σ to P.

Since the jet extension map is not surjective we cannot expect that the representation of forces by stresses will be unique. This feature is well known in continuum mechanics and it is referred to as static indeterminacy. It is the static indeterminacy which forces the use of material properties or constitutive relations in order to be able to restrict forces to subbodies. However, as the next proposition shows, a force system can be consistent with at most one stress, i.e., if we know the force acting on each subbody we can determine the stress uniquely. This statement is a generalization of the principle in continuum mechanics according to which the stress at a point can be determined uniquely if the traction across every surface is given. In the classical case however, the result is stated for the case $p = 1$ only, and the stress tensor measure is given in terms of a tensor field whose value at a given point we want to determine.

Proposition 7.1: If a force system is consistent with the stresses σ_1 and σ_2 then, $\sigma_1 = \sigma_2$.

Proof: In order to show that $\sigma_1 = \sigma_2$, it suffices to show that their local representatives in any given chart are equal. Let A be a subbody contained in the domain of a chart in B. For any subbody P of A, let f_P be the force acting on P in the given force system which is consistent with both σ_1 and σ_2. We denote by u^i the components of the local representative of $u \in C^p((\kappa|P)^* \tau_S)$ and for the multi-index $\alpha = (\alpha_1,...,\alpha_m)$, we recall that the local representative of $j_p(u)$ is $\{D^\alpha u^i\}$, $|\alpha| = \alpha_1 + \cdots + \alpha_m \leqslant p$. Let $\mu_{i\alpha}$ and $\nu_{i\alpha}$ be the measures on $\underset{\sim}{P}$—the image of P under the chart—that represent σ_1 and σ_2, respectively. By the representation of forces by stresses we have

$$f_P(u) = \int_{\underset{\sim}{P}} \sum_{|\alpha|=0}^{p} D^\alpha u^i \, d\mu_{i\alpha} = \int_{\underset{\sim}{P}} \sum_{|\alpha|=0}^{p} D^\alpha u^i \, d\nu_{i\alpha}$$

for every $u \in C^p((\kappa|P)^* \tau_S)$ and every subbody P.

In particular, for $j \in \{1,...,n\}$, where n is the dimension of S, let u satisfy $u^i = \delta^{ij}$. By the equation above we have

$$\mu_{j\alpha}(\underset{\sim}{P}) = \nu_{j\alpha}(\underset{\sim}{P}), \quad |\alpha| = 0,$$

for every subbody P of A. Since the two measures agree on every subbody we have $\mu_{j\alpha} = \nu_{j\alpha}, |\alpha| = 0$.

Now, given j, β, with $|\beta| = 1$, let u satisfy $u^i = \delta^{ij} x^\beta$, where (x^k) are the local coordinates in the given chart. We have

$$\int_{\underset{\sim}{P}} \sum_{|\alpha|\leqslant 1} D^\alpha u^i \, d\mu_{i\alpha} = \int_{\underset{\sim}{P}} \sum_{|\alpha|\leqslant 1} D^\alpha u^i \, d\nu_{i\alpha}$$

as the higher-order derivatives vanish. Since $\mu_{i\alpha} = \nu_{i\alpha}$ for $|\alpha| = 0$, and since $D^\alpha u^i \neq 0$ only for $i = j$, $\alpha = \beta$, we have $\mu_{j\beta}(\underset{\sim}{P}) = \nu_{j\beta}(\underset{\sim}{P})$, for every subbody P and arbitrary j, β, $|\beta| = 1$. We conclude that that $\mu_{i\alpha} = \nu_{i\alpha}$ for all i and α, with $|\alpha| = 1$.

We can continue the process evaluating the virtual work performed on the virtual displacements u such that $u^i = \delta^{ij} x^\alpha = \delta^{ij} (x^1)^{\alpha_1} (x^2)^{\alpha_2} \ldots (x^n)^{\alpha_n}$, with $|\alpha| = 2,3,...,p$ to obtain $\mu_{i\alpha} = \nu_{i\alpha}$ for all α with $|\alpha| \leqslant p$.

Proposition 7.2: Let a force system $\{f_P\}$ which is consistent with a stress σ, be given. Then, if A is a subbody contained in the domain of a chart on $\kappa^* \tau_S$ with coordinates (x^k, u^j), the local representatives $\mu_{i\alpha}$ of σ are given by the following inductive process.

Let $(\delta^{ij} x^\alpha)'$ be the section of $C^p((\kappa|A)^* \tau_S)$ whose local representatives satisfy $u^i = \delta^{ij} x^\alpha$ for given j and α. Then,

$$\mu_{j\alpha}(\underset{\sim}{P}) = f_P(\delta^{ij})', \quad |\alpha| = 0;$$

$$\mu_{j\alpha}(\underset{\sim}{P}) = \frac{1}{\alpha!} f_P(\delta^{ij} x^\alpha)' - \sum_{\beta < \alpha} \frac{1}{(\alpha - \beta)!} \int_{\underset{\sim}{P}} x^{\alpha - \beta} \, d\mu_{j\beta},$$

$$0 < |\alpha| \leqslant p,$$

where $\beta < \alpha$ means that $\beta_i \leqslant \alpha_i$ and $|\beta| < |\alpha|$.

Proof: By hypothesis

$$f_p(\delta^{ij} x^\alpha)' = \int_{\underset{\sim}{P}} \sum_{|\beta|\leqslant p} D^\beta (\delta^{ij} x^\alpha) \, d\mu_{i\beta}.$$

Since,

$$D^\beta x^\alpha = [\alpha!/(\alpha - \beta)!] x^{\alpha - \beta}$$

for $\beta < \alpha$, and $D^\beta x^\alpha = 0$, for $\alpha < \beta$, we have

$$f_P(\delta^{ij}x^\alpha)' = \delta^{ij}\alpha!\,\mu_{i\alpha}(\underset{\sim}{P}) + \sum_{\substack{\beta \neq \alpha \\ |\beta| < p}} \frac{\alpha!}{(\alpha-\beta)!} \int_{\underset{\sim}{P}} \delta^{ij} x^{\alpha-\beta}\, d\mu_{i\beta}$$

$$= \alpha!\,\mu_{j\alpha}(\underset{\sim}{P}) + \sum_{\beta < \alpha} \frac{\alpha!}{(\alpha-\beta)!} \int_{\underset{\sim}{P}} x^{\alpha-\beta}\, d\mu_{j\beta}.$$

The proposition suggests a procedure which enables one to determine whether a given force system is consistent with any stress, and to obtain the local representatives of this stress if it exists. Given any vector bundle atlas on $\kappa^*\tau_S$, one has to evaluate $f_P(\delta^{ij})'$ for all subbodies P contained in the domain of charts. Then, if for every chart, the set function $P \mapsto f_P(\delta^{ij})'$ for all subbodies contained in the domain of the chart can be extended to a measure on the domain of the chart, we can identify $\mu_{j\alpha}(\underset{\sim}{P})$, $|\alpha| = 0$, with $f_P(\delta^{ij})'$ for the various charts. We proceed by evaluating $f_P(\delta^{ij}x^\alpha)'$, $|\alpha| = 1$, and we use the relations of the last proposition and the previously obtained $\mu_{j\alpha}(\underset{\sim}{P})$, $|\alpha| = 0$, to obtain $\mu_{j\alpha}(\underset{\sim}{P})$, $|\alpha| = 1$. We check that $\mu_{j\alpha}$, $|\alpha| = 1$, can be extended to measures and we continue the process for $f_P(\delta^{ij}x^\alpha)'$, $|\alpha| > 1$, until we reach a pth step such that $\mu_{j\alpha} = 0$ for all $|\alpha| > p$. Next, we have to check that the $\mu_{j\alpha}$ satisfy the transformation rules on the intersections of charts. If the compatibility conditions are satisfied, we conclude that the $\{\mu_{j\alpha}\}$, $|\alpha| \leqslant p$, obtained are the local representatives of a stress which is consistent with the given force system.

VIII. CONSTITUTIVE RELATIONS

As we mentioned in the introduction, the problem of the restriction of forces to subbodies, which was transformed into a problem of nonunique relation between forces and stresses, leads to the specification of the material properties as additional information. The material properties are introduced via the so called constitutive relations, which in classical continuum mechanics, associate the stress at a point with the deformation gradient at that point. In this section we suggest a way by which constitutive theory may be incorporated in the structure that we developed.

We assume that the following two principles hold in continuum mechanics.

Axiom 8.1. (the principle of body self-determinism): The force acting on a body is determined by the configuration of the body, i.e., for any body B there is a section $F_B\colon Q \to T^*Q$ which we call the loading of B.

Axiom 8.2 (the principle of consistency): Given any configuration κ of the body B, the force system $\{F_P(\kappa|P);\ P$ is a subbody of $B\}$, is consistent.

Thus, by Proposition 7.1, the principle of consistency implies that any configuration of B determines a unique stress representation in $T^*C^0(\pi^P)$. The mapping $\Psi_B\colon Q \to T^*C^0(\pi^P)$ that associates stresses with the various configurations is called a constitutive relation for B.

Given a force $f \in T^*Q$ and a constitutive relation Ψ_B such that $f = T^*(j_p)(\Psi_B(\kappa))$, the measure $\Psi_B(\kappa)$ induces a unique force on any subbody and the problem of the restriction of the force is immediately solved. The general problem of continuum mechanics can be formulated now as follows. Given a loading F_B of B and a constitutive relation Ψ_B, determine the configuration κ such that $\Psi_B(\kappa)$ represents $F_B(\kappa)$, i.e., $F_B(\kappa) = T^*(j_p)(\Psi_B(\kappa))$.

It should be noted that in the general geometric framework we use, any "force" is a "follower force" in the sense that a force has meaning only when it is associated with a configuration. Thus, rather than looking for an equilibrium configuration under a given force, a meaningless problem, one has to find the equilibrium configuration for a given loading.

We can examine now the way in which the principle of local determinism restricts the constitutive relations. Let P be subbody of B and let Ψ_P, Ψ_B be constitutive relations on P and B, respectively. Since for any κ, the principle of body determinism implies that the force on P and any of its subbodies is determined by $\kappa|P$, we have $\Psi_P(\kappa|P) = \Psi_B(\kappa)|P$. Thus, we will omit the suffix and we will write Ψ when no confusion can arise. We also note that this principle implies that it is sufficient to examine the case where B is in R^m. Moreover, assuming that the constitutive relations are continuous, we can show that the constitutive relations are p-jet local in the following sense.

Proposition 8.3: Let Ψ be a continuous constitutive relation and let $x \in B$. Then, for any $\epsilon > 0$, there exists a $\delta > 0$ such that if a subbody P is contained in a ball of radius δ (in the R^m Euclidean metric) centered at x, then,

$$\|\Psi(\kappa)|P - \Psi(j_p(\kappa)(x))|P\| < \epsilon,$$

where $j_p(\kappa)(x)$ denotes the pth-order Taylor expansion of κ about x.

Proof: Given any $\epsilon > 0$, the continuity of Ψ implies that there exists a $\delta_1 > 0$ such that if $\|\kappa - j_p(\kappa)(x)\|_{C^p} < \delta_1$, then $\|\Psi(\kappa) - \Psi(j_p(\kappa)(x))\| < \epsilon$. By Taylor's theorem, given $\delta_1 > 0$, there is a $\delta > 0$ such that $\|\kappa|P - j_p(\kappa)(x)|P\|_{C^p} < \delta_1$ if P is contained in a ball of radius δ about x. Thus, by locality

$$\|\Psi(\kappa)|P - \Psi(j_p(\kappa)(x))|P\| = \|\Psi(\kappa|P) - \Psi(j_p(\kappa)(x)|P)\| < \epsilon.$$

Since there is no meaning to the value of a stress at a point, the classical locality assumption that the value of the stress at a point depends on the value of the deformation gradient at that point cannot be obtained or even conjectured. If stresses were continuous sections and if the space of stresses were given the C^1 topology, then the continuity argument of the previous proposition together with the two principles would imply that the value of the stress at a point depends only on the value of the pth jet at that point.

IX. STRESSES GIVEN BY SMOOTH DENSITIES

In this section, in order to complete the analogy with classical continuum mechanics, we obtain the representation of forces by surface forces and body forces, the equilibrium differential equations, and the boundary conditions.

Since the procedure involves integration by parts, we assume that the stresses are given in terms of smooth densities. We also assume that a connection is specified on S and that B and S have the same dimension. It follows that the connection on S induces a connection on B. Keeping κ fixed during the discussion, we identify the body with its image under κ.

We saw that if connections are given on B and S, any force can be represented in the form

$$f(u) = \sum_{k=0}^{p} \int_B \nabla^k u \, d\sigma_k,$$

where σ_k is the k th-order stress measure. Consider the vector bundle $L(L^k(\tau_B, \kappa^*\tau_S), \overset{m}{\wedge} T^*B)$. Assuming that B is orientable, a smooth section s_k of this vector bundle induces a k th-order stress measure σ_k by

$$\int_B \nabla^k u \, d\sigma_k = \int_B s_k \circ \nabla^k u,$$

where $s_k \circ \nabla^k u$ is the m-form whose value at $x \in B$ is $s_k(x)(\nabla^k u(x))$. In particular, if a volume element θ is given on B, the collection of sections $\{\mathscr{s}_k\}$, $\mathscr{s}_k \in C^\infty(L^k(\tau_B, \kappa^*\tau_S)^*)$ will induce a stress representation

$$f(u) = \sum_{k=0}^{p} \int_B \mathscr{s}_k(\nabla^k u)\theta,$$

where $\mathscr{s}_k(\nabla^k u)$ is the real function whose value at $x \in B$ is $\mathscr{s}_k(x)(\nabla^k u(x))$. More geometric structure is available in the case where both the connection and the volume element are derived from a Riemmanian metric.

In order to perform the integration by parts in the general geometric framework, we generalize the definition of the divergence of a tensor field as follows. We have the isomorphism

$$L(L^k(\tau_B, \kappa^*\tau_S), \overset{m}{\wedge} T^*B)$$
$$\cong \overset{m}{\wedge} T^*B \otimes \tau_B \otimes L^{k-1}(\tau_B, \kappa^*\tau_S)^*$$

and we define

$$\text{co: } L(L^k(\tau_B, \kappa^*\tau_S), \overset{m}{\wedge} T^*B) \to L(L^{k-1}(\tau_B, \kappa^*\tau_S), \overset{m-1}{\wedge} T^*B),$$

to be the mapping induced by the contraction of the first two factors in the tensor product above. Then, for $s_k \in C^\infty(L(L^k(\tau_B, \kappa^*\tau_S), \overset{m}{\wedge} T^*B))$, we define the divergence $\operatorname{div} s_k \in C^\infty(L(L^{k-1}(\tau_B, \kappa^*\tau_S), \overset{m}{\wedge} T^*B))$ by

$$\operatorname{div} s_k(\nabla^{k-1}u) = d(\operatorname{co}(s_k(\nabla^{k-1}u))) - s_k(\nabla^k u).$$

Using local expressions it can be shown that the divergence is well defined and that it agrees with the usual definition in the case of a Riemannian manifold.

For the case $p = 1$, let the force f be represented by smooth densities in the form

$$f(u) = \int_B s_0(u) + s_1(\nabla u),$$

where $s_i \in C^\infty(L(L^i(\tau_B, \kappa^*\tau_S), \overset{m}{\wedge} T^*B))$. Using the definition of the divergence and Stokes' theorem, one can show that f can be represented by two sections $b \in C^\infty(L(\tau_B, \overset{m}{\wedge} T^*B))$ and $t \in C^\infty(L(i^*\tau_B, \overset{m-1}{\wedge} T^*\partial B))$ (i is the embedding $\partial B \to B$) in the form

$$f(u) = \int_B b(u) + \int_{\partial B} t(u),$$

where b and t satisfy $\operatorname{div} s_1 + b = s_0$ and $t = i^* \circ \operatorname{co}(s_1)$. (We use i^* for both the pullback of differential forms and the pullback of vector bundles.)

In the case of Riemannian geometry we obtain for the three-dimensional case the usual result, i.e., if

$$f(u) = \int_B (s_{0j}u^j + s^i_{1j}\, u^j_{|i})\, dv$$

(the vertical bar denotes covariant derivative), we have

$$f(u) = \int_B \mathscr{b}_j u^j \, dv + \int_{\partial B} \mathscr{t}_j u^j \, da,$$

where $\mathscr{s}^i_{1j|i} + \mathscr{b}_j = \mathscr{s}_{0j}$, $\mathscr{t}_j = n_i \mathscr{s}^i_{1j}$, and n is the unit normal to the boundary.

Remark: The term $\mathscr{s}_0$ vanishes and the term $\mathscr{s}_1$ can be shown to be symmetric in the Euclidean geometry if we require that the force is invariant with respect to the Euclidean group (cf. Refs. 4, 21, and 22).

For the case $p = 2$, the case of second-grade continuum mechanics, we assume that the stresses are given in terms of the densities s_0, s_1, and s_2 such that

$$f(u) = \int_B (s_0(u) + s_1(\nabla u) + s_2(\nabla^2 u)).$$

It can be shown that f can be represented in the form

$$f(u) = \int_B b(u) + \int_{\partial B} (t(u) + t'(\nabla u)),$$

where b, t, and t' are in

$$C^\infty(L(\tau_B, \overset{m}{\wedge} T^*B)), \quad C^\infty(L(i^*\tau_B, \overset{m-1}{\wedge} T^*\partial B)),$$

and

$$C^\infty(L(L(i^*\tau_B, i^*(\kappa^*\tau_S)), \overset{m-1}{\wedge} T^*\partial B)),$$

respectively, and they satisfy

$$b = \operatorname{div}^2 s_2 - \operatorname{div} s_1 + s_0,$$
$$t = i^* \circ \operatorname{co}(s_1) - i^* \circ \operatorname{co}(\operatorname{div} s_2),$$
$$t' = i^* \circ \operatorname{co}(s_2).$$

A further integration by parts of the term involving t' is possible only if we have additional geometric structure. Again, for the three-dimensional Riemannian geometry, the classical results (see, e.g., Refs. 23 and 24) can be obtained.

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Moment-equation and path-integral techniques for wave propagation in random media

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Differential equations for all moments of the field of a wave propagating through a random medium are derived under the parabolic approximation and the Markov approximation, but including anisotropy in the random medium and a deterministic background refractive index. Mathematical equivalence is demonstrated between these moment equations and path-integral expressions for the moments obtained under the same approximations. A discussion of approximations that are weaker than Markov is given.

I. INTRODUCTION

Many problems in wave propagation through random media concern phenomena in which there is no significant backscatter, so that a parabolic approximation may be made to the wave equation.[1] In these cases a further approximation, called the Markov approximation,[2] leads to relatively tractable mathematical expressions for moments of the field that can be used for practical calculations. Two quite different formalisms have been used in this context: the moment-equation and path-integral techniques.

A path-integral expression for a general moment of the field of a wave propagating through an inhomogeneous, anisotropic medium in the presence of a deterministic background refractive index has been derived,[3] and the expression has been used for specific calculations.[4–6]

Moment equations in coordinate representation have been derived for homogeneous isotropic media in the absence of a deterministic background.[2] Treatments of inhomogeneity, anisotropy, and deterministic background by moment-equation techniques have heretofore been confined to special cases involving the first and second moments.[7,8]

We present here general moment equations in coordinate representation that account for inhomogeneity, anisotropy, and deterministic background, but require the Markov approximation. We derive these equations using the time-ordered-product method of Van Kampen,[9] which also provides a derivation of equations that are valid under conditions more general than the Markov approximation. The modified equations are more complicated than those that require the Markov approximation; a special case was derived by Besieris and Tappert.[10]

We also show that our new general moment equations derived under the Markov approximation are mathematically equivalent to the path-integral expressions for the moments that have been previously presented. Thus, the two popular formalisms, under the Markov approximation, are not different in content.

The plan of the paper is as follows: In Sec. II we establish notation, present our new moment equations, and present path-integral expressions for the moments in similar notation. In Sec. III we establish the mathematical equivalence between the two techniques. In Sec. IV we present the derivation of our moment equations, and, along the way, derive the modified equations. In Sec. V, for completeness, we rederive the path-integral expressions for the moments. In Sec. VI we comment on the use of different coordinate systems (such as cylindrical or spherical) in the writing of moment equations. A summary concludes the paper.

II. NOTATION AND MARKOV-APPROXIMATION RESULTS

Consider waves traveling predominantly in the z direction. Let $\mathbf{x}$ be a transverse coordinate (e.g., two-dimensional, but in fact general), and k be a reference wave number ($k = \omega/C_0$), where ω is the wave frequency and C_0 is a reference wave speed). Express the full wave field as

$$u(\mathbf{x},z,t) = \psi(\mathbf{x},z)\exp[ik(z - C_0 t)]. \tag{1}$$

Let the wave speed (a function of position only) be

$$C(\mathbf{x},z) = C_0[1 - 2U_0(\mathbf{x}) - 2\mu(\mathbf{x},z)]^{-1/2}$$
$$\approx C_0[1 + U_0(\mathbf{x}) + \mu(\mathbf{x},z)], \tag{2}$$

where U_0 represents the deterministic background and μ represents the fluctuating random medium, assumed to be a realization of a zero-mean Gaussian process.

Then, the parabolic equation (in rectangular coordinates) for the reduced wave function ψ is

$$ik\,\partial_z\psi = -\tfrac{1}{2}\nabla^2\psi + k^2U_0(\mathbf{x})\psi + k^2\mu(\mathbf{x},z)\psi, \tag{3}$$

where ∇^2 is the transverse Laplacian.

A moment Γ is the ensemble expectation value of a product of ψ's and ψ^*'s, where each ψ or ψ^* is evaluated at a different position $\mathbf{x}_j$ and wave number k_j. We write, in abbreviated form,

$$\Gamma_{mn} = \langle \psi_1^*\cdots\psi_m^*\psi_{m+1}\cdots\psi_{m+n}\rangle. \tag{4}$$

Define an operator L_0 such that

$$L_0 = \sum_{j=1}^{m+n} \pm\frac{1}{k_j}\left(-\frac{1}{2}\nabla_j^2 + k_j^2U_{0j}\right). \tag{5}$$

The terms that apply to the ψ's use the plus sign and those

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that apply to the ψ^*'s use the minus sign. The subscript j requires that ∇_j^2 operate only on $\mathbf{x}_j$ and $U_{0j} \equiv U_0(\mathbf{x}_j)$.

Define the important combination of fluctuation quantities as

$$M(z) = \sum_{j=1}^{m+n} \pm k_j \mu(\mathbf{x}_j, z). \tag{6}$$

Our general moment equation under the Markov approximation can be written

$$\partial_z \Gamma_{mn}(z) = iL_0 \Gamma_{mn}(z) - \frac{1}{2}\int_{-\infty}^{\infty} dz' \langle M(z) M_{\text{shift}}(z') \rangle \Gamma_{mn}(z), \tag{7}$$

where $M_{\text{shift}}(z')$ is obtained by evaluating $M(z)$ with all the $\mathbf{x}_j$ at z shifted by the transverse distance that a deterministic ray through $(\mathbf{x}_j, z)$ moves in traveling from z to z' (see Fig. 1). In other words $M_{\text{shift}}(z')$ is evaluated at point B, i.e., $\mathbf{x}_j = \mathbf{x}_{\text{ray}}(z')$ where the ray is forced to go through $\mathbf{x}_j(z)$. The particular ray is determined not only by the local position $(\mathbf{x}_j, z)$, but also by the initial conditions on the moment; for example, the location of a point source, or the direction of a plane wave.[11] The unphysical assumption of delta-correlated medium fluctuations along the propagation direction would imply that $M_{\text{shift}}(z')$ would be evaluated at point C, i.e., $\mathbf{x}_j(z)$ (and z'). In the isotropic case (or in the case of propagation along a principal axis of the anisotropy) the difference between evaluating $M_{\text{shift}}(z')$ at $\mathbf{x}_j(z)$ and $\mathbf{x}_{\text{ray}}(z')$ is negligible, and the delta-correlated assumption is adequate. In the anisotropic case, the necessity of defining the unperturbed ray makes (7) somewhat complicated to apply for general initial conditions. However, since (7) is a linear equation, superposition can be used whether the source is a point, an incident plane wave, or an arbitrary coherent or incoherent sum of point sources. Equation (7), which is one of the principal results of this paper, is derived in Sec. IV.

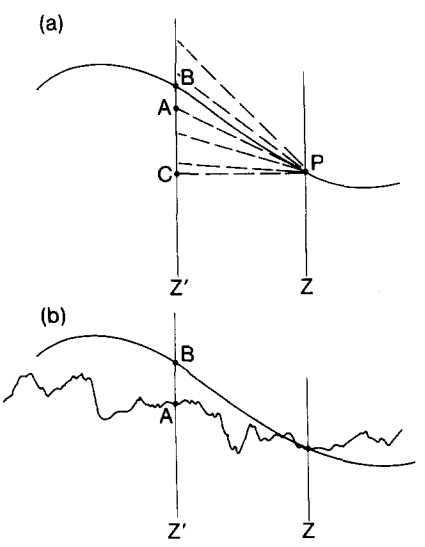

FIG. 1. (a) Moment-equation expression of the Markov approximation. The correlation should be taken between a point at z (point P) and an arbitrary point at z' (point A). Instead it is taken with the point B, obtained by extrapolating along the unperturbed ray from P. The assumption of delta-correlated medium fluctuations leads to the incorrect formulation of correlations between points P and C. The dashed lines indicate the idea of a scattering as a function of angle from point P. (b) Path-integral expression of the Markov approximation. The general path at z' (point A) is approximated by the path at z extrapolated along the unperturbed ray (point B).

We now turn to the path integral method. Equation (3) has the formal solution

$$\psi = \int D\mathbf{x}(z) e^{iS}, \tag{8}$$

where $\int D\mathbf{x}(z)$ means integration over paths, $\mathbf{x}(z)$ is a transverse vector indicating the position of the path at z, and

$$S = k\int_0^R dz \left(\frac{1}{2}\left(\frac{d\mathbf{x}}{dz}\right)^2 - U_0(\mathbf{x}) - \mu(\mathbf{x}, z)\right). \tag{9}$$

In order to obtain a given moment, expressions like (8) (or its complex conjugate) are multiplied together, and the ensemble average is taken:

$$\Gamma_{mn} = \int \prod_{j=1}^{m+n} D\mathbf{x}_j(z) \left\langle \exp\left(\sum_j \pm iS_j\right)\right\rangle. \tag{10}$$

The Markov approximation yields (see Sec. V)

$$\Gamma_{mn} = \int \prod_{j=1}^{m+n} D\mathbf{x}_j(z) \times \exp\int_0^R dz \left[\sum_j \pm ik_j \left(\frac{1}{2}\left(\frac{d\mathbf{x}_j}{dz}\right)^2 - U_{0j}\right) - \frac{1}{2}\int_{-\infty}^{\infty} dz' \langle M(z) M_{\text{shift}}(z')\rangle\right]. \tag{11}$$

We show in Sec. III that the moment equations (7) and the path-integral expressions (11) are mathematically equivalent.

III. EQUIVALENCE OF PATH INTEGRAL AND MOMENT EQUATIONS UNDER THE MARKOV APPROXIMATION

We follow the technique that Feynman[12] used to show that his path-integral expression for nonrelativistic quantum mechanics is equivalent to the Schrödinger equation. The key to this demonstration is an understanding of how the important paths behave transversely as they move in z from a particular point. Feynman found that these paths resembled random walks in that

$$|\mathbf{x}(z') - \mathbf{x}(z)| \sim (z' - z)^{1/2} \tag{12}$$

as z' gets close to z. Given this behavior, it is easy to expand (11) in a Taylor series and obtain a differential equation which will turn out to be (7). We give the demonstration of (12) in the Appendix.

The path integral is defined as the limit of an integration over a set of "phase screens." These screens are at values $z_N = N\delta z$. The derivative $d\mathbf{x}/dz$ at $z = z_N$ is defined as $(\mathbf{x}(z_N + \delta z) - \mathbf{x}(z_N))/\delta z = \delta\mathbf{x}/\delta z$. The limit $\delta z \to 0$ is taken after the integrals are evaluated. The differential equation is obtained by considering the integral over the very last phase screen. The last integral in (11) can be written in terms of $\mathbf{x}_j' = \mathbf{x}_j(R - \delta z)$ and $\mathbf{x}_j = \mathbf{x}_j(R)$. Also, we define $\delta\mathbf{x}_j \equiv \mathbf{x}_j - \mathbf{x}_j'$. Then Γ_{mn} can be expressed as

$$\Gamma_{mn}(\{\mathbf{x}\}, R) = N\int \prod_j d\mathbf{x}_j' \exp\left(\delta z\left[\sum_j \pm ik_j\left(\frac{1}{2}\left(\frac{\delta\mathbf{x}_j}{\delta z}\right)^2 - U_{0j}\right) - \frac{1}{2}\int dz' \langle M(R) M_{\text{shift}}(z')\rangle\right]\right)\Gamma_{mn}(\{\mathbf{x}'\}, R - \delta z), \tag{13}$$

where $\{\mathbf{x}\}$ denotes the set of $(m+n)$ $\mathbf{x}_j$'s. The first term in the exponent, $\pm (ik_j/2)[(\delta \mathbf{x}_j)^2/\delta z]$, is $O(1)$ for small δz, because of (12). The exponent of the remaining terms can be expanded, since they have an explicit δz, as well as higher-order terms. This results in

$$\Gamma_{mn}(\{\mathbf{x}\},R) = N\int \prod_j \left(d\delta \mathbf{x}_j \exp\left\{ \frac{\pm ik_j(\delta \mathbf{x}_j)^2}{2\delta z} \right\} \right) \times \left[1 - \delta z \left(\sum_j \pm ik_j U_{0j}(R) + \frac{1}{2}\int_{-\infty}^{\infty} dz' \langle M(R) M_{\text{shift}}(z') \rangle \right) \right] \times \Gamma_{mn}(\{\mathbf{x}'\}, R-\delta z) + O(\delta z^{3/2}). \tag{14}$$

We now have a relationship between the moment at R and the moment at $R-\delta z$, which we derived from our path-integral expression. But since the moment is a differentiable function we can find another relationship by Taylor expansion as follows:

$$\Gamma_{mn}(\{\mathbf{x}'\}, R-\delta z) = \left[1 - \delta z\, \partial_R - \sum_j \delta \mathbf{x}_j \cdot \nabla_j + \frac{1}{2}\left(\sum_j \delta \mathbf{x}_j \cdot \nabla_j \right)^2 \right] \times \Gamma_{mn}(\{\mathbf{x}\}, R) + O(\delta z^{3/2}). \tag{15}$$

Substituting (15) into (14) we find

$$\Gamma_{mn}(\{\mathbf{x}\},R) = N\int \prod_j \left(d\,\delta \mathbf{x}_j \exp\left\{ \pm \frac{ik_j(\delta \mathbf{x}_j)^2}{2\,\delta z} \right\} \right) \times \left\{ 1 - \sum_j \delta \mathbf{x}_j \cdot \nabla_j + \frac{1}{2}\left(\sum_j \delta \mathbf{x}_j \cdot \nabla_j \right)^2 - \delta z\, \partial_R - \delta z \left(\sum_j \pm ik_j U_{0j}(R) + \frac{1}{2}\int_{-\infty}^{\infty} dz' \langle M(R) M_{\text{shift}}(z') \rangle \right) \right\} \times \Gamma_{mn}(\{\mathbf{x}\}, R) + O(\delta z^{3/2}). \tag{16}$$

The term linear in $\Sigma_j \delta \mathbf{x}_j \cdot \nabla_j$ is odd in $\delta \mathbf{x}_j$ and therefore gives 0 due to the $\delta \mathbf{x}_j$ integral. The term that is quadratic in $\delta \mathbf{x}_j$ can be integrated by parts, yielding, to order δz

$$\Gamma_{mn}(\{\mathbf{x}\},R) = N\int \prod_j \left(d\delta \mathbf{x}_j \exp\left\{ \frac{\pm ik_j(\delta \mathbf{x}_j)^2}{2\,\delta z} \right\} \right) \times \left\{ 1 + \delta z \left[-\partial_R - \frac{1}{2}\sum_j \frac{1}{\pm ik_j}\nabla_j^2 - \sum_j \pm ik_j U_{0j}(R) - \frac{1}{2}\int_{-\infty}^{\infty} dz' \langle M(R) M_{\text{shift}}(z') \rangle \right] \right\} \times \Gamma_{mn}(\{\mathbf{x}\}, R). \tag{17}$$

The only way (17) can be true for all δz is for the coefficient of δz within the curly brackets operating on Γ_{mn} to give zero. Therefore, setting $R \to z$,

$$\partial_z \Gamma_{mn}(\{\mathbf{x}\},z) = -i\sum \pm \frac{1}{k_j}\left(-\frac{1}{2}\nabla_j^2 + k_j^2 U_{0j} \right)\Gamma_{mn}(\{\mathbf{x}\},z) - \frac{1}{2}\int_{-\infty}^{\infty} dz' \langle M(z) M_{\text{shift}}(z') \rangle \Gamma_{mn}(\{\mathbf{x}\},z), \tag{18}$$

which is identical to (7), as required. Thus, we have derived the moment equation (7) from the path-integral expression (11). This shows that the path-integral expression (11) is a solution of the moment equation (7) and hence the two techniques are equivalent.

IV. MOMENT EQUATION DERIVATION

We derive our moment equations by the method of Van Kampen.[9] The advantage of his method is that the physical basis for each approximation is readily apparent. He bases his method on techniques that were developed for quantum mechanics.

We shall find that the Markov approximation requires that the dimensionless number $L_p^2 M_t^2$ be small where L_p is the medium correlation length in the direction of the wave propagation, and M_t is the "typical" value of M, defined by (6) and called the "interaction strength." For the first moment $M = k\mu$, but for higher moments M is the sum and difference of a number of $k\mu$'s at different positions, and with different values of k.

We start with the parabolic wave equation (3) and the definition of L_0 and M, and write

$$i\,\partial_z \psi_1^* \psi_2^* \cdots \psi_{m+n} = (L_0 + M)\psi_1^* \psi_2^* \cdots \psi_{m+n}. \tag{19}$$

The "interaction representation" is defined by

$$(\psi_1^* \psi_2^* \cdots \psi_{m+n})_I = e^{iL_0 z}\psi_1^* \psi_2^* \cdots \psi_{m+n} \tag{20}$$

and

$$M_I(z) = e^{iL_0 z} M(z) e^{-iL_0 z}. \tag{21}$$

With these definitions, (19) becomes

$$i\,\partial_z (\psi_1^* \psi_2^* \cdots \psi_{m+n})_I = M_I(z)(\psi_1^* \psi_2^* \cdots \psi_{m+n})_I. \tag{22}$$

This equation is linear and has the formal solution

$$(\psi_1^* \psi_2^* \cdots \psi_{m+n})_I = T\exp\left(-i\int_0^z M_I(z')dz' \right)\Gamma_{mn}(0), \tag{23}$$

where $\Gamma_{mn}(0)$ is the initial condition. The "time-ordering" symbol T requires explanation. One notices that M_I is an operator, not just a function of space. Thus, $M_I(z_1)$ and $M_I(z_2)$ do not, in general, commute. If they did the solution of (22) would be given by (23) without the T symbol. The T symbol means that a product of operators to the right is not applied in the usual order, but in such a way that operators with smaller values of z' are to be applied first. Thus there is an ordering in z. (The T symbol was invented for solving problems in quantum mechanics where the analog of the longitudinal direction z is the time.) For example,

$$T\exp\left(-i\int_0^z M_I(z')dz' \right) = \left[T\exp\left(-i\int_{z_1}^z M_I(z')dz' \right) \right] \times \left[T\exp\left(-i\int_0^{z_1} M_I(z')dz' \right) \right], \tag{24}$$

for $0 \leqslant z_1 \leqslant z$. Another example is

$$T\frac{(-i)^k}{k!}\left[\int_0^z M_I(z')dz'\right]^k$$
$$= (-i)^k \int M_I(z_k)\cdots M_I(z_2)M_I(z_1)dz_1\, dz_2\cdots dz_k, \tag{25}$$

where the integration region on the right side of (25) is $0 < z_1 < z_2 < \cdots < z_k < z$, which is $k!$ times smaller than that of the left side, canceling the factor of $k!$. Using either (24) or (25), one readily checks that (23) is a formal solution of (22).

We are assuming that M is a Gaussian process. The result that the expectation of the exponential of a zero-mean Gaussian random variable is the exponential of half the variance follows from combinatorial factors and remains true for a time-ordered exponential. Thus

$$(\Gamma_{mn})_I = T\exp\left[-\frac{1}{2}\left\langle\left(\int_0^z M_I(z')dz'\right)^2\right\rangle\right]\Gamma_{mn}(0). \tag{26}$$

Although this is a formal expression for Γ_{mn}, it is not immediately useful for calculations, since there is no simple algorithm for evaluating a time-ordered exponential (in contrast to a normal exponential). Van Kampen proceeds by differentiating (26):

$$\partial_z(\Gamma_{mn})_I = -T\left\langle M_I(z)\int_0^z dz'\, M_I(z')\right\rangle$$
$$\times\exp\left[-\frac{1}{2}\left\langle\left(\int_0^z M_I(z'')dz''\right)^2\right\rangle\right]\Gamma_{mn}(0). \tag{27}$$

The $M_I(z)$ has the largest z, so it is written in the proper ordered position. The $M_I(z')$ that it is correlated with, however, might occur anywhere relative to the $M_I(z'')$'s in the exponential. If $L_p^2 M_t^2 \ll 1$, very little error is made by assuming that the first two M_I's are in the proper order, so that the T symbol can be brought through the first expectation value, yielding

$$\partial_z(\Gamma_{mn})_I = -\left\langle M_I(z)\int_0^z dz'\, M_I(z')\right\rangle(\Gamma_{mn})_I. \tag{28}$$

This may be shown by expanding the exponential operators in (26) or (27) and discussing the order of M's in each term. The Nth term in the expansion has $2N$ occurrences of M_I, and is of a magnitude

$$\left\langle\left(\int_0^z M_I\, dz'\right)^2\right\rangle^N / N!, \tag{29}$$

where typical eigenvalues of the operators are implied. The terms beyond

$$N \approx 4\left\langle\left(\int_0^z M_I\, dz'\right)^2\right\rangle \tag{30}$$

become negligible compared to the original exponential in (26), so we have to deal with at most N pairs of M_I's from source to range z. The two M_I's in a correlated pair must be within L_p of each other to give a nonzero correlation. The number of pairs may be estimated as

$$N \approx 4L_p z M_t^2, \tag{31}$$

where M_t^2 is a typical value of M_I^2. (See Fig. 2 for a schematic representation.) Our approximation reduces to saying it is unlikely to find a third occurrence of an M_I in between a pair that are within L_p of each other. This probability is roughly

$$\text{Probability} \approx L_p N/z \approx L_p^2 M_t^2. \tag{32}$$

Thus if the fluctuations are weak enough ($L_p M_t \ll 1$), the approximation is valid, and (28) is justified.

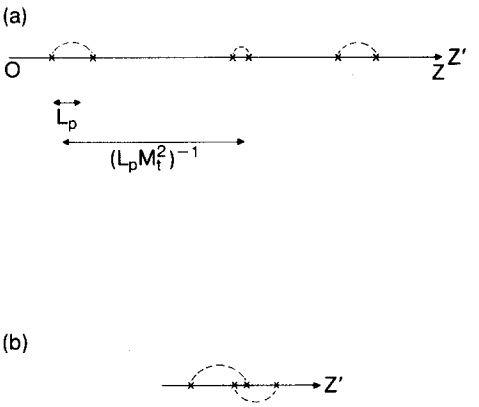

FIG. 2. (a) Typical z values of the interactions from a Taylor series term in (9) are indicated by $\times$'s. Dashed lines show which interactions are correlated. It is assumed that $L_p^2 M_t^2 \ll 1$. (b) A portion of a contribution to (9) which is improperly ordered in "first-order perturbation theory." Such contributions are small if $L_p^2 M_t^2 \ll 1$.

We call (28) "first-order perturbation theory." In typical situations, z is much larger than L_P, and the lower limit can be replaced by $-\infty$, making the equation independent of the source position. Moreover, the integral from $-\infty$ to z can be replaced by half the integral from $-\infty$ to ∞, when the correlation is a much slower function of $\frac{1}{2}(z+z')$ than of $z-z'$. The result is used, not in the interaction representation, but in the original representation. The exponentials of (20) and (21) are removed, giving

$$\partial_z\Gamma_{mn}(z) = -iL_0\Gamma_{mn}(z) - \int_{-\infty}^{z} dz'\langle M(z)e^{-iL_0(z-z')}$$
$$\times M(z')e^{iL_0(z-z')}\rangle\Gamma_{mn}(z). \tag{33}$$

For the second moment, this equation is related to an expression of Besieris and Tappert.[10] Although their work was for the second moment, we can generalize it directly; therefore in the rest of our comments we treat the general moment Γ_{mn} where Besieris and Tappert treated only Γ_{11}. Their equation (3.2) was expressed in a Fourier transformed domain, but can be expressed in our notation as

$$\partial_z\Gamma_{mn}(z) = -iL_0\Gamma_{mn}(z)$$
$$-\int_{-\infty}^{z} dz'\langle M(z)e^{-iL_0(z-z')}M(z')\rangle\Gamma_{mn}(z'). \tag{34}$$

This equation is equivalent to (33) to order $L_p^2 M_t^2$, and it should be noted that both (33) and (34) are invalid if $L_p^2 M_t^2$ is not small. Unlike (33), (34) implies a "memory" effect in which the gradient of the moment depends explicitly on the moment at all previous z's. The Markov approximation leads to (7), which eliminates the memory effect and requires only a correlation function of the medium along a specified (shifted) direction. Besieris and Tappert pointed out that a

weaker approximation, called the "long-time Markov" approximation leads to a local (nonmemory) equation (their Eq. 3.3), that in our notation is expressed as

$$\partial_z \Gamma_{mn} = -iL_0\Gamma_{mn}(z) - \left\{\int_{-\infty}^{z} dz' \langle M(z)e^{-iL_0(z-z')}M(z')\rangle\right\}\Gamma_{mn}(z), \tag{35}$$

where the L_0 operator acts only on $M(z')$, not on $\Gamma_{mn}(z)$, in the last term. We have derived (35) by use of the Wigner-function notation of Besieris and Tappert. We are only considering situations in which the parabolic wave equation is valid. It has been shown that in that case the long-time Markov approximation is valid,[10] and therefore (35) is as valid as (33).

Because L_0 is an operator, the integrals in (33)–(35) involve the medium correlation function in all directions, or, in the Fourier-transform domain, require a scattering kernel as a function of scattering angle. The Markov approximation to (33) consists of simplifying the deterministic propagation operator $e^{-iL_0(z-z')}$ for $z-z'$ on the order of L_P. Instead of correlating $M(z)$ with all possible transverse positions of $M(z')$, the Markov approximation corresponds to choosing only one transverse position for $M(z')$. (See Fig. 1, where point A represents an arbitrary transverse position.) If the wave represented by $\Gamma_{mn}(z)$ were the unperturbed solution, then deterministic propagation would move the phase in the direction of the unperturbed ray. If the wave energy is traveling close to the unperturbed ray this operator retains its behavior to first approximation. As a result, deterministic propagation approximates a shift along the unperturbed ray to point B, i.e., $\mathbf{x}(z') = \mathbf{x}_{\text{ray}}(z')$, where the ray is forced to go through $\mathbf{x}(z)$. Hence $e^{-iL_0(z-z')}M(z')e^{iL_0(z-z')}$ can be approximated by $M_{\text{shift}}(z')$. This is the appropriate definition of the Markov approximation (rather than assuming the medium is delta correlated along the z axis) and it immediately yields (7) from (33). In practice, instead of using the actual unperturbed ray, the tangent to the ray at z is often used.

If the delta-correlated assumption were made, it would correspond to evaluating $M_{\text{shift}}(z')$ at point C, which is strictly valid only if there is a single unperturbed ray traveling along the z axis. If the medium fluctuations are isotropic, the correlation of any point at z' with the point P at z will give the same result because of the parabolic approximation, and hence the delta-correlated assumption is as good as any other choice. However, for an anisotropic medium it is important that point B [and hence (7)] be used, even when the Markov approximation is invoked. Note that (7) can be used in the presence of a deterministic background refractive index.

The difference between (33) and (7) can be caused by directions different from the unperturbed ray becoming important. It is in this sense that (33)–(35), which never refer to unperturbed rays, are more general than (7), which does. A transverse wave number k_T, coming, for example, from M, causes the angle to change by $\delta\theta = k_T/k$. A transverse error in position of about $k_T L_P/k$ is made by assuming the direction of the unperturbed ray. Thus, in order for the Markov approximation to be valid, it is required that $k_T L_P/k \ll L_T$, where L_T is the transverse scale of concern. Since $L_T \approx 1/k_t$, the Markov approximation fails at sufficiently small $k \approx L_P/L_T^2$. The parameter $\alpha = kL_T^2/L_P$ introduced by Beran and McCoy[13] and discussed further in Flatté[4] reflects these considerations. For small α, one can use (33) or its equivalent.

V. PATH-INTEGRAL DERIVATION

We recapitulate the derivation of the path-integral expression (7) from (10). Using the assumed Gaussian behavior of the fluctuations, we obtain from (10)

$$\Gamma_{mn} = \int \prod_{J=1}^{n} D\mathbf{x}_J(z) \exp\left(\sum_j \pm iS_{0j}\right) e^V, \tag{36}$$

where S_0 is the part of S in (9) that does not involve μ, and

$$V = -\frac{1}{2}\int dz\, dz' \langle M(z)M(z')\rangle. \tag{37}$$

The expression (36) is an exact representation of the moment of the solution of the parabolic equation with Gaussian fluctuations. It is not used in practice as it stands because V depends on the paths at two values of z, namely z and z'.

The Markov approximation for the path integral comes from assuming that the paths do not stray far in transverse space over a distance L_P; they all move approximately parallel to the unpertubed ray. Thus, in the Markov approximation

$$V = -\frac{1}{2}\int dz\, dz' \langle M(z)M_{\text{shift}}(z')\rangle \tag{38}$$

which only requires knowledge of the path at z. The final result (11) follows directly.

VI. COORDINATE SYSTEMS

Moment equations can be formulated in a variety of coordinate systems, while path integrals require a rectangular coordinate system. There has been a fair amount of effort expended on using polar coordinate systems, especially for point source problems.

The same results (for point sources among others) can be obtained in either polar or rectangular coordinates. Thus, the results of Shishov[14] on the intensity correlation, derived in spherical polar coordinates, can be seen to be identical (after an appropriate transformation) to the results of Codona *et al.*,[15] derived in rectangular coordinates. It was necessary for Shishov to make small-angle approximations in addition to the parabolic approximation of dropping the second derivative in the propagation direction, whereas Codona *et al.* only require the single parabolic approximation.

VII. SUMMARY

We have derived moment equations in coordinate representation under the Markov approximation that apply in anisotropic, inhomogeneous media with deterministic background. The derivation shows the relationship between these moment equations and modified equations that are valid under approximations weaker than Markov; the second-moment equation of Besieris and Tappert is a special case of these modified equations.

In a hierarchy of approximations we begin with the

parabolic wave equation itself. A path integral with nonlocal exponent can be written as an exact solution, although it is not yet useful in practice. The next level is the approximation that the interaction strength over a correlation length is small—this "first-order perturbation theory" leads to the modified moment equations, and in homogeneous, isotropic media, to the standard moment equations and path-integral expressions. In anisotropic, inhomogeneous media, however, a further approximation is necessary to obtain the moment equations and path integral expressions. This further approximation is that the significant flow of wave energy, or the important paths, are parallel to the unperturbed ray; we call this the Markov approximation because its violation implies the appearance of correlations between successive scatterings. We have shown that the moment equations and the path-integral expressions for the moments are mathematically equivalent under the Markov approximation. Thus the two formalisms have exactly the same physical content. In an anisotropic medium, the moment equation involves a shift operation to calculate the medium correlation function along the unperturbed ray; this form of the moment equation has not been given before.

We have also pointed out that all appropriate formulas can be derived in a rectangular coordinate system (even for point sources).

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APPENDIX

We must show that the scaling $|\delta \mathbf{x}_j| \sim (\delta z)^{1/2}$ holds for integrals of the form

$$\int \prod d\delta\, \mathbf{x}_j \exp\left(\sum \pm ik_j \frac{\delta x_j^2}{2\delta_z}\right) F(\mathbf{x}_j). \tag{A1}$$

If F is expandable in a power series (even if the radius of convergence is zero) this result follows immediately. One expands F and integrates term by term, obtaining a power series in $(\delta z)^{1/2}$. By standard methods in the theory of asymptotic expansions, only the low order terms need to be retained as $\delta z \to 0$.

For singular functions, a demonstration is not as simple. One may worry about cancellations between terms in the exponent, since the signs might differ.

We will content ourselves with a demonstration in the case likely to arise in practice. It is common to model a random medium as having a power-law structure function. Thus as two x's become equal, a singularity $|x_i - x_j|^p$ with $p > 0$ might occur in the integrand. In order to have possible cancellations in the exponent, we assume that $k_i = k_j = k$, and the exponential factor is $\exp(ik\,(\delta x_i^2 - \delta x_j^2)/2\,\delta z)$. We assume, for simplicity, that x_i and x_j are one dimensional; higher-dimensional singularities are effectively weaker.

Define $\nu = (\delta x_i + \delta x_j)/2$, $\mu = \delta x_i - \delta x_j$, and $\alpha = x_i - x_j$. The singularity from the previous step, $x_j' = x_j - \delta x_j$ is $|\mu - \alpha|^p$. The integral to be evaluated is

$$\int d\mu\, d\nu\, e^{ik\mu\nu/\delta z} f(\alpha,\mu,\nu)|\mu - \alpha|^p. \tag{A2}$$

We would like to ignore the μ dependence in f. However, spurious large-μ contributions would arise, even though we are only interested in contributions from μ close to α. To drop the μ dependence of f and also to simplify the analysis, we introduce a convergence factor $\exp(-a(\mu^2 + \nu^2)/\delta z^{1-\epsilon})$. As long as $\mu,\nu, \sim \delta z^{1/2}$, this factor does not change the integral as $\delta z \to 0$ (we are assuming $\epsilon > 0$). Conversely, if the integral in the limit $\delta z \to 0$ does not depend on a and ϵ, then μ and ν are of order $\delta z^{1/2}$.

The integral is then

$$I = \int d\mu\, d\nu\, e^{ik\mu\nu/\delta z} \times \exp[-a(\mu^2 + \nu^2)/\delta z^{1-\epsilon}]|\mu - \alpha|^p f(\alpha,\nu). \tag{A3}$$

The μ integral can be done, yielding

$$I = C_1 \int d\nu\, e^{ik\alpha\nu/\delta z} \exp[-a(\alpha^2 + \nu^2)/\delta z^{1-\epsilon}] \times f(\alpha,\nu) a^{-(1+p)/2} \delta z^{(1+p)(1-\epsilon)/2} \times M\left(\frac{p+1}{2}, \frac{1}{2}, -\frac{(\nu + 2i\delta z^{\epsilon} a\alpha)^2}{4a\delta z^{1+\epsilon}}\right), \tag{A4}$$

where M is a confluent hypergeometric function and C_1 is a constant independent of $\delta z, \epsilon$, and a (as are C_2 and C_3, below). The hypergeometric function has a part that behaves as the exponential of its argument for large (positive) values of its argument, a part that falls as a power [since $(p+1)/2$ is positive] and a part at small values of the argument. These last two parts can be combined into a bounded part. We show that the exponential part gives the leading behavior and the bounded part is a higher power of δz.

The contribution I_1 from the exponential asymptotic part of M is

$$I_1 = C_2 \int d\nu\, e^{ik\alpha\nu/\delta z} \exp[-a(\alpha^2 + \nu^2)/\delta z^{1-\epsilon}] \times f(\alpha,\nu) a^{-(1+p)/2} \delta z^{(1+p)(1-\epsilon)/2} \times \exp\left(\frac{(2\delta z^{\epsilon} a\alpha - ik\nu)^2}{4a\delta z^{1-\epsilon}}\right). \tag{A5}$$

The exponential from M cancels much of the first two exponentials

$$I_1 = C_2 \int d\nu \exp\left\{-\nu^2\left[\frac{a}{\delta z^{1-\epsilon}} + \frac{k^2}{4a\delta z^{1+\epsilon}}\right]\right\} \times f(\alpha,\nu) a^{-(1+p)/2} \delta z^{(1+p)(1-\epsilon)/2}, \tag{A6}$$

which can be done explicitly. Only the first term in the exponential survives as $\delta z \to 0$. The result is independent of a and ϵ, and is

$$I_1 = C_3 \delta z\, f(\alpha,0)|\alpha|^p, \tag{A7}$$

exactly as would be obtained from the Taylor series expansion for I.

We now turn to the contribution I_2 from the bounded part of M. We show I_2 has a higher power of δz than I_1. We can set ϵ to any positive value. At large ϵ we depend on the fact that $e^{ik\alpha\nu/\delta z}$ averages to zero for $\nu \sim \delta z^{1+\delta}$ for any positive δ, but it would be necessary to examine the detailed behavior of M to use this fact. On the other hand, for small

enough ϵ, it suffices to bound the integral by the integral of the absolute value of the integrand. The convergence factor provides a cutoff at $\nu \sim \delta z^{1-\epsilon/2}$. Thus $\int d\nu \exp[-a\nu^2/\delta z^{1-\epsilon}] f(\alpha,\nu)$ gives a contribution scaling like $\delta z^{1-\epsilon/2}$. Thus I_2 is bounded by an expression which scales as

$$I_2 \sim \delta z^{(1-\epsilon)/2+(1+p)(1-\epsilon)/2} = \delta z^{(1+p/2)(1-\epsilon)}. \tag{A8}$$

As long as we have chosen ϵ small enough, the exponent of δz is larger than 1, and I_2 can be neglected relative to I_1. Thus we have established the necessary scaling of μ and ν even in the singular case.

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Reconstruction of dynamics from an eigenstate

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For Hamiltonians that have a formal (canonical) decomposition $H = -\frac{1}{2}\Delta + V(x)$, $V(x)$ being a multiplication operator, the definition of the dynamics by a ground state measure leads to an energy (Dirichlet) form formulation of quantum mechanics that is more general than the operator Schrödinger approach. Here, the question of reconstruction of the dynamics from an eigenstate when the potential is not restricted to the class of multiplication operators is analyzed. By explicit analysis of several examples, it is found that, once a particular operator class is chosen, the potential and the energy form are, to some extent, determined by the eigenstate. However, depending on the type of operator the potential is chosen to be, many distinct dynamics can be associated to the same fixed eigenstate. The nature of the stochastic processes associated with each reconstructed dynamic is also discussed, as well as a generalization of the stochastic dynamics formalism allowing for nonlocal potentials.

I. INTRODUCTION

Consider a Schrödinger operator $H = -\frac{1}{2}\Delta + V(x)$, where $V(x)$ is a multiplication operator, and a real function $\phi(x) \in L^2_{\text{loc}}(\mathbb{R}^n)$, such that $(-\frac{1}{2}\Delta + V - E)\phi = 0$. Let Ω be an open set in the support of the measure $d\nu = \phi^2\, dx$ and $\mathscr{H}_\nu(\Omega)$ the closed subspace of $L^2(\Omega, d\nu)$ obtained by closing $C_0^\infty(\Omega)$ in the $L^2(\Omega, d\nu)$ norm. For $f_1, f_2 \in C_0^1(\Omega)$, the quadratic form

$$\epsilon(f_1, f_2) = \frac{1}{2}\int \overline{\nabla f_1} \cdot \nabla f_2\, d\nu \tag{1.1}$$

is a local Markovian symmetric form on $L^2(\Omega, d\nu)$. If ϕ is such that the form ϵ is closable in $\mathscr{H}_\nu(\Omega)$ then its closure $\bar{\epsilon}$ is a local regular Dirichlet form.[1] Several closability conditions are known.[2–4] For example, $\phi > 0$ locally uniformly; $\phi = 0$ at most on a set of Lebesgue measure zero ($n = 1$) plus some regularity.

Conversely if $\bar{\epsilon}(f_1, f_2)$ is a densely defined symmetric positive closed form there is a positive self-adjoint operator H such that [2,5,6]

$$\bar{\epsilon}(f_1, f_2) = (H^{1/2} f_1, H^{1/2} f_2). \tag{1.2}$$

One has, therefore, a way to describe quantum dynamics through (energy) forms alternative to the conventional operator Schrödinger approach. In sufficiently well-behaved situations the two approaches are equivalent. In particular, if $\nabla\phi, \nabla\phi/\phi, \Delta\phi/\phi \in L^2_{\text{loc}}(\Omega)$, then $H = -\frac{1}{2}\Delta + V - E$ with

$$V - E = \tfrac{1}{2}\phi^{-1}\Delta\phi. \tag{1.3}$$

The Dirichlet approach is, however, more general in the sense that through regular Dirichlet forms one can describe dynamic situations which formally would correspond to potentials more singular than distributions.

The Dirichlet approach faces a uniqueness question, since $\epsilon(f_1, f_2) = \frac{1}{2}\int \overline{\nabla f_1} \cdot \nabla f_2\, d\nu$ is first defined on a dense domain, but for the characterization of quantum dynamics one needs a self-adjoint operator. In principle, distinct quantum dynamics would correspond to the possible nonequivalent extensions of ϵ. A certain number of uniqueness results are available, in particular when the operator associated with ϵ is essentially self-adjoint in $C_0^\infty(\Omega)$.[7,8]

In this paper, a different nonuniqueness question is discussed. This relates not to the equivalence of the Dirichlet and Schrödinger approaches as formulated above, but to the question of whether the ground state determines the dynamics uniquely.

The sense in which the eigenstate ϕ determines the dynamics is apparent in the potential equation (1.3) or in the fact that given, for example, $\phi \in L^2_{\text{loc}} \neq 0$ almost everywhere and $\nabla\phi \in L^2_{\text{loc}}(\mathbb{R}^n - N)$ (N a closed null set), then the form is closable and the positive self-adjoint operator H of Eq. (1.2) is unique. This uniqueness, however, is a consequence of the implicit assumption that V is a multiplication operator or equivalently that the energy form is the closure of a form of the type (1.1). Physically this assumption makes sense if one has grounds to believe in the assumed (canonical) decomposition of the Hamiltonian. This may be the case when reconstruction from the vacuum is used in models where the fundamental dynamic laws are presumed to be known, for example, lattice QED or QCD.[9]

In (nonrelativistic) many-body problems the situation may be quite different. In nuclear physics, for example, there is often more information on the nature of the ground state than on the form of the interaction potentials. It is also true that when the fundamental forces are known but many particles are in interaction, to determine experimentally without ambiguity the ground state structure may be easier than the effective one-body potential. Even when some parts of the potential correspond to known particle exchanges, it is only the leading static contribution that can be described by a multiplication potential. Higher-order contributions have a nonlocal nature.

When detailed information on the dynamic laws is lacking, a sensible question to address is the characterization of the possible dynamics compatible with a given (zero) energy eigenstate (or a finite set of known eigenstates). Defined in such a generality the question has infinitely many nonequivalent answers. One should somehow restrict the classes of operators one uses as candidate potentials.

In the Schrödinger and the Dirichlet approaches one

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deals, respectively, with the spaces $L^2(\mathbb{R}^n,dx)$ and $L^2(\mathbb{R}^n,dv)$, $dv=\phi^2dx$, the unitary map U_ϕ between them being multiplication by ϕ^{-1}:

$$g\in L^2(\mathbb{R}^n,dx)\xrightarrow{U_\phi} g\phi^{-1}\in L^2(\mathbb{R}^2,dv).$$

A natural restriction on the operators of the theory would be to require a simple operation on the product of functions, i.e., a multiplication law

$$V(g\phi)=F[g,\phi,Vg,V\phi]. \tag{1.4}$$

From linearity it follows that F is a homogeneous function of order 2. Linear operators with a multiplication law (1.4) are called Bourlet operators and have been studied extensively.[10,11]

Under fairly general conditions it can be shown that there are three types of Bourlet operators, namely multipliers V_M, derivations V_D, and substitution operators V_H. In $\mathbb{R}$, for example,

$$(V_Mg)(x)=\omega(x)g(x),$$

$$(V_Dg)(x)=\omega(x)\frac{d}{dx}g(x)-cg(x),$$

$$(V_Hg)(x)=(1/A)g[Av(x)]+\mu g(x).$$

Unfortunately, derivation and substitution operators are not symmetric in general and their symmetrized versions no longer obey the simple multiplication law (1.4). Therefore symmetrized derivation and substitution operators will be used, but we will not be restricted to these classes only.

The plan of the paper is the following: The potential V is considered to belong to one of the following operator classes: finite rank operators, second order (Sturm–Liouville) operators, symmetrized derivations, or symmetrized substitution operators. In each case, ϕ is considered to be a (zero-) energy eigenstate of the dynamics

$$(-\tfrac{1}{2}\Delta+V)\phi=0,$$

and V is determined in the assumed class. The nature of the (reconstructed) dynamics is then characterized by spectral analysis and (or) construction of the associated stochastic process through the Beurling–Deny formula. For explicit calculations and examples one concentrates on the one-dimensional case. As an illustrative example ϕ is taken to be the harmonic oscillator wave function $e^{-x^2/2}$. One finds in all operator classes distinct dynamics that contain this ϕ as a zero-energy eigenstate.

II. FINITE RANK POTENTIALS

An operator O is of finite rank if it can be written as

$$Of=\sum_{i=1}^{N}(g_i,f)h_i, \tag{2.1}$$

where $\{g_i,h_i\}$ are $2N$ vectors in a Hilbert space. Here one considers potentials that are sums of a constant with a symmetric finite rank operator

$$V_{RN}=c+\sum_{i,j=1}^{N}|h_i\rangle b_{ij}\langle h_j|, \tag{2.2}$$

where $b_{ij}^*=b_{ji}$ and c is a constant $\geqslant 0$. Let ϕ be a zero-energy eigenstate of $H_{RN}=-\tfrac{1}{2}\Delta+V_{RN}$. The state ϕ determines the potential uniquely only if $N=1$. Then one knows that

$$H_{R1}=-\tfrac{1}{2}\Delta+c-|h\rangle\langle h|=-\tfrac{1}{2}\Delta+V_{R1}, \tag{2.3a}$$

where

$$h=(\phi,(-\tfrac{1}{2}\Delta+c)\phi)^{-1/2}(-\tfrac{1}{2}\Delta+c)\phi. \tag{2.3b}$$

[For example if ϕ is the harmonic oscillator ground state $\phi\sim\exp(-x^2/2)$, then

$$h=\{(c+\tfrac{1}{4})u_0-\sqrt{2}/4u_2\}(c+\tfrac{1}{4})^{-1/2}, \tag{2.4}$$

where

$$u_n=(\sqrt{\pi}2^n n!)^{-1/2}H_n(x)e^{-x^2/2} \tag{2.5}$$

are the normalized eigenstates of the (multiplicative) harmonic oscillator.]

The spectral properties of a Hamiltonian H_{R1} with rank-one potential are known.[6,12] It has at most one eigenvector (bound state) and because the potential is a compact perturbation of $-\tfrac{1}{2}\Delta+c$ the continuous spectrum is $[c,\infty)$.

For the harmonic oscillator example, the corresponding (local) Hamiltonian with multiplicative potential is

$$H_M=-\frac{1}{2}\frac{d^2}{dx^2}+\frac{1}{2}(x^2-1).$$

Here H_M has a pure point spectrum $\{0,1,2,\ldots\}$, whereas the rank-one potential which has u_0 as a zero-energy eigenstate has very different spectral properties.

The basic qualitative difference between local (multiplicative) and finite rank potentials, even when they share one (or several) eigenvalues, becomes clearer if one examines the corresponding stochastic processes.

A local Hamiltonian with a zero-energy eigenstate $\phi(x)$ corresponds to a diffusion process with diffusion measure $\phi^2(x)d^nx$. To characterize the stochastic process associated with H_{R1}, one compares the (energy) form $\epsilon(f,g)=(f\phi,H_{R1}g\phi)$, f and g being real functions, with the Beurling–Deny formula

$$\begin{aligned}\epsilon(f,g)&=\frac{1}{2}\int\nabla f\cdot\nabla g\phi^2\,d^nx\\&\quad+\int f\phi\{V_{R1}(g\phi)-gV_{R1}\phi\}d^nx\\&=\frac{1}{2}\int\nabla f\cdot\nabla g\phi^2\,d^nx\\&\quad-\int f(x)\phi(x)h(x)\{g(y)\\&\quad-g(x)\}h(y)\phi(y)d^nx\,d^ny.\end{aligned} \tag{2.6}$$

For comparison purposes, one writes the Beurling–Deny formula

$$\begin{aligned}\epsilon(f,g)&=\int\partial_i f\,\partial_j g\mu_{ij}(dx)\\&\quad+\int(f(x)-f(y))(g(x)-g(y))\sigma(dx,dy)\\&\quad+\int f(x)g(x)k(dx)\end{aligned} \tag{2.7}$$

as follows:

$$\epsilon(f,g)=\int\partial_i f\,\partial_j g\mu_{ij}(x)dx + \int f(x)g(x)\left\{k(x)+2\int dy\,\sigma(x,y)\right\}dx - 2\int f(x)g(y)\sigma(x,y)dx\,dy, \tag{2.8}$$

where the measures are not necessarily absolutely continuous. Notice that when comparing Eq. (2.6) with (2.8), $\sigma(x,y)$ is defined only up to $\gamma(x)\,\delta(x-y)$, where $\gamma(x)$ is an arbitrary function. To obtain the actual jumping measure density one has to extract all terms proportional to $\delta(x-y)$.

Comparing (2.6) with (2.8) one concludes that the stochastic process associated with H_{R1} has diffusion, jumping, and killing measure densities, respectively,

$$\mu_{ij}(x)=\tfrac{1}{2}\phi^2(x)\delta_{ij}, \tag{2.9a}$$

$$\sigma(x,y)=\tfrac{1}{2}\phi(x)h(x)\phi(y)h(y), \tag{2.9b}$$

$$k(x)=0, \tag{2.9c}$$

with $h(x)$ a function of $\phi(x)$ [Eq. (2.3b)].

Intuitively, one might think that if one considered a rank N potential which coincided with a local potential in its action on N distinct functions, the jumping measure would vanish in the limit $N\to\infty$. This intuition turns out to be right only under particular conditions.

Let the Hamiltonian $H_N=H_0+\Sigma_{i,j=0}^{N-1}|i\rangle b_{ij}\langle j|$ share N eigenstates $\{\phi_i,\ i=0,\ldots,N-1\}$ with the local $H=H_0+V(x)$, i.e.,

$$H_N\phi_i=H\phi_i=E_i\phi_i. \tag{2.10}$$

Then it follows[13] that H_N has the form

$$H_N=H_0+\sum_{i,j=0}^{N-1}V|\phi_i\rangle(\mathscr{V}^{-1})_{ij}\langle\phi_j|V, \tag{2.11}$$

where $\mathscr{V}^{-1}$ is the inverse of the matrix $\mathscr{V}_{ij}=\langle\phi_i|V|\phi_j\rangle$. Comparing the energy form $\epsilon(f,g)=(f\phi_0,H_N g\phi_0)$ with the Beurling–Deny formula, as before, one obtains

$$\sigma(x,y)=-\frac{1}{2}\sum_{i,j=0}^{N-1}\phi_0(x)V(x)\phi_i(x)\times(\mathscr{V}^{-1})_{ij}\phi_j(y)V(y)\phi_0(y). \tag{2.12}$$

In the $N\to\infty$ limit the jumping disappears only if $\sigma(x,y)$ becomes proportional to $\delta(x-y)$,

$$\sum_{i,j=0}^{\infty}\phi_i(x)(\mathscr{V}^{-1})_{ij}\phi_j(y)\sim\delta(x-y) \tag{2.13}$$

(which holds if $\{\phi_i\}$ is a complete orthonormal set).

So far, the stochastic process associated with the Hamiltonian operator H has meant the Markov process with transition functions leading to the same semigroup as that generated by H. The Markov transition functions represent, therefore, the behavior of the Schrödinger equation in imaginary time.

Another connection between the Schrödinger equation and probabilistic notions is established in the framework of stochastic mechanics,[14] which concerns the time evolution of the probability density $\rho(x,t)=|\psi(x,t)|^2$ in real time. Consideration of nonlocal potentials requires an extension of the stochastic mechanics formalism, which is sketched below.

From the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi=-\frac{\hbar^2}{2m}\Delta\psi+V\psi \tag{2.14}$$

and its adjoint, one obtains

$$\frac{\partial\rho}{\partial t}=-\nabla\{b\rho\}+\frac{\hbar}{2m}\Delta\rho+\mathrm{Im}\int\Sigma(x,y)\rho(y,t)d^n y, \tag{2.15}$$

where

$$b=\frac{\hbar}{m}\nabla\ln|\psi|+\frac{\hbar}{m}\nabla\arg\psi=u+v, \tag{2.16a}$$

$$(V\psi)(x)=\int V(x,y)\psi(y)d^n y, \tag{2.16b}$$

$$\Sigma(x,y)=\frac{2}{\hbar}\psi^*(x,t)V(x,y)\frac{1}{\psi^*(y,t)}, \tag{2.16c}$$

and $V(x,y)=V^*(y,x)$. From (2.16a)–(2.16c), one sees that once a solution $\psi(x,t)$ of the Schrödinger equation is known, all parameters in (2.15) are known. However, one can interpret (2.15) as the forward equation of a stochastic process and use it, together with the equations of motion for u, v, and Σ, to define the dynamics without explicit reference to the Schrödinger equation. This is the point of view of stochastic mechanics.

The equations of motion for u, v, and Σ are

$$\dot u=-\frac{\hbar}{2m}\nabla_x(\nabla_x\cdot v)-\nabla_x(u\cdot v) - \frac{\hbar}{2m}\,\mathrm{Im}\,\nabla_x\int\Sigma(y,x)d^n y, \tag{2.17a}$$

$$\dot v=\frac{1}{2}\nabla_x(u^2-v^2)+\frac{\hbar}{2m}\nabla_x(\nabla_x\cdot u) - \frac{\hbar}{2m}\,\mathrm{Re}\,\nabla_x\int\Sigma(y,x)d^n y, \tag{2.17b}$$

$$\dot\Sigma(x,y)=\Sigma(x,y)\Big[\Big\{-\frac{m}{\hbar}u\cdot v(x)-\frac{1}{2}\nabla\cdot v(x) - \frac{im}{2\hbar}(u^2(x)-v^2(x)) - \frac{i}{2}\nabla\cdot u(x)+\frac{i}{2}\int\Sigma(z,x)d^n z\Big\}-\{x\leftrightarrow y\}\Big]. \tag{2.17c}$$

In the local (multiplicative) operator case $V(x,y)=V(x)\delta(x-y)$ and the kernel Σ is

$$\Sigma_M(x,y)=(2/\hbar)V(x)\delta(x-y).$$

Then $\dot\Sigma_M(x,y)=0=\mathrm{Im}\,\Sigma_M(x,y)$ and the only contribution is the usual $(1/m)\nabla V(x)$, in the equation for $\dot v$.

For the case of the rank N potential of Eq. (2.2), the kernel has nontrivial dynamics. In terms of the solution of the Schrödinger equation, $\Sigma_{RN}(x,y)$ is

$$\Sigma_{RN}(x,y)=(2/\hbar)c\delta(x-y) + \frac{2}{\hbar}\sum_{i,j=1}^{N}\psi^*(x,t)h_i(x)b_{ij}h_j^*(y)\frac{1}{\psi^*(y,t)}. \tag{2.18}$$

III. STURM–LIOUVILLE POTENTIAL

Let the potential be a second-order differential operator with real coefficients. Symmetry restricts the operator to the general form

$$V_{SL} = -K^{ij}(x)\frac{\partial^2}{\partial x^i\,\partial x^j} - \left(\frac{\partial}{\partial x^i}K^{ij}(x)\right)\frac{\partial}{\partial x^j} + G(x), \tag{3.1}$$

with $K^{ij}(x) = K^{ji}(x)$. This is called a Sturm–Liouville operator. Some of the nonlocal potentials used in nuclear physics[15,16] are of this type.

Of particular interest are the one-dimensional and the spherically symmetric three-dimensional cases. In three dimensions, with spherical symmetry $K^{ij}(x) = K(r)\delta^{ij}$, $G(x) = G(r)$, and writing the wave function as

$$\psi(r,\theta,\phi) = (u(r)/r)Y_{lm}(\theta,\phi),$$

one obtains for the radial eigenvalue equation

$$\left\{\left(\frac{1}{2}+K(r)\right)\left(-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}\right) - \frac{dK}{dr}\frac{d}{dr}+\frac{1}{r}\frac{dK}{dr}+G(r)-E\right\}u(r)=0. \tag{3.2}$$

As before $\hbar = m = 1$, for simplicity, otherwise the factor $\frac{1}{2}+K(r)$ should be replaced by $\hbar^2/2m + K(r)$.

Let ϕ be a zero-energy eigenvalue

$$H_{SL}\phi = (-\tfrac{1}{2}\Delta + V_{SL})\phi = 0. \tag{3.3}$$

Using (3.3) to compute the energy form $\epsilon(f,g)$ one obtains

$$\epsilon(f,g) = (f\phi, H_{SL}g\phi) = \int \partial_i f\left\{\frac{1}{2}\delta^{ij}+K^{ij}(x)\right\}\partial_j g\,\phi^2\,d^n x. \tag{3.4}$$

Hence, in the Sturm–Liouville case, the associated stochastic process is (as in the multiplication potential case) a pure diffusion with a (modified) diffusion measure density

$$\mu_{ij}(x) = \{\tfrac{1}{2}\delta^{ij} + K^{ij}(x)\}\phi^2(x). \tag{3.5}$$

This refers to the stochastic process associated with the imaginary time Schrödinger equation. In real time, the equation of motion for the probability density $\rho(x,t) = |\phi(x,t)|^2$, Eq. (2.15), is in this case

$$\frac{\partial\rho}{\partial t} = -\partial_i\{b^i\rho\} + \partial_i\{\nu^{ij}(x)\partial_j\rho\}, \tag{3.6}$$

with

$$b^i = \frac{2}{\hbar}\left(\frac{\hbar^2}{2m}\delta^{ij}+K^{ij}(x)\right)(\partial_j \arg\psi + \partial_j \ln|\psi|) \tag{3.7a}$$

$$\nu^{ij} = \frac{1}{\hbar}\left(\frac{\hbar^2}{2m}\delta^{ij}+K^{ij}(x)\right), \tag{3.7b}$$

i.e., a generalized Fokker–Planck equation with a space dependent diffusion.

Nonlocalities of the Sturm–Liouville type are relatively mild in the sense that the stochastic processes associated with imaginary time evolution and with the stochastic mechanics description are both generalized diffusions.

Nonlocal potentials of the type studied in this section can be transformed to a form which may be handled by the same computational techniques as local potentials. For the one-dimensional (or the radial) equation one performs the transformation[17]

$$\psi = (\tfrac{1}{2}+K)^{-1/2}\chi \tag{3.8}$$

in

$$\left\{-\left(\frac{1}{2}+K\right)\frac{d^2}{dx^2} - K'\frac{d}{dx}\right\}\psi + G\psi = E\psi \tag{3.9}$$

to obtain

$$-\chi'' + \left\{\left(G+\frac{K''}{2}-E\right)\left(\frac{1}{2}+K\right)^{-1} - \frac{K'^2}{4}\left(\frac{1}{2}+K\right)^{-2}\right\}\chi = 0. \tag{3.10}$$

The nonlocal eigenvalue problem is therefore transformed into the search for the zero-energy eigenvalue of a local energy-dependent potential.

The requirement (3.3) that ϕ be a zero-energy eigenstate leads to an equation

$$\partial_j\phi\,\partial_i K^{ij} + \partial_i\,\partial_j\phi K^{ij} = G\phi - \tfrac{1}{2}\Delta\phi, \tag{3.11}$$

which for each ϕ, determines $G(x)$ once $K^{ij}(x)$ is fixed, or conversely.

To learn about the nature of the dynamics that are reconstructed when nonlocalities of the Sturm–Liouville type are chosen, one analyzes briefly the one-dimensional case.

Let ϕ be the harmonic oscillator ground state $\exp\{-x^2/2\}$.

When $K(x)$ is a constant (K) the coefficient of d/dx in (3.1) vanishes and H_{SL} with $G(x)$ obtained from (3.11) is simply the Hamiltonian of a harmonic oscillator multiplied by the factor $(1+2K)$. The eigenstates are the same, with the scale factor $(1+2K)$ multiplying the eigenvalues.

A nonconstant $K(x)$ may be interpreted as a description of space inhomogeneity of the oscillator parameters. Defining

$$m(x) = (1+2K(x))^{-1}, \tag{3.12}$$

one rewrites Eq. (3.9) as

$$\left\{-\frac{1}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{1}{dx}\right)+G(x)\right\}\psi = E\psi, \tag{3.13}$$

which can be interpreted as describing the motion of a variable mass particle in the potential $G(x)$. However, if dm/dx is large this intuitive interpretation may be misleading because the contribution of the derivative terms may become more important than the static potential $G(x)$.

With the same zero-energy eigenstate, one can associate very many distinct Sturm–Liouville operators. For example both

$$K = x^2;\quad G = x^4 - \tfrac{5}{2}x^2 - \tfrac{1}{2} \tag{3.14}$$

and

$$K = \tfrac{1}{2}(e^{x^2}-1);\quad G = -\tfrac{1}{2}(x^2+1)e^{x^2} \tag{3.15}$$

have $\phi = e^{-x^2/2}$ as a zero-energy eigenstate, although their static potentials are quite different. In (3.14) it is a double well, whereas in (3.15) the static potential is not bounded from below. However, in (3.15) the derivative part of the potential is sufficiently strong to overcome the static negative unbounded contribution. In particular it is easy to prove

that the negative real axis belongs to the resolvent set.

The Hamiltonian operator associated with the choice (3.15) is

$$H_{SL} = -\frac{1}{2} e^{x^2}\left(x+\frac{d}{dx}\right)^2 = -\frac{1}{2} e^{x^2/2}\frac{d^2}{dx^2} e^{x^2/2}. \quad (3.16)$$

This operator is, at least from a mathematical point of view, sufficiently interesting to deserve further study. H_{SL} is symmetric in $C_0^\infty(\mathbb{R})$ and commutes with complex conjugation. By von Neumann's theorem[18] it has self-adjoint extensions, which one characterizes by specifying the boundary conditions at $\pm\infty$. From

$$\int \psi_2^* H_{SL}\psi_1\, dx = \int (H_{SL}\psi_2)^*\psi_1\, dx - \frac{1}{2} e^{x^2/2}\left\{\psi_2^*\frac{d}{dx}(e^{x^2/2}\psi_1) - \frac{d}{dx}(e^{x^2/2}\psi_2)^*\psi_1\right\}\Big|_{-\infty}^{\infty}$$

one is led to define the following domain for the self-adjoint extensions:

$$D(H_{SL}^{(\theta)}) = \left\{\psi \in L^2 \mid H_{SL}\psi \in L^2;\ \lim_{x\to\infty} e^{x^2/2}\psi = e^{i\theta}\lim_{x\to-\infty} e^{x^2/2}\psi,\ \lim_{x\to\infty}\frac{d}{dx}(e^{x^2/2}\psi) = e^{i\theta}\lim_{x\to-\infty}\frac{d}{dx}(e^{x^2/2}\psi)\right\}. \quad (3.17)$$

Requiring $\phi = e^{-x^2/2}$ to be an eigenstate one is led to choose the self-adjoint extension $H_{SL}^{(0)}$. Notice that H_{SL} has a two-dimensional subspace of zero energy eigenstates, namely $(c_1 x + c_2)e^{-x^2/2}$. The choice of a particular self-adjoint extension selects one vector in this subspace.

The negative real axis belongs to the resolvent set of $H_{SL}^{(0)}$ and there is a point spectrum contained in $[0,\infty)$. This analysis is divided into two parts.

A. $\forall\lambda<0$, $\lambda\notin\sigma(H_{SL}^{(0)})$

According to Weyl's criterion $\lambda\in\sigma(H_{SL}^{(0)})$ if and only if there is a sequence ψ_n in $D(H_{SL}^{(0)})$, with $\|\psi_n\| = 1$, such that $\lim_{n\to\infty}\|(H_{SL}^{(0)} - \lambda)\psi_n\| = 0$.

Defining

$$\psi_n = e^{-x^2/2}\gamma_n, \quad (3.18)$$

and using the boundary conditions in $D(H_{SL}^{(0)})$ to perform the partial integrations, one obtains

$$\|(H_{SL}^{(0)} - \lambda)\psi_n\|^2 = \int dx\left\{\frac{e^{x^2}}{4}|\gamma_n''|^2 - \lambda|\gamma_n'|^2 + \lambda^2 e^{-x^2}|\gamma_n|^2\right\}.$$

If $\lambda<0$, the right-hand side is a sum of positive quantities and is $\neq 0$ because

$$\int dx\, e^{-x^2}|\gamma_n|^2 = \|\psi_n\| = 1.$$

Therefore any $\lambda<0$ belongs to the resolvent set of $H_{SL}^{(0)}$.

B. $\lambda\geqslant 0$

Using (3.18) one writes

$$(H_{SL}^{(0)} - \lambda)\psi_n = e^{x^2/2}\left\{-\frac{1}{2}\frac{d^2}{dx^2} - \lambda e^{-x^2}\right\}\gamma_n. \quad (3.19)$$

The question of whether λ belongs to the spectrum of $H_{SL}^{(0)}$ is therefore related to the zero eigenvalue problem for the operator

$$B_\lambda = -\frac{1}{2}\frac{d^2}{dx^2} - \lambda e^{-x^2}.$$

Because λe^{-x^2} is an L^2 perturbation, $\sigma_{ess}(B_\lambda) = \sigma_{ess}(-d^2/dx^2)$, which implies $0\in\sigma(B_\lambda)$. Because zero is in the spectrum of B_λ, there is a sequence γ_n with $\|\gamma_n\| = 1$ such that $\|B_\lambda\gamma_n\|\to 0$. However this does not guarantee that $\|e^{x^2/2}B_\lambda\gamma_n\|\to 0$, nor that $\|e^{-x^2/2}\gamma_n\|$ remains $\neq 0$ in the $n\to\infty$ limit.

Instead, one analyzes directly the equation

$$\left\{\frac{d^2}{dx^2} + 2\lambda e^{-x^2}\right\}\gamma(x) = 0. \quad (3.20)$$

In a neighborhood of $\pm\infty$, this equation has an asymptotic solution $\alpha_\pm x + \beta_\pm$. If one requires that $\psi = e^{-x^2/2}\gamma\in D(H_{SL}^{(0)})$, then $\alpha_\pm = 0$ and $\beta_+ = \beta_-$.

Fix $\gamma\to\beta_-$ and $\gamma'\to 0$ when $x\to-\infty$ as initial conditions. Because e^{-x^2} is continuous in $(-\infty,\infty)$ the existence–uniqueness theorem for second-order linear homogeneous equations[19] implies, for any λ, the existence of a solution to (3.20), which at $x\to+\infty$ grows at most linearly. Therefore, the problem $(H_{SL}^{(0)} - \lambda)\psi = 0$ has an L^2 solutions for any λ. This does not imply that all λ's are in the spectrum because in general ψ will not belong to the domain $D(H_{SL}^{(0)})$. ψ is in $D(H_{SL}^{(0)})$ only if $\lim_{x\to\infty}\gamma(x) = \beta_-$. The λ values for which this condition holds are the elements of the point spectrum of $H_{SL}^{(0)}$. Below, the first seven such values obtained by numerical integration of (3.20) are listed:

0 4.33 15.07 32.14

55.52 85.21 121.19 ...

Qualitatively they follow the same pattern as $\lambda\sim\pi n^2$, which is obtained from the semiclassical approximation

$$\gamma(x)\sim\cos\int_{-\infty}^{x}\sqrt{2\lambda}\, e^{-\eta^2/2}d\eta.$$

IV. SYMMETRIZED DERIVATION

The potential that is to be studied in this section is required to have the form

$$V_D = \left\{a(x), i\frac{\partial}{\partial x}\right\}_+ + W(x) = 2ia(x)\frac{\partial}{\partial x} + i\frac{da}{dx} + W(x), \quad (4.1)$$

where $a(x)$ and $W(x)$ are real functions in $\mathbb{R}$.

Let $\phi(x)$ be a real zero energy eigenstate

$$H_D\phi = \left(-\frac{1}{2}\frac{d^2}{dx^2} + V_D\right)\phi = 0.$$

Then one obtains

$$a(x) = (c/2)\phi^{-2}(x), \tag{4.2a}$$

$$W(x) = \frac{1}{2\phi(x)}\frac{d^2\phi}{dx^2}, \tag{4.2b}$$

c being an arbitrary constant. For the harmonic oscillator ground state $\phi = e^{-x^2/2}$,

$$V_D = \frac{c}{2}\left\{e^{x^2}, i\frac{\partial}{\partial x}\right\}_+ + \frac{1}{2}(x^2-1)$$
$$= cie^{x^2}\left(x + \frac{d}{dx}\right) + \frac{1}{2}(x^2-1). \tag{4.3}$$

Even when c is small the term $c[e^{x^2}, i(\partial/\partial x)]_+$ cannot be considered a perturbation of the (multiplicative) harmonic oscillator, because the operator V'

$$V' = ie^{x^2}\left(x + \frac{\partial}{\partial x}\right) = e^{x^2/2} i\frac{d}{dx} e^{x^2/2} \tag{4.4}$$

has divergent matrix elements in the $\{u_n\}$ basis. More precisely, except for u_0 all other u_n's are not in the domain of V':

$$V'u_n = ie^{x^2}\sqrt{2n}\,u_{n-1} \notin L^2(\mathbb{R}), \quad \text{if } n \neq 0.$$

The operator $H_D = -\frac{1}{2}(d^2/dx^2) + V_D$ is symmetric in $C_0^\infty(\mathbb{R})$ and unitarily equivalent (see below) to a real potential. It has a one-parameter family of self-adjoint extensions which one characterizes by the boundary conditions at $\pm\infty$. From

$$\int \psi_2^* ie^{x^2}\left(x + \frac{d}{dx}\right)\psi_1\, dx$$
$$= i\psi_2^* e^{x^2}\psi_1\Big|_{-\infty}^{\infty} + \int\left[ie^{x^2}\left(x + \frac{d}{dx}\right)\psi_2\right]^*\psi_1\, dx$$

one obtains the following domains for the self-adjoint extensions

$$D(H_D^{(\theta)}) = \{\psi \in L^2 \mid H_D\psi \in L^2,$$
$$\lim_{x\to\infty} e^{x^2/2}\psi = e^{i\theta}\lim_{x\to-\infty} e^{x^2/2}\psi\}. \tag{4.5}$$

The self-adjoint extension that contains $e^{-x^2/2}$ in its domain, as required, is $H_D^{(0)}$. Although it shares this zero energy eigenstate with the harmonic oscillator, the dynamic is otherwise of a completely different nature. This becomes apparent if one considers the isometric map

$$\psi(x) \to (U_c\psi)(x) = \exp\left\{-ic\int_0^x e^{\xi^2}\, d\xi\right\}\psi(x). \tag{4.6}$$

Then

$$H' = U_c H_D U_c^{-1} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(x^2-1) - \frac{c^2}{2}e^{2x^2} \tag{4.7}$$

is the harmonic oscillator Hamiltonian plus a negative unbounded potential.

To H_D is associated a singular jumping measure. Computing the energy form $\epsilon(f,g) = (f\phi, H_D g\phi)$ and comparison with the Beurling–Deny formula as in (2.6)–(2.8) leads to

$$\mu_{ij}(x) = \tfrac{1}{2}\phi^2(x)\delta_{ij}, \tag{4.8a}$$

$$\sigma(x,y) = (-ic/2)\delta'(x-y), \tag{4.8b}$$

$$k(x) = 0. \tag{4.8c}$$

The kernel $\Sigma_D(x,y)$ for the stochastic mechanics equation (2.15) is

$$\Sigma_D(x,y) = \frac{2}{\hbar}\left\{W(x) + i\frac{da}{dx} - 2ia(x)\frac{d}{dx}\ln\psi^*(x)\right\}\delta(x-y)$$
$$+ \frac{4}{\hbar}ia(x)\delta'(x-y). \tag{4.9}$$

V. POTENTIALS WITH SUBSTITUTION OPERATORS

Symmetrized substitution operators may also be of some interest in the description of effective nuclear interactions.[20] They have the general form

$$(V_s\psi)(x) = \frac{1}{\omega(x)}\psi(\nu(x))$$
$$+ \frac{1}{\omega^*(\nu^{-1}(x))}\left(\frac{d\nu^{-1}}{dx}\right)^*\psi(\nu^{-1}(x)) + q(x)\psi(x). \tag{5.1}$$

Using $H_s\phi = (-\frac{1}{2}\Delta + V_s)\phi = 0$ one can, as before, compute the energy form $\epsilon(f,g) = (f\phi, H_s g\phi)$ and compare with the Beurling–Deny formula to obtain for the diffusion, jumping, and killing

$$\mu_{ij}(x) = \tfrac{1}{2}\phi^2(x)\delta_{ij}, \tag{5.2a}$$

$$\sigma(x) = -\frac{1}{2}\left\{\frac{1}{\omega(x)}\delta(y-\nu(x))\right.$$
$$\left. + \frac{1}{\omega^*(y)}\left(\frac{d\nu^{-1}}{dx}\right)^*\delta(y-\nu^{-1}(x))\right\}\phi(x)\phi(y), \tag{5.2b}$$

$$k(x) = 0. \tag{5.2c}$$

Example: Let $\phi = e^{-x^2/2}$, $\omega(x) = 1$, and the substitution function be a translation $\nu(x) = x + b$.

Then

$$q(x) = \tfrac{1}{2}(x^2-1) - 2e^{-b^2/2}\cosh bx. \tag{5.3}$$

Because the translation operators can be written in differential form, the Hamiltonian is

$$H_s = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(x^2-1) + 2\cosh\left(b\frac{d}{dx}\right)$$
$$- 2e^{-b^2/2}\cosh bx. \tag{5.4}$$

From the fact that $H_s u_n \in L^2$ it follows that, in principle and for small b, the two last terms in (5.4) can be treated as a perturbation. From

$$H_s = (1-2b^2)\left\{-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(x^2-1)\right\} + O(b^4),$$

one concludes that in leading order the effect of the perturbation is a scale change in the harmonic oscillator spectrum.

VI. RECONSTRUCTION FROM A STOCHASTIC PROCESS

If $\epsilon(f,g)$ is a closed positive symmetric form densely defined in $L^2(\Omega, d\mu)$ ($\Omega \subset \mathbb{R}^n$ open) there is a unique self-adjoint operator $\hat{H}$ such that $\epsilon(f,g) = (\hat{H}^{1/2}f, \hat{H}^{1/2}g)_{d\mu}$, where $(\cdot)_{d\mu}$ is the scalar product in $L^2(\Omega, d\mu)$. Here one is concerned not with $\hat{H}$ but with the operator H in the corresponding Schrö-

dinger form. Given a (Dirichlet) form by its measure densities, H is an operator such that

$$\epsilon(f,g) = (f,\hat{H}g)_{d\mu} = (\psi_f, H\psi_g)_{dx}, \tag{6.1}$$

where dx denotes the "flat" Lebesgue measure, and ψ_f, ψ_g are related to f,g by unitary equivalence.

Let ϵ be defined as in (2.7) by the measure densities $\mu_{ij}(x)$, $\sigma(x,y)$, $k(x)$, and

$$H = -\tfrac{1}{2}\Delta + V. \tag{6.2}$$

Assume that $\mu_{ij}(x) = \mu(x)\delta_{ij}$ and $\mu(x) > 0$ everywhere. The states in $L^2(\Omega,d\mu)$ and $L^2(\Omega,dx)$ are related by

$$f \xrightarrow{U_\mu} \psi_f = f\sqrt{2\mu}, \tag{6.3}$$

thus one obtains by a straightforward calculation using (6.1) and (2.8)

$$(V(\mu,\sigma,k)\psi)(x) = \left[\frac{1}{2}\frac{\Delta\sqrt{2\mu(x)}}{\sqrt{\mu(x)}} + \frac{1}{2\mu(x)}\left\{k(x) + 2\int \sigma(x,y)d^n y\right\}\right]\psi(x) - \int \frac{\sigma(x,y)}{\sqrt{\mu(x)\mu(y)}}\psi(y)d^n y. \tag{6.4}$$

From (6.4) it would seem that nonlocal potential effects can only be associated to the jumping measure. However one should notice that the potential in (6.2) is not uniquely defined, it depends on the choice of the unitary transformation U between $L^2(\Omega,d\mu)$ and $L^2(\Omega,dx)$. Let us decompose $\mu(x) = \alpha(x) + \beta(x)$ where now one requires only $\alpha(x) > 0$. Using now

$$f \xrightarrow{U_\alpha} \psi_f = f\sqrt{2\alpha}, \tag{6.5}$$

one obtains for the potential in (6.2)

$$V = V(\alpha,\sigma,k) - \frac{\beta}{2\alpha}\Delta - \nabla\left(\frac{\beta}{2\alpha}\right)\cdot\nabla - \frac{1}{\sqrt{2\alpha}}\nabla\cdot\left(\beta\nabla\frac{1}{\sqrt{2\alpha}}\right). \tag{6.6}$$

The nonlocal part in (6.6) that is not related to the jumping measure is of the Sturm–Liouville type.

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Continued fractions and Rayleigh–Schrödinger perturbation theory at large order

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Concern with the continued fraction representations of divergent Rayleigh–Schrödinger perturbation expansions in quantum mechanics is expressed. The following relation between the large-order behavior of the continued fraction coefficients c_n and the perturbation series coefficients $E^{(n)}$ is shown to exist: If $E^{(n)} \sim (-1)^{n+1}\Gamma(pn+a)$, $p = 0,1,2,...$, as $n \to \infty$, then $c_n = O(n^p)$ as $n \to \infty$. The case $p = 1$ is studied in detail here, using the problems of the quartic anharmonic oscillator and the hydrogen atom in a linear radial potential as illustrative examples. For $p = 1$ the asymptotics of the c_n are shown to be linked to the infinite field limit $E(\lambda) \sim F^{(0)}\lambda^{\alpha}$, predicting α and providing convergent estimates of $F^{(0)}$.

I. INTRODUCTION AND MOTIVATION

Perturbation methods have been an indispensible tool of applied mathematics and theoretical physics. The fundamental work of Lord Rayleigh[1] and of Schrödinger[2] provided a basis for the important quantum mechanical perturbation that bears their names. Suppose that we have a quantum mechanical system characterized by a Hamiltonian operator $\hat{H}^{(0)}$ with known energy eigenvalues $E_m^{(0)}$. Now let this system be perturbed, for example, by an external magnetic field, so that it is now represented by the Hamiltonian $\hat{H}(\lambda) = \hat{H}^{(0)} + \lambda\hat{V}$, where $\hat{V}$ represents the perturbation and λ, the coupling constant, represents its strength. The question is, "What are the eigenvalues $E_m(\lambda)$, if any, of $\hat{H}(\lambda)$?" Generally, the perturbed eigenvalue problem is not exactly solvable and approximation methods must be employed. Rayleigh–Schrödinger perturbation theory (RSPT) represents the unknown energy (and wave function) as a Taylor series in the coupling constant

$$E(\lambda) = E^{(0)} + \sum_{n=1}^{\infty} E^{(n)}\lambda^n . \tag{1.1}$$

The expansion coefficients $E^{(n)}$ are determined by well defined procedures. One of the questions of large-order perturbation theory (LOPT) is, "How do the $E^{(n)}$ behave as $n \to \infty$?"

Traditionally, physicists and chemists have been content to compute perturbation expansions to only one or two terms, for a number of reasons. In most situations, this number of terms is sufficient to remove any degeneracy of the unperturbed problem, so the physics associated with the perturbation has been revealed. Moreover, in most laboratory applications, $\lambda \ll 1$ and these terms provide good estimates of $E(\lambda)$. Another reason is that the calculation of higher-order terms, even for simple systems such as the hydrogen atom, may be very tedious. However, developments over the last twenty years have changed the status of perturbation calculations. In many physical situations, e.g., intense magnetic fields observed on the surfaces of neutron stars, the coupling constant may assume values reaching several orders of magnitude. In addition, computers have made it possible to calculate perturbation expansions for a variety of simple quantum mechanical problems to large order. Some of the oldest perturbation problems of nonrelativistic quantum mechanics, e.g., the anharmonic oscillator, the Stark and quadratic Zeeman effects in hydrogen, have been found to yield divergent perturbation series. Only relatively recently was the perturbation expansion of the classical quartic anharmonic oscillator studied in detail by Bender and Wu,[3–5] Loeffel *et al.*,[6] Simon,[7] and others. Since then, LOPT, concerned with the nature of these expansions and their summability, has evolved into an intense and ongoing area of research in mathematical, theoretical, as well as atomic and molecular physics.[8] Much of the stimulus for this research has come from quantum field theory where perturbation methods are essential. Simple perturbation problems of nonrelativistic quantum mechanics, such as those mentioned above, are similar in nature to the problems encountered in field theory. For example, the problems of the hydrogen molecule-ion and double-welled oscillators are of relevance to quantum field theories with degenerate vacuum states. Many such problems have revealed a rich mathematical structure and provide excellent testing grounds for the development of efficient and accurate summability methods.

Many of the perturbation expansions encountered in theoretical physics are divergent and their large-order behavior is given typically by

$$E^{(n)} \sim (-1)^{n+1} A\Gamma(pn+a)k^n , \quad \text{as } n \to \infty , \tag{1.2}$$

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where A, p, a, and k are constants. Titchmarsh[9] and Kato[10] showed many years ago that such nonconvergent expansions may still be asymptotic. In special cases the perturbation expansions may be shown to be rigorously Borel summable or, in the case of Stieltjes series, Padé summable.[11]

In this paper, we focus on continued fraction (CF) representations of the RS perturbation series in Eq. (1.1) and (1.2), having the form

$$E(\lambda) = E^{(0)} + \lambda C(\lambda)$$
$$= E^{(0)} + \cfrac{c_1\lambda}{1 + \cfrac{c_2\lambda}{1 + \cfrac{c_3\lambda}{1 + \ddots}}} \tag{1.3}$$

The function $C(z)$ is referred to as a RITZ (rotation-inversion-translation-z) fraction.[12] More specifically, we are concerned with the large-order behavior of the c_n, which shall be abbreviated as CFLO (continued fractions at large order).

The continued fraction representations of some standard perturbation expansions whose coefficients exhibit the asymptotic behavior in (1.2) demonstrate two noteworthy features: (1) all $c_n > 0$, hence $C(\lambda)$ is a Stieltjes fraction,[12] a consequence of the Stieltjes nature of the perturbation series, and (2) $c_n \sim Dn^{\rho}$, as $n \to \infty$, where D is a constant. For convenience, we refer to such continued fractions as $S_{(\rho)}$ fractions. The function $E(\lambda)$ is typically analytic in the cut plane $\tilde{\mathbb{C}} = \{\lambda : |\arg\lambda| < \pi\}$, and for $\rho \leqslant 2$, the expression in Eq. (1.3) converges to $E(\lambda)$ uniformly on compact subsets of $\tilde{\mathbb{C}}$. In this way, the S fraction is seen to be a much more natural representation of $E(\lambda)$ than its perturbation series counterpart.

In an earlier study,[13] this gross asymptotic connection was numerically exploited to provide very good estimates of the eigenvalue $E(\lambda)$ for rather high values of the coupling constant λ; in other words, to serve as an effective numerical summability method. Since that report, the asymptotic relation between LOPT and CFLO has been refined for a number of problems yielding $S_{(1)}$ fraction representations.[14–16] Asymptotic analysis reveals that significant information is encoded in these CF representations.

The organization of this paper is as follows: In Sec. II are presented the main features of RITZ continued fractions and their representations of formal power series, S fractions, and the Stieltjes moment problem. In Sec. III, Simon's theory of the Stieltjes nature of perturbation expansions is outlined along with a synopsis of the Bender–Wu method of determining the large-order behavior of the coefficients $E^{(n)}$. The connection between CFLO and LOPT is then discussed. In Sec. IV we look at the $S_{(1)}$ fraction representations afforded by two well-known perturbation problems: the quartic anharmonic oscillator and the hydrogen atom in a linear radial potential. The large-λ behavior for a particular class of $S_{(1)}$ fractions, including the examples cited above, is shown in Sec. V to be related to the asymptotics of the c_n. This in turn implies a relationship between CFLO and the infinite field expansion of the perturbation problem concerned. Specifically, if the infinite field expansion has the form $E(\lambda) \sim F^{(0)}\lambda^{\alpha}$, as $\lambda \to \infty$, and the c_n behave asymptotically as $c_n \sim \frac{1}{2}kn + A^{(i)} + o(1)$, as $n \to \infty$, where $i = (1,2)$, if n is (even,odd), then $\alpha = \frac{1}{2} - (A^{(1)} - A^{(2)})/k$. Moreover, asymptotic expansions of the $S_{(1)}$ fraction representations afford converging estimates of the leading coefficient $F^{(0)}$. The examples cited above will be analyzed in Sec. VI to show that a simple relationship analogous to feature (2) does not exist for subdominant terms in the CFLO and LOPT expansions. We mention that some of these results were announced in a preliminary report.[15]

II. RITZ CONTINUED FRACTION REPRESENTATIONS OF FORMAL POWER SERIES

A. RITZ fractions

In this section are outlined some important properties of the RITZ fractions defined in Eq. (1.3). Theorems are presented here without proof. Discussions and proofs can be found in the standard texts on continued fractions[17–19] and Padé approximants.[20,21] The book by Henrici[12] contains a presentation of RITZ and S fractions most relevant to this study.

The continued fraction function in Eq. (1.3), $C(z)$: $\mathbb{C} \to \mathbb{C}$, which we write in the following fashion:

$$C(z) = \cfrac{c_1}{1 + \cfrac{c_2 z}{1 + \cfrac{c_3 z}{1 + \cdots}}}, \tag{2.1}$$

and abbreviate as

$$C(z) = z^{-1} \mathop{\mathrm{K}}_{n=1}^{\infty} \frac{c_n z}{1},$$

is referred to as a RITZ (rotation-inversion-translation-z) fraction since it may be formally defined as a composition of linear fractional transformations with complex parameter z. If $C(z)$ is a *terminating fraction*, i.e., $c_k = 0$ for $k > n$, then it is a rational function of z. If $C(z)$ is *nonterminating*, which is to be assumed throughout the course of this paper, it may be truncated by setting $c_k = 0$, $k > n$, to produce a set of rational functions, $w_n(z)$, the nth *convergents* or *approximants* to $C(z)$,

$$w_n(z) = \cfrac{c_1}{1 + \cfrac{c_2 z}{1 + \cfrac{c_3 z}{1 + \cdots + \cfrac{c_n z}{1}}}}$$
$$= \frac{A_n(z)}{B_n(z)}. \tag{2.2}$$

The polynomials $A_n(z)$ and $B_n(z)$ are the nth *numerator and denominator*, respectively, of $C(z)$. They satisfy the recurrence relations

$$A_n(z) = A_{n-1}(z) + c_n z A_{n-2}(z),$$
$$B_n(z) = B_{n-1}(z) + c_n z B_{n-2}(z), \quad n = 2,3,4,\ldots, \tag{2.3}$$

with initial values $A_0 = 0$, $B_0 = 1$, $A_1 = c_1$, $B_1 = 1$. Moreover, it may easily be shown that $L = \deg\{A_n(z)\} = [(n-1)/2]$ and $M = \deg\{B_n(z)\} = [n/2]$, where $[x]$ denotes the greatest integer contained in x. If we let a_{nj}, $0 \leqslant j \leqslant L$, and b_{nk}, $0 \leqslant k \leqslant M$, represent the coefficients of x^j and x^k in the polynomials $A_n(z)$ and $B_n(z)$, respectively, then Eq. (2.3) implies the recurrence relations

$$a_{nj} = a_{n-1,j} + c_n a_{n-2,j-1}, \quad j = 0,1,\ldots,[(n-1)/2],$$
$$b_{nj} = b_{n-1,j} + c_n b_{n-2,j-1}, \quad j = 0,1,\ldots,[n/2], \tag{2.4}$$

TABLE I. Numerator and denominator polynomial coefficients a_{nj} and b_{nj} of the RITZ fraction convergents $w_n(z)$ defined in Eq. (2.2). These coefficients are expressed in terms of the RITZ fraction coefficients c_n and obey the recursion relations in Eq. (2.4).

a_{nj}

n \ j	0	1	2	3
1	c_1			
2	c_1			
3	c_1	c_1c_3		
4	c_1	$c_1c_3 + c_1c_4$		
5	c_1	$c_1c_3 + c_1c_4 + c_1c_5$	$c_1c_3c_5$	
6	c_1	$c_1c_3 + c_1c_4 + c_1c_5 + c_1c_6$	$c_1c_3c_5 + c_1c_3c_6 + c_1c_4c_6$	
7	c_1	$c_1c_3 + c_1c_4 + c_1c_5 + c_1c_6 + c_1c_7$	$c_1c_3c_5 + c_1c_3c_6 + c_1c_4c_6 + c_1c_3c_7 + c_1c_4c_7 + c_1c_5c_7$	$c_1c_3c_5c_7$

b_{nj}

n \ j	0	1	2	3
1	1			
2	1	c_2		
3	1	$c_2 + c_3$		
4	1	$c_2 + c_3 + c_4$	c_2c_4	
5	1	$c_2 + c_3 + c_4 + c_5$	$c_2c_4 + c_2c_5 + c_3c_5$	
6	1	$c_2 + c_3 + c_4 + c_5 + c_6$	$c_2c_4 + c_2c_5 + c_3c_5 + c_2c_6 + c_3c_6 + c_4c_6$	$c_2c_4c_6$
7	1	$c_2 + c_3 + c_4 + c_5 + c_6 + c_7$	$c_2c_4 + c_2c_5 + c_3c_5 + c_2c_6 + c_3c_6 + c_4c_6 + c_2c_7 + c_3c_7 + c_4c_7 + c_5c_7 + c_6c_7$	$c_2c_4c_6 + c_2c_4c_7 + c_2c_5c_7 + c_3c_5c_7$

where $a_{00} = 0$, $b_{00} = 1$; $a_{0i} = b_{0i} = 0$, for $i > 0$; $a_{10} = c_1$, $b_{10} = 1$. Clearly, these polynomial coefficients are expressible solely in terms of the CF coefficients c_n. Closed-form expressions for $n \leqslant 7$ are presented in Table I.

Theorem 2.1: For each convergent $w_n(z)$ of $C(z)$, the polynomials $A_n(z)$ and $B_n(z)$ have no common zeroes.

The continued fraction $C(z)$ is said to *converge* at a point z_0 if $\lim_{n\to\infty} w_n(z_0)$ exists and is finite. Theorems which relate the regions of convergence of $C(z)$ to the behavior of the c_n are given in Refs. 17–20.

B. RITZ fractions and corresponding power series

Clearly, the approximants $w_n(z)$ in Eq. (2.2) are rational functions analytic at $z = 0$. The following theorem is important in establishing a correspondence between RITZ fractions and formal power series.

Theorem 2.2: The first n terms of the Taylor series expansions of $w_{n+k}(z)$, $k = 0,1,2,\ldots$ are identical.

The formal power series,

$$P(z) = a_0 + a_1 z + a_2 z^2 + \cdots, \tag{2.5}$$

and the continued fraction $C(z)$ are said to correspond to each other if

$$P(z) - w_n(z) = O(z^n). \tag{2.6}$$

From Eq. (2.3) this is equivalent to the condition

$$P(z) - A_n(z)/B_n(z) = O(z^{L+M+1}), \tag{2.7}$$

which is precisely the relation defining the unique $[L,M]$ Padé approximant[20,21]

$$[L,M](z) = \frac{p_0 + p_1 z + \cdots + p_L z^L}{1 + q_1 z + \cdots + q_M z^M}, \tag{2.8}$$

to the series $P(z)$. Thus $w_{2N}(z) = [N-1,N](z)$ and $w_{2N+1}(z) = [N,N](z)$ so that the sequence $\{w_n(z)\}_{n=0}^{\infty}$ generates a stepwise descent of the Padé table of $P(z)$.

Remarks: There is an immediate computational advantage afforded by RITZ representations over their Padé counterparts—a *single* sequence of RITZ coefficients c_n generates the two diagonal Padé sequences. In order to move from $w_{2N}(z)$ to $w_{2N+1}(z)$, we need only add the coefficient c_{2N+1} to the sequence $\{c_n\}_{n=1}^{2N}$. As will be shown below, this computation requires the additional series coefficient a_{2N}. This is not the situation for Padé approximants, where a new set of $L + M + 1$ coefficients need to be calculated for each $[L,M]$ Padé.

Theorem 2.3: A necessary and sufficient condition for the existence of a unique RITZ fraction representation $C(z)$ of the formal power series in Eq. (2.5) is that $P(z)$ be *normal*, i.e., that the Hankel determinants defined by $H_0^{(0)} = 1$ and

$$H_k^{(n)} = \begin{vmatrix} a_n & a_{n+1} & \cdots & a_{n+k-1} \\ a_{n+1} & a_{n+2} & \cdots & a_{n+k} \\ \vdots & \vdots & & \vdots \\ a_{n+k-1} & a_{n+k} & \cdots & a_{n+2k-2} \end{vmatrix} \tag{2.9}$$

satisfy $H_k^{(n)} \neq 0$ for $n = 0,1$ and $k = 1,2,\ldots$. The CF coefficients c_n are then given by $c_1 = a_0$ and

$$\begin{aligned} c_{2m} &= -H_m^{(1)} H_{m-1}^{(0)} / H_{m-1}^{(1)} H_m^{(0)}, \\ c_{2m+1} &= -H_{m+1}^{(0)} H_{m-1}^{(1)} / H_m^{(0)} H_m^{(1)}. \end{aligned} \tag{2.10}$$

These equations are quite unsuitable for numerical computation of the CF coefficients, however. As in the case of

Padé approximants, the evaluation of such determinants is tedious and very sensitive to the roundoff error associated with fixed point arithmetic. There exist a number of simpler, but also numerically unstable, algorithms which exploit, either directly or indirectly, the relationships between neighboring Hankel determinants to calculate the c_n. We now outline the *quotient-difference* (QD) algorithm of Rutishauser,[22] which has been employed in this study. The notation scheme employed here differs slightly from the usual one presented in books.[12,17,23]

For the power series $P(z)$ defined in Eq. (2.5), the QD algorithm defines the two-dimensional sequences e_{nm} and q_{nm} with the initial values

$$e_{n0} = 0\,, \quad n = 1,2,3,\ldots\,, \qquad (2.11)$$
$$q_{n1} = -a_n/a_{n-1}\,, \quad n = 1,2,\ldots\,,$$

and the following recursion relations, the so-called "rhombus rules,"

$$e_{nm} = q_{n+1,m} - q_{nm} + e_{n,m-1}\,, \qquad (2.12a)$$
$$q_{nm} = e_{n,m-1}\,q_{n,m-1}/e_{n-1,m-1}\,, \qquad (2.12b)$$
$$n = 2,3,\ldots\,, \quad m = 2,3,\ldots,n\,.$$

These sequences are traditionally presented as a set of interwoven two-dimensional arrays known as the *QD table*, which is shown schematically in Fig. 1. Any four elements of the table which form a unit rhombus are connected by the recursion relations of (2.12).

Theorem 2.4: If the power series $P(z)$ is normal, then its RITZ fraction representation is uniquely defined by the "diagonal" elements of the QD table, i.e.,

$$C(z) = \cfrac{a_0}{1 + \cfrac{q_{11}z}{1 + \cfrac{e_{11}z}{1 + \cfrac{q_{22}z}{1 + \cfrac{e_{22}z}{1 + \cdots}}}}}\,. \qquad (2.13)$$

The QD algorithm represents a convenient method of determining the RITZ fraction representation (if it exists) of a formal power series. The first column e_{n0} is filled with zeroes, and the next column q_{n1} is filled with the negative ratios of successive power series coefficients. Equations (2.12) are then used to calculate a QD triangle outward to the diagonal as in Fig. 1. This method is known as the *forward QD algorithm*. Each additional series coefficient a_n allows the determination of an additional CF coefficient c_n. In this way a one-to-one correspondence is seen to exist between the a_n and the c_n.

The QD scheme, as other algorithms designed to calculate RITZ CF coefficients from power series coefficients, is numerically unstable by virtue of the alternating procedures of division and subtraction. Practical calculations of RITZ coefficients to large order are thus impeded by this sensitivity to roundoff error. It is found that roughly one digit of accuracy in the c_n is lost for every two orders of calculation, implying that even in IBM quadruple precision (32 significant digits), coefficients beyond about c_{60} are totally meaningless. As a result, all calculations performed in the course of this work have been accomplished with the use of a multiple-precision software routine,[24] which allows decimal numbers to be represented by arbitrarily large numbers of digits. In these calculations, each decimal number—including those involved in the calculation of the perturbation coefficients—was represented by, typically, 200 digits. This would ensure a 32-digit accuracy of the c_n to at least $n = 100$.

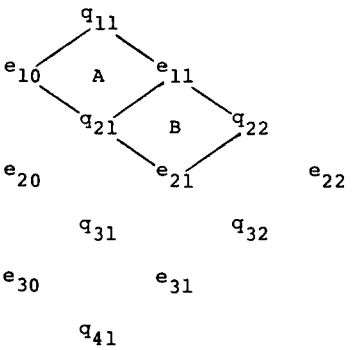

FIG. 1. The quotient-difference (QD) table, illustrating two particular unit rhombi. The elements defining rhombus A satisfy Eq. (2.12a) with $m = n = 1$. The elements of rhombus B satisfy Eq. (2.12b) with $m = n = 2$. From these equations, the rightmost elements of any rhombus may be calculated from the other three elements. The first two columns are initialized as in Eq. (2.11), permitting the calculation of the triangular lattice shown in this figure. This procedure is known as the *forward QD scheme*. The diagonal entries q_{nn} and e_{nn} define the coefficients c_n of the RITZ continued fraction representation of the formal power series concerned.

C. S fractions and the Stieltjes moment problem

A *Stieltjes* or *nonrational positive symmetric function* $f(z)$ may be defined by the Stieltjes integral,

$$f(z) = \int_0^\infty \frac{d\psi(t)}{1+zt}\,, \qquad (2.14)$$

where $\psi(t)$ is a bounded, nondecreasing real valued function with infinitely many points of increase on $[0,\infty)$. The function $f(z)$ is said to be the Stieltjes transform of ψ, $f = \mathcal{S}\psi$, and obeys the following four basic properties: (i) $f(z)$ is analytic in the cut plane $\tilde{\mathbb{C}} = \{z:|\arg z| < \pi\}$, (ii) $f(x) > 0$ for $x > 0$, i.e., $f(z)$ is *real positive symmetric*, (iii) if $U = \{z|\mathrm{Im}(z) > 0\}$ and $L = \{z|\mathrm{Im}(z) < 0\}$, then $f(L) \subset U$ and $f(U) \subset L$, i.e., $-f(z)$ is Herglotz,[7] and (iv) $f(z)$ admits an asymptotic expansion as $z \to 0$.

A formal expansion of the denominator of the integrand in Eq. (2.14) followed by term-by-term integration gives the series expansion

$$f(z) = \sum_{n=0}^{\infty} \mu_n z^n\,, \qquad (2.15)$$

where the μ_n are real and finite moments of the measure $d\psi(t)$:

$$\mu_n = (-1)^n \int_0^\infty t^n d\psi(t)\,, \quad n = 0,1,2,\ldots\,. \qquad (2.16)$$

The series in Eq. (2.15), termed a *Stieltjes series*, may or may not converge for $z \neq 0$, but is asymptotic to $f(z)$ as $z \to 0$. Given a sequence of real numbers $\{\mu_n\}_{n=0}^{\infty}$, the *Stieltjes moment problem* consists of finding a real valued, bounded, and nondecreasing function $\psi(t)$ with infinitely many points of increase on $[0,\infty)$ whose moments are the μ_n.

We now define an S *(Stieltjes) fraction* as a nonterminat-

ing RITZ fraction of Eq. (2.1) for which $c_n > 0$, $n = 1,2,3,\ldots$.

Theorem 2.5: The RITZ fraction representation corresponding to a series of Stieltjes is an S fraction.

Theorem 2.6: The sequence of convergents $\{w_n(z)\}$ of an S fraction contains a subsequence which converges uniformly on any compact subset S of the cut plane $\tilde{\mathbb{C}}$. The limit function of this convergent subsequence will be analytic in S.

If $C(z)$ converges for $z \in S$, then $\lim_{n\to\infty} w_n(z)$ exists and all subsequences converge to the same limit function, called the *value function* (VF) of $C(z)$. If $C(z)$ does not converge for some $z \in S$, then it is possible that different subsequences of $w_n(z)$ converge to different *generalized value functions* (GVF) of $C(z)$.

Theorem 2.7: Corresponding to each GVF of an S fraction, we may construct a bounded nondecreasing function $\psi(t)$ satisfying Eq. (2.14). The function $\psi(t)$ must have an infinite number of points of increase.

Theorem 2.8: The even and odd approximants of an S fraction which corresponds to the asymptotic expansion in (2.15) obey the following bounding properties for $x > 0$:

$$w_{2N}(x) = [N-1,N](z) < f(x) < [N,N](z) = w_{2N+1}(x), \quad N = 1,2,\ldots . \tag{2.17}$$

If $C(z)$ converges, then its value function is equal to $f(z)$ for all $z \in \tilde{\mathbb{C}}$. A unique function ψ generates the moment sequence $\{\mu_n\}$ and the Stieltjes moment problem is said to be *determinate*. If $C(z)$ diverges, it will have two generalized value functions, the limits of the subsequences $w_{2n}(z)$ and $w_{2n+1}(z)$ as $n \to \infty$ and the moment problem is *indeterminate*. The convergence is uniform on every compact subset of $\tilde{\mathbb{C}}$. An infinite number of functions ψ_i yield the same moment sequence, each of which produces a Stieltjes transform, but only two of these are generalized value functions of $C(z)$. The determinacy of the moment problem is thus seen to boil down to the convergence of the S fraction $C(z)$. The following theorems are of paramount importance in the studies of LOPT and CFLO.

Theorem 2.9: An S fraction $C(z)$ whose coefficients c_n obey the relation

$$\sum_{n=1}^{\infty} c_n^{-1/2} = \infty \tag{2.18}$$

converges uniformly on all compact subsets of $\tilde{\mathbb{C}}$.

Theorem 2.10: (Carleman condition) A sufficient condition for the determinacy of the moment problem, hence the convergence of $C(z)$, is that

$$\sum_{n=1}^{\infty} |\mu_n|^{-1/2n} = \infty , \tag{2.19}$$

where the μ_n are the given moments of Eq. (2.15).

By Theorem 2.7, determinacy of the moment problem ensures Padé summability of the power series. In fact, for Stieltjes series, the Padé sequences $[N+k,N](z)$, $k = -1,0,1,\ldots$ converge in the limit as $N \to \infty$ to $f(z)$ uniformly on compact subsets of the cut plane $\tilde{\mathbb{C}}$.[20]

III. RAYLEIGH–SCHRÖDINGER PERTURBATION SERIES AND THEIR S FRACTION REPRESENTATIONS AT LARGE ORDER

We now return to the following general class of bound state eigenvalue problems: Given the unperturbed problem $\hat{H}^{(0)}\psi_m^{(0)} = E_m^{(0)}\psi_m^{(0)}$, $m = 0,1,2,\ldots$, we consider the perturbed problem

$$[\hat{H}^{(0)} + \lambda\hat{V}]\psi_m = E_m(\lambda)\psi_m = [\hat{E}_m^{(0)} + \Delta E(\lambda)]\psi_m , \quad m = 0,1,2,\ldots , \tag{3.1}$$

where $\hat{V}$ is a positive (self-adjoint) perturbation and it is assumed that $\psi_m \to \psi_m^{(0)}$ and $\Delta E(\lambda) \to 0$ as $\lambda \to 0$. For a large number of perturbation problems, the function $\lambda^{-1}\Delta E(\lambda)$ may be shown to satisfy the four properties of a Stieltjes function given in Sec. II C. The asymptotic series to $E(\lambda)$ corresponds to the Rayleigh–Schrödinger perturbation series of Eq. (1.1). In his detailed treatment of the quartic anharmonic oscillator, Simon[7] showed that if $E(\lambda) \sim |\lambda|^q$, as $|\lambda| \to \infty$, the coefficients $E^{(n)}$ constitute a negative Stieltjes series for $n > q$. More precisely, the $E^{(n)}$ obey the dispersion relation

$$E^{(n)} = \pi^{-1}\int_{-\infty}^{0} \frac{Im(E+i0)}{\lambda^{n+1}}\,d\lambda , \quad n > q . \tag{3.2}$$

Bender–Wu theory[5] exploits Eq. (3.2) to establish the large-order behavior of the $E^{(n)}$ as $n \to \infty$. For n very large, the dominant contribution to the integral comes from the region $\lambda \sim 0$. The quantity $\mathrm{Im}(E)$ is proportional to the tunneling factor for the unstable state, whose asymptotics as $\lambda \to 0$ are determined by WKB methods. The LOPT of a number of problems has been studied in this way and it is found that typically

$$\mathrm{Im}(E+i0) \sim C(-\lambda)^b e^{B/\lambda^c}[1 + O(\lambda^d)] , \quad \text{as } \lambda \to 0^- . \tag{3.3}$$

Substitution of (3.3) into (3.2) gives

$$E^{(n)} \sim (-1)^{n+1}\frac{AB^{b/c}}{\pi c}(B^{-1/c})^n\Gamma\left(\frac{n-b}{c}\right) \times [1 + O(n^{-d/c})] , \quad \text{as } n \to \infty , \tag{3.4}$$

which we shall write in a more general form as

$$E^{(n)} \sim (-1)^{n+1}A\Gamma(pn+a)k^n[1 + O(n^{-r})] , \quad \text{as } n \to \infty , \tag{3.5}$$

where A, p, a, k, and r are constants specific to the problem studied.

From Carleman's condition in Eq. (2.19), the moment problem associated with the RS perturbation coefficients in Eq. (3.5) is guaranteed determinate for $p \leqslant 2$. Padé summability of the series is thus ensured. Borel ($p = 1$) and generalized Borel ($p > 1$) methods may also be possibly established.[11]

We now focus on the RITZ fraction representations of these generic RS perturbation series. From Eq. (3.1) and the fact that $0 < q < 1$ for many problems, we construct represen-

tations of the form

$$E_m(\lambda) = E_m^{(0)} + \lambda C^m(\lambda), \tag{3.6}$$

where

$$C^m(\lambda) = \frac{c_1^m}{1 + \quad 1 \quad + \quad 1 \quad + \quad 1 \quad + \ \ldots}$$

The index m represents any quantum number labeling of states and will generally be suppressed below. In these generic perturbation problems, $C(z)$ is an S fraction, i.e., $c_n > 0$ for $n = 1,2,3,\ldots$.

An interesting relationship is generally observed between the large-order behavior of the RS series coefficients $E^{(n)}$ and their S-fraction counterparts c_n. If the $E^{(n)}$ behave asymptotically as in Eq. (3.5), then

$$c_n \sim Dn^p, \quad \text{as } n \to \infty, \tag{3.7}$$

where D is a constant. We shall refer to this asymptotic property as the *continued-fractions-at-large-order* (CFLO) relation. For convenience, we refer to S fractions whose coefficients behave asymptotically like (3.7) as $S_{(p)}$ fractions. The case $p = 0$ corresponds to representations of geometric power series for which the c_n approach a constant.

The behavior in Eq. (3.7) could be expected from a look at the extended QD table for the perturbation series, discussed in the Appendix. Its rows and columns grow asymptotically as $O(E^{(n+1)}/E^{(n)}) = O(n^p)$. The diagonal elements q_{nn} and e_{nn} also behave in this way as $n \to \infty$ although some work is required to obtain the coefficients of the leading term. In this paper, we restrict ourselves to an analysis of the relatively simple relation for $p = 1$, relevant to the study of $S_{(1)}$ representations presented below. The following result is proved in the Appendix.

Proposition 3.1: Given that the $E^{(n)}$ form a negative Stieltjes series for $n > 1$ and behave as in Eq. (3.5) with $p = 1$ and $r \geqslant 1$, then the coefficients of its S-fraction representation in Eq. (3.6) behave as $c_n \sim kn/2$, as $n \to \infty$.

Illustrative example—The generalized Euler series: The following modification of the classical Euler series,[12,20] $E(z) = 0! - 1!z + 2!z^2 - \cdots$, is relevant to the analysis of $S_{(1)}$ fractions presented in Sec. V:

$$F(z) = 1 + \sum_{n=1}^{\infty} (-1)^{n+1} \Gamma(n + a)\, k^n z^n. \tag{3.8}$$

This series has been constructed in a form which corresponds to the typical leading behavior of $n!$-type perturbation expansions [e.g., $k = 3, a = K + \frac{1}{2}$ for the QAHO series in Eq. (4.4)]. It is the asymptotic expansion of the Stieltjes transform

$$G(z) = 1 + kz \int_0^{\infty} \frac{e^{-t} t^a}{1 + kzt}\, dt \tag{3.9}$$

for $z \to 0$ in the cut plane $|\arg z| < \pi$.

The coefficients of the S-fraction representation,

$$F(z) = 1 + \frac{b_1 z}{1 + \quad 1 \quad + \quad 1 \quad + \quad 1 \quad + \ \ldots}, \tag{3.10}$$

are easily determined in closed form by constructing the QD table (Fig. 1) for the expansion in (3.8):

$$b_1 = k\Gamma(1 + a),$$

$$b_{n,\text{even}} = \tfrac{1}{2} kn + ka, \tag{3.11}$$

$$b_{n,\text{odd}} = \tfrac{1}{2} kn - k/2.$$

The special case $k = 1, a = 0$ corresponds to the Euler series.

The CFLO property in (3.7) provides a consistency relation between the moment conditions in Eqs. (2.8) and (2.9). In both cases, the moment problem is determinate for $p \leqslant 2$ in Eqs. (3.5) and (3.7).

From a computational viewpoint, a knowledge of $S_{(p)}$-fraction asymptotics for $p = 1,2$ has proven useful[13] in the estimation of energy eigenvalues $E(\lambda)$ for rather larger values of the coupling constant λ. For $S_{(1)}$ fractions, an extrapolation of a small number of accurately known c_n, produces an approximate "tail" of $C(\lambda)$. The approximants $w_n(\lambda)$ associated with this CF are then evaluated to sufficiently high order to ensure convergence of the fraction, i.e., $|w_{n+1}(\lambda) - w_n(\lambda)| < \epsilon$ for a given $\epsilon > 0$. Excellent estimates of $E(\lambda)$ for large λ are obtained. In the case of $S_{(2)}$ fractions, a similar extrapolation of the c_n is performed. The convergence of the $w_n(\lambda)$ is extremely slow. A suitably constructed extrapolation of even (lower bound) and odd (upper bound) approximants yields a common limit which again approximates $E(\lambda)$ very well for even large λ. Some numerical results are presented in Ref. 13.

We mention that the importance of CFLO has already been realized for the case of $S_{(0)}$ fractions, i.e., $c_n \to a$, as $n \to \infty$, where a is a constant. These types of fractions have been encountered in solid state physics[25,26] in the approximation of densities of states of periodic and aperiodic systems as well as in atomic and molecular physics[27,28] for the determination of optical dispersion profiles. In both cases, one is interested in the location of a branch cut of singularities in the complex energy plane as well as the discontinuity across the cut. The asymptotic value a is important in light of an extension of a theorem due to Van Vleck.[18]

Theorem 3.1: Let $C(z)$ be an S fraction such that $\lim_{n\to\infty} c_n = a \neq 0$, where a is a complex constant and let $\mathbb{C}_a = \{z: |\arg(az + \frac{1}{4})| < \pi\}$. The continued fraction $C(z)$ converges to a function $f(z)$, which is either meromorphic in $\mathbb{C}_a$ or identically infinity.

The region $\mathbb{C}_a$ represents the complex plane $\mathbb{C}$ cut along the line which passes through the point $z_c = -(4a)^{-1}$ and the origin. The cut begins at the point z_c and extends outward to infinity. In the context of photoabsorption studies,[28] the continued fraction corresponding to the Stieltjes series for complex polarizability $\alpha(z)$ (having nonzero radius of convergence) is constructed and the (real) asymptotic value a is estimated. The distance from the origin to the cut, $|z_c|$, corresponds to the *photoionization threshold frequency* for the atomic or molecular system concerned.

The subject of $S_{(0)}$ representations of perturbation series, including the well-known problem of a rigid dipole rotor in an electric field, will be discussed in a future report.

TABLE II. The first 105 coefficients c_n of the S-fraction representation, Eq. (4.4), of the ground-state Rayleigh–Schrödinger perturbation series for the energy $E(\lambda)$ of the quartic anharmonic oscillator in Eq. (4.1).

n	c_n	n	c_n
1	0.750 000 000 000 000 000 000 000 000 000 $D+00$	54	0.406 586 405 522 041 706 283 769 067 693 $D+02$
2	0.175 000 000 000 000 000 000 000 000 000 $D+01$	55	0.411 421 268 655 535 125 766 943 934 596 $D+02$
3	0.221 428 571 428 571 428 571 428 571 421 $D+01$	56	0.421 580 132 542 199 212 702 235 748 957 $D+02$
4	0.328 067 396 313 364 055 299 539 170 507 $D+01$	57	0.426 418 233 947 834 481 230 612 157 025 $D+02$
5	0.368 842 779 459 679 897 367 783 849 295 $D+01$	58	0.436 574 196 271 822 690 130 688 022 839 $D+02$
6	0.473 804 188 521 881 063 707 142 639 340 $D+01$	59	0.441 415 356 393 589 419 024 936 020 957 $D+02$
7	0.517 612 209 347 468 499 579 930 828 597 $D+01$	60	0.451 568 567 683 689 989 026 434 041 269 $D+02$
8	0.622 046 670 654 721 646 752 711 278 894 $D+01$	61	0.456 412 622 835 465 321 760 882 311 956 $D+02$
9	0.666 893 242 501 742 590 748 909 803 938 $D+01$	62	0.466 563 221 133 621 513 614 705 133 795 $D+02$
10	0.770 863 415 363 561 254 700 818 557 412 $D+01$	63	0.471 410 021 611 420 740 202 843 289 912 $D+02$
11	0.816 435 361 582 525 381 761 294 381 692 $D+01$	64	0.481 558 133 870 169 732 229 550 002 981 $D+02$
12	0.920 033 250 189 205 270 860 568 794 018 $D+01$	65	0.486 407 542 342 811 785 880 668 124 362 $D+02$
13	0.966 091 975 248 318 987 231 089 675 743 $D+01$	66	0.496 553 285 628 456 366 775 785 329 355 $D+02$
14	0.106 941 039 059 420 442 884 222 717 620 $D+02$	67	0.501 405 175 758 083 127 125 447 075 667 $D+02$
15	0.111 582 703 907 225 187 463 106 182 106 $D+02$	68	0.511 548 658 291 584 962 866 225 233 352 $D+02$
16	0.121 891 786 716 627 292 093 981 465 150 $D+02$	69	0.516 402 913 545 210 988 616 740 602 626 $D+02$
17	0.126 561 481 600 439 307 617 042 237 015 $D+02$	70	0.526 544 235 606 717 905 492 047 637 396 $D+02$
18	0.136 851 666 800 951 687 340 583 597 644 $D+02$	71	0.531 400 748 227 523 481 657 986 922 305 $D+02$
19	0.141 543 905 856 510 535 100 790 729 557 $D+02$	72	0.541 540 002 945 683 876 082 634 129 675 $D+02$
20	0.151 818 201 881 278 086 509 898 007 004 $D+02$	73	0.546 398 673 058 640 534 948 768 719 363 $D+02$
21	0.156 529 036 609 641 454 734 415 308 722 $D+02$	74	0.556 535 947 102 096 253 126 954 317 229 $D+02$
22	0.166 789 725 929 183 986 105 190 000 238 $D+02$	75	0.561 396 681 933 142 450 130 413 395 460 $D+02$
23	0.171 516 250 463 633 149 014 914 506 289 $D+02$	76	0.571 532 056 118 585 474 617 123 149 510 $D+02$
24	0.181 765 110 007 862 677 187 948 391 759 $D+02$	77	0.576 394 769 310 252 475 830 880 035 511 $D+02$
25	0.186 505 099 422 477 445 005 670 089 919 $D+02$	78	0.586 528 319 139 005 802 204 136 059 178 $D+02$
26	0.196 743 558 645 901 433 503 889 886 225 $D+02$	79	0.591 392 930 148 347 636 208 678 651 578 $D+02$
27	0.201 495 258 388 647 959 134 768 165 616 $D+02$	80	0.601 524 726 281 461 064 295 401 471 352 $D+02$
28	0.211 724 487 343 025 978 350 805 140 175 $D+02$	81	0.606 391 159 848 526 671 653 170 951 027 $D+02$
29	0.216 486 487 913 904 719 665 323 624 721 $D+02$	82	0.616 521 268 528 770 627 915 137 953 121 $D+02$
30	0.226 707 455 165 976 782 269 398 642 140 $D+02$	83	0.621 389 454 205 790 738 151 998 196 930 $D+02$
31	0.231 478 606 456 887 946 340 101 511 963 $D+02$	84	0.631 517 937 633 613 814 640 723 299 693 $D+02$
32	0.241 692 123 421 839 163 178 236 803 349 $D+02$	85	0.636 387 809 366 651 971 458 620 241 430 $D+02$
33	0.246 471 472 775 375 599 234 607 439 973 $D+02$	86	0.646 514 726 036 083 720 705 508 426 670 $D+02$
34	0.256 678 227 429 547 402 476 297 926 381 $D+02$	87	0.651 386 221 792 192 662 882 270 236 493 $D+02$
35	0.261 464 975 059 643 661 428 067 741 878 $D+02$	88	0.661 511 626 791 776 902 003 228 269 454 $D+02$
36	0.271 665 556 836 904 330 890 567 928 711 $D+02$	89	0.666 384 688 225 765 166 563 320 358 766 $D+02$
37	0.276 459 023 629 938 404 499 119 327 073 $D+02$	90	0.676 508 633 508 864 441 634 996 399 357 $D+02$
38	0.286 653 941 970 252 042 903 449 281 275 $D+02$	91	0.681 383 205 664 658 379 358 696 010 237 $D+02$
39	0.291 453 545 655 385 564 489 559 777 508 $D+02$	92	0.691 505 740 292 848 656 085 278 687 390 $D+02$
40	0.301 643 244 245 166 299 113 381 212 607 $D+02$	93	0.696 381 771 335 167 227 892 366 108 653 $D+02$
41	0.306 448 481 268 505 030 447 360 406 552 $D+02$	94	0.706 502 941 697 920 626 433 180 581 495 $D+02$
42	0.316 633 349 237 015 931 994 160 481 653 $D+02$	95	0.711 380 382 670 592 101 404 492 697 713 $D+02$
43	0.321 443 780 714 774 978 038 609 561 019 $D+02$	96	0.721 500 232 684 006 573 528 150 279 693 $D+02$
44	0.331 624 161 540 972 554 682 971 634 140 $D+02$	97	0.726 379 037 291 769 538 599 407 518 198 $D+02$
45	0.336 439 402 247 503 199 580 128 679 770 $D+02$	98	0.736 497 608 578 733 388 621 936 009 027 $D+02$
46	0.346 615 600 894 529 650 256 854 210 487 $D+02$	99	0.741 377 732 989 796 844 663 583 318 223 $D+02$
47	0.351 435 310 544 054 420 561 746 757 623 $D+02$	100	0.751 495 065 043 661 298 463 454 064 922 $D+02$
48	0.361 607 599 219 648 367 281 669 394 216 $D+02$	101	0.756 376 467 710 664 171 010 360 108 025 $D+02$
49	0.366 431 475 489 866 424 186 492 282 574 $D+02$	102	0.766 492 598 044 229 348 950 781 251 158 $D+02$
50	0.376 600 098 342 814 395 223 790 757 194 $D+02$	103	0.771 375 239 541 549 915 310 285 838 617 $D+02$
51	0.381 427 871 230 572 481 752 179 401 097 $D+02$	104	0.781 490 203 822 940 836 992 120 212 793 $D+02$
52	0.391 593 048 217 481 625 609 338 844 893 $D+02$	105	0.786 374 046 698 570 669 023 801 627 046 $D+02$
53	0.396 424 475 425 589 626 214 906 981 943 $D+02$		

IV. $S_{(1)}$-FRACTION REPRESENTATIONS OF THE QUARTIC ANHARMONIC OSCILLATOR AND CHARMONIUM PERTURBATION SERIES

In this section we focus on two perturbation problems whose Rayleigh–Schrödinger expansions yield $S_{(1)}$-fraction representations: (1) the quartic anharmonic oscillator (QAHO) and (2) the hydrogen atom in a linear radial potential or the charmonium model. The LOPT of these expansions is known. In both cases, the S-fraction coefficients for the first few bound state levels have been computed accurately to high order, typically $n = 100$, to facilitate numerical analysis of their asymptotic behavior. Details of numerical aspects are presented in Refs. 13, 15, and 16.

A. The quartic anharmonic oscillator

The quartic anharmonic oscillator, whose perturbation expansions were first studied in detail by Bender and Wu[3–5]

(with a different normalization), Loeffel *et al.*,[6] and Simon,[7] is given by the eigenvalue problem

$$\left[-\frac{d^2}{dx^2}+x^2+\beta x^4-E(\beta)\right]\psi(x)=0\,, \tag{4.1}$$

with boundary conditions $\psi(x)\to 0$, $|x|\to\infty$, $x\in\mathbf{R}$. The unperturbed eigenvalues are given by $E_K^{(0)}=2K+1$, $K=0,1,2,\ldots$. The perturbation expansion for the Kth level of Eq. (4.1) will be denoted by

$$E_K(\beta)=2K+1+\sum_{n=1}^{\infty}E_K^{(n)}\beta^n\,. \tag{4.2}$$

The large-order behavior of the RS coefficients is given by[4]

$$E_K^{(n)}\sim(-1)^{n+1}\frac{12^K}{K!}\left(\frac{6}{\pi^3}\right)^{1/2}\Gamma(n+K+\tfrac{1}{2})\,(\tfrac{3}{2})^n \times\left[1-\frac{1}{n}\left(\frac{95}{72}+\frac{29}{12}K+\frac{17}{12}K^2\right)+O\left(\frac{1}{n^2}\right)\right]. \tag{4.3}$$

The perturbation series is negative Stieltjes[7] for $n\geq 1$. This guarantees its Padé, hence S fraction, summability to $E_K(\beta)$ in the cut plane $|\arg\beta|<\pi$.

We now consider S-fraction representations of the QAHO perturbation series having the form

$$E_K(\beta)=E_K^{(0)}+\beta C^K(\beta)\,, \tag{4.4}$$

where

$$C^K(\beta)=\frac{c_1^K}{1}+\frac{c_2^K\beta}{1}+\frac{c_3^K\beta}{1}+\cdots\,. \tag{4.5}$$

The coefficients c_n^K have been calculated from the RS coefficients $E_K^{(n)}$ to $n=100$ for the levels $K=1$, 2, and 3. The first 100 coefficients for the ground state, $K=0$, are presented in Table II, accurate to all digits shown.

From Eq. (3.7) it is expected that $c_n^K\sim\frac{3}{4}n$, as $n\to\infty$, which is observed numerically. On the basis of more detailed numerical analysis,[14,15] the asymptotic behavior of the c_n^K is conjectured to be

$$c_n^K\sim\tfrac{3}{4}(n+K)\pm\tfrac{1}{8}+R_n^{(i)}\,,\quad i=\begin{cases}1\,, & n\text{ even}\,,\\ 2\,, & n\text{ odd}\,,\end{cases} \tag{4.6}$$

where $R_n^{(i)}\to 0$, as $n\to\infty$, and it is conjectured that $R_n^{(i)}=O(n^{-1/2})$. The constant terms in Eq. (4.6) are not *a priori* correction terms—in fact, no general asymptotic expansion beyond the leading term is guaranteed. Nevertheless, numerical analysis strongly suggests these terms. Moreover, the analysis in Sec. V attests to their validity.

Before concluding this discussion, we mention that Reid[29] performed the first calculation of continued fraction representations of QAHO perturbation series. His calculations appeared well before Refs. 3–7, the latter two of which established the Stieltjes nature and Padé summability of the series. Reid did, however, realize the power of continued fraction summability of divergent Stieltjes series, using the classical Euler series as an example. His representations involved *J fractions*,[17,18] having the form

$$E_K(\beta)=E_K^{(0)}+J^K(\beta)$$
$$=E_K^{(0)}+\frac{a_1\beta}{1+b_1\beta-}\,\frac{a_2\beta^2}{1+b_2\beta-}\,\frac{a_3\beta^2}{1+b_3\beta\cdots}\,. \tag{4.7}$$

The coefficients a_i, b_i, $i=1,2,\ldots,10$, were calculated for a number of levels in multiple precision and, for all cases, were found to be positive.

The J fraction in Eq. (4.7) is actually the *even part* of the S fraction in Eq. (4.5).[12] Its sequence of approximants coincides with the approximants of even order, $w_{2n}(\beta)$, of the S fraction. This fact is revealed in Reid's calculations of the first ten approximants of the J fraction for various values of β. All sequences of approximants approach the exact values $E(\beta)$ monotonically from below. The coefficients a_k and b_k are related to the c_n as follows:

$$a_1=c_1\,,\quad b_1=c_2\,,$$
$$a_i=c_ic_{i+1}\,,\quad b_i=c_{i+1}+c_{i+2}\,,\quad i=2,3,4,\ldots\,. \tag{4.8}$$

The calculation of a_i and b_i to $i=10$ is thus seen to be equivalent to determining the c_n to c_{20}. A look at the tables of J-fraction coefficients presented by Reid reveals that the a_i grow quadratically and that the b_i grow linearly, in accordance with Eqs. (4.6) and (4.8).

B. Charmonium—The hydrogen atom in a linear radial potential

The problem of a hydrogenic atom in a linear radial potential, one of many nonrelativistic quark-confinement models,[30–32] is given by the Hamiltonian (in atomic units)

$$\hat{H}(\lambda)=-\tfrac{1}{2}\nabla^2-Z/r+\lambda r\,. \tag{4.9}$$

With no loss of generality, we consider the problem for $Z=1$. The RS perturbation expansion for the energy of a given level will be denoted by

$$E_{NLM}(\lambda)=-\frac{1}{2N^2}+\sum_{n=1}^{\infty}E_{NLM}^{(0)}\lambda^n\,. \tag{4.10}$$

The indices N, L, and M denote, respectively, the principal, orbital-angular momentum, and magnetic quantum numbers of the unperturbed hydrogenic state giving rise to the level.

The large-order behavior of the RS coefficients is given by[16]

$$E_{NLM}^{(n)}\sim\frac{(-1)^{n+1}3^{2N}2^{2N-1}\exp[-3N+L(L+1)/N]}{\pi N^3(N+L)!(N-L-1)!} \times(\tfrac{3}{2}N^3)^n\Gamma(n+2N)[1+A/n+O(n^{-2})] \tag{4.11}$$

The coefficient A has been computed for a number of states but no general formula has been conjectured. The numerical evidence strongly indicates that for the S-wave states, i.e., $L=M=0$,

$$A=-\tfrac{1}{9}(21N^2+18N+10)\,. \tag{4.12}$$

The coefficients form a negative Stieltjes series[16] for $n>1$.

We now consider S-fraction representations to the charmonium series having the same form as Eq. (4.5), and let c_n^{NLM} denote the CF coefficients. These coefficients have

been calculated to at least 32 digit precision to order $n = 100$ for the hydrogenic states $N \leqslant 3$, $0 \leqslant L \leqslant N-1$, $M = 0$. From Eq. (4.11) and Proposition 3.1, it is expected that $c_n \sim \frac{3}{4} N_n^3$, as $n \to \infty$, which is observed numerically. A more detailed numerical analysis[16] leads to the following conjectured behavior for the S-fraction coefficients:

$$c_n^{NLM} \sim \tfrac{3}{4} N^3 (n+2N) - \tfrac{1}{2} N^3 + R_n^{(1),NLM}, \quad n \text{ even}, \tag{4.13}$$

$$c_n^{NLM} \sim \tfrac{3}{4} N^3 (n+2N) - \tfrac{1}{4} N^3 + R_n^{(2),NLM}, \quad n \text{ odd},$$

where $R_n^{(i)} \to 0$, as $n \to \infty$. As in the case of the QAHO, numerical extrapolation techniques strongly suggest that the $R_n^{(i)} = O(n^{-1/2})$.

V. ASYMPTOTICS OF $S_{(1)}$ FRACTIONS AND THE INFINITE FIELD LIMIT

A. General formulation

The infinite field expansion for many standard perturbation problems assumes the form

$$E(\lambda) \sim \lambda^{\alpha} \sum_{n=0} F^{(0)} \lambda^{-n\gamma}, \quad \text{as } |\lambda| \to \infty, \tag{5.1}$$

and may often be obtained by real-valued dilation transformations, usually referred to as Symanzik transformations.[7] For example, in the case of generalized anharmonic oscillators, where $\hat{H}_m = \hat{p}^2 + x^2 + \lambda x^{2m}$, $m = 2,3,4,...$, the scaling transformation $x = rx$, r real, yields $\alpha = 1/(m+1)$, $\gamma = 2/(m+1)$. The leading term coefficients $F_K^{(0)}$ represent the K th eigenvalues of the oscillator with Hamiltonian $\hat{H} = \hat{p}^2 + x^{2m}$.

The infinite field limit is reflected in the large-order behavior of certain $S_{(1)}$-fraction representations. In the examples below, for which

$$c_n \sim \tfrac{1}{2} kn + A^{(i)} + o(1), \quad i = \begin{cases} 1, & n \text{ even}, \\ 2, & n \text{ odd}, \end{cases} \tag{5.2}$$

where the $A^{(i)}$ are constants, it will be shown that the exponent α in Eq. (5.1) is given by

$$\alpha = \tfrac{1}{2} - \Delta A / k, \tag{5.3}$$

where

$$\Delta A = A^{(1)} - A^{(2)}. \tag{5.4}$$

First, consider the continued fraction

$$\tilde{w}_{N-1}(z) = \frac{c_1}{1} + \frac{c_2 z}{1} + \cdots + \frac{c_{N-1} z g_N(z)}{1}, \tag{5.5}$$

where

$$g_N(z) = \frac{1}{1} + \frac{\tilde{c}_N z}{1} + \frac{\tilde{c}_{N+1} z}{1} + \cdots, \tag{5.6}$$

and

$$\tilde{c}_n = \tfrac{1}{2} kn + A^{(i)}, \quad n \geqslant N. \tag{5.7}$$

In other words, $\tilde{w}(z)$ is constructed by replacing the infinite tail of $C(z)$ with one whose coefficients $\tilde{c}_n$ ignore the terms of $R_n^{(i)}$ in Eq. (5.2). For N even, we produce the *odd convergent approximation* $\tilde{w}_{N-1}(z)$ to $C(z)$; for N odd we produce the *even convergent approximation*.

The function $g_N(z)$ in Eq. (5.6) is an $S_{(1)}$ fraction formally representing a Stieltjes transform and converging uniformly to it over compact subsets of the cut plane $\tilde{\mathbb{C}}$. We first determine the asymptotics of $g_N(z)$ as $|z| \to \infty$, $z \in \tilde{\mathbb{C}}$, by means of the following classical relation[17,21] between contiguous Gauss hypergeometric functions:

$$\frac{{}_2F_0(a,b+1,-z)}{{}_2F_0(a,b,-z)} = \frac{1}{1} + \frac{az}{1} + \frac{(b+1)z}{1} + \frac{(a+1)z}{1} + \cdots, \tag{5.8}$$

where $a \notin [0,1,2,...]$ and $b \notin [-1,-2,...]$. The ratio of the two series on the left-hand side of Eq. (5.8) formally represents the function

$$G(z) = \frac{\int_0^{\infty} (e^{-t} t^{a-1}/(1+zt)^{b+1})\, dt}{\int_0^{\infty} (e^{-t} t^{a-1}/(1+zt)^{b})}, \tag{5.9}$$

which is analytic for $z \in \tilde{\mathbb{C}}$, provided that $\mathrm{Re}(a) > 0$. By Theorem 2.8 the S fraction in Eq. (5.8) converges uniformly to $G(z)$ on $\tilde{\mathbb{C}}$. We now analyze the odd and even truncations individually.

Odd convergent truncation, $N = 2n$: From Eqs. (5.6) and (5.7), it follows that

$$g_{2n}(z) = \frac{{}_2F_0(n + A^{(1)}/k, n + \tfrac{1}{2} + A^{(2)}/k; -kz)}{{}_2F_0(n + A^{(1)}/k, n - \tfrac{1}{2} + A^{(2)}/k; -kz)} \tag{5.10}$$

$$= \frac{U(n + A^{(1)}/k, \tfrac{1}{2} + \Delta A/k; (kz)^{-1})}{U(n + A^{(1)}/k, \tfrac{3}{2} + \Delta A/k; (kz)^{-1})}, \tag{5.11}$$

where $U(a,b;z)$ is a solution of Kummer's confluent hypergeometric equation,[33,34]

$$z \frac{d^2 w}{dz^2} + (b - z) \frac{dw}{dz} - aw = 0. \tag{5.12}$$

We now employ the relation[34]

$$U(a,b;x) = \frac{\Gamma(1-b)}{\Gamma(1+a-b)} {}_1F_1(a;b;x) + \frac{\Gamma(b-1)}{\Gamma(a)} x^{1-b} {}_1F_1(1+a-b;2-b;x), \quad x \in \tilde{\mathbb{C}}, \tag{5.13}$$

to expand the Kummer functions in Eq. (5.11) for $x = (kz)^{-1} \to 0^+$. The leading asymptotic behavior of the $U(a,b;x)$, in terms of the arguments a and b, is tabulated in Refs. 33 and 34. However, Eq. (5.13) is useful for the calculation of more terms in the asymptotic expansion. One special case requires care: For $b = 1$,

$$U(a,b;x) \sim -[1/\Gamma(a)][\ln(z) + \psi(a)] + O(|z \ln(z)|), \tag{5.14}$$

where $\psi(x)$ denotes the psi (digamma) function.[35] Temporarily ignoring this case, we rewrite Eq. (5.11) as

$$g_{2n}(z) = \frac{\sum_{i=1} p_i z^{-a(i)}}{\sum_{i=1} q_i z^{-b(i)}}, \tag{5.15}$$

where $0 < a(1) < a(2) < \cdots$, and $0 < b(1) < b(2) \cdots$. Clearly, these exponents are sensitive to the values of a and b in Eq. (5.13), which are, in turn, defined by the asymptotic coefficients in Eqs. (5.2) and (5.4).

Formal division in Eq. (5.15) yields the relation

$$g_{2n}(z) = D_1^{(2n)} z^{r(1)} + D_2^{(2n)} z^{r(2)}, \quad |z| \to \infty, \quad z \in \tilde{\mathbb{C}}, \tag{5.16}$$

where $r(1) = b(1) - a(1) > r(2) > r(3) \cdots$. Only two terms of the expansion in (5.15) are used since two terms in the expansion of the c_n, cf. (5.7), are employed.

The function $\tilde{w}_{N-1}(z)$ in Eq. (5.5) may be interpreted as a terminating fraction—the generalized odd approximant $\tilde{w}_{2n-1}(z)$ which may be written as

$$\tilde{w}_{2n-1}(z) = \frac{A_{2n-2}(z) + c_{2n-1} z g_{2n}(z) A_{2n-3}(z)}{B_{2n-2}(z) + c_{2n-1} z g_{2n}(z) B_{2n-3}(z)}. \tag{5.17}$$

The $A_k(z)$ and $B_k(z)$, $k \leqslant 2n-2$ are, respectively, the lower-order partial numerators and denominators of $C(z)$. We now expand these polynomials in terms of the coefficients in (2.4) and substitute Eq. (5.16) into Eq. (5.17). Formal multiplication of powers in z, rearrangement of terms, and subsequent division yields an expansion of the form

$$\tilde{w}_{2n-1}(z) = W_1^{(2n-1)} z^{u(1)} + W_2^{(2n-1)} z^{u(2)} + \cdots, \quad \text{as } |z| \to \infty, \tag{5.18}$$

where $u(1) > u(2) > \cdots$. Substitution of Eq. (5.18) into Eq. (5.5) produces the approximation

$$\tilde{E}_{2n-1}(z) = E^{(0)} + W_1^{(2n-1)} z^{u(1)+1} + W_2^{(2n-1)} z^{u(2)+1} + \cdots, \quad \text{as } |z| \to \infty, \tag{5.19}$$

for $z \in \tilde{\mathbb{C}}$.

Even convergent truncation, $N=2n+1$: In this case it follows from Eqs. (5.6) and (5.7) that

$$g_{2n+1}(z) = \frac{{}_2F_0(n + \tfrac{1}{2} + A^{(2)}/k, n + 1 + A^{(1)}/k; -kz)}{{}_2F_0(n + \tfrac{1}{2} + A^{(2)}/k, n + A^{(1)}/k; -kz)} \tag{5.20}$$

$$= \frac{U(n + \tfrac{1}{2} + A^{(2)}/k, \tfrac{1}{2} - \Delta A/k; (kz)^{-1})}{U(n + \tfrac{1}{2} + A^{(2)}/k, \tfrac{3}{2} - \Delta A/k; (kz)^{-1})} \tag{5.21}$$

Proceeding in the same manner as above, we expand the Kummer functions in Eq. (5.21) to ultimately obtain an asymptotic series for $g_{2n+1}(z)$ analogous to Eq. (5.16),

$$g_{2n+1}(z) = D_1^{(2n+1)} z^{s(1)} + D_2^{(2n+1)} z^{s(2)} + \cdots, \quad \text{as } |z| \to \infty, \quad z \in \tilde{\mathbb{C}}, \tag{5.22}$$

where $s(1) > s(2) > \cdots$. The function $\tilde{w}_{N-1}(z)$ in Eq. (5.5) is now written as a generalized even approximant $\tilde{w}_{2n}(z)$ [replace $2n-1$ by $2n$, etc., in Eq. (5.17)]. This ratio of two series again yields an expansion analogous to Eq. (5.18),

$$\tilde{w}_{2n}(z) = W_1^{(2n)} z^{v(1)} + W_2^{(2n)} z^{v(2)} + \cdots, \quad \text{as } |z| \to \infty, \tag{5.23}$$

where $v(1) > v(2) \cdots$. When substituted into Eq. (5.5), Eq. (5.23) yields the approximation

$$\tilde{E}_{2n}(z) = E^{(0)} + W_1^{(2n)} z^{v(1)+1} + W_2^{(2n)} z^{v(2)+1} + \cdots, \quad \text{as } |z| \to \infty, \tag{5.24}$$

where $z \in \tilde{\mathbb{C}}$.

Several remarks concerning the above truncations are now to be made. First, the expansion for $g_{2n+1}(z)$ in (4.22) could also have been derived from that of $g_{2n}(z)$ in (4.16) (or *vice versa*) by using the defining property

$$g_{2n}(z) = [1 + \tilde{c}_{2n} z g_{2n+1}(z)]^{-1} = [1 + (kn + A^{(1)}) z g_{2n+1}(z)]^{-1}. \tag{5.25}$$

Both leading exponents in (5.16) and (5.22) satisfy the inequality $-1 < x < 0$. Furthermore, from (5.25), the exponents in these two expansions obey the relations $r(1) = -1 - s(1)$, $r(2) = -1 - 2s(1) - s(2)$. Additional manipulation reveals that expansions (5.19) and (5.24) possess the same power-law behavior, i.e.,

$$u(1) = v(1), \quad u(2) = v(2). \tag{5.26}$$

We now consider the approximate convergents of Eqs. (5.19) and (5.24), written in the more general form

$$\tilde{E}_N(z) = E^{(0)} + z\tilde{w}_N(z). \tag{5.27}$$

Their asymptotic expansions will be denoted by

$$\tilde{E}_N(z) \sim E^{(0)} + W_1^{(N)} z^{\mu(1)} + W_2^{(N)} z^{\mu(2)} + \cdots, \quad \text{as } |z| \to \infty, \tag{5.28}$$

where $\mu(1) = u(1) + 1$ and $\mu(2) = u(2) + 1$. As N increases, i.e., as the infinite tail of the true $S_{(1)}$ fraction is replaced farther down, better estimates of $E(z)$ are obtained. This is expressed more precisely in the following theorem.

Theorem 5.1: The approximate convergents $\tilde{E}_N(z)$ in (5.28) converge uniformly to $E(z)$ over compact subsets of the cut plane $\tilde{\mathbb{C}}$.

Proof: Consider the $S_{(1)}$-fraction representations of the RS perturbation series having the form $E(z) = E^{(0)} + zC(z)$. The approximants $w_n(z)$ of $C(z)$ converge uniformly to an analytic function $f(z)$ on compact subsets of $\tilde{\mathbb{C}}$. Moreover, the bounding properties in Eq. (2.17) hold on the positive real axis. The $\tilde{w}_N(z)$ defined in Eq. (5.5) are $S_{(1)}$ fractions analytic in the cut plane $\tilde{\mathbb{C}}$. The functions $g_N(z)$ in (5.6) are also $S_{(1)}$ fractions and have the properties $g_N(0) = 1$, $0 \leqslant g_N(x) \leqslant 1$, $x \in \mathbb{R}$. The following relations are also satisfied on the positive real axis:

$$w_{2N-2}(x) \leqslant \tilde{w}_{2N}(x) \leqslant w_{2N-1}(x), \qquad w_{2N}(x) \leqslant \tilde{w}_{2N+1}(x) \leqslant w_{2N-1}(x). \tag{5.29}$$

These properties arise from the relation

$$\min\left[\frac{a_1}{b_1}, \frac{a_2}{b_2}\right] \leqslant \frac{a_1 + ta_2}{b_1 + tb_2} \leqslant \max\left[\frac{a_1}{b_1}, \frac{a_2}{b_2}\right], \quad a_i, b_i > 0, \quad t \geqslant 0, \tag{5.30}$$

where the following correspondences have been made: $t = c_n z g_n(x)$, $a_1 = A_{n-1}(x)$, $b_1 = B_{n-1}(x)$, $a_2 = A_{n-2}(x)$, $b_2 = B_{n-2}(x)$, and $n = 2N$ or $2N+1$. Uniform convergence of the $w_n(x)$ implies uniform convergence of the $\tilde{w}_N(x)$ to $f(x)$ on $\mathbb{R}$. By analytic continuation the $\tilde{w}_N(z)$ converge uniformly to $f(z)$ on compact subsets of $\tilde{\mathbb{C}}$, and the theorem is proved.

Relation (5.29) actually implies that the uniform convergence of the $\tilde{w}_N(z)$ to $f(z)$ is guaranteed if the tail of $C(z)$ is replaced by any real positive symmetric function $g_{N-1}(z)$. The exact association of the functions $\tilde{E}_N(z)$ with the infinite field expansion (5.1) may now be stated.

Theorem 5.2: In the asymptotic expansion of the $\tilde{E}_N(z)$ in Eq. (5.28), the exponents $\mu(1)$ and $\mu(2)$, which are independent of N, coincide with the leading two powers in the

infinite field expansion

$$E(z) - E^{(0)} \sim H_1 z^{\mu(1)} + H_2 z^{\mu(2)}, \quad \text{as } |z| \to \infty ,$$

obtained from Eq. (5.1). Moreover, the coefficients $W_1^{(N)}$ and $W_2^{(N)}$ converge uniformly to H_1 and H_2, respectively, as $N \to \infty$.

Proof: This theorem follows from the results of Theorem 5.1 and from the original construction in Eq. (5.27).

Uniform convergence of the approximate convergents $\tilde{E}_N(z)$ in (5.27) implies that the asymptotic expansion coefficients $W_i^{(N)}$, $i = 1,2$, converge to the coefficients of the corresponding terms in the infinite field expansion (5.1) as $N \to \infty$.

B. Application to *S*-fraction representations of the quartic anharmonic oscillator

The goal of this section is to employ the above procedures to recover the leading terms in the infinite field expansion (5.1) for the QAHO,[7] for which $\alpha = \frac{1}{3}$ and $\gamma = \frac{2}{3}$. The coefficients $F_K^{(0)}$ represent the K th eigenvalues of the quartic oscillator $\hat{H} = \hat{p}^2 + x^4$. We determine the asymptotic expansion of

$$\tilde{E}_N(z) = E^{(0)} + z\tilde{w}_N(z), \quad \text{as } z \to \infty , \tag{5.31}$$

where the modified CF, $\tilde{w}_N(z)$, is constructed as in Sec. V A. It shall always be understood that $z \in \tilde{\mathbb{C}}$.

From Eq. (4.6), we define the relevant parameters

$$k = \tfrac{3}{2}, \quad A^{(1)} = \tfrac{1}{8} + \tfrac{3}{4}K, \quad A^{(2)} = -\tfrac{1}{8} + \tfrac{3}{4}K, \quad \Delta A/k = \tfrac{1}{6} . \tag{5.32}$$

The analysis to follow will be applicable to ground and excited states. The important property $0 < (\Delta A/k) < \frac{1}{2}$, for all states, will be implicitly assumed since it plays a role in the ordering of powers of z, for example, in Eq. (5.17).

For the *odd convergent truncation*, Eqs. (5.10), etc., yield the expansion

$$g_{2n}(z) = D_1^{(2n)} z^{-s} + D_2^{(2n)} z^{-1} + D_3^{(2n)} z^{-2s} + \cdots , \tag{5.33}$$

where $s = \frac{1}{2} + \Delta A/k$ and

$$\begin{aligned} D_1^{(2n)} &= \frac{\Gamma(\frac{1}{2} - \Delta A/k)\Gamma(n + A^{(1)}/k)}{\Gamma(\frac{1}{2} + \Delta A/k)\Gamma(n + \frac{1}{2} + A^{(2)}/k)} \\ &\quad \times k^{-(1/2 + \Delta A/k)}, \\ D_2^{(2n)} &= k^{-1}(-\tfrac{1}{2} + \Delta A/k)^{-1} . \end{aligned} \tag{5.34}$$

We note that $g_{2n}(z) = O(z^{-2/3})$, as $|z| \to \infty$. Substitution of Eq. (5.33) into (5.17) and multiplication by z yield the formal expansion

$$z\tilde{w}_{2n-1}(z) \sim W_1^{(2n-1)} z^{1/2 - \Delta A/k} + W_2^{(2n-1)} + \cdots , \tag{5.35}$$

where

$$\begin{aligned} W_1^{(2n-1)} &= \frac{c_{2n-1} D_1^{(2n)} a_{2n-3,n-2}}{b_{2n-2,n-1}}, \\ W_2^{(2n-1)} &= [b_{2n-2,n-1}]^{-1} \\ &\quad \times [a_{2n-2,n-2} + c_{2n-1} D_2^{(2n)} a_{2n-3,n-2}] . \end{aligned} \tag{5.36}$$

It is immediately noticed that the dominant behavior in Eq. (5.35) is given by $O(z^{1/3})$, in agreement with the infinite field limit.

We now consider the coefficient $W_1^{(2n-1)}$ for a general level of the QAHO, continuing to suppress the index K for notational ease. A look at the closed form expressions in Table I as well as the recursion relations (2.4) reveal that the polynomial coefficients which occur in Eq. (5.36) have the simple form

$$\begin{aligned} a_{2n-3,n-2} &= c_1 c_3 c_5 \cdots c_{2n-3} , \\ b_{2n-2,n-1} &= c_2 c_4 c_6 \cdots c_{2n-2} . \end{aligned} \tag{5.37}$$

The leading coefficient in Eq. (5.35) for the K th level becomes

$$\begin{aligned} W_1^{(2n-1),K} &= \left[\prod_{i=1}^{n=1} \frac{c_{2i-1}^K}{c_{2i}^K} \right] c_{2n-1}^K \\ &\quad \times \frac{\Gamma(\frac{1}{3})\Gamma(n + \frac{1}{12} + K/2)}{\Gamma(\frac{2}{3})\Gamma(n - \frac{1}{12} + K/2)} k^{-2/3} . \end{aligned} \tag{5.38}$$

From Theorem 5.2, it follows that $W_1^{(2n-1),K} \to F_K^{(0)}$, as $n \to \infty$, where the $F_K^{(0)}$ were defined at the beginning of this section. This behavior is observed numerically and will be discussed at the end of this section.

We now focus on the second term of the expansion in (5.35). For the QAHO, no constant terms are present in the infinite field expansion (5.1). From Theorem 5.2, however, we expect that $W_2^{(2n-1),K} \to -E_K^{(0)} = -(2K+1)$, as $n \to \infty$.

Returning to the *even convergent truncation procedure*, Eqs. (5.10), etc., yield the expansion

$$g_{2n+1}(z) \sim D_1^{(2n+1)} z^{-t} + D_2^{(2n+1)} z^{-2t} + D_3^{(2n+1)} z^{-1} + \cdots , \tag{5.39}$$

where $t = \frac{1}{2} - \Delta A/k$ and

$$\begin{aligned} D_1^{(2n+1)} &= \frac{\Gamma(\frac{1}{2} + \Delta A/k)\Gamma(n + \frac{1}{2} + A^{(2)}/k)}{\Gamma(\frac{1}{2} - \Delta A/k)\Gamma(n + 1 + A^{(1)}/k)} k^{-1/2 + \Delta A/k}, \\ D_2^{(2n+1)} &= \frac{\Gamma(n + A^{(1)}/k)}{(\frac{1}{2} - \Delta A/k)} [D_1^{(2n+1)}]^2 . \end{aligned} \tag{5.40}$$

We now substitute the above into Eq. (5.17), where $2n-1$ is replaced by $2n$, etc., and multiply by z to find that

$$z\tilde{w}_{2n}(z) \sim W_1^{(2n)} z^{1/2 - \Delta A/k} + W_2^{(2n)} + \cdots , \tag{5.41}$$

where

$$\begin{aligned} W_1^{(2n)} &= a_{2n-1,n-1} [c_{2n} D_1^{(2n+1)} b_{2n-2,n-1}]^{-1} , \\ W_2^{(2n)} &= \left[a_{2n-2,n-2} - \frac{a_{2n-1,n-1}(n + A^{(1)}/k)}{c_{2n}(\frac{1}{2} - \Delta A/k)} \right] \\ &\quad \times [b_{2n-2,n-1}]^{-1} . \end{aligned} \tag{5.42}$$

The exponents in (5.41) agree with those of the odd convergent expansion in Eq. (5.35). Proceeding as before, the leading term coefficient for the K th level may be simplified to

$$W_1^{(2n),K} = \left[\prod_{i=1}^{n} \frac{c_{2i-1}^K}{c_{2i}^K} \right] \frac{\Gamma(\frac{1}{3})\Gamma(n + \frac{13}{12} + K/2)}{\Gamma(\frac{2}{3})\Gamma(n - \frac{1}{12} + K/2)} k^{1/3} . \tag{5.43}$$

Again, it is expected that $W_1^{(2n)} \to F_K^{(0)}$, as $n \to \infty$. In fact, the common limiting behavior of the two leading term coeffi-

TABLE III. The leading term coefficients $W_1^{(2n-1)}$ and $W_1^{(2n)}$ in Eqs. (5.38) and (5.43), respectively, for odd and even truncation expansion of the ground state ($K=0$) quartic anharmonic oscillator S fraction. These coefficients were calculated from the c_n presented in Table II. The exact asymptotic value corresponds to the ground state energy of the quartic oscillator, accurately calculated in Ref. 36.

n	$W_1^{(2n-1)}$	$W_1^{(2n)}$
1	1.224 047 7874	1.136 615 8026
2	1.184 372 7691	1.128 172 1211
3	1.147 912 1127	1.120 524 8180
4	1.131 702 1008	1.114 333 6496
5	1.121 723 1409	1.109 553 1035
6	1.114 927 2483	1.105 798 2023
7	1.109 924 9553	1.102 752 7649
8	1.106 050 6539	1.100 227 0571
9	1.102 941 5164	1.098 092 4465
10	1.100 377 3017	1.096 258 9783
11	1.098 216 7152	1.094 662 9230
12	1.096 364 8471	1.093 257 8234
13	1.094 755 2164	1.092 008 8703
14	1.093 339 6745	1.090 889 4343
15	1.092 082 4154	1.089 878 7881
16	1.090 956 2079	1.088 960 5397
17	1.089 939 9310	1.088 121 5369
18	1.089 016 9206	1.087 351 0914
19	1.088 173 8319	1.086 640 4182
20	1.087 399 8377	1.085 982 2236
25	1.084 302 1726	1.083 294 1739
30	1.082 061 9832	1.081 298 6219
35	1.080 346 3128	1.079 742 6098
40	1.078 978 6658	1.078 485 8784
45	1.077 855 7235	1.077 443 6524
50	1.076 912 4936	1.076 561 3088
Exact	1.060 362 0905	1.060 362 0905

cients may be seen by examining the ratio

$$\frac{W_1^{(2n)}}{W_1^{(2n-1)}} = \frac{k\Gamma(n+1+A^{(1)}/k)}{c_{2n}\Gamma(n+A^{(1)}/k)} = \frac{kn+A^{(1)}}{c_{2n}} \to 1, \quad \text{as } n\to\infty, \tag{5.44}$$

where the final limit follows from Eq. (5.2).

It is also expected that $W_2^{(2n)} \to -E_K^{(0)}$, as before. Here, a ratio analogous to (5.44) exists between coefficients obtained from odd and even truncations.

TABLE IV. The leading term coefficients $W_1^{(N),K}$ in Eqs. (5.38) and (5.43) for odd and even truncation expansion of the QAHO excited states, $K=1$ and 2, calculated from exact S-fraction coefficients c_n^K. The entries denoted "Extrap" are obtained from a Thiele–Padé extrapolation of the numerical values for $n<40$. The exact values correspond to the eigenvalues $E_K^{(0)}$ of the first and second excited states of the quartic oscillator, as calculated in Ref. 36.

n	$W_1^{(2n-1),1}$	$W_1^{(2n),1}$	$W_1^{(2n-1),2}$	$W_1^{(2n),2}$
10	4.167 460 1887	4.112 230 5151	9.331 761 4599	8.687 772 5465
15	4.086 243 5971	4.056 467 9529	8.605 787 0279	8.372 579 4890
20	4.041 365 6060	4.022 161 4546	8.192 793 1484	8.110 471 3017
25	4.012 117 4604	3.998 449 3352	8.099 262 4616	8.040 537 0703
30	3.991 198 6065	3.980 844 6770	8.033 011 7261	7.988 468 4132
35	3.975 315 0468	3.967 126 7485	7.983 089 7907	7.947 836 1085
40	3.962 740 8882	3.956 058 0405	7.943 812 7059	7.915 026 9928
Extrap	3.800	3.799 6	7.46	7.456
Exact	3.799 673 0298	3.799 673 0298	7.455 697 9380	7.455 697 9380

Numerical results: The values of the leading term coefficients $W_1^{(2n-1)}$ and $W_1^{(2n)}$ in Eqs. (5.38) and (5.43), calculated from the exact coefficients c_n of Table II, are presented in Table III. A regular monotonic behavior toward the exact value[36] $F_0^{(0)} = 1.060\,362\,09...$ is observed for both sequences. For $n=52$, the coefficients are in error by about 1.5%. The accurate estimation of this constant from LOPT has been a subject of some interest.[13,37] A number of extrapolation techniques were adopted to determine whether these sequences could predict the exact values more accurately.

In one method, the sequence of S-fraction coefficients c_n was artificially extended by a Thiele–Padé CF extrapolation which employed the asymptotics of Eq. (4.6). The approximate coefficients $\hat{c}_n$ were calculated to $n=18\,000$. Eqs. (5.38) and (5.43) were then evaluated by employing the leading three terms of an asymptotic relation for the ratio of the $\Gamma(n)$ functions. The result was $\hat{W}_1^{(18\,000)} = 1.061\,550\,0$, which is in error by 0.11%. Needless to say, this method converges very slowly—a 180-fold increase in the number of c_n yields only a tenfold increase in accuracy.

TABLE V. Numerical values of the coefficients $W_2^{(N),K}$ for odd and even convergent expansions of the QAHO, $K=0$ and 1 states, as calculated from exact S-fraction coefficients c_n^K using Eqs. (5.36) and (5.42). The entries denoted "Extrap" are obtained from a Thiele–Padé extrapolation of the numerical values. The exact values correspond to $-E_K^{(0)} = -(2K+1)$, the negatives of the unperturbed harmonic oscillator eigenvalues.

n	$W_2^{(2n-1),0}$	$W_2^{(2n),0}$	$W_2^{(2n-1),1}$	$W_2^{(2n),1}$
10	−1.319 182 0604	−1.307 525 7128	−5.797 418 9494	5.638 473 0622
15	−1.295 084 5542	−1.287 925 1310	−5.562 695 7668	5.464 876 2762
20	−1.279 587 8618	−1.274 511 5840	−5.415 005 9102	5.345 663 1522
25	−1.268 236 7160	−1.264 445 2638	−5.309 333 3028	5.256 213 5888
30	−1.259 587 9252	−1.256 454 5210	−5.228 033 6260	5.185 296 6200
35	−1.252 476 9026	−1.249 867 1622	−5.162 492 9676	5.126 926 9212
40	−1.246 515 1018	−1.244 287 2144	−5.107 904 0762	5.077 564 8328
Extrap	-1.00 ± 0.02	-1.00 ± 0.02	-3.0 ± 0.2	-2.9 ± 0.2
Exact	−1	−1	−3	−3

A final attempt to accelerate the slow convergence of this sequence was to Thiele-extrapolate the approximate $\hat{W}_1^{(N)}$ values of above to their infinite limit. Sets of $[n,n]$ Thiele–Padé approximants were constructed from all sets of $2n+1$ consecutive members of the sequence $\hat{W}_1^{(N)}$, $N = 1000, 2000, \ldots, 18\,000$. The common limit of these extrapolations for $n = 3,4,5$, and 6 was 1.060 362 075, a result in error by less than 0.000 000 02. This represents the most accurate calculation of the infinite coupling constant limit from LOPT. The accuracy surpasses the calculations of Refs. 13 and 37.

A similar behavior is observed for the sequences of leading term coefficients for excited state representations. Some values from the sequences corresponding to the levels $K = 1$ and 2 are presented in Table IV. Also given are estimated limits of the sequences as predicted by a Thiele–Padé extrapolation of the elements of these sequences only.

Table V presents some values of the coefficients $W_2^{(N)}$ for both odd and even convergent expansions associated with the ground and first excited states, $K = 0$ and 1, respectively. These values were calculated from the exact S-fraction coefficients. Their convergence to the theoretical values $-E_K^{(0)}$ is not as rapid as for the leading term coefficients. Also presented are Thiele–Padé CF extrapolations of these sequences which are in good agreement with the theoretical values.

C. S-fraction representations of charmonium

The infinite field expansion for the charmonium model has the form of Eq. (5.1) with $\alpha = \frac{2}{3}$ and $\gamma = \frac{1}{3}$. The leading term coefficients $F_{NLM}^{(0)}$ represent eigenvalues of a three-dimensional Airy-type differential equation.[16,30] We now construct a CF representation analogous to Eq. (5.31) and investigate its large field asymptotics.

The asymptotic behavior of the charmonium $S_{(1)}$-fraction coefficients was given in Eq. (4.13). The parameters relevant to the following analysis are

$$\begin{aligned} &k = \tfrac{3}{2}N^3, \\ &A^{(1)} = N^3(-\tfrac{1}{2} + \tfrac{3}{2}N), \\ &A^{(2)} = N^3(-\tfrac{1}{4} + \tfrac{3}{2}N), \\ &\Delta A/k = -\tfrac{1}{6}. \end{aligned} \tag{5.45}$$

We summarize the results of both truncation procedures below.

Odd convergent truncation: Referring to Eq. (5.16), we have $r(1) = -\frac{1}{3}$ and $r(2) = -\frac{2}{3}$ and

$$\begin{aligned} &D_1^{(2n)} = \frac{\Gamma(\frac{2}{3})\Gamma(n - \frac{1}{3} + N)}{\Gamma(\frac{1}{3})\Gamma(n + \frac{1}{3} + N)} \left(\frac{2}{3}\right)^{1/3} N^{-1}, \\ &D_2^{(2n)} = 3(n - \tfrac{2}{3} + N)[D_1^{(2n)}]^2. \end{aligned} \tag{5.46}$$

The net result is

$$z\tilde{w}_{2n-1}(z) \sim W_1^{(2n-1)} z^{2/3} + W_2^{(2n-1)} z^{1/3} + \cdots, \tag{5.47}$$

where

$$\begin{aligned} &W_1^{(2n-1)} = \frac{c_{2n-1} D_1^{(2n)} a_{2n-3,n-2}}{b_{2n-2,n-1}}, \\ &W_2^{(2n-1)} = W_1^{(2n-1)} \left[\frac{D_2^{(2n)}}{D_1^{(2n)}} - W_1^{(2n-1)} \frac{b_{2n-3,n-2}}{a_{2n-3,n-2}} \right]. \end{aligned} \tag{5.48}$$

Even convergent truncation: Referring to Eq. (5.22), we have $s(1) = \frac{2}{3}$, $s(2) = 1$, and

$$\begin{aligned} &D_1^{(2n+1)} = \frac{\Gamma(\frac{1}{3})\Gamma(n + \frac{1}{3} + N)}{\Gamma(\frac{2}{3})\Gamma(n + \frac{2}{3} + N)} (\tfrac{2}{3})^{2/3} N^{-2/3}, \\ &D_2^{(2n+1)} = -3/k. \end{aligned} \tag{5.49}$$

The net result is

$$z\tilde{w}_{2n}(z) \sim W_1^{(2n)} z^{2/3} + W_2^{(2n)} z^{1/3} + \cdots, \tag{5.50}$$

where

$$\begin{aligned} &W_1^{(2n)} = \frac{a_{2n-1,n-1}}{c_{2n} D_1^{(2n+1)} b_{2n-2,n-1}}, \\ &W_2^{(2n)} = W_1^{(2n)} \left[-\frac{D_2^{(2n+1)}}{D_1^{(2n+1)}} - W_1^{(2n)} \frac{b_{2n-1,n-1}}{a_{2n-1,n-1}} \right]. \end{aligned} \tag{5.51}$$

We immediately notice that the leading exponent $\alpha = \frac{2}{3}$ is obtained from the term $\frac{1}{2} - \Delta A/k$. The leading term coefficients $W_1^{(2n-1)}$ and $W_2^{(2n)}$ have the same generic form as their QAHO counterparts in Eqs. (5.38) and (5.43). For a general

TABLE VI. Numerical values of the leading term coefficients $W_1^{(k)}$ in Eqs. (5.52) and (5.53) for truncations of the ground state charmonium S fraction. The exact value is the ground state of an Airy differential equation.

n	$W_1^{(2n-1)}$	$W_1^{(2n)}$
1	0.502 195 6152	1.255 489 0381
2	1.255 489 0381	1.365 191 9638
3	1.397 286 2825	1.452 522 4410
4	1.468 149 2263	1.506 058 7769
5	1.515 535 3965	1.543 038 1825
6	1.549 352 0460	1.570 587 0907
7	1.575 100 4133	1.592 108 1965
8	1.595 479 8492	1.609 502 3004
9	1.612 117 7745	1.623 936 6885
10	1.626 021 2941	1.636 157 5755
11	1.637 856 5953	1.646 674 8240
12	1.648 085 4000	1.655 848 0979
13	1.657 037 1400	1.663 938 9765
14	1.664 954 3381	1.671 143 2758
15	1.672 020 0523	1.677 610 7481
16	1.678 375 1994	1.683 458 0510
17	1.684 130 2254	1.688 777 6125
18	1.689 373 0844	1.693 643 7351
19	1.694 174 7790	1.698 116 9063
20	1.698 593 3221	1.702 246 9261
25	1.716 369 0297	1.718 992 1717
30	1.729 305 5925	1.731 305 1658
35	1.739 252 2482	1.740 841 1185
40	1.747 201 9267	1.748 503 5446
45	1.753 740 9885	1.754 932 4751
50	1.759 240 6071	1.760 172 9309
Exact	1.855 757 081	1.855 757 081

TABLE VII. Results of a Thiele–Padé estimation of the limits of leading term coefficients $W_1^{(k)}$ in Eqs. (5.52) and (5.53), as $k\to\infty$, k even and odd, for the six lowest-lying charmonium states. The limits $W_1^{(\infty)}$ are presented to the number of digits shared by estimates for even-k and odd-k sequences. The exact values $F_{NL}^{(0)}$, which correspond to the (N,L) state eigenvalues of a three-dimensional Airy differential equation, are taken from Ref. 30.

State	N	L	$W_1^{(\infty)}$	$F_{NL}^{(0)}$
$1S$	1	0	1.855 75	1.855 757
$2S$	2	0	3.24	3.244 6
$2P$	2	1	2.668	2.667 9
$3S$	3	0	4.4	4.381 7
$3P$	3	1	3.9	3.876 8
$3D$	3	2	3.37	3.371 8

state $|N,L,M\rangle$, they assume the explicit form

$$W_1^{(2n-1),NLM}=\left[\prod_{i=1}^{n-1}\frac{c_{2i-1}^{NLM}}{c_{2i}^{NLM}}\right]c_{2n-1}^{NLM}\times\frac{\Gamma(\frac{2}{3})\Gamma(n-\frac{1}{3}+N)}{N\Gamma(\frac{1}{3})\Gamma(n+\frac{1}{3}+N)}\left(\frac{2}{3}\right)^{1/3},\tag{5.52}$$

$$W_1^{(2n),NLM}=\left[\prod_{i=1}^{n}\frac{c_{2i-1}^{NLM}}{c_{2i}^{NLM}}\right]\frac{\Gamma(\frac{2}{3})\Gamma(n+\frac{2}{3}+N)}{\Gamma(\frac{1}{3})\Gamma(n+\frac{1}{3}+N)}N^2\left(\frac{3}{2}\right)^{2/3}.\tag{5.53}$$

An analysis of the same form as in Eq. (5.44) reveals that the above constants approach a common limit as $n\to\infty$. From Eq. (5.1), it is expected that this common limit is $F_{NLM}^{(0)}$.

Numerical results: The values of the leading term coefficients $W_1^{(2n-1)}$ and $W_2^{(2n)}$ in Eq. (5.52), corresponding to the ground state $N=1$, $L=M=0$, are presented in Table VI. A regular monotone behavior approaching the exact value $F^{(0)}=1.855\,757\,081$ is observed for both sequences. A Thiele–Padé extrapolation of values from each sequence affords approximate limits which are in excellent agreement with the exact results. Table VII presents the results of these extrapolations for all states $1\leqslant N\leqslant 3$, $L=0,1,2,\ldots,N$. The estimates are presented to the number of digits shared by extrapolations of even and odd sequences. In all cases, the estimated limits are in good agreement with the exact values taken from Ref. 30.

TABLE VIII. Numerical values of the second term coefficients $W_2^{(k)}$ in Eqs. (5.48) and (5.51) for ground state charmonium, as obtained from exact S-fraction coefficients c_n^{100}. The entries denoted "Extrap" are obtained from Thiele extrapolation of the sets of numerical values. They represent estimates of the expectation value of the negative Coulomb potential over the unperturbed ground state Airy function.

n	$W_2^{(2n-1)}$	$W_2^{(2n)}$
10	0.727 593 170 3	0.706 640 967 7
15	0.623 259 099 7	0.608 708 767 3
20	0.549 905 928 8	0.538 892 017 4
25	0.493 981 747 5	0.485 182 577 5
30	0.449 114 911 4	0.441 823 389 1
35	0.411 841 069 4	0.405 637 637 0
40	0.380 080 166 3	0.374 696 598 4
Extrap	-0.26 ± 0.02	-0.26 ± 0.03

Table VIII presents some values of the coefficients $W_2^{(2n-1)}$ and $W_2^{(2n)}$ corresponding to the ground state, along with the Thiele–Padé extrapolated limits of both sequences. Interestingly, the limits of these positive and monotone decreasing sequences are negative, which is to be expected, since they correspond to the expectation value of a negative Coloumb potential over the unperturbed Airy eigenfunctions.

VI. THE RELATION BETWEEN SUBDOMINANT TERMS IN LOPT AND CFLO FOR $S_{(1)}$ FRACTIONS

Here we show, by example, that a simple relationship does not exist between $n!$-type Stieltjes series coefficients and their $S_{(1)}$-fraction counterparts as far as subdominant terms are concerned. We shall refer to the relevant expansions for the quartic anharmonic oscillator, Eqs. (4.4) and (4.6), and inquire whether a relationship exists between the $1/n$ correction term in Eq. (4.4) and the constant terms in Eq. (4.6). The knowledge of these terms in closed form serves as a motivation. The following treatment will be centered around the QAHO problem, and special reference to the charmonium model will be made at the end.

For convenience, we consider the following scaled QAHO perturbation coefficients,

$$E_K^{(n)}=(-1)^{n+1}\Gamma(n+K+\tfrac{1}{2})[1+A_K n^{-1}+O(n^{-2})],\tag{6.1}$$

where

$$A_K=-(\tfrac{95}{72}+\tfrac{29}{12}K+\tfrac{17}{12}K^2)\tag{6.2}$$

and the geometric factor $k=\frac{3}{2}$ is combined with the coupling constant β to produce the expansion parameter $z=k\beta$. The multiplicative factor has also been ignored as it will only contribute to c_1^K. The coefficients of the $S_{(1)}$ fraction which represents the scaled series beginning with term $E_K^{(1)}$ are given by

$$c_n^K=n/2+K/2\pm\tfrac{1}{12}+R_n^{(i),K},\qquad n\geq 2,\quad i=\begin{cases}1, & n \text{ even},\\ 2, & n \text{ odd},\end{cases}\tag{6.3}$$

where it has been conjectured that $R_n^{(i),K}=O(n^{-1/2})$. Let us now consider the "model" perturbation series whose coefficients contain only the dominant terms of the $E_K^{(n)}$ in (4.1), i.e.,

$$\overline{E}(z)=1+\sum_{n=1}^{\infty}\overline{E}_K^{(n)}z^n=1+\sum_{n=1}^{\infty}(-1)^{n+1}\Gamma\left(n+K+\frac{1}{2}\right)z^n.\tag{6.4}$$

From Eq. (3.11), the coefficients of the S-fraction representation, $\overline{E}(z)=1+z\overline{C}(z)$, are given by

$$\overline{c}_1^K=\Gamma(K+\tfrac{3}{2}),\qquad \overline{c}_{n,\text{even}}^K=n/2+K+\tfrac{1}{2},\qquad \overline{c}_{n,\text{odd}}^K=n/2-\tfrac{1}{2}.\tag{6.5}$$

A comparison between Eqs. (6.3) and (6.5) gives the interest-

ing set of relations,

$$c_n^K = \bar{c}_n^K + (-1)^{n+1}\epsilon^K + R_n^{(i),K}$$
$$= d_n^K + R_n^{(i),K}, \quad n \geq 2, \tag{6.6}$$

where

$$\epsilon^K = K/2 + \tfrac{5}{12}. \tag{6.7}$$

In other words, the "true" QAHO coefficients c_n are obtained by perturbing the model hypergeometric $\bar{c}_n^K$ with a constant term alternating in sign and correction terms of order $o(1)$. One may well ask whether the oscillating perturbation alone could account for the appearance of the term A_K/n in (6.1), which, in turn, arises from a transformation of the series in (6.4). In other words, given the formal CF-power series correspondence,

$$\mathop{\mathbf{K}}_{n=1}^{\infty} \frac{d_n^K z}{1} = \sum_{n=1}^{\infty} (-1)^{n+1}\Gamma\left(n + K + \frac{1}{2}\right) \times\left(1 + \frac{B_K}{n} + \cdots\right) z^n, \tag{6.8}$$

does $B_K = A_K$?

In order to answer this question, we define

$$F(z,\epsilon) = 1 + z\Gamma(a-\epsilon)\Gamma(1+\epsilon)\frac{{}_2F_0(a-\epsilon, 1+\epsilon, -z)}{{}_2F_0(a-\epsilon, \epsilon, -z)}, \tag{6.9}$$

where $a = K + \frac{3}{2}$ so that $F(z,0) = \bar{E}(z)$. For ease of notation, the index K will be supressed in the following presentation. From Eq. (5.8), the function $F(z,\epsilon)$ is seen to admit the S-fraction representation

$$F(z,\epsilon) = 1 + \mathop{\mathbf{K}}_{n=1}^{\infty} \frac{\bar{c}_n^K + (-1)^{n+1}\epsilon}{1}. \tag{6.10}$$

We now expand $F(z,\epsilon)$ as a power series in z,

$$F(z,\epsilon) = 1 + \sum_{n=1}^{\infty} F^{(n)} z^n, \tag{6.11}$$

and seek to express the coefficients $F^{(n)}$ as

$$F^{(n)} \sim (-1)^{n+1}\Gamma(n+a-1)[1 + B/n + \cdots], \tag{6.12}$$

where B will be determined in terms of a and ϵ. We let

$${}_2F_0(a-\epsilon, 1+\epsilon; -z) = \sum_{n=0}^{\infty} a_n z^n, \tag{6.13}$$

$${}_2F_0(a-\epsilon, \epsilon; -z) = \sum_{n=0}^{\infty} b_n z^n \tag{6.14}$$

$$= \left[\sum_{n=0}^{\infty} p_n z^n\right]^{-1}. \tag{6.15}$$

The general coefficient $F^{(n)}$ in Eq. (6.11) will have the formal Cauchy composition

$$F^{(n)} = \Gamma(a-\epsilon)\Gamma(1+\epsilon)(a_0 p_{n-1} + a_1 p_{n-2} + \cdots + a_{n-2} p_1 + a_{n-1} p_0). \tag{6.16}$$

Formal expansion of the hypergeometric function in Eq. (6.13) and use of the relation[38]

$$\Gamma(n+r) \sim \Gamma(n+s) n^{r-s}[1 + (r-s)(r+s-1)/(2n) + O(n^{-2})], \quad \text{as } n \to \infty, \tag{6.17}$$

yields

$$a_{n-1} = (-1)^{n-1}\Gamma(n+a-1)/\Gamma(a-\epsilon)\Gamma(1+\epsilon) \times [1 + (\epsilon^2 - (a-1)\epsilon)/n + O(n^{-2})]. \tag{6.18}$$

Furthermore, $c_0 = 1$, so we have determined the contribution from $p_0 a_{n-1}$ in (6.16). In order to find the contribution from $a_{n-2} p_1$, we use the fact that $p_1 = \epsilon(a-\epsilon)$ and apply relation (6.17) to (6.13) to obtain

$$a_{n-2} p_1 = (-1)^n\Gamma(n+a-1)/(\Gamma(a-\epsilon)\Gamma(1+\epsilon)) \times [(a-\epsilon)\epsilon/n + O(n^{-2})]. \tag{6.19}$$

The term $a_{n-3} p_2$ contributes terms of order $O(n^{-2})$ to (6.16) and, along with lower terms, need not be considered, with the exception of the final term $a_0 p_n$.

To determine the asymptotic behavior of the coefficients p_n of the inverse series in Eq. (6.15), we employ the method discussed by Bender.[39] It is sufficient to show that if (i) $b_n \neq 0$, $b_{n-1} = o(b_n)$, and (ii) there exists an $R > 0$ such that for n sufficiently large

$$S_R \equiv \sum_{k=R}^{n-R} |b_k b_{n-k}| = O(b_{n-R}),$$

then the coefficients p_n are given by

$$p_n = \sum_{k=0}^{R-1} g_k b_{n-k} + O(b_{n-R}),$$

where the g_k are coefficients of the power series expansion

$$-\left[\sum_{n=0}^{\infty} b_n z^n\right]^{-2} = \sum_{n=0}^{\infty} g_n z^n.$$

The above properties are easily established from the exact form of the b_n coefficients and the final result is

$$p_n = \frac{(-1)^{n+1}}{\Gamma(a-\epsilon)\Gamma(\epsilon)}\Gamma(n+a)\left[\frac{1}{n} + O(n^{-2})\right]. \tag{6.20}$$

The net contribution from Eqs. (6.18), (6.19), and (6.20) to Eq. (6.16) is

$$B_K = 2\epsilon^2 - 2a\epsilon. \tag{6.21}$$

For the quartic anharmonic oscillator, $\epsilon = K/2 + \frac{5}{12}$ and $a = K + \frac{3}{2}$, so that

$$B_K = -(\tfrac{65}{72} + \tfrac{3}{2}K + \tfrac{1}{2}K^2). \tag{6.22}$$

Numerical results for $K = 0, 1, 2, 3$, and 4 are in exact agreement with this expression. Clearly, this term does not equal the true asymptotic correction for the QAHO perturbation coefficients in (6.2).

Turning to the $L = 0$ charmonium representations, we consider the scaled series coefficients

$$E_N^{(n)} = (-1)^{n+1}\Gamma(n+2N) \times [1 - \tfrac{1}{9}(10 + 18N + 21N^2)(1/n) + O(n^{-2})]. \tag{6.23}$$

The expansion parameter becomes $z = \frac{3}{2}N^3\lambda$. The associated S-fraction coefficients have the form

$$c_n^N = \frac{n}{2} + \begin{cases} N - \frac{1}{3} \\ N - \frac{1}{6} \end{cases} + R_n^{(i),N}, \quad \begin{cases} n \text{ even}, \\ n \text{ odd}. \end{cases} \tag{6.24}$$

The relevant parameters in Eq. (6.21) are $a = 2N + 1$ and $\epsilon = N + \frac{1}{3}$. Thus, we have

$$B_N = -(\tfrac{4}{9} + 2N + 2N^2), \tag{6.25}$$

again in disagreement with the LOPT result in (6.23).

This represents the limit of any closed-form analysis. Numerical experiments suggest that all subdominant terms in $R_n^{(j)}$ contribute to the $1/n$ correction to the perturbation series. The experiments and mechanism will be discussed elsewhere.

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APPENDIX: PROOF OF PROPOSITION 3.1

In this section we prove Proposition 3.1 [c.f. Eq. (3.7)]: Given a Stieltjes series $f(z)$ whose coefficients behave asymptotically as

$$a_n \sim (-1)^{n+1}\Gamma(n+a)k^n(1+A/n+\cdots), \quad \text{as } n\to\infty, \tag{A1}$$

where a, k, and A are real constants, then the coefficients of its S-fraction representation $f(z)=a_0+zC(z)$ behave asymptotically as

$$c_n \sim \tfrac{1}{2}kn, \quad \text{as } n\to\infty. \tag{A2}$$

We now consider this quotient-difference (QD) table for the above series, as defined by Eqs. (2.11) and (2.12) and illustrated in Fig. 1. The existence and uniqueness of the QD table, hence the c_n, is guaranteed from the hypothesis that $f(z)$ is Stieltjes. From Eq. (2.11) it follows that the elements of the column q_{n1} behave asymptotically as

$$q_{n1} = k(n+a)+O(n^{-1}), \quad \text{as } n\to\infty. \tag{A3}$$

The following expansions are now assumed for the columns,

$$\begin{aligned} q_{nm} &= n[B_{0m}+B_{1m}/n+B_{2m}/n^2+\cdots], \\ &\quad m=1,2,..., \quad \text{as } n\to\infty, \\ e_{nm} &= C_{0m}+C_{1m}/n+C_{2m}/n^2+\cdots, \\ &\quad m=1,2,..., \quad \text{as } n\to\infty. \end{aligned} \tag{A4}$$

From Eq. (A3), we have $B_{0m}=k$.

Substitution of the above expansions into the rhombus rules, Eq. (2.12) shows that the first four expansion coefficients are given by

$$\begin{aligned} &C_{0m}=mB_{01}, && B_{0m}=B_{0,m-1}=\cdots=B_{01}, \\ &C_{1m}=0, && B_{1m}=B_{1,m-1}=\cdots=B_{11}, \\ &C_{2m}=-mB_{21}, && B_{2m}=B_{2,m-1}=\cdots=B_{21}, \\ &C_{3m}=-2m^2-m(2B_{31}+B_{21}), && B_{3m}=B_{30}+2mB_{21}. \end{aligned} \tag{A5}$$

In other words, the elements of the q_{nm} columns are growing linearly downward as $B_{01}n$, while those of the e_{nm} columns approach the constants C_{0m}. However, these constants $C_{0m}=mB_{01}$ grow linearly as we move outward horizontally.

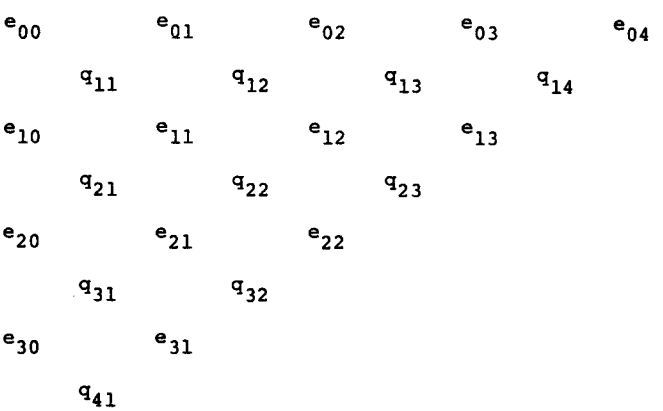

FIG. 2. The *extended* QD table associated with the QD table presented in Fig. 1. The upper triangle array represents the quotient-difference array for the inverse power series. The rows e_{0m} and q_{1m} are initialized according to Eqs. (A6). The rhombus rules in Eq. (A8) permit a downward calculation of the array from these rows to the diagonal elements q_{nn} and e_{nn}. This constitutes the *extended QD scheme*.

We now consider an extension[23] of the QD array of Fig. 1 to produce a rectangular array as shown in Fig. 2. All elements obey the rhombus rules as before. The elements of the first two rows of the extended array are given by

$$\begin{aligned} &q_{11} = -a_1/a_0 = b_1/b_0, \\ &q_{1m} = 0, \quad m=2,3,4,..., \\ &e_{1m} = -b_{m+1}/b_m, \quad m=2,3,4,..., \end{aligned} \tag{A6}$$

where the b_i are coefficients of the reciprocal power series,

$$[a_0+a_1z+a_2z^2+\cdots]^{-1} = b_0+b_1z+b_2z^2+\cdots. \tag{A7}$$

All elements of the QD array in Fig. 2 may, in fact, be calculated from the initial values in Eq. (A6) by rearranging the rhombus rules as follows:

$$\begin{aligned} e_{nm} &= e_{n-1,m}q_{n,m+1}/q_{nm}, \\ q_{nm} &= q_{n-1,m}+e_{n-1,m}-e_{n-1,m-1}, \\ &\quad m=2,3,..., \quad n=2,3,... . \end{aligned} \tag{A8}$$

This method of calculating the QD array is known as the *extended QD scheme*.

From the asymptotic analysis of reciprocal series described in Ref. 39 and outlined in Sec. VI, it follows that the coefficients b_i of the inverse power series in (A6) behave asymptotically as

$$b_n \sim (-1)^n\Gamma(n+a)k^n(1+B/n+\cdots), \quad \text{as } n\to\infty. \tag{A9}$$

It follows that the elements of the first nonzero row e_{1m} behave asymptotically as

$$e_{1m} \sim k(n+a)+O(n^{-1}), \quad \text{as } n\to\infty. \tag{A10}$$

We now consider row-wise asymptotic expansions, analogous to (A4), and having the form

$$\begin{aligned} e_{nm} &= m[\tilde{B}_{n0}+\tilde{B}_{n1}/m+\tilde{B}_{n2}/m^2+\cdots], \quad \text{as } m\to\infty, \\ q_{nm} &= \tilde{C}_{n0}+\tilde{C}_{n1}/m+\tilde{C}_{n2}/m^2+\cdots, \quad \text{as } m\to\infty. \end{aligned} \tag{A11}$$

These expansions exploit the fundamental symmetry property of the extended QD scheme: q-columns behave as e-rows, and e-columns behave as q-rows. The following rela-

tions between expansion coefficients also reflect this property:

$$\begin{aligned}
&\tilde{C}_{n0} = n\tilde{B}_{10}, && \tilde{B}_{n0} = \tilde{B}_{n-1,0} = \cdots = \tilde{B}_{10}, \\
&\tilde{C}_{n1} = 0, && \tilde{B}_{n1} = \tilde{B}_{n-1,1} = \cdots = \tilde{B}_{11}, \\
&\tilde{C}_{n2} = -n\tilde{B}_{12}, && \tilde{B}_{n2} = \tilde{B}_{n-1,2} = \cdots = \tilde{B}_{12}, \\
&\tilde{C}_{n3} = -2n^2 - n(2\tilde{B}_{12} + \tilde{B}_{02}), && \tilde{B}_{n3} = \tilde{B}_{03} + 2n\tilde{B}_{12}.
\end{aligned} \tag{A12}$$

Thus, for the upper triangular section of the extended QD scheme, the e_{nm} rows grow outward linearly as $\tilde{B}_{10}m$ while the q_{nm} rows approach constants $\tilde{C}_{n0}$. However, these constants grow linearly as $\tilde{B}_{10}n$ as we move downward.

The growth rates for rows and columns of upper and lower triangles of the extended QD array are now seen to match, implying that the diagonal elements grow as $q_{nn} = B_{01}n$, $e_{nn} = B_{01}n$. Since $B_{01} = k$ and $c_{2n} = q_{nn}$, $c_{2n+1} = e_{nn}$, it follows that $c_n \sim kn/2$.

The condition that the a_n have an asymptotic expansion in powers of $1/n$ in Eq. (A1) is evidently strong but not necessary. We have relied on the observation that many of the typical perturbation coefficients encountered in quantum mechanics possess such expansions. This enables us to assume the expansions in (A4) and (A11).

Before closing this section, let us make one final remark concerning the application of the above analysis to other $S_{(k)}$ fractions. For $S_{(2)}$ fractions, the expansions analogous to (A4) and (A7) involve quadratic growth of the q-columns and linear growth of the e-columns. There is a net quadratic growth of entries both horizontally and vertically but the elucidation of the constant coefficient from the relations analogous to Eqs. (A5) and (A12) is much more complicated. Unlike in the $S_{(1)}$ case, all terms B_{nm} and C_{nm} contribute to this constant. This feature will be discussed in a future report.

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A possible explanation for the probabilities of quantum mechanics

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It is shown that a lack of knowledge about the measurements of a physical system gives rise to a nonclassical probability calculus for this physical system. It is also shown that the nonclassical probability calculus of quantum mechanics can be interpreted as being the result of a lack of knowledge about the measurements. Examples are given of macroscopic real systems that have a nonclassical probability calculus. A macroscopic real system that has a quantum probability calculus is also given, and more specifically a model for the spin of a spin-$\frac{1}{2}$ particle is constructed. These results are analyzed in light of the old hidden variable problem.

I. INTRODUCTION

It is an opinion that the probabilities appearing in quantum mechanics do not arrive as a consequence of our lack of knowledge, but are inherent in nature and hence ontological. This opinion was present from the advent of quantum mechanics as a consequence of one of the possible interpretations of the Heisenberg uncertainty relations. Some physicists, however, did not agree with this interpretation and wondered whether it would not be possible to imbed quantum mechanics into a classical theory. They had in mind what happened with thermodynamics. Indeed, the theory of thermodynamics is independent of classical mechanics, and has its own set of observables such as pressure, volume, temperature, energy, and entropy and its own set of states. It was, however, possible to introduce an underlying theory of classical mechanics. To do this one assumes that every thermodynamical system consists of a large number of molecules and the real pure state of the system is determined by the positions and momenta of all these molecules. A thermodynamic state of the system is then a mixed state of the underlying theory. It was possible and it was a great success to derive the laws of thermodynamics in this way from Newtonian mechanics. The theory that resulted was called statistical mechanics.

Is it possible to do something similar for quantum mechanics? Is it possible to introduce extra variables into quantum mechanics such that these extra variables would define new states, and the description of the system based on these new states and the same observables would be classical? Moreover, quantum mechanics would be the statistical theory that results by averaging over these variables. A theory that has such extra variables and a procedure for averaging over these extra variables is usually called a "hidden variable theory." Because we want to have the same observables and only new, better defined states, the algebraic structure of the observables has to be conserved in this hidden variable theory.

Von Neumann gave the first proof of the impossibility of hidden variables for quantum mechanics.[1] One of the assumptions made by Von Neumann is that the expectation value of a linear combination of two observables is the linear combination of the expectation values of the observables. As remarked by Bell in Ref. 2, this assumption is not justified for noncompatible observables, such that, indeed, Von Neumann's proof cannot be considered to be conclusive. Bell constructs in the same reference[2] a hidden variable model for the spin-$\frac{1}{2}$, and shows that indeed Von Neumann's assumption is not satisfied in this model. Bell also criticizes in the same paper two other proofs of the nonexistence of hidden variables, the proof by Jauch and Piron[3] and the proof by Gleason.[4] Bell correctly points out the danger of demanding extra assumptions to be satisfied without knowing exactly what these assumptions mean physically. The extra mathematical assumptions criticized by Bell were introduced in all these approaches to express the physical idea that it must be possible to find, in the hidden variable description, the original observables and their basic algebra. We think that this physical idea was expressed correctly, without extra mathematical assumptions, and used in the impossibility proof of Kochen–Specker.[5] Gudder[6] gave an impossibility proof along the same lines as the one by Jauch and Piron, but now carefully avoiding the assumption criticized by Bell.

One could conclude by stating that every one of these impossibility proofs consists of showing that a hidden variable theory gives rise to a certain mathematical structure for the observables (in Refs. 1, 4, and 5) or for the properties (in Refs. 3 and 6) of the physical system under consideration. The observables or the properties of a quantum system do not have this mathematical structure. Therefore it is impossible to replace quantum mechanics by a hidden variable theory. To be more specific, if one works in the category of observables, then a hidden variable theory always has a commutative algebraic structure for the set of observables, while the algebra of observables of a quantum system is never commutative. If one works in the category of properties (yes–no observables) then a hidden variable theory always has a Boolean lattice structure for the set of properties, while the lattice of properties of a quantum system is never Boolean.

Recently this structural difference between classical systems and quantum systems has been studied by Accardi in another category, namely the category of probability models.[7] Accardi gives a definition of a Kolmogorovian probability model, which is the probability model of a classical system, and a quantum probability model, which is the probability model of a quantum system. Again these two probability models have completely different mathematical structures. What is more powerful in this probability ap-

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proach, compared to the algebraic or lattice theoretic approach, is that probability models can be compared with experimental results. To make this possible, Accardi derives a set of inequalities that characterizes the Kolmogorovian model and shows that these inequalities can always be violated by experiments with a quantum system. Accardi even manages to derive inequalities that can discriminate between a complex and a real Hilbert-space model, which shows the power of this approach.[8] Again this probability approach shows the fundamental difference between a classical theory and a quantum theory.

A lot of physicists, once aware of this fundamental structural difference between a classical theory and a quantum theory, gave up hope that it would ever be possible to replace quantum mechanics by a hidden variable theory; and I admit that I was one of them. I should like to show in this paper that the state of affairs is, however, more complicated.

Some time ago I managed to build a macroscopic classical system that violates Bell inequalities.[9,10] On the other hand, Accardi had shown that Bell inequalities are equivalent to his inequalities characterizing a Kolmogorovian probability model. Since my example did violate Bell inequalities, it should also violate Accardi's inequalities characterizing a Kolmogorovian probability model. This is indeed the case. But then I had given an example of a macroscopic "classical" system having a non-Kolmogorovian probability model. This was very amazing, and the classification made by a lot of physicists of a microworld described by quantum mechanics and a macroworld described by classical physics was challenged completely. This system violating Bell inequalities and having a non-Kolmogorovian probability model is presented in Ref. 10. The reason macroscopic systems can have non-Kolmogorovian probability models is what I want to analyze in this paper. I shall show that the state of affairs is the following: If we have a physical system S and we have a lack of knowledge about the state of S, then a theory describing this situation is necessarily a classical statistical theory having a classical Kolmogorovian probability model. If we have a physical system S and a measurement e on this physical system S, and the situation is such that we do not have a lack of knowledge about the state of S, but we do have a lack of knowledge about the measurement e, then we cannot describe this situation by a classical statistical theory, because the probability model that arises is non-Kolmogorovian. Hence, lack of knowledge about the measurements leads to a non-Kolmogorovian probability model. What do we mean by "lack of knowledge about the measurement e ?" Well, we mean that the measurement e is in fact not a "pure" measurement, in the sense that there are hidden measurements e_λ such that the measurement e consists of choosing in one way or another between the measurements e_λ and then performing the chosen measurement.

We can ask now whether it is possible to get a quantum probability model in this way. That this can indeed be done is shown in Sec. III, based on a macroscopic example. The example in Sec. III has a non-Kolmogorovian probability model of the spin of a spin-$\frac{1}{2}$ particle, and is constructed by introducing a lack of knowledge about the measurements.

It is shown in Sec. IV, based on another macroscopic example, that this physical situation of lack of knowledge about the measurements does not only give rise to a quantum probability model, but can also deliver a probability model that is neither Kolmogorovian nor quantum.

We can wonder now whether every quantum system can be described by a model with a lack of knowledge about the measurements. That this is indeed the case is shown in Sec. V.

In Ref. 5 Kochen and Specker give a classical statistical model for the spin of a spin-$\frac{1}{2}$ particle. Because we show in Sec. III that a spin model is a non-Kolmogorovian model, this seems to contradict the result of Kochen and Specker. We analyze this situation in Sec. VI.

Now, what is the relation of our model with lack of knowledge about the measurement to the attempts to build a hidden variable model? Well, our model with a lack of knowledge about the measurements can also be regarded as a hidden variable model. The hidden variables are not then hidden variables of the system, but hidden variables of the measuring apparatus. But, for each measuring apparatus we then have a different set of hidden variables. As I came to know recently, it was shown by Gudder that a hidden variable model, where a different set of variables is allowed for each measurement, can reconstruct the probabilities of quantum mechanics.[11] It seems, however, that nobody wanted to take into consideration these kinds of hidden variables. This is certainly because no interpretation was given to these hidden variables, and the theorem of Gudder was only considered to be an interesting mathematical result.

If we accept our explanation for the probabilities of quantum mechanics, namely that they are due to a lack of knowledge about the measurements, then these probabilities are not more ontological than ordinary probabilities. They form a nonclassical probability model because they correspond to a different physical situation, namely the physical situation where we lack knowledge about the measurements and not about the state of the system. It is clear that such a physical situation can be found, as well, in the macroworld. We have shown this based on our examples. We can now ask why nonclassical probabilities only appeared in the microworld. In light of our hypothesis, the answer would be that the type of measurement, introducing nonclassical probabilities, is never used to describe a macroscopic system, because we have enough other measurements to replace them. This is no longer the case in the microworld.

II. CLASSICAL AND QUANTUM PROBABILITY MODELS

We will, in this paper, always consider the following situation: We have a physical system S. This physical system can be in different states $p, q, r, \ldots$. We denote the set of states by Σ. We can perform measurements $e, f, g, \ldots$ on this physical system. We denote the set of measurements by $\mathcal{M}$. We suppose for sake of simplicity that all measurements have an outcome set which is a discrete set of real numbers. Hence a measurement e has possible outcomes $\{e_1, e_2, \ldots\}$.

If the system S is a classical system, then for a state p, a measurement e has a determined outcome $e(p)$, and measurements can, in this case, be represented by real valued functions (random variables) on Σ. If we have a lack of knowledge

about the state of this classical system, then this lack of knowledge is described by a probability measure μ on Σ such that if D is a measurable subset of Σ, then $\mu(D)$ is the probability that the state of S is in D. This is the description of a classical system by means of a statistical theory, and often μ is called a mixed state of the system S. We then have

$$P(e = e_i) = \mu(E_i),$$

where $P(e = e_i)$ means the probability of finding the outcome e_i if the measurement e is performed, and E_i is the set of states for which the measurement e gives outcome e_i.

If the system S is a quantum system, then measurements are represented by self-adjoint operators on a Hilbert space H. Since we considered only measurements with a discrete set of outcomes, we will have corresponding self-adjoint operators with a discrete spectrum. If e is such a measurement, with possible outcomes $\{e_1, e_2, \ldots\}$, then the corresponding self-adjoint operator always has an orthonormal basis $\{\phi_1, \phi_2, \ldots\}$ of eigenvectors. The state p of the system is represented by a normalized vector ψ. We then have

$$P(e = e_i | \psi) = |\langle \phi_i, \psi \rangle|^2,$$

where $P(e = e_i | \psi)$ means the probability of finding the outcome e_i when the measurement e is performed and when the system is in a state ψ.

These two descriptions, classical and quantum, both give rise to a probability model. We would like to compare these two models. To do this we have to find a concept that exists in both descriptions. We would also like to compare both models with physical experimental examples. Therefore, the common concept must have a physical meaning independent of the theories. For this purpose we will use the concept of conditional probability $P(e = e_i | f = f_j)$.

We will attribute the following physical meaning to $P(e = e_i | f = f_j)$: The probability of finding the outcome e_i when we perform the measurement e, when the state of the system is such that if we performed the measurement f we would find the outcome f_j. Hence we do not have to perform the measurement f. There is only a condition on the state of the system such that an eventual measurement of f would give us the outcome f_j. We insist on making this remark, because often the conditional probability $P(e = e_i | f = f_j)$ is given the following meaning: The probability of finding the outcome e_i for a measurement e if a measurement f has been performed and has given outcome f_j. If the performance of the measurement f creates the good conditioning on the state of the system, namely the condition that if we performed f (again) we would find the outcome f_j, then the two meanings are equivalent. This is the case for measurements of the first kind in quantum mechanics. But it is certainly not true for general measurements. Indeed, often a measurement destroys the system if one of the outcomes is obtained (e.g., measurement of the polarization of a photon). In such cases it usually makes no sense to perform the measurement e after we have performed f.

Let us see how we can find this conditional probability in both theories.

If S is the classical system with lack of knowledge about the states described by the probability measure μ, then

$$P(e = e_i | f = f_j) = \mu(E_i \cap F_j)/\mu(F_j),$$

where E_i is the set of states for which the measurement e gives the outcome e_i, and F_j is the set of states for which the measurement f gives the outcome f_j. This equality is often introduced as a definition of the conditional probability in Kolmogorovian probability theory. We have, however, given a physical meaning to the conditional probability such that this conditional probability can be derived from the experimental results. Therefore we shall consider this equality as one of the characterizations of the Kolmogorovian probability model. If considered in this way, the equality is often called Bayes axiom.

If S is a quantum system, then the condition that the state of the system S must be such that a measurement of f would give the outcome f_j, can be expressed by asking that the state of S must be an eigenstate ψ_j of the self-adjoint operator corresponding to f, an eigenstate corresponding to the eigenvalue f_j. Then

$$P(e = e_i | f = f_j) = |\langle \phi_i, \psi_j \rangle|^2.$$

Let us now give the mathematical definitions for a classical and a quantum probability model as proposed by Accardi in Refs. 7 and 8.

Definition 1: A Kolmogorovian (classical) model for the family of conditional probabilities $\{P(e = e_i | f = f_j);\ e, f \in \mathcal{M}\}$ is defined by a set Σ, a set β of measurable subsets of Σ which has the structure of a σ-algebra, and the probability measure $\mu: \beta \to [0,1]$. For every $e \in \mathcal{M}$ and for every outcome e_i of e, there exists a set $E_i \in \beta$ such that for e, f

$$P(e = e_i | f = f_j) = \mu(E_i \cap F_j)/\mu(F_j).$$

Definition 2: A complex (resp. real or quaternonian) Hilbert-space model for the family of conditional probabilities $\{P(e = e_i | f = f_j);\ e, f \in \mathcal{M}\}$ is defined by a complex (resp. real or quaternonian) Hilbert space H. For every $e \in \mathcal{M}$ there exists an orthonormal basis $\{\phi_i\}$ such that

$$P(e = e_i | f = f_j) = |\langle \phi_i, \psi_j \rangle|^2,$$

if $\{\phi_i\}$ and $\{\psi_j\}$ are the bases corresponding to e and f.

In Sec. III we will give an example of a macroscopic system with lack of knowledge about the measurements that has a quantum probability model.

III. EXAMPLE OF A MACROSCOPIC PHYSICAL SYSTEM WITH A QUANTUM DESCRIPTION; CONSTRUCTION OF A SPIN-½ MODEL

We will give, in this section, an example of a macroscopic physical system that gives a model for the spin-½.

We consider a particle with positive charge q that is located on a sphere with radius r at a point (r, θ, ϕ). The measurement $e_{\alpha\beta}$ consists of the following operation: We choose two particles with negative charges q_1 and q_2 such that $q_1 + q_2 = Q$. The charge q_1 is chosen at random between 0 and Q. This represents the lack of knowledge about the measurement. Once the charges q_1 and q_2 are chosen we put the two particles diametrically on the sphere, such that q_1 is in the point (r, α, β) and q_2 is in the point $(r, \pi - \alpha, \pi + \beta)$. Let us call F_1 and F_2 the Coulomb forces of q_1 on q and of q_2 on q. If the magnitude of F_1 is bigger than the magnitude of F_2, we give the outcome e_1 to the measurement $e_{\alpha\beta}$. If the

magnitude of F_2 is bigger than the magnitude of F_1 we give the outcome e_2 to the measurement $e_{\alpha\beta}$. (See Fig. 1.)

The forces F_1 and F_2 are in the plane through (r, θ, ϕ), (r, α, β), and $(r, \pi-\alpha, \pi+\beta)$. (See Fig. 2.)

Let us call γ the angle between (r, θ, ϕ) and (r, α, β). Then

$$\|F_1'\| = \frac{q_1 \cdot q}{4\pi\epsilon_0 r^2 \sin^2(\gamma/2)},$$

and

$$\|F_2'\| = \frac{q_2 \cdot q}{4\pi\epsilon_0 r^2 \cos^2(\gamma/2)}.$$

Let us now calculate the probability that we get the outcome e_1 for $e_{\alpha\beta}$ if the particle q is in state (θ, ϕ).

$$P(\|F_1\| > \|F_2\|)$$
$$= P\left(\frac{q_1 \cdot q}{4\pi\epsilon_0 r^2 \sin^2(\gamma/2)} > \frac{q_2 \cdot q}{4\pi\epsilon_0 r^2 \cos^2(\gamma/2)}\right)$$
$$= P(q_1 \cos^2(\gamma/2) > q_2 \sin^2(\gamma/2))$$
$$= P(q_1 \cos^2(\gamma/2) > (Q - q_1) \sin^2(\gamma/2))$$
$$= P(q_1 > Q \sin^2(\gamma/2))$$
$$= [Q - Q \sin^2(\gamma/2)]/Q = \cos^2(\gamma/2).$$

This is exactly the probability that we would find if $e_{\alpha\beta}$ represented the measurement of the spin of a spin-$\frac{1}{2}$ particle in the (α, β) direction while the particle had spin in the (θ, ϕ) direction.

We can describe this system by means of a two-dimensional complex Hilbert space. We then represent the state of the particle q in the (θ, ϕ) direction by means of the vector

$$x_{\theta,\phi} = (e^{-i\phi/2} \cos(\theta/2), e^{i\phi/2} \sin(\theta/2)),$$

and the measurement $e_{\alpha\beta}$ by means of the self-adjoint operator

$$S_{\alpha,\beta} = \frac{1}{2}\begin{pmatrix} \cos\alpha & e^{-i\beta}\sin\alpha \\ e^{i\beta}\sin\alpha & -\cos\alpha \end{pmatrix}.$$

We can then apply the calculus of quantum mechanics to the description of our system. Let us remark again that the state of the particle q is a pure state and the probability only comes from a lack of knowledge about the measurement $e_{\alpha\beta}$.

Let us now consider the physical situation where we also have a lack of knowledge about the state of the system. More specifically, we suppose that the charge q (or the spin of the spin-$\frac{1}{2}$ particle) is in every direction (θ,ϕ) with equal probability. We consider three measurements e, f, and g such that $e = e_{0,0}$, $f = e_{\pi/3,0}$, and $g = e_{2\pi/3,0}$ (see Fig. 3). Then clearly $P(e = e_1) = P(f = f_1) = P(g = g_1) = P(e = e_2) = P(f = f_2) = P(g = g_2) = \frac{1}{2}$. Let us now show that there does not exist a classical Kolmogorovian probability model for this system.

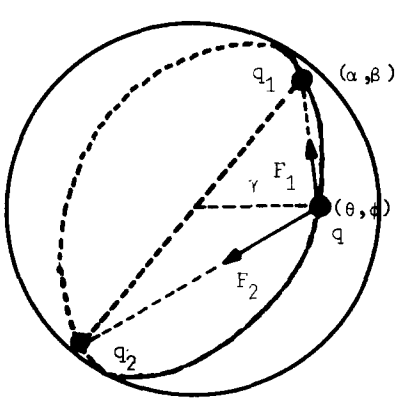

FIG. 1. A positive charge q is located on the sphere at (r,θ,ϕ) and two negative charges q_1 and q_2 are chosen as explained in the text and located on the sphere at points (r,α,β) and $(r,r-\alpha,r+\beta)$.

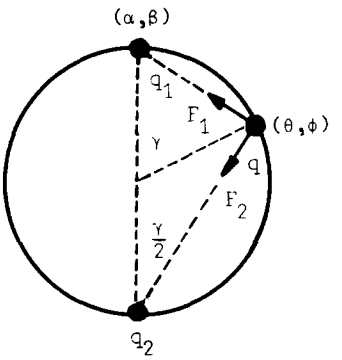

FIG. 2. We consider the three charges of Fig. 1 as they are located in one plane.

If there does exist a classical description, then we must have a probability measure μ and

$$\mu(E_1) = \mu(E_2) = \mu(F_1) = \mu(F_2) = \mu(G_1) = \mu(G_2) = \tfrac{1}{2}.$$

Using Bayes axiom and the properties of the probability measure we have

$$\tfrac{1}{2}P(f = f_1 | g = g_1) = \mu(F_1 \cap G_1) = \mu(E_1 \cap F_1 \cap G_1) + \mu(E_2 \cap F_1 \cap G_1),$$
$$\tfrac{1}{2}P(e = e_1 | g = g_1) = \mu(E_1 \cap G_1) = \mu(E_1 \cap F_1 \cap G_1) + \mu(E_1 \cap F_2 \cap G_1).$$

Now $P(f = f_1 | g = g_1)$ is the probability that a measurement of f gives the outcome f_1 if the state of the system is such that an eventual measurement of g would give the outcome g_1. The only state of the system with the property that a measurement of g would always give g_1, is the state where the charge q is at $(r, 2\pi/3, 0)$ [or the spin of the spin-$\frac{1}{2}$ particle is in direction $(2\pi/3, 0)$].

Hence

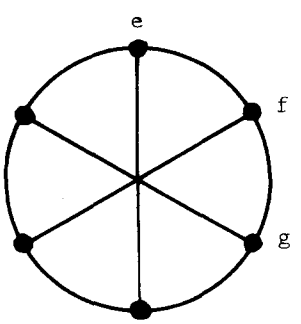

FIG. 3. The three measurements e, f, and g that are considered to show that the system of Fig. 1 does not allow a Kolmogorovian probability model.

$$P(f=f_1|g=g_1)=\cos^2(\pi/6)=\tfrac{3}{4},$$

and

$$P(e=e_1|g=g_1)=\cos^2(\pi/3)=\tfrac{1}{4}.$$

Hence

$$\mu(E_1\cap F_1\cap G_1)+\mu(E_2\cap F_1\cap G_1)=\tfrac{3}{8},$$

and

$$\mu(E_1\cap F_1\cap G_1)+\mu(E_1\cap F_2\cap G_1)=\tfrac{1}{8}.$$

From this, it follows that

$$\mu(E_2\cap F_1\cap G_1)=\tfrac{1}{4}+\mu(E_1\cap F_2\cap G_1).$$

Hence

$$\mu(E_2\cap F_1\cap G_1)\geqslant\tfrac{1}{4}.$$

On the other hand, we have

$$\tfrac{1}{2}P(e=e_2|f=f_1)$$
$$=\mu(E_2\cap F_1)=\mu(E_2\cap F_1\cap G_1)+\mu(E_2\cap F_1\cap G_2),$$

and

$$P(e=e_2|f=f_1)=\cos^2(\pi/3)=\tfrac{1}{4}.$$

Hence

$$\tfrac{1}{8}=\mu(E_2\cap F_1\cap G_1)+\mu(E_2\cap F_1\cap G_2),$$

which shows that

$$\mu(E_2\cap F_1\cap G_1)\leqslant\tfrac{1}{8}.$$

It is not possible to have $\mu(E_2\cap F_1\cap G_1)\geqslant\frac{1}{4}$ and $\mu(E_2\cap F_1\cap G_1)\leqslant\frac{1}{8}$ and so this shows that the spin-$\frac{1}{2}$ probability model cannot be replaced by a Kolmogorovian probability model.

The fact that the quantum spin-$\frac{1}{2}$ system cannot be described by a Kolmogorovian model is also a consequence of the general analysis made by Accardi in Ref. 7, but we thought it would be interesting to present a specific proof here, particularly because we want to understand the apparent contradiction with the result of Kochen and Specker[5] who claim to have built a Kolmogorovian model for the spin-$\frac{1}{2}$.

In our model for the spin-$\frac{1}{2}$ we defined the outcomes for a measurement $e_{\alpha\beta}$ as follows: $e_{\alpha\beta}$ has outcome e_1 if $\|F_1\|>\|F_2\|$ and $e_{\alpha\beta}$ has outcome e_2 if $\|F_1\|<\|F_2\|$. It would be interesting if we could relate a motion of the charge q to these two outcomes. To do this we can proceed as follows: We suppose the charge q to be on the sphere when the measurement starts. Once the measurement has started, the charge q can only move on the line between q_1 and q or on the line between q_2 and q (see Fig. 4). Then it is clear that if $\|F_1\|>\|F_2\|$, q will move towards q_1 and if $\|F_1\|<\|F_2\|$, q will move towards q_2. With this extra condition our macroscopic system not only gives the same probability model as the spin-$\frac{1}{2}$, but also gives the change of the state by means of the measurement with a Stern–Gerlach apparatus on a spin-$\frac{1}{2}$ particle.

One could ask why we had to make such a rather complicated mechanical picture for the motion of the charge q. Why not just let it move on the sphere? Well, the forces that control the motion on the sphere are not F_1 and F_2, but the projections of F_1 and F_2 on the tangent plane at q. In Sec. IV we will consider the macroscopic system consisting of the same charge q on the sphere with the same measurements $e_{\alpha\beta}$ and the same lack of knowledge about these measurements, but now we define the outcomes as follows: $e_{\alpha\beta}$ has outcome e_1 if q moves towards q_1 on the sphere (not on the line) and $e_{\alpha\beta}$ has outcome e_2 if q moves towards q_2 on the sphere. We will then show that this macroscopic system admits neither a classical Kolmogorovian nor a quantum Hilbert-space probability model.

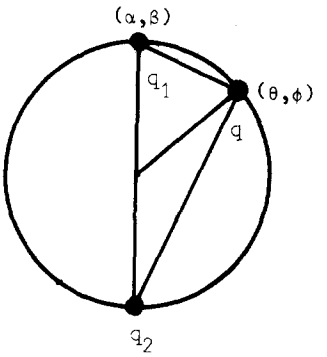

FIG. 4.

IV. EXAMPLE OF A MACROSCOPIC PHYSICAL SYSTEM THAT ADMITS NEITHER A CLASSICAL NOR A QUANTUM PROBABILITY MODEL

We consider again a particle with positive charge q that is located on a sphere with radius r at a point (r, θ, ϕ). The measurement consists of the following operation: We choose two particles with negative charges q_1 and q_2 such that $q_1+q_2=Q$. The charge q_1 is chosen at random between O and Q. This represents the lack of knowledge about the measurement. Once the charges q_1 and q_2 are chosen we put them diametrically on the sphere at points (r, α, β) and $(r, \pi-\alpha, \pi+\beta)$. We call F_1 and F_2 the Coulomb forces of q_1 on q and of q_2 on q. The charge q can move on the sphere. (See Fig. 5.) We call F_1' and F_2' the projections of F_1 and F_2 on the tangent plane at (r, θ, ϕ). If $\|F_1'\|>\|F_2'\|$, q will move towards q_1, and then we will give outcome e_1 to $e_{\alpha\beta}$. If $\|F_1'\|<\|F_2'\|$, q will move towards q_2, and then we will give outcome e_2 to $e_{\alpha\beta}$.

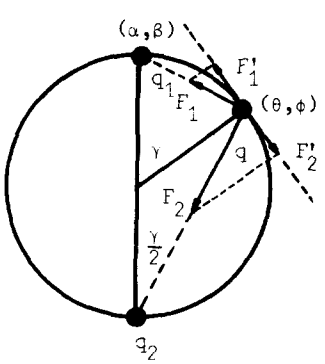

FIG. 5. The same physical situation as Fig. 1, but now the charge q is only allowed to move on the sphere.

Let us now calculate the probability of getting e_1 for $e_{\alpha\beta}$ if the particle q is in state (θ, ϕ). Again we call γ the angle between (r, θ, ϕ) and (r, α, β). Then

$$\|F_1'\| = \frac{q_1 \cdot q}{4\pi\epsilon_0 r^2 \sin^2(\gamma/2)} \cdot \cos\frac{\gamma}{2},$$

$$\|F_2'\| = \frac{q_2 \cdot q}{4\pi\epsilon_0 r^2 \cos^2(\gamma/2)} \cdot \sin\frac{\gamma}{2},$$

$$\begin{aligned} P(\|F_1'\| > \|F_2'\|) &= P\left(\frac{q_1 \cdot q}{4\pi\epsilon_0 r^2 \sin^2(\gamma/2)} \cdot \cos\frac{\gamma}{2} > \frac{q_2 \cdot q}{4\pi\epsilon_0 r^2 \cos^2(\gamma/2)} \cdot \sin\frac{\gamma}{2}\right) \\ &= P(q_1 \cos^3(\gamma/2) > q_2 \sin^3(\gamma/2)) \\ &= P(q_1 \cos^3(\gamma/2) > (Q - q_1)\sin^3(\gamma/2)) \\ &= P\left(q_1 > \frac{Q \sin^3(\gamma/2)}{\cos^3(\gamma/2) + \sin^3(\gamma/2)}\right) \\ &= \frac{\cos^3(\gamma/2)}{\cos^3(\gamma/2) + \sin^3(\gamma/2)}. \end{aligned}$$

We can, in the same way as for the macroscopic system of Sec. III, prove that this macroscopic system cannot be described by means of a Kolmogorovian probability model. We will not repeat this proof because it is completely analogous to the proof in Sec. III.

The macroscopic system in Sec. III could be given a quantum description. Let us now show that for the physical system in this section this cannot be done anymore. Hence this physical system has a probability model which is neither classical nor quantal.

We consider the measurements e, f, and g such that $e = e_{0,0}$, $f = e_{2\pi/3,0}$ and $g = e_{-2\pi/3,0}$ (see Fig. 6). Clearly with our choice of measurements

$$\begin{aligned} P(g = g_1 | e = e_1) &= P(g = g_1 | f = f_1) = P(f = f_1 | e = e_1) \\ &= P(g = g_2 | e = e_2) = P(g = g_2 | f = f_2) \\ &= P(f = f_2 | e = e_2) \\ &= \frac{\cos^3(\pi/3)}{\cos^3(\pi/3) + \sin^3(\pi/3)} = \frac{1}{3\sqrt{3} + 1}, \end{aligned}$$

$$\begin{aligned} P(g = g_1 | e = e_2) &= P(g = g_1 | f = f_2) = P(f = f_1 | e = e_2) \\ &= P(f = f_1 | g = g_2) = P(e = e_1 | f = f_2) \\ &= P(e = e_1 | g = g_2) \\ &= \frac{\sin^3(\pi/3)}{\cos^3(\pi/3) + \sin^3(\pi/3)} = \frac{3\sqrt{3}}{3\sqrt{3} + 1}. \end{aligned}$$

If there exists a Hilbert-space model, then it must be possible to find three orthonormal bases $\{\phi_1, \phi_2\}$, $\{\psi_1, \psi_2\}$, and $\{\chi_1, \chi_2\}$ such that

$$\begin{aligned} |\langle\phi_1,\psi_1\rangle|^2 &= |\langle\psi_1,\chi_1\rangle|^2 = |\langle\chi_1,\phi_1\rangle|^2 \\ &= |\langle\phi_2,\psi_1\rangle|^2 = |\langle\psi_2,\chi_1\rangle|^2 \\ &= |\langle\chi_2,\phi_1\rangle|^2 = 1/(3\sqrt{3} + 1), \end{aligned}$$

and

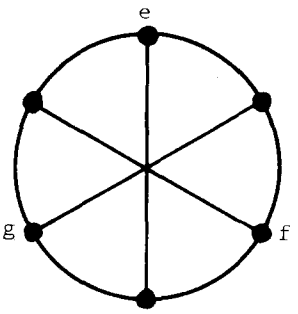

FIG. 6.

$$\begin{aligned} |\langle\phi_1,\psi_2\rangle|^2 &= |\langle\psi_1,\chi_2\rangle|^2 = |\langle\chi_1,\phi_2\rangle|^2 \\ &= |\langle\phi_2,\psi_1\rangle|^2 = |\langle\psi_2,\chi_1\rangle|^2 \\ &= |\langle\chi_2,\phi_1\rangle|^2 = 3\sqrt{3}/(3\sqrt{3} + 1). \end{aligned}$$

Let us show that this is not possible. We put

$$\lambda = \sqrt{1/(3\sqrt{3} + 1)} \quad \text{and} \quad \mu = \sqrt{3\sqrt{3}/(3\sqrt{3} + 1)}.$$

Then there must exist real numbers $\theta_1, \theta_2, \theta_3, \theta_4, \theta_5$ such that

$$\begin{aligned} &\langle\chi_1,\phi_1\rangle = \lambda e^{i\theta_1}, \quad \langle\chi_1,\psi_1\rangle = \lambda e^{i\theta_2}, \\ &\langle\psi_1,\phi_1\rangle = \lambda e^{i\theta_3}, \quad \langle\chi_1,\psi_2\rangle = \mu e^{i\theta_4}, \\ &\langle\psi_2,\phi_2\rangle = \mu e^{i\theta_5}. \end{aligned}$$

Using the fact that $\{\psi_1,\psi_2\}$ is an orthonormal basis we also have

$$\langle\chi_1,\phi_1\rangle = \langle\chi_1,\psi_1\rangle\langle\psi_1,\phi_1\rangle + \langle\chi_1,\psi_2\rangle\langle\psi_2,\phi_1\rangle.$$

Hence

$$\lambda e^{i\theta_1} = \lambda^2 e^{i(\theta_2 + \theta_3)} + \mu^2 e^{i(\theta_4 + \theta_5)},$$

and

$$\lambda e^{-i\theta_1} = \lambda^2 e^{-i(\theta_2 + \theta_3)} + \mu^2 e^{-i(\theta_4 + \theta_5)}.$$

Hence

$$\begin{aligned} \lambda^2 &= \lambda^4 + \mu^4 + \lambda^2\mu^2 e^{i(\theta_2 + \theta_3 - \theta_4 - \theta_5)} + \lambda^2\mu^2 e^{-i(\theta_2 + \theta_3 - \theta_4 - \theta_5)}, \\ \lambda^2 &= \lambda^4 + \mu^4 + 2\lambda^2\mu^2 \cos(\theta_2 + \theta_3 - \theta_4 - \theta_5). \end{aligned}$$

So $\cos(\theta_2 + \theta_3 - \theta_4 - \theta_5) = (\lambda^2 - \lambda^4 - \mu^4)/2\lambda^2\mu^2$.

Let us now calculate $(\lambda^2 - \lambda^4 - \mu^4)/2\lambda^2\mu^2$:

$$\begin{aligned} \frac{\lambda^2 - \lambda^4 - \mu^4}{2\lambda^2\mu^2} &= \frac{1/(3\sqrt{3} + 1) - [1/(3\sqrt{3} + 1)]^2 - [3\sqrt{3}/(3\sqrt{3} + 1)]^2}{2[1/(3\sqrt{3} + 1)][3\sqrt{3}/(3\sqrt{3} + 1)]} \\ &= \frac{3\sqrt{3} + 1 - 1 - (3\sqrt{3})^2}{6\sqrt{3}} = \frac{3\sqrt{3} - 27}{6\sqrt{3}} \\ &= -2.098\,076\,4\ldots. \end{aligned}$$

This shows that it is not possible to find real numbers $\theta_1, \theta_2, \theta_3, \theta_4$, and θ_5 that would satisfy the equalities, since $\cos(\theta_2 + \theta_3 - \theta_4 - \theta_5) > -1$ for all $\theta_2, \theta_3, \theta_4$, and θ_5; and as a consequence it is not possible to find a Hilbert-space model for this macroscopic system.

The example of Sec. III shows that we can find the quantum probability calculus of the spin-$\frac{1}{2}$ by supposing a lack of knowledge about the measurements. The example of Sec. IV shows that a lack of knowledge about the measurements can also, however, give rise to a nonclassical probability calculus which is nonquantal. In both examples there is no lack of knowledge about the state of the system. So we could say that the states are pure states; and it is clear that it will not be possible to build a hidden variable model if one wants the hidden variables to be hidden variables of the systems.

V. A MODEL WITH LACK OF KNOWLEDGE ABOUT THE MEASUREMENTS FOR A GENERAL QUANTUM SYSTEM

The example of Sec. III shows that lack of knowledge about the measurements can lead to a quantum mechanical probability model. We wonder whether we can make a model for a general quantum mechanical system. We will give in this section a construction that shows that this can indeed be done. In this construction we will only consider quantum mechanical systems described in an n-dimensional Hilbert space. An analogous reasoning can be made, however, for the case of an infinite-dimensional Hilbert space.

So we have a physical system S described in an n-dimensional Hilbert space H. A measurement e on this physical system is represented by a self-adjoint operator A. With this self-adjoint operator correspond n eigenvectors $v_1,...,v_n$ and eigenvalues $a_1,...,a_n$. If w is an arbitrary state of the system, we can write

$$w = \sum_{i=1}^{n} \langle w,v_i\rangle v_i ,$$

because $\{v_1,...,v_n\}$ is chosen to be orthonormal. Now $x_i = |\langle w,v_i\rangle|^2$ is the probability that by measurement of e we find the value a_i if the system is in state w. So we can represent this state w by means of these n probabilities $\{x_1,...x_n\}$. Hence all the states can be represented in this way by n-tuples

$$x = (x_1,...,x_n),$$

such that $\Sigma_{i=1}^{n} x_i = 1$ and $0 \leqslant x_i \leqslant 1$.
These are the points of the simplex S_n in $\mathbf{R}^n$ spanned by the canonical base vectors $h_1 = (1,0,...,0)$, $h_2 = (0,1,0,...,0),...$, $h_i = (0,0,...,1,...,0),...$, $h_n = (0,...,1)$. Hence

$$x = \sum_i x_i h_i .$$

We now have to show that it is possible to construct a set of measurements e_λ all with the same outcomes $(a_1,...,a_n)$ such that the measurement e consists of (i) choosing at random one of the measurements e_λ, and (ii) performing this chosen measurement. Moreover the measurements e_λ have to be classical measurements, which means that they give a determined outcome for a given state of the system.

We will construct these hidden measurements as follows: We will label the measurements by λ where λ is an n-tuple $\lambda = (\lambda_1,...,\lambda_n)$ such that $\Sigma_{i=1}^{n} \lambda_i = 1$, and $0 \leqslant \lambda_i \leqslant 1$. Suppose that we have a given state represented by the n-tuple $x = (x_1,...,x_n)$. Let us call A_i the convex closure of $\{x, h_1,...,h_{i-1}, h_{i+1},...,h_n\}$. Then clearly $S_n = \cup_{i=1}^{n} A_i$ (see Fig. 7). We define the measurements e_λ as follows: If $\lambda \in A_i$, then the measurement e_λ gives the outcome a_i if the system is in the state x. If λ is a point of the boundary of A_i and, hence, also a point of A_{i-1} or of A_{i+1}, then the outcome of e_λ is indeterminate, but indeterminate in the classical sense (as, for example, in the case of a classical unstable equilibrium). The probability of choosing λ on such a boundary is, however, zero. So these boundary situations do not contribute to the final probabilities.

Let us now calculate the probability of choosing λ in the simplex A_i. This probability is given by

$$m^n(A_i)/m^n(S_n) ,$$

where m^n is the trace on S_n of the Lebesgue measure on $\mathbf{R}^n$. For example, if $n = 3$ (see Fig. 7), then we have to calculate the surface of A_i and divide by the surface of S_3. Clearly

$$m^n(A_i) = [1/(n-1)]m^{n-1}(S^i_{n-1})l_n ,$$

where S^i_{n-1} is the convex closure of $h_1,...,h_{i-1}, h_{i+1},...,h_n$, and l_n is the distance from x to S^i_{n-1}. A point of S^i_{n-1} can be written as follows: $(y_1,...,y_{i-1},0,y_{i+1},...,y_n)$, with $\Sigma_{i=1}^{n} y_i = 1$ and $0 \leqslant y_i \leqslant 1$. The line through this point and the point $(x_1,...,x_n)$ is carried by the vector $(x_1 - y_1,...,x_{i-1} - y_{i-1}, x_{i+1} - y_{i+1},...,x_n - y_n)$. To find l_n on this line, this vector has to be orthogonal on the vectors $h_k - h_m$, for all k and m different from i. This means that $x_k - y_k = x_m - y_m$, for all k and m different from i. We also have

$$y_1 + \cdots + y_{i-1} + y_{i+1} + \cdots + y_n = 1 ,$$
$$x_1 + \cdots + x_{i-1} + x_{i+1} + \cdots + x_n = 1 - x_i .$$

Hence

$$(y_1 - x_1) + \cdots + (y_{i-1} - x_{i-1}) + (y_{i+1} - x_{i+1}) + \cdots + (y_n - x_n) = x_i .$$

From this, it follows that $y_k - x_k = x_i/(n-1)$ for all $k \neq i$. Hence $y_k = x_k + x_i/(n-1)$ for all $k \neq i$. So

$$l_n = \left|\left|(x_1,...,x_n) - \left(x_1 + \frac{x_i}{n-1},...,x_{i-1} + \frac{x_i}{n-1},0, x_{i+1} + \frac{x_i}{n-1},...,x_n + \frac{x_i}{n-1}\right)\right|\right|$$
$$= \left|\left|\left(\frac{-x_i}{n-1},\frac{-x_i}{n-1},...,x_i,...,\frac{-x_i}{n-1}\right)\right|\right|$$
$$= \sqrt{n/(n-1)}x_i .$$

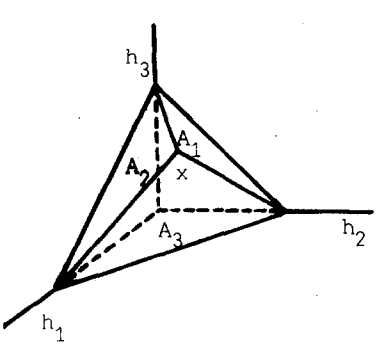

FIG. 7.

Hence $m^n(A_n) = [1/(n-1)]m^{n-1}(S^i_{n-1}) \cdot \sqrt{n/(n-1)}x_i$, and as a consequence,

$$m^n(A_i)/m^n(S_n) = x_i \, .$$

This shows that if the system is in the state x, and we perform the measurement e, then the probability of choosing e_λ such that $e_\lambda(x) = a_i$ is exactly given by x_i. For each measurement f we can construct such a collection of hidden measurements f_λ. Let us call these hidden measurements the "pure measurements." Is it possible to characterize the collection of all pure measurements? We can do this in the following way.

We have a physical system S. The pure states of S are represented by normalized vectors of an n-dimensional complex Hilbert space H. The pure measurements can also be represented by the normalized vectors of the same n-dimensional complex Hilbert space H. Let us denote by p_w a pure state represented by the vector w, and by e_u a pure measurement represented by the vector u. To derive quantum mechanics we adopt the following rules.

If we want to perform a measurement of a system, then first we choose a system and a measurement. This choice corresponds to choosing an orthonormal basis $\{v_1,...,v_n\}$ of the Hilbert space H, and a set of possible outcomes $\{a_1,...,a_n\}$ (or a self-adjoint operator). This choice is of course not governed by a probability rule, it is just the choice of the context of the measurement. The system will, however, be in a certain pure state p_w represented by the vector w, and the measurement will be a certain pure measurement e_u represented by the vector u. The outcome of this pure measurement e_u is determined for the state p_w in the following way.

Let us put

$$b_i = |\langle w,v_i\rangle|/|\langle u,v_i\rangle| \, ,$$

and let us consider the set of real numbers $B = \{b_1,...,b_n\}$. If $\langle u,v_i\rangle = 0$ and $\langle w,v_i\rangle \neq 0$, then $b_i = +\infty$. If $\langle u,v_i\rangle = \langle w,v_i\rangle = 0$, then b_i is not taken into consideration. If B has a maximum, for example the number b_j, then the outcome of the measurement e_u when the system is in the state p_w is always a_j. If B has no maximum, then the outcome of the measurement e_u when the system is in the state p_w is indeterminate in the classical sense (as, for example, in the case of a classical unstable equilibrium).

If we now want to know the probability that (in the measurement context, represented by the orthonormal basis $\{v_1,...,v_n\}$ and the system being in the state p_w) we find the outcome a_j, then this probability will be given by $|\langle w,v_j\rangle|^2$. Indeed, if we put $\lambda_i = |\langle u,v_i\rangle|^2$, then $\lambda = (\lambda_1,...,\lambda_n)$ will be a point of the simplex A_j if and only if b_j is a maximum of B.

VI. COMPARING OUR SPIN MODEL WITH THE MODEL OF KOCHEN AND SPECKER

In Ref. 5 Kochen and Specker construct a spin model which has a classical statistical mathematical structure. This seems to contradict our result of Sec. III where we explicitly show that every spin model will have a non-Kolmogorovian probability model. Let us analyze this situation. The model of Kochen and Specker is mathematically more complicated than ours, but we can construct a model equivalent to the one of Kochen and Specker which is very similar to our model and can easily be compared. Let us do this first. In the model that we proposed in Sec. III, the lack of knowledge that gives rise to the probabilities is about the measurements. We can, however, in the same spirit build a model where the lack of knowledge is about the state of the system. To obtain this we consider the measuring apparatus of the example in Sec. III as the physical system and we consider the system as measuring apparatus. The model that we get in this way is completely equivalent to the model proposed by Kochen and Specker. But let us see now that it is in fact not really a spin model; so the physical system consists of two negative charges q_1 and q_2 such that $q_1 + q_2 = Q$, that are located diametrically on a sphere with radius r at points (r, α, β) and $(r, \pi - \alpha, \pi + \beta)$. The pure state of the system can be described by the direction (α, β) and the charge q_1. Hence the pure states can be represented by a point of the sphere and a point in $[0,Q]$. We now suppose that we have a lack of knowledge about these states, in the sense that we do not know the charges q_1 and q_2. The mixed states are described by the directions (α, β), and q_1 is a hidden variable. The measurement $e_{\theta,\phi}$ consists of putting a positive charge q in a point (r, θ, ϕ). Let us call F_1 and F_2 the two Coulomb forces between q_1 and q and between q_2 and q (see Fig. 8). If the magnitude of F_1 is bigger than the magnitude of F_2 we give the outcome e_1 to the measurement $e_{\theta,\phi}$ and if the magnitude of F_1 is smaller than the magnitude of F_2 we give the outcome e_2 to the measurement $e_{\theta,\phi}$. If we call γ the angle between (r, α, β) and (r, θ, ϕ), then we find with the same calculation as in Sec. III that

$$P(\|F_1\| > \|F_2\|) = \cos^2(\gamma/2) \, .$$

So for one measurement $e_{\theta,\phi}$ we find the good probability of the spin-$\frac{1}{2}$. But let us see what happens if we make a second measurement $e_{\theta',\phi'}$ after $e_{\theta,\phi}$ in the direction (θ',ϕ') which makes an angle δ with the direction (θ,ϕ). We also suppose that (r, α, β), (r, θ, ϕ), and (r', θ', ϕ') lie in the same plane (see Fig. 9). So, we now suppose that the state (mixture) of the system was (α, β) and we have performed $e_{\theta,\phi}$ and gotten the outcome e_1. After this we perform the measurement $e_{\theta',\phi'}$ and we want to calculate the probability that we get the outcome e_1 for $e_{\theta',\phi'}$. Let us denote this probability as follows:

$$P(e_{\theta',\phi'} = e_1 | e_{\theta,\phi} = e_1) \, .$$

Then, because we have a classical statistical situation,

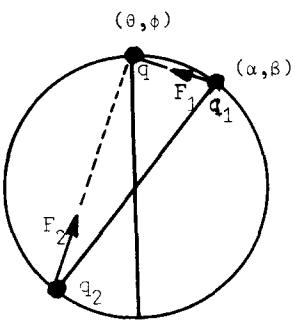

FIG. 8.

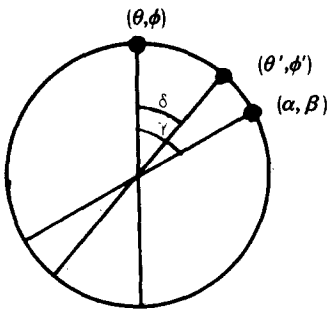

FIG. 9.

$$P(e_{\theta',\phi'} = e_1 | e_{\theta,\phi} = e_1) = \frac{P(e_{\theta',\phi'} = e_1 \text{ and } e_{\theta,\phi} = e_1)}{P(e_{\theta,\phi} = e_1)}.$$

Now

$$P(e_{\theta,\phi} = e_1) = \cos^2(\gamma/2),$$

and

$$\begin{aligned} &P(e_{\theta',\phi'} = e_1 \text{ and } e_{\theta,\phi} = e_1) \\ &\quad = P(q_1 > \sin^2(\gamma/2) \text{ and } q_1 > \sin^2(\gamma - \delta/2)) \\ &\quad = 1 - \max(\sin^2(\gamma/2), \sin^2(\gamma - \delta/2)) \\ &\quad = \min(\cos^2(\gamma/2), \cos^2(\gamma - \delta/2)). \end{aligned}$$

Hence

$$P(e_{\theta',\phi'} = e_1 | e_{\theta,\phi} = e_1) = \frac{\min(\cos^2(\gamma/2), \cos^2(\gamma - \delta/2))}{\cos^2(\gamma/2)}.$$

If $e_{\theta',\phi'}$ and $e_{\theta,\phi}$ would be spin measurements in the (θ',ϕ') and (θ,ϕ) direction, then

$$P(e_{\theta',\phi'} = e_1 | e_{\theta,\phi} = e_1) = \frac{\min(\cos^2(\gamma/2), \cos^2(\gamma - \delta/2))}{\cos^2(\gamma/2)}.$$

So this calculation shows that if we perform two measurements one after the other, the model that we propose here does not agree with the spin-$\frac{1}{2}$ model. This explains the apparent contradiction between our results and those of Kochen and Specker.

The reason the model proposed in this section is not a spin model is because the hidden variable q_1 does not get distributed at random again after one measurement. Kochen and Specker were clearly aware of this difficulty in their model, and, therefore, they add the extra condition that after a measurement the hidden variable must in one way or another get distributed at random again. If this extra condition is added, then the model is a spin model; but of course it is easy to see that if one adds the extra condition that the hidden variable gets distributed at random again after the measurement, then the hidden variable is in fact a hidden variable of the measurement, and hence with this extra condition we really are in a physical situation as the one described in this paper, namely the physical situation that we lack knowledge about the measurement, and this is no classical statistical situation.

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The Cauchy problem for the coupled Maxwell–Schrödinger equations

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The Cauchy problem for the coupled Maxwell–Schrödinger equations in $\mathbb{R}^d$ in the Lorentz gauge is considered. The viscosity method is used to establish local existence. In one and two space dimensions, global solutions are obtained.

I. INTRODUCTION

Due in part to the developments of lasers, there has been a revived interest in the theory of the interaction of the radiation and nonrelativistic charged particles in recent years.[1] In this paper we shall study the Cauchy problem for the closely related minimally coupled Maxwell–Schrödinger equations, by specializing to the Lorentz gauge. These equations are the classical approximation to the quantum field equations for an electrodynamical nonrelativistic many body system,[2] and may be written as

$$\partial^\mu F_{\mu\nu} = J_\nu, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \tag{1.1}$$

$$(iD_0 + D_j D_j)\psi = V\psi, \quad D_\mu = \partial_\mu - iA_\mu \tag{1.2}$$

with the components $A_\mu(t,x)$'s of the electromagnetic real vector potential and the complex scalar field $\psi(t,x)$ of nonrelativistic charged particles. Here $x\in\mathbb{R}^d$, μ,ν range over $0,1,...,d$, j ranges over $1,...,d$ (repeated indices always imply summation), $\partial^0 = \partial_0 = \partial/\partial t$, $(-\partial^1,...,-\partial^d) = (\partial_1,...,\partial_d) = \nabla$, $V = V(x)$ is a given real external potential, and the J_ν are the charge-current densities given by

$$J_0 = -\bar{\psi}\psi, \quad J_j = -i(\bar{\psi}D_j\psi - \psi\overline{D_j\psi}), \quad j = 1,...,d.$$

The Lorentz gauge condition is expressed as

$$\partial^\mu A_\mu = 0. \tag{1.3}$$

In Sec. II, we shall show that the Cauchy problem for Eqs. (1.1)–(1.3) with $d\geqslant 1$ has a local solution, provided the initial data and the external potential V are sufficiently regular. Our local existence argument uses the viscosity method (see, e.g., Refs. 3–5) to deal with the difficulty arising from the presence of highly singular derivative coupling terms in the Schrödinger equation.

In Sec. III, we prove the global existence of solutions in the cases of one and two space dimensions. The needed *a priori* estimates for the solutions will be obtained by using the energy method in the form developed in Ref. 6, together with the covariant Sobolev inequalities. See the preliminary version of the present paper[7] for an L^p–L^q approach.

Throughout this paper we shall use Greek indices $\mu,\nu,...$ to run from 0 to d Latin indices $j,k,...$ to run from 1 to d, and the summation convention for both types of indices. We use the standard notation H^s for the Sobolev space of order s and exponent 2. If X is a normed space, we write $\|\cdot\|_X$ for its norm, and if X is also an inner product space, $(\cdot,\cdot)_X$ for its inner product. The L^p norm will be denoted simply by $\|\cdot\|_p$, and C_b^m will denote the space of functions in $C^m(\mathbb{R}^d)$ bounded with their first m derivatives.

II. LOCAL EXISTENCE

Introducing the momenta $P_\mu = \partial_0 A_\mu$ and the vector notation $\mathbf{f} = (f_1,...,f_d)$, we write Eqs. (1.1)–(1.3), with initial data $A_0^0, P_0^0, \mathbf{A}^0, \mathbf{P}^0, \psi^0$, in the form

$$\frac{du}{dt} + Zu = K(u), \quad u = (A_0,P_0,\mathbf{A},\mathbf{P},\psi), \tag{2.1}$$

$$P_0 - \partial_j A_j = 0, \tag{2.2}$$

$$u(0) = u_0 = (A_0^0, P_0^0, \mathbf{A}^0, \mathbf{P}^0, \psi^0),$$

where the components A_μ, P_μ, and ψ of the unknown u take values in L^2, and the operator Z and the function $K(\cdot)$ are, respectively, defined by

$$Zu = (-P_0, -\Delta A_0, -\mathbf{P}, -\Delta\mathbf{A}, -i\Delta\psi),$$

$$K(u) = (0,J_0,0,\mathbf{J}, -iV\psi + iA_0\psi + P_0\psi + 2A_j\partial_j\psi - iA_jA_j\psi),$$

the indicated differential operators being defined by Fourier transformation. Use has been made of the side condition Eq. (1.3) to convert Eqs. (1.1) and (1.2) into Eq. (2.1). Equations (2.1) and (2.2) impose the following initial value constraints on the components of the data u_0:

$$P_0^0 - \partial_j A_j^0 = 0, \quad \partial_j P_j^0 - \Delta A_0^0 + \bar{\psi}^0\psi^0 = 0. \tag{2.3}$$

Next we form for $s\geqslant 1$ the direct sum Hilbert spaces

$$X^s = H^{s+1}(\mathbb{R}^d;\mathbb{R}) \oplus H^s(\mathbb{R}^d;\mathbb{R}) \oplus H^s(\mathbb{R}^d;\mathbb{R}^d) \oplus H^{s-1}(\mathbb{R}^d;\mathbb{R}^d) \oplus H^s(\mathbb{R}^d;\mathbb{C}),$$

$$Y^s = H^{s+1}(\mathbb{R}^d;\mathbb{R}) \oplus H^s(\mathbb{R}^d;\mathbb{R}) \oplus H^s(\mathbb{R}^d;\mathbb{R}^d) \oplus H^{s-1}(\mathbb{R}^d;\mathbb{R}^d) \oplus H^{s-1}(\mathbb{R}^d;\mathbb{C}).$$

We now state the main result of this section. We will denote by $[p]$ the integer part of $p\in\mathbb{R}^+$. Let $d\geqslant 1$.

Theorem 2.1: Let m be an integer satisfying $m\geqslant[d/2+2]$, and let $V\in H^m(\mathbb{R}^d;\mathbb{R})$. Let u_0 be any initial data lying in X^m, not necessarily satisfying (2.3). Then Eq. (2.1) has a unique solution u on $[0,T)$ for some T, $0<T\leqslant\infty$, such that $u\in C([0,T);X^m)\cap C^1([0,T);Y^{m-1})$ and $u(0)=u_0$, where we may assume that either $T=\infty$ or $\lim_{t\to T}\|u(t)\|_{X^{[d/2+2]}} = \infty$; the solution u depends continuously on the initial data u_0, in the sense that if $\|u\|_{X^{[d/2+2]}}\leqslant C$ on $[0,T']$ for some fixed $C,T'>0$ when u_0 converges to some $u_0'\in X^m$ weakly in X^m, strongly in X^{m-1}, then the solution u' of Eq. (2.1) corresponding to the data u_0' also exists on $[0,T']$, and u converges to u' weakly in X^m uniformly on $[0,T']$. Furthermore, if in addition the data u_0 satisfies the initial value constraints (2.3), the solution u satisfies Eq. (2.2).

The proof of Theorem 2.1 depends on the following lemma.

Lemma 2.2: Let m and V be as in Theorem 2.1, and let $0\leqslant\alpha\leqslant 1$. Then

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$$\|K(u)-K(u')\|_{X^{m-\alpha}}$$
$$\leqslant \omega(\|u\|_{X^{m-\alpha}},\|u'\|_{X^{m-\alpha}})\|u-u'\|_{X^{m-\alpha}}, \quad u,u'\in X^{m-\alpha}, \tag{2.4}$$

$$\mathrm{Re}(K(u),u)_{X^m}$$
$$\leqslant c\{1+\|u\|_{X^{[d/2+2]}}+\|u\|^2_{X^{[d/2+2]}}\}\|u\|^2_{X^m}, \quad u\in X^{m+1}, \tag{2.5}$$

$$\mathrm{Re}(K(u)-K(u'),u-u')_{X^{m-1}}$$
$$\leqslant \omega(\|u\|_{X^m},\|u'\|_{X^m})\|u-u'\|^2_{X^{m-1}}, \quad u,u'\in X^m, \tag{2.6}$$

where $\omega(a,b)=c\{1+a+b+a^2+b^2\}$.

Proof: The inequality (2.4) immediately follows from the multiplication lemma

$$\|fg\|_{H^s}\leqslant c\|f\|_{H^{s_1}}\|g\|_{H^{s_2}},$$
$$\text{if } s_1,s_2\geqslant s>0 \text{ and } s_1+s_2-d/2>s, \tag{2.7}$$

which implies that

$$\|fg\|_{H^{s-1}}\leqslant c\|f\|_{H^s}\|g\|_{H^{s-1}}, \quad \text{for } s>d/2.$$

In proving (2.5) and (2.6), we may assume that u and u' are C_0^∞ vectors in view of (2.4). Let m be an integer satisfying $m\geqslant[d/2+2]$. To show (2.5), we make use of the following inequality:

$$\|\partial^\alpha(fg)-f\,\partial^\alpha g\|_2\leqslant c\{\|f\|_{H^m}\|g\|_{H^{[d/2+1]}}+\|f\|_{H^{[d/2+2]}}\|g\|_{H^{m-1}}\},$$
$$f,g\in C_0^\infty, \tag{2.8}$$

where $|\alpha|\leqslant m$. For $|\alpha|\leqslant d/2+1$, (2.8) (the right side becomes simpler in this case) results from (2.7) after an application of Leibnitz rule. For the case $d/2+1<|\alpha|\leqslant m$, see, e.g., Ref 8. Now let k be any integer satisfying $0\leqslant k\leqslant m$. Then (2.8) in particular implies that

$$\|fg\|_{H^k}\leqslant c\{\|f\|_{H^m}\|g\|_{H^{[d/2+1]}}+\|f\|_{H^{[d/2+2]}}\|g\|_{H^{m-1}}+\|f\|_{H^{[d/2+1]}}\|g\|_{H^k}\} \tag{2.9}$$

since for $|\alpha|=k$,

$$\|f\,\partial^\alpha g\|_2\leqslant\|f\|_\infty\|g\|_{H^k}\leqslant c\|f\|_{H^{[d/2+1]}}\|g\|_{H^k}.$$

A repeated application of (2.9) yields

$$\|f_1f_2f_3\|_{H^k}$$
$$\leqslant c\sum\|f_{j_1}\|_{H^{[d/2+2]}}\|f_{j_2}\|_{H^{[d/2+2]}}\|f_{j_3}\|_{H^m},$$
$$f_1,f_2,f_3\in C_0^\infty, \tag{2.10}$$

where the sum is taken over all cyclic permutations (j_1,j_2,j_3)'s of (1,2,3). Except for the term $\mathrm{Re}(A_j\,\partial_j\psi,\psi)_{H^m}$, the inequality (2.5) can be proved by using (2.9) and (2.10) in the left-hand side, after an application of Schwartz inequalities. To estimate the term $\mathrm{Re}(A_j\partial_j\psi,\psi)_{H^m}$ we shall use (2.8) directly. We write

$$\mathrm{Re}(A_j\,\partial_j\psi,\psi)_{H^m}$$
$$=\mathrm{Re}\sum_{|\alpha|\leqslant m}(\partial^\alpha(A_j\,\partial_j\psi)-A_j\,\partial^\alpha\partial_j\psi,\partial^\alpha\psi)_{L^2}$$
$$+\mathrm{Re}\sum_{|\alpha|\leqslant m}(A_j\,\partial^\alpha\partial_j\psi,\partial^\alpha\psi)_{L^2}. \tag{2.11}$$

Applying (2.8) to the first term on the right side in the obvious manner, and noting in the second term that, by an integration by parts,

$$\mathrm{Re}(A_j\,\partial^\alpha\partial_j\psi,\partial^\alpha\psi)_{L^2}=-\tfrac{1}{2}(\partial_jA_j\,\partial^\alpha\psi,\partial^\alpha\psi)_{L^2},$$

and that $\|\partial_jA_j\|_\infty\leqslant c\|\partial_jA_j\|_{H^{[d/2+1]}}$, we find that the right side of (2.11) is bounded by a constant times $\|u\|_{X^{[d/2+2]}}\times\|u\|^2_{X^m}$. Thus (2.5) follows.

The proof of the inequality (2.6) is, except for the term $\mathrm{Re}(A_j\,\partial_j\psi-A'_j\partial_j\psi',\psi-\psi')H_{m-1}$, straightforward, and in fact reduces to that of (2.4). We now write

$$\mathrm{Re}(A_j\,\partial_j\psi-A'_j\partial_j\psi',\psi-\psi')_{H^{m-1}}$$
$$=\mathrm{Re}((A_j-A'_j)\partial_j\psi',\psi-\psi')_{H^{m-1}}+\mathrm{Re}\sum_{\substack{|\alpha|\leqslant m-1\\0<|\beta|<|\alpha|}}c_{\alpha\beta}$$
$$\times(\partial^\beta A_j\,\partial^{\alpha-\beta}\partial_j(\psi-\psi'),\partial^\alpha(\psi-\psi'))_{L^2}$$
$$+\mathrm{Re}\sum_{|\alpha|\leqslant m-1}(A_j\,\partial^\alpha\partial_j(\psi-\psi'),\partial^\alpha(\psi-\psi'))_{L^2}.$$

Using (2.7) in the first and the second term on the right side after the application of Schwartz inequalities, and estimating the last term in the same way as in the last part of the proof of (2.5), one finds that the right side of the above equality is bounded by a constant times $\{\|u\|_{X^m}+\|u'\|_{X^m}\}\|u-u'\|^2_{X^{m-1}}$ and obtains (2.6).

Proof of Theorem 2.1: Let m and V be as in the statements of Theorem 2.1, and assume first that the initial data u_0 is an arbitrary element of X^m. In order to construct the solution of Eq. (2.1) corresponding to the data u_0, we shall introduce the following approximate Cauchy problem:

$$\frac{du}{dt}+B_\epsilon u=F(u), \quad u(0)=u_0, \tag{2.12}$$

where $\epsilon>0$, and $B_\epsilon=\epsilon T+S$, $F(u)=-Mu+K(u)$, with $T=I-\Delta$ and

$$Mu=(-P_0,-\Delta A_0,-\mathbf{P},-\Delta\mathbf{A},0),$$
$$Su=(0,0,0,0,-i\Delta\psi)$$

(so that $M+S=Z$). Note that the norms $\|\cdot\|_{X^{1+2\alpha}}$ and $\|B^\alpha_\epsilon(\cdot)\|_{X^1}$ are equivalent for each $\alpha\geqslant0$, B^α_ϵ's being the fractional powers of B_ϵ. The operator B_ϵ generates a holomorphic semigroup on $X^{[d/2+1]}$, and by (2.4),

$$\|F(u)-F(u')\|_{X^s}\leqslant\omega(\|u\|_{X^{s+1}},\|u'\|_{X^{s+1}})\|u-u'\|_{X^{s+1}},$$

for any $s\geqslant[d/2+1]$, where $\omega(a,b)=c\{1+a+b+a^2+b^2\}$. Thus it follows from the well-established theory of semilinear parabolic equations (see, e.g., Ref. 9) that Eq. (2.12) has a unique solution u_ϵ on some nonempty interval $[0,T_\epsilon)$ such that $u_\epsilon\in C([0,T_\epsilon);X^m)\cap C^1((0,T_\epsilon);X^{m-1})\cap C((0,T_\epsilon);X^{m+1})$ and $u_\epsilon(0)=u_0$, and here we may assume that either $T_\epsilon=\infty$ or $\lim_{t\to T_\epsilon}\|u_\epsilon(t)\|_{X^{[d/2+2]}}=\infty$.

We shall now consider the convergence of u_ϵ, $\epsilon>0$, in the limit $\epsilon\to0$. Taking the X^m-inner product of Eq. (2.12) (for u_ϵ) with u_ϵ and adding the complex conjugate of the result, we have

$$\frac{1}{2}\frac{d}{dt}\|u_\epsilon\|^2_{X^m}+\epsilon(Tu_\epsilon,u_\epsilon)_{X^m}=\mathrm{Re}(K(u_\epsilon),u_\epsilon)_{X^m}. \tag{2.13}$$

Using (2.5) and noting that the second term on the left-hand side is non-negative, we obtain

$$\frac{d}{dt}\|u_\epsilon\|_{X^m} \leqslant P(\|u_\epsilon\|_{X^{[d/2+2]}})\|u_\epsilon\|_{X^m},$$

where $P(a) = c\{1 + a + a^2\}$. It follows that

$$\|u_\epsilon(t)\|_{X^m} \leqslant \|u_\epsilon(0)\|_{X^m} \exp\left[\int_0^t P(\|u_\epsilon(s)\|_{X^{[d/2+2]}})ds\right], \quad (2.14)$$

on $[0,T_\epsilon)$.

With the solution b of the scalar Cauchy problem

$$\frac{db}{dt} = P(b), \quad b(0) = L \geqslant \|u_0\|_{X^{[d/2+2]}},$$

which exists and is bounded on a time interval $[0,T_0]$, $T_0 = T_0(L) > 0$, it also follows that $\|u_\epsilon(t)\|_{X^{[d/2+2]}} \leqslant b(t)$ on $[0,T_\epsilon) \cap [0,T_0]$, from which we may assume that $T_\epsilon > T_0$. Then by (2.14),

$$\|u_\epsilon(t)\|_{X^m} \leqslant \|u_0\|_{X^m} e^{Ct}, \quad \text{on } [0,T_0], \quad (2.15)$$

where C is a positive constant independent of ϵ.

Next let $0 < \epsilon_1 < \epsilon_2$, and put $w = u_{\epsilon_1} - u_{\epsilon_2}$. From (2.12) we have

$$\frac{dw}{dt} + B_{\epsilon_1} w = (\epsilon_2 - \epsilon_1) T u_{\epsilon_2} - Mw + K(u_{\epsilon_1}) - K(u_{\epsilon_2}). \quad (2.16)$$

Taking the X^{m-1}-inner product of this equation with w and adding the complex conjugate of the result, we get

$$\frac{1}{2}\frac{d}{dt}\|w\|^2_{X^{m-1}} + \epsilon_1 (Tw,w)_{X^{m-1}} = (\epsilon_1 - \epsilon_2)\mathrm{Re}(Tu_{\epsilon_2},w)_{X^{m-1}} + \mathrm{Re}(K(u_{\epsilon_1}) - K(u_{\epsilon_2}),w)_{X^{m-1}}.$$

Noting that the second term on the left side is non-negative and using (2.6) and (2.15), we obtain

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|w\|^2_{X^{m-1}} &\leqslant (\epsilon_2 - \epsilon_1)\|u_{\epsilon_2}\|_{X^m}\|w\|_{X^m} + \omega(\|u_{\epsilon_1}\|_{X^m}, \|u_{\epsilon_2}\|_{X^m})\|w\|^2_{X^{m-1}} \\ &\leqslant c\epsilon_2 + c\|w\|^2_{X^{m-1}}. \end{aligned} \quad (2.17)$$

Application of Gronwall's inequality then gives $\|w(t)\|^2_{X^{m-1}} \leqslant c\epsilon_2$ on $[0,T_0]$ since $w(0) = 0$. Thus by letting $\epsilon_2 \to 0$, we find a function $u \in C([0,T_0];X^{m-1})$ such that $u_\epsilon \to u$ in X^{m-1} uniformly on $[0,T_0]$ as $\epsilon \to 0$. By (2.15), it also follows that $u \in L^\infty([0,T_0];X^m)$ with $\|u(t)\|_{X^m} \leqslant \|u_0\|_{X^m} e^{Ct}$, that $u_\epsilon \to u$ weakly in X^m uniformly on $[0,T_0]$ as $\epsilon \to 0$, and that u is weakly continuous from $[0,T_0]$ to X^m.

Now let ϕ be a smooth element of Y^{m-1}. Then we have

$$(-B_\epsilon u_\epsilon + F(u_\epsilon),\phi)_{Y^{m-1}} = -\epsilon(u_\epsilon, T\phi)_{Y^{m-1}} + (u_\epsilon, Z\phi)_{Y^{m-1}} + (K(u_\epsilon),\phi)_{Y^{m-1}}.$$

This together with (2.4) implies that $(-B_\epsilon u_\epsilon + F(u_\epsilon),\phi)_{Y^{m-1}}$ converges to $(-Zu + K(u),\phi)_{Y^{m-1}}$ uniformly on $[0,T_0]$. Thus, integrating the equality $(-(du_\epsilon/dt) - B_\epsilon u_\epsilon + F(u_\epsilon),\phi)_{Y^{m-1}} = 0$ on a time interval in $[0,T_0]$, and changing the order of the inner product and the time integral after taking the limit $\epsilon \to 0$, we find that u is a solution of Eq. (2.1) lying in the class $C([0,T_0];X^{m-1}) \cap L^\infty([0,T_0];X^m)$. By taking the X^{m-1}-inner product of Eq. (2.1) with u and using (2.6) and Gronwall's inequality, we also find that the solution u is unique in this class. Note that u is strongly continuous in X^m at $t = 0$ since u is weakly continuous in X^m at $t = 0$ and $\limsup_{t \to 0} \|u(t)\|_{X^m} \leqslant \|u_0\|_{X^m}$. The fact that Eq. (2.1) is time translational then implies that the solution corresponding to the initial data $u(t_0)$, given at $t = t_0 > 0$, is also right continuous in X^m at $t = t_0$. By the above uniqueness result, it follows that u is right continuous in X^m at any t in $[0,T_0]$. Since Eq. (2.1) is also time reversible (in a suitable sense), we deduce that $u \in C([0,T_0];X^m)$. Note that the choice of T_0 was uniform for all initial data u_0 satisfying $\|u_0\|_{X^{[d/2+2]}} \leqslant L$, for each fixed $L > 0$. Thus the above solution u extends to some larger interval $[0,T)$ in such a way that $u \in C([0,T);X^m)$ with either $T = \infty$ or $\lim_{t \to T} \|u(t)\|_{X^{[d/2+2]}} = \infty$. From the equation, it also follows that $u \in C^1([0,T);Y^{m-1})$.

To prove the continuous dependence of the solution u of Eq. (2.1) on the initial data u_0, let $\{u_{n0}\}_{n=1}^\infty$ be a sequence in X^m that converges to u_0 weakly in X^m strongly in X^{m-1}, and let u_n be the solution of Eq. (2.1) corresponding to the initial data u_{n0}, for each n. Suppose that $\{u_n\}$ satisfies $\|u_n\|_{X^{[d/2+2]}} \leqslant C$ of $[0,T']$ for some constants $C, T' > 0$ independently of n. Now an argument similar to that which led from (2.13) to (2.15) (but now setting $\epsilon = 0$ and replacing u_0 by u_{n0}) shows that $\|u_n\|_{X^m} \leqslant \|u_{n0}\|_{X^m} e^{Ct}$ on $[0,T']$ for some constant $C > 0$ independent of n. An analysis similar to that which led from (2.17) to (2.18) then shows that $\|u_n(t) - u_{n'}(t)\|_{X^{m-1}} \leqslant C\|u_{n0} - u_{n'0}\|_{X_{m-1}}$ on $[0,T']$ again for some constant $C > 0$ independent of n and n'. Then by the same argument as above, we deduce that $u_n \to u$ weakly in X^m uniformly on $[0,T']$.

It remains to show the last part of the theorem. To see this, assume further that u_0 satisfies (2.3), and let $u = (A_0, P_0, \mathbf{A}, \mathbf{P}, \psi)$ be the corresponding solution of Eq (2.1). Put

$$f = P_0 - \partial_j A_j, \quad g = \partial_j P_j - \Delta A_0 + \bar{\psi}\psi.$$

From Eq. (2.1) we have

$$\frac{df}{dt} = -g, \quad \frac{dg}{dt} = -\Delta f + 2\bar{\psi}\psi f.$$

Using these equations, we obtain

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\{\|f\|_2^2 + \|\nabla f\|_2^2 + \|g\|_2^2\} &= \int_{\mathbf{R}^d} (2\bar{\psi}\psi - 1) f g \, dx \\ &\leqslant \{\tfrac{1}{2} + \|\psi\|_\infty^2\}\{\|f\|_2^2 + \|g\|_2^2\},\end{aligned}$$

on the interval of existence $[0,T)$ of u. Since $\|\psi\|_\infty \leqslant \|\psi\|_{H^{[d/2+1]}} \leqslant c(T')$ on each $[0,T']$, $T' < T$, and $f(0) = g(0) = 0$ by assumption, it follows that $\|f\|_2^2 + \|\nabla f_2^2\| + \|g\|_2^2 = 0$ on $[0,T)$. Thus $f \equiv 0$, which is the desired result.

III. GLOBAL EXISTENCE IN ONE AND TWO SPACE DIMENSIONS

In this section we shall prove the following theorem.

Theroem 3.1: Let $d \in \{1,2\}$, m an integer satisfying

$m \geqslant [d/2+4]$, and $V \in H^m(\mathbf{R}^d;\mathbf{R})$. Let u_0 be any initial data lying in X^m and satisfying the constraints (2.3). Then Eqs. (2.1) and (2.2) have a unique solution u on $[0,\infty)$ such that $u \in C([0,\infty);X^m) \cap C^1([0,\infty);Y^{m-1})$ and $u(0)=u_0$.

The proof of Theorem 3.1 depends on the energy and the charge conservation laws, which we shall state here as a lemma. Note that we have the identities

$$\partial_\mu(f\bar{g}) = D_\mu f \bar{g} + f\,\overline{D_\mu g},$$
$$D_\mu(fg) = \partial_\mu f g + f D_\mu g,$$
$$D_\mu D_\nu f = D_\nu D_\mu f + iF_{\nu\mu} f,$$
$$\partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} + \partial_\lambda F_{\mu\nu} = 0,$$

whenever f, g, and the A_μ are smooth in (t,x) and the A_μ are real valued.

Lemma 3.2: Let $(A_0, A_1, \ldots, A_d, \psi)$ be a smooth solution of Eqs. (1.1) and (1.2) with V smooth, and assume that A_0, $A_1,\ldots,A_d,\psi,V$ and their derivatives (of suitable order) are square integrable on $\mathbf{R}^d$. Then the energy E_1 and the charge Q of the solution, that is,

$$E_1 = \int_{\mathbf{R}^d} \{D_j\psi\,\overline{D_j\psi} + V\psi\bar{\psi} + \tfrac{1}{2}F_{j0}F_{j0} + \tfrac{1}{4}F_{jk}F_{jk}\}dx,$$

$$Q = \int_{\mathbf{R}^d} \psi\bar{\psi}dx,$$

are finite constant functions of time.

Proof: In fact, we have from the equations that $(d/dt)E_1 = (d/dt)Q = 0$. The proof is facilitated by using the above identities for the D_μ and the $F_{\mu\nu}$.

Proof of Theorem 3.1: We shall prove the theorem under slightly weaker assumptions. We replace the condition $m \geqslant [d/2+4]$ by $m \geqslant [d/2+2]$, and assume the existence of a sequence $\{u_{n0}\}$ of initial data in X^k, with $k \geqslant \max\{m,[d/2+4]\}$, such that $u_{n0} \to u_0$ strongly in X^m weakly in X^{m-1}, and that each u_{n0} satisfies the constraints (2.3). Let $\{V_n\}$ be a sequence of external potentials in $H^k(\mathbf{R}^d;\mathbf{R})$, k being as above, that converges to V in H^m, and for each n, let $u_n \in C([0,T_n);X^k)$ be the solution of Eqs. (2.1) and (2.2) corresponding to the initial data u_{n0} and the external potential V_n, given by Theorem 2.1. We shall show that for such $\{u_n\}$, there is a locally bounded function $C(\cdot)$ on $[0,\infty)$, which can be chosen independently of n, such that $\|u_n(t)\|_{X^{[d/2+2]}} \leqslant C(t)$ on $[0,T_n)$. One can then show, by an obvious change of the proof of the previous result on continuous dependence of solutions on initial data (to include the dependence on the external potential), that, for every $T>0$, the solution u of Eqs. (2.1) and (2.2), corresponding to the initial data u_0 and the external potential V, exists in $C([0,T];X^m)$ as the uniform limit of $\{u_n\}$ on $[0,T]$ in the weak topology of X^m, and thus conclude the desired global existence result.

To derive the above estimate, we will use the covariant Sobolev inequality (see, e.g., Ref. 10, Appendix)

$$\|f\|_p \leqslant K\left\{\sum_{1\leqslant j\leqslant d}\|D_j f\|_q\right\}^a \|f\|_r^{1-a}, \quad D_j = \partial_j - iA_j,$$

where $1/p = a(1/q - 1/d) + (1-a)(1/r)$, with $d \geqslant 1$, $1 \leqslant p \leqslant \infty$, $1 \leqslant q \leqslant \infty$, $1 \leqslant r < \infty$, and $0 \leqslant a \leqslant 1$ (if $p=\infty$, only $a<1$ is allowed), $K = K(d,p,q,r)$, and the A_j are real and f is complex valued, with $f \in L^r$, $\partial_j f \in L^q$, and $A_j f \in L^q$. We will need the following particular estimates:

$$\|f\|_4 \leqslant K\|Df\|_2^{d/4}\|f\|_2^{1-d/4}, \quad d=1,2, \tag{3.1}$$
$$\|f\|_\infty \leqslant K\|Df\|_2^{1/2}\|f\|_2^{1/2}, \quad d=1, \tag{3.2}$$
$$\|f\|_\infty \leqslant K\|D^2 f\|_2^{\epsilon/2}\|Df\|_2^{1-\epsilon}\|f\|_2^{\epsilon/2}, \quad 0<\epsilon<1, \quad d=2, \tag{3.3}$$

and also use the usual estimates obtained by setting $A_j = 0$ for all j in (3.1)–(3.3). Here as in the following, we write $\|D^s f\|_2$ for $\{\Sigma_{j_1,\ldots,j_s}\|D_{j_1}\cdots D_{j_s}f\|_2^2\}^{1/2}$ We will also use the notation $\|\partial^s f\|_2$ to designate $\{\Sigma_{j_1,\ldots,j_s}\|\partial_{j_1}\ldots\partial_{j_s}f\|_2^2\}^{1/2}$.

We shall denote u_n simply as u, and any positive locally bounded function of $t \in [0,\infty)$ (including any positive constant), which can be chosen independently of n by the same letter C. Note that $u = (A_0,P_0,\mathbf{A},\mathbf{P},\psi) \in C([0,T_n);X^k)$ implies that $A_0 \in C^l([0,T_n)\ H^{k+1-l})$, $A_j \in C^l([0,T_n);H^{k-l})$ $(j=1,\ldots,d)$ and $\psi \in C^l([0,T_n);H^{k-2l})$, for $l=0,1,\ldots,[k/2]$. The identities for the D_μ and the $F_{\mu\nu}$ will be freely used in the following arguments.

Lemma 3.2 and the fact that the sequence of initial data with which we are concerned is bounded in X^m first give

$$E_1 < C, \quad \|\psi\|_2 < C. \tag{3.4}$$

Consider now the second-order pseudoenergy E_2 defined by

$$E_2 = \int_{\mathbf{R}^d}\{D_jD_j\psi\,\overline{D_kD_k\psi} + \tfrac{1}{2}\partial_k F_{j0}\,\partial_k F_{j0} + \tfrac{1}{2}\partial_k F_{jl}\,\partial_k F_{jl}\}dx.$$

We note that (3.1) and (3.4) imply

$$\begin{aligned}\|D^2\psi\|_2^2 &= \int_{\mathbf{R}^d} D_jD_k\psi\,\overline{D_jD_k\psi}\,dx \\ &= \int_{\mathbf{R}^d}\{D_jD_j\psi\,\overline{D_kD_k\psi} \\ &\quad + 2iF_{jk}D_j\psi\,\overline{D_k\psi} + i\partial_jF_{jk}\psi\,\overline{D_k\psi}\}dx \\ &\leqslant \|D_jD_j\psi\|_2^2 + \|F_{jk}\|_2\|D_j\psi\|_4\|D_k\psi\|_4 \\ &\quad + \|\partial_jF_{jk}\|_2\|\psi\|_4\|D_k\psi\|_4 \\ &\leqslant E_2 + C\|D^2\psi\|_2^{d/2} + CE_2^{1/2}\|D^2\psi\|_2^{d/4},\end{aligned}$$

so that

$$\|D^2\psi\|_2^2 \leqslant CE_2 + C. \tag{3.5}$$

We compute the time derivative of E_2 using Eqs. (1.1) and (1.2), and then estimate the result by means of (3.1)–(3.5). The result is that

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}E_2 &= \mathrm{Re}\int_{\mathbf{R}^d}\{2iF_{j0}D_k\psi\,\overline{D_kD_j\psi} \\ &\quad - i\partial_j\partial_jV\psi\,\overline{D_kD_k\psi} \\ &\quad - 2i\partial_jVD_j\psi\,\overline{D_kD_k\psi} - \partial_kF_{j0}F_{jk}\psi\bar{\psi}\}dx \\ &\leqslant 2\|F_{j0}\|_4\|D_k\psi\|_4\|D_kD_j\psi\|_2 \\ &\quad + \|\partial_j\partial_jV\|_2\|\psi\|_\infty\|D_kD_k\psi\|_2 \\ &\quad + 2\|\partial_jV\|_4\|D_j\psi\|_4\|D_kD_k\psi\|_2 \\ &\quad + \|\partial_kF_{j0}\|_2\|F_{jk}\|_4\|\psi\|_4\|\psi\|_\infty \\ &\leqslant CE_2 + C.\end{aligned}$$

(The $\|\partial_jV\|_4, \|F_{j\mu}\|_4$ are estimated by the usual Sobolev ine-

quality.) Recalling that the sequence of initial data is bounded in X^m, we obtain

$$E_2 < C. \tag{3.6}$$

In a completely analogous way, we further estimate for $d = 2$ the third order pseudoenergy

$$E_3 = \int_{\mathbf{R}^2} \{D_l D_j D_j \psi \overline{D_l D_k D_k \psi} + \tfrac{1}{2} \partial_l \partial_k F_{j0} \partial_l \partial_k F_{j0} + \tfrac{1}{4} \partial_l \partial_k F_{jn} \partial_l \partial_k F_{jn}\} dx,$$

by using the covariant and the usual Sobolev inequalities and the above estimates. One first finds that

$$\begin{aligned}
\|D^3\psi\|_2^2 &= \int_{\mathbf{R}^2} D_j D_k D_l \psi \overline{D_j D_k D_l \psi}\, dx \\
&= \int_{\mathbf{R}^2} \{D_l D_j D_j \psi \overline{D_l D_k D_k \psi} \\
&\quad + iF_{kj} D_l \psi \overline{D_j D_k D_l \psi} \\
&\quad - iF_{kj} D_j D_l \psi \overline{D_k D_l \psi} + i \partial_j F_{lj} \psi \overline{D_k D_k D_l \psi} \\
&\quad + 2iF_{lj} D_j \psi \overline{D_k D_k D_l \psi} - i \partial_k F_{lk} D_l D_j D_j \psi \bar{\psi} \\
&\quad - 2iF_{lk} D_l D_j D_j \psi \overline{D_k \psi}\} dx \\
&\leqslant CE_3 + C\|D^3\psi\|_2 + C
\end{aligned}$$

and thus obtains

$$\|D^3\psi\|_2^2 \leqslant CE_3 + C. \tag{3.7}$$

Using Eqs. (1.1) and (1.2) and noting this estimate, one has

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt} E_3 &= \int_{\mathbf{R}^d} \{(2iF_{j0} D_l D_j \psi + iF_{l0} D_j D_j \psi + 2i \partial_l F_{j0} D_j \psi \\
&\quad + i \partial_j F_{j0} D_l \psi + i \partial_l \partial_j F_{j0} \psi - i \partial_l \partial_j V \psi \\
&\quad - i \partial_j \partial_j V D_l \psi - 2i \partial_l \partial_j V D_j \psi \\
&\quad - 2i \partial_j V D_l D_j \psi \\
&\quad - i \partial_l V D_j D_j \psi) \overline{D_l D_k D_k \psi} \\
&\quad + (iD_j \psi \overline{D_l D_k \psi} + iD_l D_j \psi \overline{D_k \psi} \\
&\quad + iD_k D_j \psi \overline{D_l \psi} + iD_l D_k D_j \psi \bar{\psi}) \partial_l \partial_k F_{j0}\} dx \\
&\leqslant CE_3 + C,
\end{aligned}$$

which gives

$$E_3 < C. \tag{3.8}$$

The results (3.4)–(3.8) show that

$$\|\psi\|_2 < C, \quad \|D^s\psi\|_2 < C, \quad s = 1,\ldots,[d/2+2], \tag{3.9}$$

$$\|F_{\mu\nu}\|_{H^{[d/2+1]}} < C, \quad \mu,\nu = 0,1,\ldots,d, \tag{3.10}$$

for $d = 1,2$. To derive the needed bound on $(A_0, \partial_0 A_0, \mathbf{A}, \partial_0 \mathbf{A}, \psi)$, we shall consider the following quantities:

$$\begin{aligned}
E_{A_0} &= \|\mathbf{A}\|_2^2 + \|A_0\|_{H^{[d/2+3]}}^2 + \|\partial_0 A_0\|_{H^{[d/2+2]}}^2 \\
&= \int_{\mathbf{R}^d} A_\mu A_\mu\, dx + \sum_{|\alpha| < [d/2+2]} \int_{\mathbf{R}^d} \partial^\alpha \partial_\mu A_0\, \partial^\alpha \partial_\mu A\, 0\, dx, \\
E_{\mathbf{A}} &= \|\partial \mathbf{A}\|_{H^{[d/2+1]}}^2 + \|\partial_0 A\|_{H^{[d/2+1]}}^2 \\
&= \sum_{|\alpha| < [d/2+1]} \int_{\mathbf{R}^d} \partial^\alpha \partial_\mu A_j\, \partial^\alpha \partial_\mu A_j\, dx.
\end{aligned}$$

Here we use the notation ∂^α in the usual sense; thus $\partial^\alpha = \partial_{j_1} \cdots \partial_{j_s}$ with $|\alpha| = s$. Equations (1.1), (1.3), and (3.10) give

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt} E_{A_0} &= -\int_{\mathbf{R}^d} F_{j0} A_j\, dx \\
&\quad - \sum_{|\alpha| < [d/2+2]} \int_{\mathbf{R}^d} \partial^\alpha \partial_0 A_0\, \partial^\alpha \partial_j F_{j0}\, dx \\
&\leqslant \|F_{j0}\|_2 \|A_j\|_2 + \|\partial_0 A_0\|_{H^{[d/2+2]}} \||\psi|^2\|_{H^{[d/2+2]}} \\
&\leqslant \{C + \||\psi|^2\|_{H^{[d/2+2]}}\} E_{A_0}^{1/2}.
\end{aligned}$$

But from (3.1)–(3.3) and (3.9) one obtains

$$\begin{aligned}
&\||\psi|^2\|_2 \leqslant \|\psi\|_4^2 < C, \\
&\|\partial |\psi|^2\|_2 \leqslant 2\|\psi\|_4 \|D\psi\|_4 < C, \\
&\|\partial^2 |\psi|^2\|_2 \leqslant 2\|\psi\|_\infty \|D^2\psi\|_2 + 2\|D\psi\|_4^2 < C, \\
&\|\partial^3 |\psi|^2\|_2 \leqslant 2\|\psi\|_\infty \|D^3\psi\|_2 + 6\|D\psi\|_4 D^2\psi\|_4 < C \quad (d = 2),
\end{aligned}$$

the last estimate being needed only for $d = 2$. Thus it follows that $E_{A_0} < C$. Equations (1.3) and (3,10) and this result yield

$$\begin{aligned}
E_{\mathbf{A}} &= \sum_{|\alpha| < [d/2+1]} \int_{\mathbf{R}^d} \{\partial^\alpha F_{\mu j}\, \partial^\alpha \partial_\mu A_j \\
&\quad + \partial^\alpha \partial_j A_0\, \partial^\alpha \partial_0 A_j + \partial^\alpha \partial_0 A_0\, \partial^\alpha \partial_0 A_0\} dx \\
&\leqslant \|F_{\mu j}\|_{H^{[d/2+1]}} \|\partial_\mu A_j\|_{H^{[d/2+1]}} \\
&\quad + \|\partial_j A_0\|_{H^{[d/2+1]}} \|\partial_0 A_0\|_{H^{[d/2+1]}} \\
&\quad + \|\partial_0 A_0\|_{H^{[d/2+1]}}^2 \\
&\leqslant C E_{\mathbf{A}}^{1/2} + C,
\end{aligned}$$

giving $E_{\mathbf{A}} < C$. Therefore,

$$\|A_0\|_{H^{[d/2+3]}} < C, \quad \|\partial_0 A_0\|_{H^{[d/2+2]}} < C,$$

$$\|\mathbf{A}\|_{H^{[d/2+2]}} < C, \quad \|\partial_0 \mathbf{A}\|_{H^{[d/2+1]}} < C$$

Finally, from the definition of the D_μ one has

$$\begin{aligned}
&\partial_j \psi = D_j \psi + iA_j \psi \\
&\partial_j \partial_k \psi = D_j D_k \psi + i \partial_j A_k \psi + iA_k \partial_j \psi + iA_j D_k \psi, \\
&\partial_j \partial_k \partial_l \psi = D_j D_k D_l \psi + i \partial_j \partial_k A_l \psi \\
&\qquad + i \partial_k A_l \partial_j \psi + i \partial_j A_l \partial_k \psi \\
&\qquad + iA_l \partial_j \partial_k \psi + i \partial_j A_k D_l \psi + iA_k \partial_j \partial_l \psi \\
&\qquad + A_k \partial_j A_l \psi - A_k A_l \partial_j \psi - iA_j D_k D_l \psi.
\end{aligned}$$

Using these expressions, one finds, with the help of (3.1)–(3.3) and the usual Sobolev inequalities, that (3.9) and the above estimate on $\mathbf{A}$ imply that $\|\psi\|_{H^{[d/2+2]}} < C$, which completes the proof of the desired global result.

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The propagator of the time-dependent forced harmonic oscillator with time-dependent damping

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By using the Caldirola–Kanai Hamiltonian and by applying Feynman polygonal paths, exact evaluation of the propagator of one-dimensional time-dependent forced and damped harmonic oscillator, based on the work of Montroll in deriving the propagator of the harmonic oscillator with time-dependent frequency, is possible. The results are compared with previously found results.

I. INTRODUCTION

As is well known in nonrelativistic quantum mechanics, the propagator[1–6] can be expressed as the path integral in phase space,[7]

$$K(x'',t'';x',t') = \int \exp\left\{\left(\frac{i}{\hbar}\right)[p\dot{x} - H(p,x,t)]dt\right\} Dp\,Dx$$
$$= \lim_{n\to\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\frac{dp'}{(2\pi\hbar)^{1/2}}\prod_{j=1}^{n}\frac{dp_j\,dx_j}{(2\pi\hbar)^{1/2}}$$
$$\times\exp\left\{\frac{i}{\hbar}\sum_{j=1}^{n-1}[p_j(x_{j+1}-x_j) - H(p_j,x_j,t_j)]\right\}, \quad (1.1)$$

where $H(p,x,t)$ is the time-dependent Hamiltonian of the one-dimensional dynamical system considered, and $Dp\,Dx$ is the usual Feynman differential measure in two-dimensional phase space. For later convenience we have set $T = t'' - t'$, $\tau = T/n$, $r_j = r(t' + j\tau)$, $r' = r(t')$, and $r'' = r(t'')$ for any function $r(t)$ of time t.

Now we use the Caldirola–Kanai Hamiltonian[8,9]

$$H(p,x,t) = (p^2/2m)e^{\gamma(t)} + V(x)e^{-\gamma(t)}, \quad (1.2)$$

for the quantum dissipative system, where $V(x)$ and $\gamma(t)$ are the potential energy and the time-dependent dissipative coefficient. Substituting (1.2) into (1.1) and then integrating over all the momenta in phase space, we obtain

$$K(x'',t'';x',t') = \int \exp\left\{\frac{i}{\hbar}\int_{t'}^{t''}L(\dot{x},x,t)dt\right\} D_{\gamma(t)}x$$
$$= \lim_{n\to\infty}\left(\frac{me^{\gamma'}}{2\pi i\hbar\tau}\right)^{1/2n-1}\prod_{j=1}^{n}\left(\frac{me^{\gamma_j}}{2\pi i\hbar\tau}\right)^{1/2}$$
$$\times\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left\{\frac{i\tau}{\hbar}\sum_{j=1}^{n-1}\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\tau}\right)^2 - V(x_j)\right]e^{\gamma_j}\right\}dx_j, \quad (1.3)$$

with the Lagrangian

$$L(\dot{x},x,t) = [(m/2)\dot{x}^2 - V(x)]e^{\gamma(t)}, \quad (1.4)$$

since

$$\frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}\exp\left\{\frac{i}{\hbar}\left[p_j(x_{j+1}-x_j) - \frac{\tau p_j^2}{2m}e^{-\gamma_j}\right]\right\}dp_j$$
$$= \left(\frac{me^{\gamma_j}}{i\tau}\right)^{1/2}\exp\left[\frac{im\tau}{2\hbar}\left(\frac{x_{j+1}-x_j}{\tau}\right)^2\right]. \quad (1.5)$$

Here, $D_{\gamma(t)}x$ is designed to indicate the modified, one-dimensional Feynman polygonal path differential measure by including the time-dependent dissipative effects in configuration space.[10,11] For the case of $\gamma(t) = \gamma t$, Eq. (1.3) has already been used for evaluating the propagator of the time-dependent forced harmonic oscillator with constant damping by Khandekar and Lawande[12] and by Cheng,[13] respectively.

For the quadratic Lagrangian, Eq. (1.3) can, however, be calculated by first transforming it into the following Gaussian integral:

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp[i(Y^TAY + 2B^TY)]\prod_{j=1}^{n}dy_j$$
$$= (i\pi)^{n/2}(\det A)^{-1/2}\exp(-iB^TA^{-1}B), \quad (1.6)$$

multiplied by a function of x'', x', and τ (where A is an $n\times n$ matrix, Y and B are $n\times 1$ matrices, and Y^T and B^T are, respectively, the transpose matrices of Y and B) and then by calculating (1.6) in the limit as $n\to\infty$ (or $\tau\to 0$). Montroll[14] carries out such calculations for the propagator of the harmonic oscillator with time-dependent frequency. Recently, we are able to generalize his results for the time-dependent forced harmonic oscillator with constant damping.[13] In this paper we use the same method to evaluate the propagator of the harmonic oscillator with time-dependent damping and we compare our results with those of Dodonov *et al.*[15] and of Urrutia and Hernández.[16]

II. FORMULATION

For our dynamical system, the Lagrangian has the form

$$L(\dot{x},x,t) = \{(m/2)[\dot{x}^2 - \omega^2(t)x^2] + q(t)x\}e^{\gamma(t)}, \quad (2.1)$$

where $\omega(t)$ and $q(t)$ are the time-dependent angular frequency and perturbative force, respectively. Substituting (2.1) into (1.3), we have

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$$K(x'',t'';x',t')$$

$$= \lim_{n\to\infty}\left[\prod_{j=1}^{n}\left(\frac{me^{\gamma_j}}{2\pi i\hbar}\right)^{1/2}\right]$$

$$\times\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left\{\frac{i\tau}{2\hbar}\left[m\sum_{j=1}^{n}\left(\frac{x_j-x_{j-1}}{\tau}\right)^2 e^{\gamma_j}\right.\right.$$

$$\left.\left.-\sum_{j=0}^{n-1}(m\omega_j^2x_j^2-2q_jx_j)e^{\gamma_j}\right]\right\}\prod_{j=1}^{n-1}dx_j, \tag{2.2}$$

by using Feynman's polygonal paths. The extra factor $\exp(\gamma_j)$ is necessary for including time-dependent dissipative effect. Making the transformation $y_j=(me^{\gamma_j}/2\hbar\tau)^{1/2}x_j$, Eq. (2.2) can be rewritten as

$$K(x'',t'';x',t')$$

$$= \lim_{n\to\infty}(i\pi)^{-n/2}\exp\left\{\frac{i\tau}{2h}[m\tau^{-2}(e^{\gamma_1}x'^2+e^{\gamma''}x''^2)\right.$$

$$\left.-e^{\gamma'}(m\omega'^2x'^2+2q'x')]\right\}$$

$$\times\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\left\{i\left[\sum_{j=1}^{n-1}(1+e^{\dot\gamma_j\tau}-\omega_j^2\tau^2)y_j^2\right.\right.$$

$$-2\sum_{j=0}^{n-1}e^{\dot\gamma_j\tau/2}y_jy_{j+1}+\left(\frac{2\tau^3}{m\hbar}\right)^{1/2}$$

$$\left.\left.\times\sum_{j=1}^{n-1}e^{\gamma_j/2}q_jy_j\right]\right\}\prod_{j=1}^{n-1}dy_j, \tag{2.3}$$

since $dx_j=(2\hbar\tau e^{-\gamma_j}/m)^{1/2}dy_j$.

By comparing (1.6) and (2.3) the matrix A is of the form

$$A=\begin{pmatrix} a_1 & -d_1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0\\ -d_1 & a_2 & -d_2 & 0 & \cdots & 0 & 0 & 0 & 0\\ 0 & -d_2 & a_3 & -d_3 & \cdots & 0 & 0 & 0 & 0\\ \vdots & & & & & & & & \vdots\\ 0 & 0 & 0 & 0 & \cdots & -d_{n-4} & a_{n-3} & -d_{n-3} & 0\\ 0 & 0 & 0 & 0 & \cdots & 0 & -d_{n-3} & a_{n-2} & -d_{n-2}\\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -d_{n-2} & a_{n-1}\end{pmatrix} \tag{2.4}$$

with $a_j=1+e^{\dot\gamma_j\tau}-\omega_j^2\tau^2$ and $d_j=-e^{\dot\gamma_j\tau/2}$. The column matrix B has the elements

$$b_1=-y'e^{\dot\gamma\tau/2}+(\tau^3/2m\hbar)^{1/2}Q_1$$

$$=-c\tau^{-1/2}e^{\gamma_1/2}x'^2+a\tau^{3/2}Q_1, \tag{2.5}$$

$$b_j=a\tau^{3/2}Q_j \quad (j=2,3,\ldots,n-2),$$

and

$$b_{n-1}=-y''e^{\dot\gamma_{n-1}\tau/2}+(\tau^3/2m\hbar)^{1/2}Q_{n-1}$$

$$=-c\tau^{-1/2}e^{(\gamma''+\dot\gamma_{n-1}\tau)/2}x''^2+a\tau^{3/2}Q_{n-1}$$

and the matrix Y has elements y_j $(j=1,2,\ldots,n-1)$. Here we have set $Q_j=\exp(\gamma_j/2)q_j$, $c=(m/2\hbar)^{1/2}$, and $a=(2m\hbar)^{-1/2}$. Using (1.6), (2.4), and (2.5), we obtain from (2.3)

$$K(x'',t'';x',t')=\lim_{\tau\to0}\left(\frac{me^{\gamma''}}{2\pi i\hbar\tau\det A}\right)^{1/2}\exp[iB(x'',x',\tau)], \tag{2.6}$$

with

$$B(x'',x',\tau)=(m/2\hbar\tau)(e^{\gamma_1}x'^2+e^{\gamma''}x''^2)-B^TA^{-1}B. \tag{2.7}$$

We have already assumed the factor $\exp[(i\tau/2\hbar)(2q'x'-m\omega'^2x'^2)e^{\gamma'}]$ in (2.3) to be 1 as $\tau\to0$. Now we are left only to calculate the limit values of $\tau\det A$ and $B(x'',x',\tau)$ as $\tau\to0$. These calculations will be carried out in the next section.

III. CALCULATION

From the matrix A, we define f_j and g_j as the following determinates:

$$f_n=\tau,\quad f_{n-1}=\tau a_{n-1},$$

$$f_{n-2}=\tau\begin{vmatrix} a_{n-2} & -d_{n-2}\\ -d_{n-2} & a_{n-1}\end{vmatrix},$$

$$f_{n-3}=\tau\begin{vmatrix} a_{n-3} & -d_{n-3} & 0\\ -d_{n-3} & a_{n-2} & -d_{n-2}\\ 0 & -d_{n-2} & a_{n-1}\end{vmatrix},\ldots,$$

$$f_1=\tau\det A, \tag{3.1}$$

and

$$g_0=\tau,\quad g_1=\tau\begin{vmatrix} a_1 & -d_1\\ -d_1 & a_2\end{vmatrix},$$

$$g_3=\tau\begin{vmatrix} a_{n-3} & -d_{n-3} & 0\\ -d_{n-3} & a_{n-2} & -d_{n-2}\\ 0 & -d_{n-2} & a_{n-1}\end{vmatrix},\ldots,$$

$$g_{n-1}=\tau\det A.$$

Now it can be shown easily that f_j and g_j satisfy the recurrence relations

$$f_{j-1}=a_{j-1}f_j-d_j^2f_{j+1}\quad(1<j<n-2), \tag{3.2}$$

and

$$g_{j+1}=a_{j+1}g_j-d_j^2g_{j-1}\quad(2<j<n-1), \tag{3.3}$$

with the following end conditions:

$$(f_{n-2}-f_{n-1})/\tau$$

$$=[a_{n-1}(1-a_{n-2})+d_{n-1}^2]/\tau\simeq-1, \tag{3.4}$$

and

$$(g_2-g_1)/\tau=[a_1(a_2-1)-d_1^2]/\tau\simeq1. \tag{3.5}$$

With the help of the definitions of a_j and d_j, and of end conditions (3.4) and (3.5), Eqs. (3.2) and (3.3) can be reduced to the following differential equations:

$$\ddot{f}+\dot{\gamma}\dot{f}+\omega^2 f=0, \quad f''=0, \quad \dot{f}''=-1, \tag{3.6}$$

and

$$\ddot{g}-\dot{\gamma}\dot{g}+(\omega^2-\ddot{\gamma})g=0, \quad g'=0, \quad \dot{g}'=1, \tag{3.7}$$

respectively, as $\tau\to 0$. Therefore we have

$$g''\cong\lim_{\tau\to 0} g_{n-1}=\lim_{\tau\to 0}(\tau \det A)=\lim_{\tau\to 0} f_1\cong f'. \tag{3.8}$$

From (3.2) and (3.3) we also find that f_j and g_j are related through the formula

$$\begin{aligned} &f_{j+1}g_j-d_{j+2}^2 f_{j+2}g_{j-1}\\ &\quad=f_j g_{j-1}-d_j^2 f_{j+1}g_{j-2}\\ &\quad=\cdots=\tau^2 \det A=\tau f_1=\tau g_{n-1}. \end{aligned} \tag{3.9}$$

Hence

$$\begin{aligned} g_j&=\tau f_1 f_{j+2}\left[(f_{j+2}f_{j+1})^{-1}+d_{j+1}^2 f_{j+2}g_{j-1}/f_{j+1}\right]\\ &=\tau f_1 f_{j+2}\left[(f_{j+2}f_{j+1})^{-1}+d_{j+1}^2(f_{j+1}f_j)^{-1}\right.\\ &\quad\left.+d_{j+1}^2 d_j^2 f_{j+1}g_{j-2}/f_j\right]\\ &=\cdots=\tau f_1 f_{j+2}\sum_{k=1}^{j+1}\left[(f_k f_{k+1})^{-1}\prod_{i=k+1}^{n+1} d_i^2\right]. \end{aligned} \tag{3.10}$$

For $j=n-2$, we have

$$\tau^2\sum_{k=1}^{n-1}\left[(f_k f_{k+1})^{-1}\prod_{i=k+1}^{n-1} d_i^2\right]=\frac{g_{n-2}}{g_{n-1}}. \tag{3.11}$$

However, the elements of A^{-1}, represented by a_{jk}^{-1}, are determined by finding the cofactor of the matrix A. Therefore we have from (2.4) that

$$a_{jk}^{-1}=\frac{g_{k-1}f_{j+1}}{\tau f_1}\prod_{i=k}^{j-1} d_i, \quad j>k,$$

and

$$a_{jk}^{-1}=(g_{j-1}f_{k+1}/\tau f_1)\prod_{i=j}^{k-1} d_i, \quad j\leqslant k. \tag{3.12}$$

Using (3.10) and (3.11), we obtain

$$\begin{aligned} B^T A^{-1}B&=\sum_{j,k=1}^{n-1} b_j a_{jk}^{-1} b_k\\ &=\sum_{j=1}^{n-1}\left(f_{j+1}f_j\prod_{i=1}^{j} d_i^2\right)^{-1}\left[\sum_{k=j}^{n-1} b_k f_{k+1}\prod_{i=1}^{k} d_i\right]^2, \end{aligned} \tag{3.13}$$

after lengthy algebraic manipulations. With the help of Eqs. (2.5) and (3.12), Eq. (2.7) has the form

$$\begin{aligned} &B(x'',x',\tau)\\ &\quad=A_\tau x'^2+B_\tau x'x''+C_\tau x''^2+D_\tau x'+E_\tau x''+F_\tau, \end{aligned} \tag{3.14}$$

after lengthy, but straightforward, calculations. As $\tau\to 0$, we obtain

$$\begin{aligned} \lim_{\tau\to 0} A_\tau&=\lim_{\tau\to 0}\left(\frac{me^{\gamma_1}}{2\hbar\tau}\right)\left(1-\frac{f_2}{f_1}\right)=-\frac{me^{\gamma'}\dot{f}'}{2\hbar f'},\\ \lim_{\tau\to 0} B_\tau&=\lim_{\tau\to 0}\left(\frac{m}{\hbar f_1}\right)\left[\frac{-\exp(\gamma''+\dot{\gamma}_{n-1}\tau+\gamma_{n-1})}{2}\right]\\ &=-\frac{me^{\gamma''}}{\hbar f'},\\ \lim_{\tau\to 0} C_\tau&=\lim_{\tau\to 0}\left(\frac{me^{\gamma''}}{2\hbar\tau}\right)\left[1-e^{\dot{\gamma}_{n-1}\tau}\frac{g_{n-2}}{g_{n-1}}\right]\\ &=\lim_{\tau\to 0}\left(\frac{me^{\gamma''}}{2\hbar\tau}\right)\left[1-(1+\dot{\gamma}_{n-1}\tau)\frac{g_{n-2}}{g_{n-1}}\right]\\ &=\left(\frac{me^{\gamma''}}{2\hbar}\right)\left[\frac{\dot{g}''}{g''}-\dot{\gamma}''\right], \end{aligned} \tag{3.15}$$

$$\lim_{\tau\to 0} D_\tau=\frac{1}{\hbar f'}\int_{t'}^{t''} q(t)f(t)e^{\gamma(t)}dt,$$

$$\lim_{\tau\to 0} E_\tau=\frac{e^{\gamma''}}{\hbar f'}\int_{t'}^{t''} q(t)g(t)dt,$$

$$\lim_{\tau\to 0} F_\tau=-\frac{1}{m\hbar f'}\int_{t'}^{t''} q(t)f(t)e^{\gamma(t)}dt\int_{t'}^{t} q(\theta)g(\theta)d\theta.$$

However, we should mention that the relation $\gamma_{j+1}=\gamma_j+\dot{\gamma}_j\tau$ has been used in deriving the above equations and the reader must read the similar derivations in Ref. 13 for detail.

Substituting (3.8), (3.14), and (3.15) into (2.6), we finally obtain our principal result

$$\begin{aligned} &K(x'',t'';x',t')\\ &=\left(\frac{me^{\gamma''}}{2\pi i\hbar f'}\right)^{1/2}\exp\left\{\frac{m}{2i\hbar f'}\left[\dot{f}'x'^2e^{\gamma''}+2e^{\gamma''}x'x''\right.\right.\\ &\quad\left.\left.+(\dot{\gamma}''f'-\dot{g}'')e^{\gamma''}x''^2\right]\right\}\\ &\quad\times\exp\left\{\frac{i}{\hbar f'}\left[x'\int_{t'}^{t''} q(t)f(t)e^{\gamma(t)}dt\right.\right.\\ &\quad+e^{\gamma''}x''\int_{t'}^{t''} q(t)g(t)dt\\ &\quad\left.\left.-\frac{1}{m}\int_{t'}^{t''} q(t)f(t)e^{\gamma(t)}dt\int_{t'}^{t} q(\theta)g(\theta)d\theta\right]\right\}. \end{aligned} \tag{3.16}$$

For excluding catastrophic phenomenon we have assumed that $f'=g''\neq 0$. In the case of $\gamma(t)=\gamma t$, (3.16) reduces exactly to (3.24) in Ref. 13 as we expect.

It can be shown easily that the solutions of (3.6) and (3.7) are of the form

$$f(t)=s(t)e^{-[\gamma(t)-\gamma'']/2}\sin[\nu''-\nu(t)], \tag{3.17}$$

and

$$g(t)=s(t)e^{-[\gamma-\gamma(t)]/2}\sin[\nu(t)-\nu']. \tag{3.18}$$

Furthermore, in order to satisfy their boundary conditions, we must have

$$\begin{aligned} &\ddot{s}(t)-s'^2 s^{-3}(t)+[\omega^2(t)-\dot{\gamma}^2/4-\ddot{\gamma}/2]s(t)=0,\\ &s^2(t)\dot{\nu}(t)=s'. \end{aligned} \tag{3.19}$$

We also have $s'=s''$, $\dot{\nu}'=\dot{\nu}''$, and $\dot{s}'\dot{\nu}''=\dot{s}''\dot{\nu}''=1$ since $f'=g''$. With the help of (3.17)–(3.19), Eq. (3.16) can be rewritten in the following form:

$$K(x'',t'';x',t') = \left(\frac{me^{(\gamma''+\gamma')/2}\dot{\nu}'}{2\pi i\hbar \sin\Phi(t'',t')}\right)^{1/2} \exp\left\{\frac{m\dot{\nu}'}{4i\hbar}[(2\dot{s}' - \dot{\gamma}'s')x'^2 - (2\dot{s}'' - \dot{\gamma}''s'')x''^2]\right\}$$
$$\times \exp\left\{\frac{im\dot{\nu}'}{2\hbar}[x_\gamma'^2 + x_\gamma''^2]\cot\Phi(t'',t') - 2x_\gamma' x_\gamma'' \csc\Phi(t'',t')\right\}$$
$$\times \exp\left\{\frac{i\dot{\nu}'}{\hbar \sin\Phi(t'',t')}\left[x_\gamma' \int_{t'}^{t''} q(t)s(t)e^{\gamma(t)/2}\sin\Phi(t'',t)dt + x_\gamma'' \int_{t'}^{t''} q(t)s(t)e^{\gamma(t)/2}\sin\Phi(t,t')dt\right.\right.$$
$$\left.\left. - \frac{1}{m}\int_{t'}^{t''} q(t)s(t)e^{\gamma(t)/2}\sin\Phi(t'',t)dt \int_{t'}^{t} q(\theta)s(\theta)e^{\gamma(\theta)/2}\sin\Phi(\theta,t')d\theta\right]\right\} \tag{3.20}$$

with $x_\gamma' = e^{\gamma'/2}x'$, $x_\gamma'' = e^{\gamma''/2}x''$, $\Phi(\alpha,\beta) = \nu(\alpha) - \nu(\beta)$ for any two arbitrary times α and β in between t' and t''.

IV. CONCLUSION

Recently the propagator of our dynamical system has also been obtained by Dodonov *et al.*[15] based on the connection between the integrals of motion of a quantum system with its propagator, and by Urrutia and Hernádez[16] based on the Schwinger action principle. However, it is easy to show that

$$f(t) = -\beta(t)/\dot{\beta}'' = e^{\gamma''}[\lambda_1''\lambda_3(t) - \lambda_3''\lambda_1(t)], \tag{4.1}$$

and

$$g(t) = \alpha(t)e^{\gamma(t)}/\dot{\alpha}'e^{\gamma'} = -e^{\gamma(t)}\lambda_3(t). \tag{4.2}$$

Here, $\alpha(t)$ and $\beta(t)$ are defined by (42) and (43) of Ref. 16 and $\lambda_1(t)$ and $\lambda_3(t)$ are defined by (5) of Ref. 15. Therefore our result (3.16) is exactly equivalent to (6) in Ref. 15 and to (63) in Ref. 16 as we expect. Finally, we should remark that (3.20) is independent of any boundary conditions related to the functions of $s(t)$ and $\nu(t)$ since they are connected with $f(t)$ and $g(t)$ through (3.17) and (3.18).

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Functional integrals for spin-Bose systems

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The problem of obtaining the propagator of a spin-Bose system consisting of spins-$\frac{1}{2}$ and several radiation modes in interaction is reduced to developing a bosonized Hamiltonian for the system from the propagator of which, by appropriate projection, the propagator relating to the original Hamiltonian is extracted. The analysis proceeds via functional integration involving the evaluation of two auxiliary propagators of Schrödinger equations whose Hamiltonians depend separately on radiation operators, and bosonized spin operators. These propagators are coupled through a complex field and the functional average of their product against a Gaussian measure of the field leads to the bosonized system's propagator. The procedure is applied to the propagator for a single spin-Bose system which is obtained as a power series in the spin flipping energy. The analysis is also applied for an explicit evaluation in the case of a simplified spin-Bose Hamiltonian.

I. INTRODUCTION

Interest in path integrals for spin systems has recently been revived.[1] The authors basically exploit representation properties of the spin coherent states.[2]

A central role in the development of any form of path integral giving the propagator of a system is played by the unity resolution[3] in terms of states through which the propagator is expressed. In the case of Bose coherent states, manipulations in conjunction with the unity resolution involve relatively simple procedures, whereas the task of handling operations with spin coherent states is a formidable one.

On account of facilities provided by the Bose operators a number of authors[4] have used Schwinger's Bose representation[5] of angular momentum for handling certain spin problems. In the present work Schwinger's representation will be the starting point for developing functional integrals for spin-Bose problems.

An important spin-Bose problem involves the Hamiltonian

$$H_N = \sum_{r=1}^{M} \hbar\Omega_r a_r^+ a_r + \sum_{\lambda=1}^{N} \frac{1}{2}\hbar\omega\sigma_z^{(\lambda)} + \sum_{\lambda=1}^{N}\sum_{r=1}^{M} \hbar(g_{r\lambda}^* a_r^+ + g_{r\lambda} a_r)\sigma_x^{(\lambda)}, \tag{1.1}$$

for the treatment of M modes of radiation interacting with N two-level atoms[6] or spins-$\frac{1}{2}$. It has also been used for the treatment of phase transition problems[7,8] in the case of a single spin. In (1.1) a_r^+ and a_r stand for Bose creation and annihilation operators, $g_{r\lambda}^*$ and $g_{r\lambda}$ are coupling constants of the interaction with the spins, and $\sigma_x^{(\lambda)}$ and $\sigma_z^{(\lambda)}$ are the x and z components of the λ th spin.

The present work aims at establishing a method of functional integration for spin problems and can handle the propagator associated with (1.1). Path integrals have already been used[8] for obtaining the partition function relating to (1.1) in the case of a single spin. Our method covers the case of the many-spin problem. It relies on producing a bosonized form of the original Hamiltonian from the propagator of which the appropriate spin-Bose propagator can be extracted by projection. Rules for the projection procedure will be given in the text.

Bosonization of angular momentum operators, followed by relevant projection, has been used for the treatment of spin problems.[4,5] However, when more than one spin are involved the approach cannot provide the answers to all questions about the system. Furthermore, the method fails to apply when the spins are coupled differently to the various Bose fields. The proposed method bypasses the above difficulties by introducing separate Bose operators per spin. In the case of a single spin both methods are identical. However, in the many-spin situation the projection schemes differ.

Before embarking on details of the scheme it would be helpful to describe the representation of the Bose operators (whether derived from the spins or the radiation field) which will be used throughout the present work. It is a variant of the Bargmann representation[9] in which the creation operator a^+ takes the form of a multiplicative operator α^* (α, complex variable) and the corresponding annihilation operator a takes the form $\partial/\partial\alpha^*$ (see Refs. 10 and 11). A word of caution becomes necessary in dealing with the above representation. Namely, the above operator expressions do not act on the weighting part of the associated coherent state variable. We shall avoid accompanying our wave functions with the weighting factor, which will be employed whenever the composition law is to be applied.

In Ref. 12, certain spin states labeled by as many complex variables as the number of spins in the system considered were introduced. These states differ from Radcliffe's or Arrechi's states,[2] for the latter attain full description through a single variable. The former somehow introduce an amount of complication on account of the number of variables required, but at the same time provide higher descriptive resolution in that they retain the individuality of the spins involved. The scheme of these states will be employed in the text as a basis of comparison with the results obtained by the method of bosonization and spin projection. Details of the procedure follow in Sec. II.

In Sec. III the method of functional integration will be

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used for obtaining the propagator of the spin-Bose Hamiltonian, in the case of a single spin, in the form of a series expansion in the atom excitation energy. Finally, in Sec. IV an explicit evaluation of the propagator for a much simpler Hamiltonian derived from (1.1) is given.

II. THE SPIN-BOSE PROPAGATOR PROJECTION

In this section we shall present the scheme to be used for projecting out of the fully bosonized propagator associated with the Hamiltonian (1.1) the relevant spin-Bose propagator.

We begin initially considering a two-level atom (equivalently a spin-$\frac{1}{2}$). The states for such an atom can be described by two complex variables, each of which corresponds to a different level. Let β and γ be the variables attached to the lower and upper level, respectively. For the purpose of forming propagators we shall associate the values β' and γ' with time t', and their complex conjugates β^* and γ^* with time t. It is clear that the two components u_0 and u_1 of the wave function for a spin-$\frac{1}{2}$ system can be entered into the form $u_0\beta^* + u_1\gamma^*$, where u_0 and u_1 are functions of t and the coherent state variables associated with the radiation fields present in the system. In this mode of wave-function description the Hamiltonian has to be expressed in terms of the β^* and γ^* variables. This will be done utilizing Schwinger's[5] Bose representation of σ_z and σ_x. According to the Bose operator representation adopted in this paper these matrices will be replaced by

$$\sigma_z \to \left(\gamma^* \frac{\partial}{\partial \gamma^*} - \beta^* \frac{\partial}{\partial \beta^*}\right), \quad \sigma_x \to \left(\gamma^* \frac{\partial}{\partial \beta^*} + \beta^* \frac{\partial}{\partial \gamma^*}\right). \tag{2.1}$$

Let us now consider the Hamiltonian (1.1) specialized for the case of a single spin. The index λ in the coupling constants becomes redundant and the Hamiltonian in question takes the form

$$H_1 = \sum_{r=1}^{M} \hbar\Omega_r \alpha_r^* \frac{\partial}{\partial \alpha_r^*} + \frac{1}{2}\hbar\omega\sigma_z + \sum_{r=1}^{M} \hbar\left(g_r^* \alpha_r^* + g_r \frac{\partial}{\partial \alpha_r^*}\right)\sigma_x . \tag{2.2}$$

The bosonized form of (2.2), obtained with the aid of (2.1), is

$$\mathscr{H}_1 = \sum_{r=1}^{M} \hbar\Omega_r \alpha_r^* \frac{\partial}{\partial \alpha_r^*} + \frac{1}{2}\hbar\omega\left(\gamma^* \frac{\partial}{\partial \gamma^*} - \beta^* \frac{\partial}{\partial \beta^*}\right) + \sum_{r=1}^{M} \hbar\left(g_r^* \alpha_r^* + g_r \frac{\partial}{\partial \alpha_r^*}\right)\left(\gamma^* \frac{\partial}{\partial \beta^*} + \beta^* \frac{\partial}{\partial \gamma^*}\right). \tag{2.2'}$$

A particular solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi = \mathscr{H}_1 \Psi, \tag{2.3}$$

has the form

$$U_1 = U_{00}\beta^*\beta' + U_{01}\beta^*\gamma' + U_{10}\gamma^*\beta' + U_{11}\gamma^*\gamma', \tag{2.4}$$

where the components U_{ij} satisfy the matrix equation

$$i\frac{\partial}{\partial t}\begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix} = \begin{bmatrix} \sum \Omega_r \alpha_r^* \frac{\partial}{\partial \alpha_r^*} - \frac{\omega}{2} & \sum \left(g_r^* \alpha_r^* + g_r \frac{\partial}{\partial \alpha_r^*}\right) \\ \sum \left(g_r^* \alpha_r^* + g_r \frac{\partial}{\partial \alpha_r^*}\right) & \sum \Omega_r \alpha_r^* \frac{\partial}{\partial \alpha_r^*} + \frac{\omega}{2} \end{bmatrix} \begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix}. \tag{2.5}$$

Equation (2.5) gives precisely the equations satisfied by the spin-Bose propagator elements based on the σ representation employed earlier by the author.[11] In this representation the propagator has the form $U_{00} + U_{01}\sigma^* + U_{10}\sigma' + U_{11}\sigma^*\sigma'$. So, the only thing that remains to be taken care of in order to obtain the propagator associated with the spin-Bose Hamiltonian[13] (2.2) is to fix the appropriate initial conditions, namely

$$U_{ij}|_{t=0} = \exp\left(\sum_{r=1}^{M} \alpha_r^* \alpha_r'\right)\delta_{ij} . \tag{2.6}$$

Thus, one is able to obtain the propagator for the spin-Bose system described by the Hamiltonian (2.2) as a particular solution of a fully Bose system described by the associated bosonized Hamiltonian (2.2').

We now turn our considerations to the bosonized Hamiltonian (2.2'). Since this is a fully Bose Hamiltonian we are able to apply functional integration procedures for obtaining the associated propagator. This propagator will contain, in addition to the terms involving $\beta^*\beta'$, $\beta^*\gamma'$, $\gamma^*\beta'$, and $\gamma^*\gamma'$, other powers in the variables β^*, γ^*, β', and γ'. In order to obtain the required propagator for the spin-Bose system with Hamiltonian (2.2) we have to select, from the full Bose propagator expansion, the bilinear portion of the form (2.4). This is definitely a particular solution of (2.3) and satisfies (2.5). There remains the question of whether the components U_{ij}, thus obtained, satisfy the initial conditions (2.6). If so, the above projection of the full Bose propagator onto the bilinear component (2.4) supplies the spin-Bose propagator. Indeed, the appropriate initial conditions for the projected propagator are satisfied and this is easy to see, considering that the full propagator at $t = 0$ takes the form

$$U|_{t=0} = \exp\left(\sum_{r=1}^{M} \alpha_r^* \alpha_r'\right) \exp(\beta^*\beta' + \gamma^*\gamma'), \tag{2.7}$$

which clearly leads to the required initial condition for U_1.

Before proceeding with developing procedures for handling the many-spin problem we wish to discuss a little further the β,γ representation in the case of a single spin. We notice that $(\beta^* + \gamma^*)$ is an eigenstate of the operator $\gamma^*(\partial/\partial\beta^*) + \beta^*(\partial/\partial\gamma^*)$ (bosonized form of σ_x) corresponding to the lowest nonzero eigenvalue. The product $(\beta^* + \gamma^*)(\beta' + \gamma')$ equals the expression $\beta^*\beta' + \beta^*\gamma' + \gamma^*\beta' + \gamma^*\gamma'$ from which we get the form (2.4) for the spin-Bose propagator, by introducing the amplitudes U_{00}, U_{01}, U_{10}, and U_{11} in front of the terms $\beta^*\beta'$, $\beta^*\gamma'$, $\gamma^*\beta'$,

and $\gamma^*\gamma'$. The choice of the subscripts is such that 0 goes with the β level and 1 with the γ level. This procedure will serve as a mnemonic for writing down the form of the propagator and a suitable generalization will be devised for the many-spin problem.

Let us now look into a few properties possessed by certain of our bosonized spin operators. Remembering that β^* represents the atomic state of lower energy and γ^* the one of higher energy, it is easy to verify that the bosonized forms $\gamma^*(\partial/\partial\beta^*)$ and $\beta^*(\partial/\partial\gamma^*)$ of the flip-up (S^+) and flip-down (S^-) spin operators, when acting on the states β^* and γ^* yield the defining properties of the operators S^+ and S^-. Indeed we have $\gamma^*(\partial/\partial\beta^*)\beta^* = \gamma^*$, i.e., the creation of the upper level state through the destruction of the ground level state by the flip-up operator. Further action of this operator on the upper level state gives zero. Similarly, the action of the flip-down operator on the upper level state leads to the ground level state, and further application of this operator on the state resulted above gives zero. These properties are only valid in relation to the states β^* and γ^* and in this respect only the situation is equivalent to the two-level atom described by spin or Fermi operators.

If in conjunction with our bosonized spin operators we employ wave functions that are higher-degree polynomials of the form $\gamma^{*J-m}\beta^{*J+m}(m = -J, -J+1, ..., J)$ suitably normalized, we are led to Schwinger's theory for handling angular momentum problems.[4] The case with $J = \frac{1}{2}$ gives the set of states $\{\beta^*, \gamma^*\}$, which describes precisely the states of a two-level atom, or of a single spin-$\frac{1}{2}$, and this mode of description enables the answering of all relevant questions about the single spin system. Schwinger's theory forms a precise approach to the angular momentum possessed by a system of spins-$\frac{1}{2}$. Nevertheless, certain difficulties are encountered with the angular momentum mode of description in the case of many spins, particularly when information is sought about the behavior of a particular spin coupled to various radiation modes. Thus, the necessity of extending the method to include the treatment of the many-spin problem with varying radiation couplings. We hope to return to the question of the amount of information one can get from the angular momentum mode of description when applied to many spins-$\frac{1}{2}$ coupled to radiation.

A fixed number of atoms, essentially gives each atomic state by its upper level occupancy. This, however, does not tell us which of the atoms are in the upper state. To be specific, the case of two atoms ($J = 1$) is associated with the wave functions β^{*2}, $\beta^*\gamma^*$, and γ^{*2}, corresponding to the states; both spins down, one of the two spins up, and both up. For a system of spins alone such a description is perfectly adequate and even more appealing. However, when the system of spins interacts with a radiation field the individuality of the spins may be necessary. The spin mode of description differentiates between the state spin-1 up, spin-2 down, and the state spin-1 down, spin-2 up, which in the angular momentum mode are contracted into one state represented by the wave function $\beta^*\gamma^*$.

When the atomic system interacts with a radiation field, but the coupling of the various modes does not differ from atom to atom, one can form a Hamiltonian for the combined system using either spin operators or angular momentum operators. Evidently the number of equations of motion for the various amplitudes resulting from the spin description will exceed the number of those derived from the corresponding angular momentum description. The latter can be produced from the former by adding the equations that give the rate of change of the amplitudes of those spin states that get contracted into one state in the angular momentum treatment. Under the above circumstances the individuality of the atoms is not always important. However, in a situation in which the coupling of the field modes varies from atom to atom one has to have recourse to the individuality of the spins involved. In such a case a frame incorporating this resolution is necessary, and requires an increased number of variables.

We now proceed to show how to handle the many-spin problem. As a vehicle for presentation we shall have in mind the system described by the Hamiltonian (1.1) in which the spins are differently coupled to the various radiation modes. Should we further wish to consider more than one species of two-level atoms, this can be done by replacing ω by ω_λ, but this does not really change the method and we shall proceed with (1.1) as it is.

The bosonized Hamiltonian, appropriate for the many-spin case, is obtained from (1.1) by the following operator replacements of the spin matrices

$$\begin{aligned}\sigma_z^{(\lambda)} &\to \gamma_\lambda^* \frac{\partial}{\partial\gamma_\lambda^*} - \beta_\lambda^* \frac{\partial}{\partial\beta_\lambda^*},\\ \sigma_x^{(\lambda)} &\to \gamma_\lambda^* \frac{\partial}{\partial\beta_\lambda^*} + \beta_\lambda^* \frac{\partial}{\partial\gamma_\lambda^*},\end{aligned} \tag{2.8}$$

i.e., we make use of as many pairs of variables β_λ^*, γ_λ^* as the number of spins in the system. This is the point at which we part from the angular momentum treatment. The bosonized form of the Hamiltonian derived through the above replacements is

$$\begin{aligned}\mathscr{H}_N = &\sum_{r=1}^{M} \hbar\Omega_r \alpha_r^* \frac{\partial}{\partial\alpha_r^*} + \sum_{\lambda=1}^{N} \frac{1}{2}\hbar\omega\left(\gamma_\lambda^* \frac{\partial}{\partial\gamma_\lambda^*} - \beta_\lambda^* \frac{\partial}{\partial\beta_\lambda^*}\right)\\ &+ \sum_{r=1}^{M}\sum_{\lambda=1}^{N} \hbar\left(g_{r\lambda}^* \alpha_r^* + g_{r\lambda} \frac{\partial}{\partial\alpha_r^*}\right)\\ &\times\left(\gamma_\lambda^* \frac{\partial}{\partial\beta_\lambda^*} + \beta_\lambda^* \frac{\partial}{\partial\gamma_\lambda^*}\right).\end{aligned} \tag{2.9}$$

The propagator for the spin-Bose system with Hamiltonian (1.1) forms a portion of the propagator associated with the fully bosonized Hamiltonian (2.9). This portion is obtained by projection onto the atomic basis wave functions made out of the polynomial terms resulting from expanding the product

$$\prod_{\lambda=1}^{N} (\beta_\lambda^* + \gamma_\lambda^*)(\beta_\lambda' + \gamma_\lambda'). \tag{2.10}$$

We can make the situation more transparent by working out the details in the case of two atoms. Let us also initially deal with a wave function, rather than the propagator. In this case the atomic basis wave functions are the terms of the product $(\beta_1^* + \gamma_1^*)(\beta_2^* + \gamma_2^*)$, i.e., $\beta_1^*\beta_2^*$, $\beta_1^*\gamma_2^*$, $\gamma_1^*\beta_2^*$,

and $\gamma_1^*\gamma_2^*$. We facilitate the discussion which follows by associating the above basis wave functions with the indices 0, 1, 2, and 3, respectively. Thus, the wave function for the two-spin-Bose system will be

$$\Psi_2 = u_0\beta_1^*\beta_2^* + u_1\beta_1^*\gamma_2^* + u_2\gamma_1^*\beta_2^* + u_3\gamma_1^*\gamma_2^*, \tag{2.11}$$

where the amplitudes u_j will be functions of the coherent state variables associated with the electromagnetic field operators of the Hamiltonian, and the time.

Inserting Ψ_2 into the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi = \mathscr{H}_2\Psi, \tag{2.12}$$

we are led to the following simultaneous differential equations for the amplitudes

$$\begin{aligned}
i\frac{\partial}{\partial t}u_0 &= \left(\sum \Omega_r\alpha_r^*\frac{\partial}{\partial\alpha_r^*} - \omega\right)u_0 + \sum\left(g_{r2}^*\alpha_r^* + g_{r2}\frac{\partial}{\partial\alpha_r^*}\right)u_1 + \sum\left(g_{r1}^*\alpha_r^* + g_{r1}\frac{\partial}{\partial\alpha_r^*}\right)u_2,\\
i\frac{\partial}{\partial t}u_1 &= \sum\left(g_{r2}^*\alpha_r^* + g_{r2}\frac{\partial}{\partial\alpha_r^*}\right)u_0 + \sum\Omega_r\alpha_r^*\frac{\partial}{\partial\alpha_r^*}u_1 + \sum\left(g_{r1}^*\alpha_r^* + g_{r1}\frac{\partial}{\partial\alpha_r^*}\right)u_3,\\
i\frac{\partial}{\partial t}u_2 &= \sum\left(g_{r1}^*\alpha_r^* + g_{r1}\frac{\partial}{\partial\alpha_r^*}\right)u_0 + \sum\Omega_r\alpha_r^*\frac{\partial}{\partial\alpha_r^*}u_2 + \sum\left(g_{r2}^*\alpha_r^* + g_{r2}\frac{\partial}{\partial\alpha_r^*}\right)u_3,\\
i\frac{\partial}{\partial t}u_3 &= \sum\left(g_{r1}^*\alpha_r^* + g_{r1}\frac{\partial}{\partial\alpha_r^*}\right)u_1 + \sum\left(g_{r2}^*\alpha_r^* + g_{r2}\frac{\partial}{\partial\alpha_r^*}\right)u_2 + \left(\sum\Omega_r\,\alpha_r^*\frac{\partial}{\partial\alpha_r^*} + \omega\right)u_3,
\end{aligned} \tag{2.13}$$

which are precisely the equations obtained using proper spin operators and the σ representation as in Ref. 11.

The fact that through the β, γ basis employed in (2.11) we are led to the correct equations of motion for the wave function components concludes the equivalence of the solutions obtained from the direct spin-Bose problem with those derived from the projected bosonized procedure.

Before we deal with the propagator, it is worth noticing that the state $\beta_1^*\beta_2^*$ represents the situation where both atoms are in their ground states, $\beta_1^*\gamma_2^*$ stands for the state with atom 1 in the ground state while atom 2 in its excited state, the reverse situation being described by $\gamma_1^*\beta_2^*$, and finally $\gamma_1^*\gamma_2^*$ provides the state where both atoms are in their excited states. With the above in mind one can easily fix the initial conditions.

Now, the form of the propagator is obtained by attaching amplitudes to the polynomial terms obtained from the product $(\beta_1^* + \gamma_1^*)(\beta_2^* + \gamma_2^*)(\beta_1' + \gamma_1')(\beta_2' + \gamma_2')$. They are 16 in number, and the propagator has the form

$$\begin{aligned}
U_2 = {} & U_{00}\beta_1^*\beta_2^*\beta_1'\beta_2' + U_{01}\beta_1^*\beta_2^*\beta_1'\gamma_2'\\
& + U_{02}\beta_1^*\beta_2^*\gamma_1'\beta_2' + U_{03}\beta_1^*\beta_2^*\gamma_1'\gamma_2'\\
& + U_{10}\beta_1^*\gamma_2^*\beta_1'\beta_2' + U_{11}\beta_1^*\gamma_2^*\beta_1'\gamma_2'\\
& + U_{12}\beta_1^*\gamma_2^*\gamma_1'\beta_2' + U_{13}\beta_1^*\gamma_2^*\gamma_1'\gamma_2'\\
& + U_{20}\gamma_1^*\beta_2^*\beta_1'\beta_2' + U_{21}\gamma_1^*\beta_2^*\beta_1'\gamma_2'\\
& + U_{22}\gamma_1^*\beta_2^*\gamma_1'\beta_2' + U_{23}\gamma_1^*\beta_2^*\gamma_1'\gamma_2'\\
& + U_{30}\gamma_1^*\gamma_2^*\beta_1'\beta_2' + U_{31}\gamma_1^*\gamma_2^*\beta_1'\gamma_2'\\
& + U_{32}\gamma_1^*\gamma_2^*\gamma_1'\beta_2' + U_{33}\gamma_1^*\gamma_2^*\gamma_1'\gamma_2'.
\end{aligned} \tag{2.14}$$

The rule for the indices i and j in the amplitudes U_{ij} becomes evident and is in accord with the convention adopted for the wave function (2.11).

The expression U_2 satisfies the Schrödinger equation (2.12) provided that for each column vector j, U_{ij} $(i = 0,1,2,3)$ obeys the system of equations (2.13). These are the equations of motion for the two-spin-Bose propagator. To obtain the propagator, the initial conditions (2.6) with $(i, j = 0,1,2,3)$ have to be fixed.

As pointed out earlier, Schrödinger's equation (2.12) admits solutions of zero- and higher-order polynomials in the atomic variables. However, if we choose from the full Bose propagator the form (2.14), this will constitute the required two-spin-Bose propagator. This is seen along the lines of reasoning applied to the single-spin case.

Finally the procedure for handling the situation with a higher number of spins in the system becomes evident from the above discussion.

Next, we shall carry out the evaluation of the propagator, applying functional integration in the case of the single-spin-Bose system.

III. THE SPIN-BOSE PROPAGATOR

To enable ourselves to attain a reasonable reduction in the load of symbols in the functional integral expressions we proceed by adopting the conventions below.

In a functional integral notation the symbolic expression $\Sigma_{0<\tau<t}\,\alpha^*(\tau^+)\alpha(\tau)$ will mean that when subdivision of the interval $[0, t]$ is under consideration we have $\Sigma_{j=0}^{N-1}\,\alpha^*(\tau_{j+1})\,\alpha(\tau_j)$. Essentially when τ stands for τ_j, τ^+ will stand for the next point τ_{j+1} in the subdivision. Similar-

ly $\int_0^t \mathscr{H}(\alpha^*(\tau^+),\alpha(\tau),\tau)d\tau$ will imply that in the subdivision scheme, use is made of $\Sigma_{j=0}^{N-1}\mathscr{H}(\alpha^*(\tau_{j+1}),\alpha(\tau_j),\tau_j)\Delta\tau_j$.

Furthermore, the weight, $\pi^{-1}\exp(-|\alpha(\tau)|^2)$, for a complex integration variable $\alpha(\tau)$ will be included in an appropriately weighted differential $D^2\alpha(\tau)$ as follows:

$$D^2\alpha(\tau)=\pi^{-1}\exp(-|\alpha(\tau)|^2)d^2\alpha(\tau). \tag{3.1a}$$

The path differential will be

$$\mathscr{D}^2\{\alpha\}=\prod_{0<\tau<t} D^2\alpha(\tau), \tag{3.1b}$$

where the product in (3.1b) is understood to be taken over the internal subdivision points.

With the above in mind we shall be able to avoid writing down various limiting processes leading to the functional integrals we shall be concerned with. Thus, if our Hamiltonian is in normal form, and let it be given by $\mathscr{H}(\alpha^*,\partial/\partial\alpha^*,t)$, the associated propagator, following Klauder's[3] original construction (see also Ref. 14), is given by the path integral over coherent variables as

$$G(\alpha^*,t\,|\alpha'0)=\int\exp\Big[\sum_{0<\tau<t}\alpha^*(\tau^+)\alpha(\tau)-\frac{i}{\hbar}\int_0^t\mathscr{H}(\alpha^*(\tau^+),\alpha(\tau),\tau)d\tau\Big]\mathscr{D}^2\{\alpha\},$$
$$\alpha(0)=\alpha',\alpha^*(t)=\alpha^*. \tag{3.2}$$

In what follows the end conditions, which determine the propagator variables, will always be imposed on the path integration, although explicit mention may not be made.

It should be noted that the expression for the propagator obtained through (3.2) does not include the usual factor $\pi^{-1}\exp(-\frac{1}{2}|\alpha|^2-\frac{1}{2}|\alpha'|^2)$. This is more convenient when working in the representation where the operators a^+,a take the form $\alpha^*,\partial/\partial\alpha^*$. Of course, the same applies to the matrix elements of any quantity employed. However, in an evaluation the omitted exponentials reappear through use of the differentials of the form (3.1a), which become necessary in this scheme, and so the final result remains unaffected.

Let us now employ (3.2) in the case of the fully bosonized single-spin-Bose Hamiltonian (2.2'). Thus, we obtain the propagator of Schrödinger equation (2.3) via the path integral

$$\mathscr{U}_1(\alpha^*,\beta^*,\gamma^*,t\,|\alpha',\beta',\gamma',0)=\int\exp\Big\{\sum_{0<\tau<t}\Big[\sum_{r=1}^M\alpha_r^*(\tau^+)\alpha_r(\tau)+\beta^*(\tau^+)\beta(\tau)+\gamma^*(\tau^+)\gamma(\tau)\Big]$$
$$-i\sum_{r=1}^M\int_0^t\Omega_r\,\alpha_r^*(\tau^+)\alpha_r(\tau)-i\frac{\omega}{2}\int_0^t[\gamma^*(\tau^+)\gamma(\tau)-\beta^*(\tau^+)\beta(\tau)]d\tau$$
$$-i\sum_{r=1}^M\int_0^t[g_r^*\alpha_r^*(\tau^+)+g_r\alpha_r(\tau)][\gamma^*(\tau^+)\beta(\tau)+\beta^*(\tau^+)\gamma(\tau)]d\tau\Big\}\mathscr{D}^2\{\alpha\}\mathscr{D}^2\{\beta\}\mathscr{D}^2\{\gamma\}, \tag{3.3}$$

where α denotes the vector with components α_r, and $\mathscr{D}^2\{\alpha\}$ stands for $\Pi_{r=1}^M\mathscr{D}^2\{\alpha_r\}$.

The path integrations in (3.3) are facilitated by the introduction of a complex auxiliary field $f(\tau)$, which decouples the Bose field variables α_r from the variables β and γ associated with the spin. The following functional integral identity over the field f forms the basis for decoupling:

$$\exp\Big[-i\sum_{r=1}^M\int_0^t(g_r^*\alpha_r^*(\tau^+)+g_r\alpha_r(\tau))(\gamma^*(\tau^+)\beta(\tau)+\beta^*(\tau^+)\gamma(\tau))d\tau\Big]$$
$$=\int\exp\Big[-i\sum_{r=1}^M\int_0^t f^*(\tau)(g_r^*\alpha_r^*(\tau^+)+g_r\alpha_r(\tau))d\tau\Big]\exp\Big[\int_0^t f(\tau)(\gamma^*(\tau^+)\beta(\tau)+\beta^*(\tau^+)\gamma(\tau))d\tau\Big]\mathscr{D}^2\{f\}, \tag{3.4}$$

where we have introduced the functional differential[15]

$$\mathscr{D}^2\{f\}=\exp\Big(-\int_0^t|f(\tau)|^2d\tau\Big)\prod_{0<\tau<t}\Big(\frac{d\tau}{\pi}\Big)d^2f(\tau). \tag{3.5}$$

Utilizing (3.5) the propagator (3.3) decomposes as

$$\mathscr{U}_1(\alpha^*,\beta^*,\gamma^*,t\,|\alpha',\beta',\gamma',0)$$
$$=\int G_1(\alpha^*,t\,|\alpha',0;[f^*])$$
$$\times K_1(\beta^*,\gamma^*,t\,|\beta',\gamma',0;[f])\mathscr{D}^2\{f\} \tag{3.6}$$

where G_1 and K_1 in (3.6) are the propagators associated with the Hamiltonians $\mathscr{H}_{G_1}$ and $\mathscr{H}_{K_1}$ given by

$$\mathscr{H}_{G_1}=\hbar\sum_{r=1}^M\Big[\Omega_r\,\alpha_r^*\frac{\partial}{\partial\alpha_r^*}+f^*(t)(g_r^*\alpha_r^*+g_r\alpha_r)\Big], \tag{3.7a}$$

$$\mathscr{H}_{K_1}=\tfrac{1}{2}\hbar\omega\Big(\gamma^*\frac{\partial}{\partial\gamma^*}-\beta^*\frac{\partial}{\partial\beta^*}\Big)+if(t)\Big(\gamma^*\frac{\partial}{\partial\beta^*}+\beta^*\frac{\partial}{\partial\gamma^*}\Big). \tag{3.7b}$$

The propagators G_1 and K_1 are functionals of f^* and f respectively; thus the notation employed in (3.6).

They obey the Schrödinger equations

$$i\hbar\frac{\partial}{\partial t}G_1=\mathscr{H}_{G_1}G_1,\quad i\hbar\frac{\partial}{\partial t}K_1=\mathscr{H}_{K_1}K_1, \tag{3.8}$$

under the initial conditions

$$G_1|_{t=0}=\exp\Big(\sum_{r=1}^M\alpha_r^*\alpha_r'\Big),\quad K_1|_{t=0}=\exp(\beta^*\beta'+\gamma^*\gamma'). \tag{3.9}$$

The formula for the propagator G_1 has been obtained by

path integration (e.g., Hillery and Zubairy[14]) or can be obtained solving its equation of motion under the initial condition given in (3.9). We state here the result

$$G_1(\alpha^*,t\,|\alpha',0;[f^*]) = \exp\Bigg\{\sum_{r=1}^{M}\alpha_r^*\,\alpha_r' e^{-i\Omega_r t} - \sum_{r=1}^{M}\Bigg[i g_r^*\,\alpha_r^*\int_0^t e^{-i\Omega_r(t-\tau)}f^*(\tau)d\tau + i g_r\alpha_r^*\int_0^t e^{-i\Omega_r\tau}f^*(\tau)d\tau + |g_r|^2\int_0^t\int_0^\tau e^{-i\Omega_r(\tau-\tau')}f^*(\tau)f^*(\tau')d\tau\,d\tau'\Bigg]\Bigg\}. \quad (3.10)$$

Path integral techniques can also be applied for obtaining the propagator K_1, but here we find it more suitable to proceed differently. We show that K_1 has the form

$$K_1(\beta^*,\gamma^*,t\,|\beta',\gamma',0;[f]) = \exp(Q_{00}\beta^*\beta' + Q_{01}\beta^*\gamma' + Q_{10}\gamma^*\beta' + Q_{11}\gamma^*\gamma'), \quad (3.11)$$

where the elements Q_{ij} in (3.11) are functions of t through functional dependence on f.

Indeed, introducing expression (3.11) for K_1 into the second of Eqs. (3.8), this is seen to be the case, provided the matrix Q with elements Q_{ij} obeys the equation

$$\frac{d}{dt}Q = \left(i\frac{\omega}{2}\sigma_z + f(t)\sigma_x\right)Q. \quad (3.12)$$

In order that the initial condition in (3.9) for K_1 be satisfied (3.12) must be solved under the initial condition

$$Q_{ij}(0) = \delta_{ij} \quad (i,j = 0,1). \quad (3.13)$$

The equation of motion for the matrix Q when ω is different from zero can be solved in a series or an infinite product form. In this section we shall make use of the series solution. We start with

$$Q^{(0)}(t) = \exp\left(\sigma_x\int_0^t f(\tau)d\tau\right), \quad (3.14a)$$

as the zeroth-order approximation. The complete solution can be obtained by iteration in the form

$$Q = \sum_{n=0}^{\infty} Q^{(n)}, \quad (3.14b)$$

where the terms $Q^{(n)}$ of the series (3.14b) obey the recursive relation

$$\frac{d}{dt}Q^{(n)} = f(t)\sigma_x Q^{(n)} + i\frac{\omega}{2}\sigma_z Q^{(n-1)}, \quad (3.14c)$$

which, given that $Q^{(0)}$ incorporates the initial condition (3.13), has to be solved as a differential equation for $Q^{(n)}$ under the condition $Q^{(n)}(0) = 0$ for $n \geq 1$. In this way the condition $Q(0) = I$ for the required solution is secured. This is also true to any degree of approximation.

From (3.14c), for $n = 1$ we have

$$Q^{(1)}(t) = i\frac{\omega}{2}\exp\left(\sigma_x\int_0^t f(\tau)d\tau\right)\int_0^t d\tau_1 \times\exp\left(-\sigma_x\int_0^{\tau_1} f(\tau)d\tau\right)\sigma_z\exp\left(\sigma_x\int_0^t f(\tau)d\tau\right). \quad (3.15)$$

In order to bring σ_z forward, we notice that each time σ_z overtakes an exponential, the sign in front of σ_x in that exponential has to be reversed, since $\sigma_z\,\sigma_x = -\sigma_z\,\sigma_x$. Thus, $Q^{(1)}$ finally takes the form

$$Q^{(1)}(t) = i\frac{\omega}{2}\sigma_z\int_0^t d\tau_1\exp\left[\sigma_x\left(\int_0^{\tau_1} f(\tau)d\tau - \int_{\tau_1}^t f(\tau)d\tau\right)\right]. \quad (3.15')$$

Utilizing $Q^{(1)}$ from (3.15') we find from the recursive relation (3.14c) $Q^{(2)}$, and proceeding in this way we obtain for $Q^{(n)}$ the expression

$$Q^{(n)}(t) = \left(i\frac{\omega}{2}\sigma_z\right)^n\int_0^t d\tau_n\int_0^{\tau_n} d\tau_{n-1}\cdots\int_0^{\tau_2} d\tau_1 \times\exp\left[\sigma_x\left(\int_0^{\tau_1} - \int_{\tau_1}^{\tau_2} + \cdots + (-1)^n\int_{\tau_n}^t\right)f(\tau)d\tau\right]. \quad (3.16)$$

With (3.16) we have, through (3.14b), the propagator K_1 in (3.11) as a functional of f. Now, the propagator $\mathscr{U}_1$ of the fully bosonized Schrödinger equation (2.3) for a single-spin-Bose system can be written with the aid of (3.6) as

$$\mathscr{U}_1 = \sum_{l=0}^{\infty}\int G_1\frac{1}{l!}\left[(\beta^*,\gamma^*)Q\begin{pmatrix}\beta'\\ \gamma'\end{pmatrix}\right]^l\mathscr{D}^2\{f\}, \quad (3.17)$$

where in (3.17) we have expanded the exponential expression of the propagator K_1 given by (3.11).

The propagator $\mathscr{U}_1$ in (3.17) can be viewed as a series of functional averages taken against the functional differential measure (3.5). The l th average satisfies separately the Schrödinger equation (2.3). This is so, since the monomials in β^*, γ^*, β' and γ' of the form appearing in the l th term (each of degree l) consitute a closed system against the action of the operator $(i\hbar\partial/\partial t - \mathscr{H}_1)$, and as the whole series satisfies the Schrödinger equation (2.3), each term must also do so.

The $l = 0$ solution (3.17) corresponds to the radiation field alone. The $l = 1$ term is the one that gives the required propagator associated with the single-spin-Bose Hamiltonian (2.2) in accordance with the considerations laid in Sec. II. The higher-order terms ($l \geq 2$) relate to angular momentum Bose systems. Although the angular momentum involved is associated with a spin system with a definite number of spins (say N), this does not, as pointed out earlier, form a correct description of our N-spin-Bose system in which each spin interacts differently with the various radiation modes.

We now single out the $l = 1$ term giving the required spin-Bose propagator U_1 and proceed with the functional averaging. In doing so we shall make repeated use of the δ-functional identity, employed in (3.4), namely

$$\int P[f^*]\exp\left(\int_0^t r(\tau)f(\tau)d\tau\right)\mathscr{D}^2\{f\} = P[r] \quad (3.18)$$

where P is a functional of f exclusively dependent on f^*. This facility is now provided by the linear exponential arguments appearing in the various $Q^{(n)}$ [see (3.16)] composing the matrix Q in (3.17).

Utilizing the notation

$$\langle G,Q\rangle = \int G,Q\,\mathscr{D}^2\{f\}, \quad (3.19)$$

for the functional average of QG_1 involved in (3.17), we ob-

tain, by repeated application of the δ-functional identity (3.18), the amplitudes U_{ij} $(i,j=0,1,2,3)$ of the single-spin-Bose propagator in matrix arrangement as

$$\begin{bmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{bmatrix} = \langle G_1 Q \rangle = \exp\left(\sum_{r=1}^{M} \alpha_r^* \alpha_r' e^{-i\Omega_r t}\right) \times \sum_{n=0}^{\infty} \left(i\frac{\omega}{2}\right)^n \int_0^t d\tau_n \int_0^{\tau_n} d\tau_{n-1} \cdots \int_0^{\tau_2} d\tau_1 \times F^{(n)} \begin{bmatrix} \cosh \Phi^{(n)} & \sinh \Phi^{(n)} \\ (-1)^n \sinh \Phi^{(n)} & (-1)^n \cosh \Phi^{(n)} \end{bmatrix}, \tag{3.20}$$

where

$$F^{(n)} = \exp\left\{ -\sum_{r=1}^{M} \frac{|g_r|^2}{\Omega_r^2} \left[2n + 1 - i\Omega_r t + 2\sum_{k=1}^{n} (-1)^k e^{-i\Omega_r \tau_k} + (-1)^{n+1} e^{-i\Omega_r t}\left(1 + 2\sum_{k=1}^{n} (-1)^k e^{i\Omega_r \tau_k}\right) + 4\sum_{j=2}^{n}\sum_{k=1}^{j-1} (-1)^{j+k} e^{-i\Omega_r(\tau_j - \tau_k)} \right] \right\}, \tag{3.21a}$$

and

$$\Phi^{(n)} = \sum_{r=1}^{M} (\alpha_r^* e^{-i\Omega_r t} A_r^{(n)*} + \alpha_r' A_r^{(n)}), \tag{3.21b}$$

with

$$A_r^{(n)} = -\frac{g_r}{\Omega_r}\left[1 + 2\sum_{k=1}^{n} (-1)^K e^{-i\Omega_r \tau_k} + (-1)^{n+1} e^{-i\Omega_r t} \right]. \tag{3.21c}$$

Equation (3.20) together with Eqs. (3.21a)–(3.21c) complete the evaluation for the single-spin-Bose propagator.

In the literature one finds the traced form of the propagator (3.20), over both the discrete diagonal elements and the coherent variables, which gives the partition function, Z_1, of the single-spin-Bose system, obtained by replacing t by $-i\hbar/kT$. Upon taking the trace over the discrete elements of (3.20) only the even powers in ω will survive. Furthermore, the integrations over the end coherent variables with $\alpha_r' = \alpha_r$ against the measure $\Pi_{r=1}^{M} D^2\alpha_r$ [see (3.1a)] supply the Blume *et al.* result.[8] However, in the present treatment one has the full propagator, involving the off-diagonal discrete elements.

Next, we shall proceed with an explicit evaluation of the propagator with a simplified form of the single-spin-Bose Hamiltonian.

IV. AN EXPLICIT EVALUATION

We consider the spin-Bose Hamiltonian

$$H_1' = (\hbar\omega/2)\sigma_z + \hbar g(a^+ + a)\sigma_x, \tag{4.1}$$

for which we shall obtain the propagator.

Following the bosonization and decoupling procedure developed in Sec. III we find that the propagator K_1' is the propagator K_1 given by (3.11). Furthermore the propagator G_1' in this case can be obtained as a particular case of (3.10) in which there is only one coherent state variable α, one coupling constant, i.e., $g_1 = g_1^* = g$, and $\Omega_1 = 0$. Under these circumstances we have

$$G_1'(\alpha^*, t\,|\alpha', 0; [f^*]) = \exp\left[\alpha^*\alpha' - ig(\alpha^* + \alpha')\int_0^t f^*(\tau)d\tau - \frac{1}{2}g^2\left(\int_0^t f^*(\tau)d\tau\right)^2\right]. \tag{4.2}$$

In order, now, to proceed with the present evaluation we require the matrix Q, which obeys the equation of motion (3.12) and the initial condition (3.13). This matrix was obtained in Sec. III in the form of a series given by (3.14b). However, for the purpose needed here it will prove more convenient if we obtain Q in a product from, the way we express the evolution operator to develop functional integration from first principles (e.g., Ref 16).

Thus, the solution of (3.12) satisfying (3.13) takes the form

$$Q(t) = \mathcal{T}\exp\left[-i\int_0^t \left(\frac{\omega}{2}\sigma_z + if(\tau)\sigma_z\right)d\tau\right] = \lim_{N\to\infty} \mathcal{T}\prod_{j=0}^{N-1}\left[1 - i\Delta\tau\left(\frac{\omega}{2}\sigma_z + if(\tau_j)\sigma_x\right)\right], \tag{4.3}$$

where $\mathcal{T}$ signifies time ordering, $\Delta\tau = t/N$, and $\tau_j = j\Delta\tau$.

To facilitate application of formula (3.12) for obtaining the propagator U_1' we rewrite (4.2) in the form

$$G_1' = \int \exp\left[-\frac{1}{2}(\alpha^{*2} + \alpha'^2) + \lambda(\alpha^* + \alpha') - i\lambda g\int_0^t f^*(\tau)d\tau - \frac{1}{2}\lambda^2\right]\frac{d\lambda}{\sqrt{2\pi}}. \tag{4.4}$$

Introducing (4.4), in place of G_1, into (3.19) and utilizing the form (4.3) for Q, we can easily apply the δ-functional identity (3.18) and get

$$\langle QG_1' \rangle = \int \exp\left[-i\left(\frac{\omega}{2}\sigma_z + g\lambda\sigma_1\right)t\right] \times \exp\left[-\frac{1}{2}(\alpha^{*2}\alpha'^2) + \lambda(\alpha^* + \alpha') - \frac{1}{2}\lambda^2\right] \times \frac{d\lambda}{\sqrt{2\pi}}. \tag{4.5}$$

Expanding the exponential in (4.5) involving the matrices σ_z and σ_x in power series, and taking into account that $((\omega/2)\sigma_z + g\lambda\sigma_x)^2 = (\omega^2/4 + g^2\lambda^2)I$ (I being the 2×2 unit matrix), we find, after regrouping the series terms, the following expression for the propagator associated with the Hamiltonian (4.1):

$$\begin{bmatrix} U_{00}' & U_{01}' \\ U_{10}' & U_{11}' \end{bmatrix} = \int\left\{ I\cos\left[\left(\frac{\omega^2}{4} + g^2\lambda^2\right)^{1/2} t\right] - i\left(\frac{\omega}{2}\sigma_z + g\lambda\sigma_x\right)\frac{\sin\left[(\omega^2/4 + g^2\lambda^2)^{1/2}t\right]}{(\omega^2/4 + g^2\lambda^2)^{1/2}} \times \exp\left[-\frac{1}{2}(\alpha^{*2} + \alpha'^2) + \lambda(\alpha^* + \alpha') - \frac{1}{2}\lambda^2\right]\frac{d\lambda}{\sqrt{2\pi}}. \tag{4.6}$$

The propagator (4.6) is given essentially in eigenfunction expansion form. The eigenvalues are given by $\pm(\omega^2/4+g^2\lambda^2)^{1/2}$ and the eigenfunctions are proportional to $\exp(-\frac{1}{2}\alpha^{*2}+\lambda\alpha^{*}-\frac{1}{4}\lambda^2)$, λ being a continuous quantum number.

Unfortunately, the ease with which we have been able to handle this problem ceases to exist, once the term $\Omega a^{+}a$ is present in the Hamiltonian. The solution with $\omega=0$ and $\Omega\neq 0$ can also be obtained in a closed form and is given by the zeroth term of the general case expansion (3.20).

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An algebraic approach to the exponential cosine screened Coulomb potential

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An analytical formula is obtained for the energy eigenvalues of the exponential cosine screened Coulomb potential by a method that is a combination of algebraic perturbation theory based on the Lie algebra of the SO(2,1) group and the scaling variational method. The results are found to be in excellent agreement with Padé approximation calculations.

I. INTRODUCTION

Recently a great deal of interest has been shown in algebraic perturbation theory based on the Lie algebra of some dynamical group.[1] Gerry and Togeas[2] have successfully applied this algebraic method in a number of eigenvalue problems.

In this paper we wish to apply this method to a model potential, namely exponential cosine screened Coulomb (ECSC):

$$V(r) = -(1/r)e^{-\lambda r}\cos\lambda r. \tag{1}$$

This potential is useful in describing the interaction between an electron and an ionized impurity in both metals and semiconductors.[3] Also, it can be used to describe the electron–positron interaction in a positronium atom in a solid.[4]

So far, numerous attempts both perturbative and nonperturbative have been undertaken to calculate the energies of the ECSC potential.[5–7] The Padé approximation[7] gives accurate results but it is an iterative procedure and the perturbation method[5] fails to give satisfactory agreement for large λ.

So it would be preferable to have at one's disposal an analytical formula that will give the energy eigenvalues for all the states with fairly good accuracy.

In this paper we have obtained such a formula by a simple and straightforward method, which is based on the Lie algebra of the SO(2,1) group supplemented by a variational scaling of the parameter involved.

II. DESCRIPTION OF THE METHOD

The SO(2,1) Lie algebra consists of the three generators T_3, $T_\pm = T_+ \pm iT_2$ with the commutation relations

$$[T_3, T_+] = T_+, \quad [T_3, T_-] = -T_-, \quad [T_-, T_+] = 2T_3 \tag{2}$$

and the Casimir invariant

$$Q = T_3^2 - \tfrac{1}{2}(T_+T_- + T_-T_+). \tag{3}$$

The relevant unitary irreducible representation employed here is the so-called positive discrete series D_+ such that the generator T_3 is diagonal as

$$T_3|n, l\rangle = n|n, l\rangle \tag{4}$$

and

$$Q|n, l\rangle = l(l+1)|n, l\rangle, \tag{5}$$

where n is the principal quantum number and l is the orbital angular momentum. Here, the range of n is

$$l+1, l+2,\ldots \quad \text{or} \quad n = l+1+S, \quad S = 0,1,2. \tag{6}$$

The states $|\psi\rangle = |n, l\rangle$ are called the group states. These states satisfy the orthogonality relation

$$\langle n', l'|n, l\rangle = \delta_{n'n}\delta_{l'l} \tag{7}$$

and the completeness relation [in the SO(2,1) subspace]

$$\sum_{n=l+1}^{\infty} |n, l\rangle\langle n, l| = 1. \tag{8}$$

The most useful, for our purposes, representation of T_3, T_1, T_2 is the configuration space representation[1]

$$\begin{aligned} T_1 &= -\tfrac{1}{2}(r\Delta + r), \\ T_2 &= -i\left(1 + r\frac{\partial}{\partial r}\right), \\ T_3 &= -\tfrac{1}{2}(r\Delta - r), \end{aligned} \tag{9}$$

where

$$\Delta = \frac{\partial}{\partial x_j}\frac{\partial}{\partial x_j}, \quad r = (x_j x_j)^{1/2}. \tag{10}$$

These generators act in the Hilbert space of functions and are self-adjoint not with respect to the usual scalar product of quantum mechanics $\int \psi_1^* \psi_2 \, d^3x$ but with respect to the new scalar product

$$\langle \psi_1|\psi_2\rangle = \int \psi_1^* \psi_2 \frac{1}{r} d^3x, \tag{11}$$

where $|\psi_1\rangle$ and $|\psi_2\rangle$ are the group states. This is not the physical scalar product, although this can be expressed in terms of the invariant group theoretic product.[8]

The ECSC potential can be expanded in power series of the screening parameter λ as

$$V(r) = -\frac{1}{r}\sum_{k=0}^{\infty} V_k(\lambda r)^k, \tag{12}$$

where the potential coefficients V_k are given by

$$V_1 = -1, \quad V_2 = 0, \quad V_3 = \tfrac{1}{3}, \quad V_4 = -\tfrac{1}{6}, \quad V_5 = \tfrac{1}{30}. \tag{13}$$

Here we use atomic units so that the distances are measured in $a_0 = Kh^2/m^*e^2$ and energies in m^*e^4/Kh^2, where m^* is the effective mass and K is the dielectric constant.

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The Hamiltonian equation with potential (1) reads

$$[-\tfrac{1}{2}\Delta-(1/r)e^{-\lambda r}\cos\lambda r-E\,]|\tilde{\psi}\rangle=0, \tag{14}$$

where $|\tilde{\psi}\rangle$ denotes the physical state. These physical states $|\tilde{\psi}\rangle$ are normalized and are orthogonal with respect to a different metric. In coordinate space this amount to the usual scalar product

$$\langle\tilde{\psi}_1|r|\tilde{\psi}_2\rangle=\int\tilde{\psi}_1^*\tilde{\psi}_2\,d^3x. \tag{15}$$

Now in order to relate the Lie algebra (9) to the Hamiltonian equation (14) we multiply the latter equation by r and consider a new equation

$$\tilde{\Omega}(E)|\tilde{\psi}\rangle=r(H-E)|\tilde{\psi}\rangle=0,$$

or

$$(-\tfrac{1}{2}r\Delta-e^{-\lambda r}\cos\lambda r-rE)|\tilde{\psi}\rangle=0. \tag{16}$$

Using Eqs. (12) and (13) in Eq. (16) and retaining terms only up to the order of λ^5, we get

$$\{-r\Delta-2+2\lambda r-2Er-\tfrac{2}{3}\lambda^3r^3+\tfrac{1}{3}\lambda^4r^4-\tfrac{1}{15}\lambda^5r^5\}|\tilde{\psi}\rangle=0. \tag{17}$$

We now insert (9) in Eq. (17) and obtain

$$\left\{T_3+\frac{T_+}{2}+\frac{T_-}{2}-2+(2\lambda-2E)\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)-\frac{2}{3}\lambda^3\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)^3+\frac{1}{3}\lambda^4\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)^4-\frac{1}{15}\lambda^5\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)^5\right\}|\tilde{\psi}\rangle=0. \tag{18}$$

Now we perform the usual tilting transformation,[9] which is implemented as

$$e^{-i\theta T_2}\tilde{\Omega}(E)e^{i\theta T_2}e^{-i\theta T_2}|\tilde{\psi}\rangle=0, \tag{19}$$

so that

$$|\psi\rangle=e^{-i\theta T_2}|\tilde{\psi}\rangle \tag{20}$$

is the relation between the group state and the physical state. This is a unitary transformation similar to the Foldy–Wouthuysen transformation but infinite dimensional. Here θ is allowed to depend on n and l so that the physical state $|\tilde{\psi}\rangle$ is also dependent on n, l, and θ. Hence to obtain higher-order correction terms an algebric form of perturbation theory has to be used. This will be discussed later on.

It follows from the commutation relations that

$$\begin{aligned}e^{-iT_2\theta}T_3e^{iT_2\theta}&=T_3\cosh\theta+(T_+/2+T_-/2)\sinh\theta,\\ e^{-iT_2\theta}T_+e^{iT_2\theta}&=T_+\cosh\theta+T_3\sinh\theta,\\ e^{-iT_2\theta}T_-e^{iT_2\theta}&=T_-\cosh\theta+T_3\sinh\theta.\end{aligned} \tag{21}$$

Table I. Energy eigenvalues for the $1s$ state in atomic units.

	E (present)	E (Padé)	E (Perturbation)	E (Variational)
0.06	−0.440 200	−0.440 201	−0.440 201	−0.440 201
0.08	−0.420 463	−0.420 464	−0.420 464	−0.420 464
0.10	−0.400 883	−0.400 885	−0.400 883	−0.400 885
0.20	−0.306 268	−0.306 335	−0.306 235	−0.306 334
0.30	−0.218 939	−0.219 416	−0.218 619	−0.219 411
0.40	−0.140 662	−0.142 439	−0.139 153	−0.142 418
0.50	−0.073 523	−0.077 679	−0.068 047	−0.077 606

Table II. Energy eigenvalues for the $2S$ and $2p$ states in atomic units.

		E (Present)	E (Padé)	E (perturbation)	E (Variational)
0.02	$2S$	−0.105 104	−0.105 104	−0.105 104	−0.105 104
	$2p$	−0.105 075	−0.105 075	−0.105 075	
0.04	$2S$	−0.085 769	−0.085 769	−0.085 767	−0.085 769
	$2p$	−0.085 580	−0.085 591		
0.06	$2S$	−0.067 419	−0.067 421	−0.067 385	−0.067 421
	$2p$	−0.066 767	−0.066 778		
0.08	$2S$	−0.050 382	−0.050 387	−0.050 222	−0.050 384
	$2p$	−0.048 953	−0.048 997		
0.10	$2S$	−0.034 951	−0.034 941	−0.034 425	−0.034 935
	$2p$	−0.032 330	−0.032 469	−0.032 042	

Using relations (21) in Eq. (18), we get

$$\begin{aligned}\Big\{&T_3e^{\theta}+\frac{T_+}{2}e^{\theta}+\frac{T_-}{2}e^{\theta}-2\\&+(2\lambda-2E)e^{-\theta}\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)\\&-\frac{2}{3}\lambda^3e^{-3\theta}\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)^3\\&+\frac{1}{3}\lambda^4\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)^4e^{-4\theta}\\&-\frac{1}{15}\lambda^5e^{-5\theta}\left(T_3-\frac{T_+}{2}-\frac{T_-}{2}\right)^5\Big\}|\tilde{\psi}\rangle=0.\end{aligned} \tag{22}$$

Now we use the group states $|n,l\rangle$ and write[10]

$$\langle n,l\,|\Omega(E,\theta)|n,l\rangle=0, \tag{23}$$

where $\Omega(E,\theta)=e^{-i\theta T_2}\tilde{\Omega}(E)e^{i\theta T_2}$ and $\Omega(E,\theta)$ is given by the bracketed portion of Eq. (22).

Expanding the last three terms of Eq. (22) and making use of the commutation relations (2), we get from (23) after some straightforward algebra

$$\begin{aligned}E^{(0)}_{n,l}(\theta)=&\frac{e^{2\theta}}{2}-\frac{e^{\theta}}{x}+\lambda-\frac{1}{6}\lambda^3e^{-2\theta}(5x^2-3y+1)\\&+\tfrac{1}{48}\lambda^4e^{-3\theta}(35x^4+25x^2-30x^2y+3y^2-6y)\\&-\tfrac{1}{240}\lambda^5e^{-4\theta}(63x^4+87x^2\\&+6-70x^2y-38y+15y^2),\end{aligned} \tag{24}$$

Table III. Energy eigenvalues for the $3S$, $3p$, and $3d$ states in atomic units.

		E (present)	E (Padé)	E (Perturbation)	E (Variational)
0.02	$3S$	−0.036 025	−0.036 025	−0.036 022	−0.036 025
	$3p$	−0.035 968	−0.035 968	−0.035 965	
	$3d$	−0.035 850	−0.035 851	−0.035 849	
0.04	$3S$	−0.018 847	−0.018 823	−0.018 707	−0.018 822
	$3p$	−0.018 457	−0.018 453		
	$3d$	−0.017 663	−0.017 682		
0.05	$3S$	−0.011 677	−0.011 576		
	$3p$	−0.010 954	−0.010 929	−0.010 538	
	$3d$	−0.009 493	−0.009 555	−0.009 292	
0.06	$3S$	−0.005 875	−0.005 462	−0.004 538	−0.005 454
	$3p$	−0.004 606	−0.004 472		
	$3d$	−0.002 140	−0.002 309		

Table IV. Energy eigenvalues for the $4S$, $4p$, $4d$, and $4f$ states.

		E (present)	E (Padé)	E (Perturbation)	E (variational)
0.01	$4S$	−0.021 438	−0.021 438	−0.021 436	−0.021 437
	$4p$	−0.021 424	−0.021 424	−0.021 424	
	$4d$	−0.021 398	−0.021 398	−0.021 397	
	$4f$	−0.021 358	−0.021 358	−0.021 357	
0.02	$4S$	−0.012 581	−0.012 572	−0.012 539	−0.012 572
	$4p$	−0.012 492	−0.012 486	−0.012 454	
	$4d$	−0.012 310	−0.012 310	−0.012 283	
	$4f$	−0.012 034	−0.012 038	−0.012 019	
0.03	$4S$	−0.005 382	−0.005 270		
	$4p$	−0.005 105	−0.005 033		
	$4d$	−0.004 550	−0.004 539		
	$4f$	−0.003 715	−0.003 748		

where

$$x = l + 1 + s,$$
$$y = l(l+1). \tag{25}$$

Setting

$$\frac{dE^{(0)}_{n,l}(\theta)}{d\theta} = 0, \tag{26}$$

we obtain

$$e^{6\theta} - \frac{e^{5\theta}}{x} + e^{2\theta}\frac{\lambda^3}{3}(5x^2 - 3y + 1) - \frac{1}{16x}e^{\theta}\lambda^4 \times (35x^4 + 25x^2 - 30x^2y + 3y^2 - 6y) + (\lambda^5/60)(63x^4 + 87x^2 + 6 - 70x^2y - 38y + 15y^2) = 0. \tag{27}$$

This method of treating θ as a variational parameter is just the scaling variational method since T_2 is essentially a generator of scale transformations. This has got the added advantage that the lowest approximation satisfies both the virial theorem and the Hellmann–Feynmann theorem.[11]

Equations (24) and (27) together give $E^{(0)}_{n,l}$ for various values of λ. In Tables I–IV we list the energy eigenvalues $E^{(0)}_{n,l}$ (without second-order correction) of various states for values of λ not greater than 0.5.

Higher-order correction terms can be obtained by treating the nondiagonal terms in Eq. (22) as perturbation terms and using an algebraic form of the perturbation theory first formulated by Barut and Nagel[12] and later modified by Gerry and Inomata.[13] In this perturbation scheme, one treats the nondiagonal terms as small-order terms and for a particular n value fix the θ value ($\theta = \theta_n$). It is then possible to have a closed form normalization for the perturbed states.

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Eigenvalue problem for Schrödinger's equation with repulsive potential

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Schrödinger's operator $-(\hbar^2/2m)\{d^2/dr^2+(2/r)d/dr\}+V(r)$ is studied, and what happens when $V(r)$ approaches $-\infty$ rapidly as $r\to\infty$ is shown. The cases in which $V(r)\sim -\beta r^{\delta}$ ($\beta>0$, $\delta>2$) as $r\to\infty$ are covered. If $V(r)$ approaches $-\infty$ rapidly, then the above operator is not self-adjoint and in order to get a self-adjoint operator a boundary condition must be imposed. For such a self-adjoint operator there are states that belong to the discrete energy spectrum. To obtain the discrete energy spectrum, a quantization rule that corresponds to the quantization rule of Bohr and Sommerfeld in old quantum mechanics is considered.

I. INTRODUCTION

In the literature on quantum mechanics we usually find the description that if an electron has, in classical meaning, a kinetic energy sufficient to leave an atomic system to go to infinity, then the value of the corresponding total energy belongs to the continuous spectrum of the system under consideration. It was pointed out by von Neumann and Wigner,[1] who gave two examples, that the description mentioned above is not always correct. One of their examples is as follows.

They treated the case of a particle with mass m in a centrally symmetric potential $V(r)$, and considered Schrödinger's equation

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\psi+(V(r)-E)\psi=0\,, \tag{1}$$

where E is an eigenvalue, ψ an eigenfunction, and r the distance from the origin. By direct calculation, they showed that if

$$V(r)=(\hbar^2/2m)[(\beta^2-1)/4r^2-\beta^2 r^{2\beta-2}]\quad(\beta>2)\,,$$

then the function $\psi(r)=r^{-(\beta+1)/2}\sin(r^{\beta})$ is an eigenfunction of Eq. (1) corresponding to the eigenvalue $E=0$ and, moreover, the integral $\int_0^{\infty}|\psi(r)|^2r^2\,dr$ is finite. In other words, $E=0$ is one energy level of the discrete spectrum. Furthermore, this example is also evidence against the superstition mentioned above. In fact, since the potential $V(r)$ decreases monotonically to $V(\infty)=-\infty$, all particles would go to infinity; therefore all values of energy should belong to the continuous spectrum. However, as we have already pointed out, there extists at least one energy level of the discrete spectrum.

They explained this strange phenomenon as follows: The velocity, in the meaning of classical mechanics, of a particle with total energy E is, by the principle of conservation of energy, $dr/dt=\pm\sqrt{(2/m)(E-V(r))}$. Therefore the time taken in moving from $r=R$ to $r=+\infty$ is

$$\int_R^{\infty}dr\left(\frac{dr}{dt}\right)^{-1}=m\int_R^{\infty}\frac{dr}{\sqrt{2m(E-V(r))}}\,, \tag{2}$$

where $V(R)=E$. Since $V(r)\sim r^{2\beta-2}$ ($\beta>2$) at infinity, this time is finite; hence this particle would execute a periodic motion between the points $r=R$ and $r=+\infty$, and thus a bound state is produced.

In their argument we are interested in the fact that the wave function $\psi(r)=r^{-(\beta+1)/2}\sin(r^{\beta})$ satisfies the condition

$$\int_0^{\infty}|\psi|^2r^2\,dr<\infty\,,$$

if and only if the time (2) is finite. This condition is fulfilled when $\beta>2$, otherwise it is not.

Putting $f=r\psi$, we find that Eq. (1) is equivalent to the equation $-(\hbar^2/2m)d^2f/dr^2+(V(r)-E)f=0$.

II. FORMULATION AND NOTATION

In this article we shall examine the differential operator $-(\hbar^2/2m)(d^2/dr^2)+V(r)$ ($a<r<\infty$), where the potential $V(r)$ satisfies the assumptions (a1) $V(r)$ decreases monotonically to $-\infty$, $\int_c^{\infty}|V(r)|^{-1/2}\,dr<\infty$ for a sufficiently large c; and (a2) $V'(r)/V(r)$ and $V''(r)/V(r)$ are bounded over a neighborhood of $r=+\infty$, where the prime denotes differentiation with respect to r. Assumption (a1) is essential in our argument in this article, but (a2) is not because it is automatically fulfilled in most examples in our mind.

For fixed α,β ($-\infty\leqslant\alpha<\beta\leqslant+\infty$), let $L^2(\alpha,\beta)$ be the set of all functions f such that (a) $f(r)$ is Lebesgue measurable over the interval (α,β); and (b) $\int_{\alpha}^{\beta}|f(r)|^2\,dr<+\infty$. Let $\mathfrak{D}^*$ be the set of all functions f in $L^2(a,\infty)$ such that (a) $f(r)$, $f'(r)$ are absolutely continuous on the interval (a,∞), and (b) $-(\hbar^2/2m)f''+Vf$ is in $L^2(a,\infty)$; and let T be the operator with domain $\mathfrak{D}^*$ which takes f into $-(\hbar^2/2m)f''+Vf$.

If f and g are functions in $\mathfrak{D}^*$, then we have

$$\int_b^c(Tf\times\bar{g}-f\times\overline{Tg})dr=-\frac{\hbar^2}{2m}[f'\bar{g}-f\bar{g}']_b^c\,,$$

where $a<b<c<\infty$. Hence the existence of the limits

$$\lim_{r\to a}(f(r)\bar{g}'(r)-f'(r)\bar{g}(r))\,,$$

$$\lim_{r\to\infty}(f(r)\bar{g}'(r)-f'(r)\bar{g}(r))$$

is established by the convergence of the integral of

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$Tf\times\bar{g}-f\times\overline{Tg}$ over the interval (a,∞) (where $\bar{g}$ is the complex conjugate of g).

Let $\mathfrak{D}$ be the set of all functions f in $\mathfrak{D}^*$ such that $\int_a^\infty (Tf\times\bar{g}-f\times\overline{Tg})dr=0$ for every function g in $\mathfrak{D}^*$; and let H be the operator with domain $\mathfrak{D}$ that takes f into Tf. Then we can prove the following lemma (for the proof, see Ref. 2, Theorems 10.11 and 10.12).

Lemma 1: H is a closed linear symmetric operator with the adjoint $H^\dagger = T$ and the deficiency index (m, m), where $m=0$, 1, or 2. In order that the operator T be self-adjoint, it is necessary and sufficient that m has the value 0.

In the next section, we will show that the operator T is not self-adjoint, and that we can obtain the various self-adjoint operators by restricting the domain $\mathfrak{D}^*$ of T. In Sec. IV we will obtain a rule that gives the approximate distribution of eigenvalues of the self-adjoint operators described in Sec. III. The rule corresponds to the quantization rule of Bohr and Sommerfeld in old quantum mechanics.

III. BOUNDARY CONDITIONS

In this section we shall find that T is not self-adjoint. In order to get a self-adjoint operator from T we must restrict the domain $\mathfrak{D}^*$ of T by imposing a boundary condition.

Let f be a solution of $Tf=\lambda f$, where λ is a complex number. We should begin by describing the asymptotic form of the function f in the neighborhood of $r=+\infty$. Let c be chosen so large that

$$V(r)<0, \quad \text{for all } r>c.$$

Set $x(r)=\int_c^r |V(r)|^{1/2}\,dr$, $\rho(r)=|V(r)|^{-1/4}$. Write the solution f as $f(r)=\rho(r)g(x(r))$. Then we have

$$g''(x)+(2m/\hbar^2)g(x)+q(x)g(x)=0, \tag{3}$$

where

$$q(x(r))=|V(r)|^{-1}\left[\frac{5}{16}\left\{\frac{V'(r)}{V(r)}\right\}^2-\frac{1}{4}\frac{V''(r)}{V(r)}+\frac{2m}{\hbar^2}\lambda\right].$$

By the assumptions (a1) and (a2) we have

$$\int_0^\infty |q(x)|dx\leqslant \text{const}\int_c^\infty |V(r)|^{-1/2}\,dr<\infty,$$

where

$$\text{const}=\sup_{r>c}\left[\frac{5}{16}\left\{\frac{V'(r)}{V(r)}\right\}^2-\frac{1}{4}\frac{V''(r)}{V(r)}+\frac{2m}{\hbar^2}\lambda\right].$$

Therefore Eq. (3) has two solutions that, in the neighborhood of $r=+\infty$, have the forms

$$e^{ix\sqrt{2m}/\hbar}+o(1) \quad \text{and} \quad e^{-ix\sqrt{2m}/\hbar}+o(1)$$

(see Ref. 3, p. 1408). Thus f is a linear combination of

$$|V(r)|^{-1/4}(e^{ix(r)\sqrt{2m}/\hbar}+o(1))$$

and

$$|V(r)|^{-1/4}(e^{-ix(r)\sqrt{2m}/\hbar}+o(1)),$$

so that, by the assumption (a1), we have

$$\int_c^\infty |f(r)|^2\,dr<\infty. \tag{4}$$

We now proceed to discuss the self-adjointness of the operator T. Let n_a be the number of linearly independent solutions in $L^2(a, c)$ of the differential equation $Tf=\lambda f$, where $a<c<\infty$, and let n_∞ be the number of linearly independent solutions in $L^2(c,\infty)$ of the differential equation $Tf=\lambda f$. We first observe that the numbers n_a and n_∞ are obviously independent of c and that they are also independent of λ, when λ is not real (see Ref. 2, Theorems 10.11–10.14). Moreover the number n_a must have the value 1 or 2, when λ is not real (see Ref. 2, Theorem 10.15). On the other hand, in view of (4), we have $n_\infty=2$ for all complex numbers λ. Therefore if $n_a=1$ for all λ that are not real then H has the deficiency index (1,1); if $n_a=2$ for all λ then H has the deficiency index (2, 2) (see Ref. 2, Theorems 10.20 and 10.19). In either case T is not self-adjoint by Lemma 1. Hence in order to get a self-adjoint operator from T we have to restrict the domain $\mathfrak{D}^*$ of T by imposing a boundary condition. We distinguish two cases according to whether $n_a=1$ or 2.

(i) Case $n_a=1$: We can select a function u satisfying the relations $Tu=iu$ and $\int_a^\infty |u|^2\,dr=1$. We set $v_\theta=(e^{i\theta}u-e^{-i\theta}\bar{u})/2i$, where $0\leqslant\theta<\pi$. If $\mathfrak{D}(\theta)$ is the set of all functions in $\mathfrak{D}^*$ such that

$$\lim_{r\to\infty}(f(r)v_\theta'(r)-f'(r)v_\theta(r))=0,$$

and if $H(\theta)$ is the transformation with domain $\mathfrak{D}(\theta)$, which takes f into Tf, then $H(\theta)$ is a self-adjoint extension of H; and if S is an arbitrary maximal symmetric extension of H, then S coincides with $H(\theta)$ for exactly one θ (see Ref. 2, Theorem 10.13).

(ii) Case $n_a=2$: We can introduce eigenfunctions u_1 and u_2 of T such that

$$Tu_j=iu_j \quad (j=1,2) \quad \text{and} \quad \int_a^\infty u_j\bar{u}_k\,dr=\delta_{jk}.$$

We set

$$v_{j\alpha}=u_j-\sum_{k=1}^{2}a_{jk}\bar{u}_k, \quad j=1,2,$$

where $\alpha=\{a_{jk}\}$ is a unitary matrix. If $\mathfrak{D}(\alpha)$ is the set of all functions f in $\mathfrak{D}^*$ such that

$$[f\bar{v}_{j\alpha}'-f'\bar{v}_{j\alpha}]_a^\infty=0 \quad (j=1,2),$$

and if $H(\alpha)$ is the transformation with domain $\mathfrak{D}(\alpha)$, which takes f into Tf, then $H(\alpha)$ is a self-adjoint extension of H; and if S is an arbitrary maximal symmetric extension of H, there exists a unique matrix α such that $S=H(\alpha)$ (see Ref. 2, Theorem 10.14).

IV. QUANTIZATION RULE

In Sec. III we introduced self-adjoint operators $H(\theta)$ and $H(\alpha)$. We wish to know exact eigenvalues of them. However, apart from certain privileged cases, it is a very difficult mathematical problem. In this section we shall find a rule that will give the approximate distribution of these eigenvalues.

Let us now review the WKB method. We make in Schrödinger's equation

$$\frac{\hbar^2}{2m}\frac{d^2f}{dr^2}+(E-V)f=0 \quad (E \text{ a real number})$$

the substitution

$$f=e^{(i/\hbar)\sigma}. \tag{5}$$

Then we obtain the equation

$$\sigma'^2/2m - i\hbar\sigma''/2m = E - V. \tag{6}$$

We seek σ in the form of a series,

$$\sigma = \sigma_0 + (\hbar/i)\sigma_1 + (\hbar/i)^2\sigma_2 + \cdots,$$

expanded in powers of $\hbar$. Substituting this expression for σ into (6), and neglecting in Schrödinger's equation terms of order equal to or greater than $\hbar^2$, we obtain

$$\sigma_0 = \pm\int p\,dr, \quad \sigma_1 = -\frac{1}{2}\log|p|,$$

where $p = \sqrt{2m(E-V)}$. Substituting this expression into (5), we find the solution f in the form

$$f = C_1|p|^{-1/2}\exp\left(\frac{i}{\hbar}\int p\,dr\right) + C_2|p|^{-1/2}\exp\left(-\frac{i}{\hbar}\int p\,dr\right). \tag{7}$$

The approximation made in (7) is legitimate only if

$$|m\hbar V'|/|2m(E-V)|^{3/2} \ll 1 \tag{8}$$

(see Ref. 4, Chap. VI).

In most of the examples that we treat in this article the condition (8) is fulfilled everywhere except in the vicinity of the point for which

$$E = V(r).$$

This is the turning point of the classical motion, the point where the velocity of the particle vanishes and changes sign.

Let $r = R$ be the turning point, so that $V(R) = E$. By the assumption that $V(r)$ is a decreasing function $V(r) > E$ for all $r < R$, so that the region to the left of the turning point is classically inaccessible. The general solution is a linear combination of two solutions $f_1(r,E)$ and $f_2(r,E)$ whose asymptotic forms are

$r \ll R$,

$$f_1 \sim \frac{1}{2\sqrt{|p|}}\exp\left(-\frac{1}{\hbar}\int_r^R |p|dr\right),$$

$$f_2 \sim \frac{1}{2\sqrt{|p|}}\exp\left(\frac{1}{\hbar}\int_r^R |p|dr\right);$$

$r \gg R$,

$$f_1 \sim \frac{1}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_R^r p\,dr - \frac{\pi}{4}\right),$$

$$f_2 \sim \frac{1}{2\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_R^r p\,dr + \frac{\pi}{4}\right).$$

The conditions for the validity of these formulas are as follows (see Ref. 4, Chap. VI).

(*) At the turning point the kinetic energy $E - V$ tends to zero as $(r - R)$ and remains to a good approximation proportional to $(r - R)$ in a region extending over at least one wavelength on either side. Here we define the "number of wavelengths" contained in a given interval (α, β) by the integral

$$(1/2\pi\hbar)\int_\alpha^\beta |p|dr.$$

(**) This turning region joins, on either side of its turning point, an asymptotic region in which the condition (8) is fulfilled.

We now proceed to discuss the rule which gives the approximate distribution of eigenvalues of the self-adjoint operators $H(\theta)$ and $H(\alpha)$. We distinguish two cases according to whether $n_a = 1$ or 2.

(i) Case $n_a = 1$: We first prove the following lemma.

Lemma 2: (a) $\int_a^\infty |f_1(r,E)|^2\,dr < \infty$, so that f_1 is an element in $\mathfrak{D}^*$.

(b) Each of solutions f in $\mathfrak{D}^*$ of the equation $Tf = Ef$ has the form $f(r) = \text{const} \times f_1(r,E)$.

(c) For every E there exists a unique θ $(0 < \theta < \pi)$ such that $f_1(r,E)$ is in $\mathfrak{D}(\theta)$.

Proof: $V(r)$ is a decreasing function, therefore $|p|^{-1/2}$ is bounded in a neighborhood of $r = a$. We select R_1 such that $a < R_1 < R$; then we have

$$\int_r^R |p|dr = \int_{R_1}^R |p|dr + \int_r^{R_1} |p|dr > \int_{R_1}^R |p|dr + |p(R_1)|(R_1 - r),$$

and therefore $\exp[-(1/\hbar)\int_r^R |p|dr] < \text{const} \times e^{cr}$ $(c > 0)$ in a neighborhood of $r = a$. Thus $|f_1(r,E)| < \text{const} \times e^{cr}$, and therefore $f_1(r,E)$ is square integrable in a neighborhood of $r = a$. On the other hand, as we have already shown in Sec. III, all eigenfunctions of the operator T are square integrable in a neighborhood of $r = \infty$. Therefore we have proved (a). Since the operator H has the deficiency index (1, 1), we have, applying Theorem 10.19 in Ref. 2, that the dimension of the space of all solutions in $\mathfrak{D}^*$ of the differential equation $Tf = Ef$ is less than 2. Hence, by (a) described above, we observe that this dimension is equal to 1, and therefore we have (b). Let $u(r)$, $v_\theta(r)$, and $x(r)$ be the functions described in Sec. III. Then, by the result stated in Sec. III, we have

$$u(r) \sim |V(r)|^{-1/4}(Ae^{ix(r)\sqrt{2m}/\hbar} + Be^{-ix(r)\sqrt{2m}/\hbar}),$$

$$f_1(r,E) \sim |V(r)|^{-1/4}(Ce^{ix(r)\sqrt{2m}/\hbar} + \bar{C}e^{-ix(r)\sqrt{2m}/\hbar}) \quad (r \to \infty).$$

Hence

$$\lim_{r\to\infty}(f_1 v_\theta' - f_1' v_\theta) = (2\sqrt{2m}/\hbar)\mathrm{Re}[e^{i\theta}(A\bar{C} - BC)]$$

and therefore there exists a unique θ $(0 < \theta < \pi)$ such that $\lim_{r\to\infty}(f_1 v_\theta' - f_1' v_\theta) = 0$. With this result, the proof of the lemma is complete.

We see by Lemma 2 that an E is an eigenvalue of $H(\theta)$ if and only if $\lim_{r\to\infty}(f_1 v_\theta' - f_1' v_\theta) = 0$, and that for every E there exists a unique θ such that E is an eigenvalue of $H(\theta)$.

Now let E_0 be an eigenvalue of $H(\theta)$ for fixed θ. We shall obtain a formula which gives the other eigenvalues of $H(\theta)$. It follows that $\lim_{r\to\infty}(f_1(r,E)v_\theta'(r) - f_1'(r,E)v_\theta(r)) = 0$ if and only if $\lim_{r\to\infty}(f_1(r,E)f_1'(r,E_0) - f_1'(r,E)f_1(r,E_0)) = 0$, because the former condition means that $\lim_{r\to\infty} f_1(r,E)/v_\theta(r) = \text{const}$, and the latter means that $\lim_{r\to\infty} f_1(r,E)/f_1(r,E_0) = \text{const}$. In order to calculate the limiting value of

$$f_1(r,E)f_1'(r,E_0) - f_1'(r,E)f_1(r,E_0), \tag{9}$$

we use the asymptotic form

$$f_1 \sim \frac{1}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_R^r p\,dr - \frac{\pi}{4}\right).$$

Then, using the assumption (a2), we have

$$(9) \sim \frac{1}{\hbar}\sin\left[\frac{1}{\hbar}\left(\int_R^r p\,dr - \int_{R_0}^r p_0\,dr\right)\right] \quad (r\to\infty)$$

where $p=\sqrt{2m(E-V)}$, $p_0=\sqrt{2m(E_0-V)}$, $V(R)=E$, and $V(R_0)=E_0$. Moreover, introducing R_1 such that $R_1 > \mathrm{Max}(R,R_0)$ and using the assumption (a1), we have

$$\begin{aligned}
&\int_R^r p\,dr - \int_{R_0}^r p_0\,dr \\
&\quad = \int_R^{R_1} p\,dr - \int_{R_0}^{R_1} p_0\,dr + \int_{R_1}^r (p-p_0)dr \\
&\quad = \int_R^{R_1} p\,dr - \int_{R_0}^{R_1} p_0\,dr \\
&\qquad + 2m(E-E_0)\int_{R_1}^r \{\sqrt{2m(E-V)} \\
&\qquad + \sqrt{2m(E_0-V)}\}^{-1} dr \\
&\quad \to \int_R^{R_1} p\,dr - \int_{R_0}^{R_1} p_0\,dr \\
&\qquad + 2m(E-E_0)\int_{R_1}^{\infty} \{\sqrt{2m(E-V)} \\
&\qquad + \sqrt{2m(E_0-V)}\}^{-1} dr \quad (r\to\infty).
\end{aligned}$$

Therefore if we define the function $n(E)$ by

$$n(E) = \frac{1}{\pi\hbar}\lim_{r\to\infty}\left(\int_R^r p\,dr - \int_{R_0}^r p_0\,dr\right) \quad [V(R)=E],$$

then

$$\begin{aligned}
&\lim_{r\to\infty}(f_1(r,E)f_1'(r,E_0) - f_1'(r,E)f_1(r,E_0)) \\
&\quad = (1/\hbar)\sin[n(E)\pi].
\end{aligned}$$

Hence we conclude that E is an eigenvalue of $H(\theta)$ if and only if $n(E)$ is an integer.

We can also obtain a differential equation for the function $n(E)$:

$$\begin{aligned}
n'(E) &= \frac{dn}{dR}\frac{dR}{dE} \\
&= (\pi\hbar)^{-1}V'(R)^{-1}\frac{d}{dR} \\
&\quad \times\left[\int_R^{R_1}\sqrt{2m(V(R)-V(r))}dr\right. \\
&\quad - \int_{R_0}^{R_1}\sqrt{2m(E_0-V(r))}dr \\
&\quad + \int_{R_1}^{\infty} dr\{\sqrt{2m(V(R)-V(r))} \\
&\quad \left. - \sqrt{2m(E_0-V(r))}\}\right] \\
&= \frac{2m}{2\pi\hbar}\int_R^{\infty}\frac{dr}{\sqrt{2m(E-V(r))}}.
\end{aligned}$$

On the other hand, the time T_E taken in moving from $r=R$ to $r=\infty$ and back is as follows:

$$\begin{aligned}
T_E &= 2\int_R^{\infty} dr\left(\frac{dr}{dt}\right)^{-1} = 2m\int_R^{\infty} p^{-1}\,dr \\
&= 2m\int_R^{\infty}\frac{dr}{\sqrt{2m(E-V(r))}}.
\end{aligned}$$

Thus we obtained

$$T_E = 2\pi\hbar n'(E). \tag{10}$$

Of course the formula (10) is applicable only for E such that the conditions (*) and (**) are valid. In most applications of the formula (10), these conditions are fulfilled when E has a sufficiently large negative value and therefore the formula (10) gives the approximate distribution of eigenvalues of $H(\theta)$.

Starting from the quantization rule of Bohr and Sommerfeld in the old quantum theory,

$$\oint p\,dr = 2\pi\hbar\left(n+\frac{1}{2}\right), \tag{11}$$

we can formally obtain the formula (10). In fact differentiating both sides of (11), we have

$$2\pi\hbar n'(E) = \oint\frac{\partial p}{\partial E} = T_E.$$

Here we emphasize that the left-hand side of (11) is a divergent integral.

(ii) Case $n_a = 2$: We wish to obtain a rule that gives the approximate distribution of eigenvalues of $H(\alpha)$, but for general α it is very hard. Fortunately, however, we can prove the following lemma (for the proof, see Ref. 2, Theorem 10.17).

Lemma 3: Let $a > -\infty$, and let the function $V(r)$ satisfy the condition that $V(r)$ be extensible smoothly to an interval $(a-\delta,\infty)$, $\delta>0$. Then for fixed ϕ, $0\leqslant\phi<\pi$, there is a unique function u_ϕ such that

$$\sin\phi u_\phi(a) + \cos\phi u_\phi'(a) = 0,$$

$$Tu_\phi = iu_\phi, \quad \int_a^{\infty}|u_\phi|^2 dr = 1.$$

Let $v_{\phi,\theta}$ denote the real function $(e^{i\theta}u_\phi - e^{-i\theta}\bar{u}_\phi)/2i$, where $0\leqslant\theta<\pi$; let $\mathfrak{D}(\phi,\theta)$ be the set of all functions f in $\mathfrak{D}^*$ such that

$$\sin\phi f(a) + \cos\phi f'(a) = 0,$$

$$\lim_{r\to\infty}(f(r)v_{\phi,\theta}'(r) - f'(r)v_{\phi,\theta}(r)) = 0;$$

and let $H(\phi,\theta)$ be the transformation with domain $\mathfrak{D}(\phi,\theta)$ that takes f into Tf. Then $H(\phi,\theta)$ is a self-adjoint extension of H. The transformations $H(\phi,\theta)$ constitute a proper subset of all transformations $H(\alpha)$.

In the following we restrict ourselves to treating the transformation $H(\pi/2,\theta)$, and we will obtain a formula similar to (10). Since $n_a = 2$, all eigenfunctions of the operator T are square integrable on the interval (a,∞) (cf. Sec. III); the functions f_1 and f_2 are elements in $\mathfrak{D}^*$ for every E.

Set

$$\alpha_E = \exp\left(\frac{1}{\hbar}\int_a^R |p|dr\right), \quad \beta_E = -\exp\left[-\frac{1}{\hbar}\int_a^R |p|dr\right],$$

and

$$\hat{f}_1(r,E) = \alpha_E f_1(r,E) + \beta_E f_2(r,E),$$

then we have

$$\hat{f}_1 \in \mathfrak{D}^*, \quad T\hat{f}_1 = E\hat{f}_1, \quad \hat{f}_1(a,E) = 0 .$$

Since the equation $T = E$ is a linear differential equation of second order, we conclude that

$$\{f \in \mathfrak{D}^*; \quad f(a) = 0, \quad Tf = Ef\} = \mathbb{C}\hat{f}_1(r,E), \tag{12}$$

where $\mathbb{C}$ is the set of all complex numbers. Furthermore we can see, by the same method as in Lemma 2, that for each E there exists a unique θ such that $\hat{f}_1(r,E)$ is in $\mathfrak{D}(\pi/2,\theta)$. By (12) we see that an E is an eigenvalue of $H(\pi/2,\theta)$ if and only if

$$\lim_{r\to\infty} (\hat{f}_1(r,E)v'_{\pi/2,\theta}(r) - \hat{f}_1'(r,E)v_{\pi/2,\theta}(r)) = 0 .$$

Therefore for every E there exists a unique θ such that E is an eigenvalue of $H(\pi/2,\theta)$.

Now let E_0 be an eigenvalue of $H(\pi/2,\theta)$ for fixed θ. Then an E is an eigenvalue of $H(\pi/2,\theta)$ if and only if

$$\lim_{r\to\infty} (\hat{f}_1(r,E)\hat{f}_1'(r,E_0) - \hat{f}_1'(r,E)\hat{f}_1(r,E_0)) = 0$$

[cf. case (i)]:

$$\begin{aligned}
&\hat{f}_1(r,E)\hat{f}_1'(r,E_0) - \hat{f}_1'(r,E)\hat{f}_1(r,E_0) \\
&\sim \frac{1}{\hbar}\left[\exp\frac{1}{\hbar}\left(\int_a^R |p| + \int_a^{R_0} |p_0|\right)\right. \\
&\quad \left. + \frac{1}{4}\exp\frac{1}{\hbar}\left(-\int_a^R |p| - \int_a^{R_0} |p_0|\right)\right] \\
&\quad \times \sin\frac{1}{\hbar}\left(\int_R^r p - \int_{R_0}^r p_0\right) \\
&\quad + \frac{1}{2\hbar}\left[\exp\frac{1}{\hbar}\left(\int_a^R |p| - \int_a^R |p_0|\right)\right. \\
&\quad \left. - \exp\frac{1}{\hbar}\left(\int_a^R |p| + \int_a^{R_0} |p_0|\right)\right] \\
&\quad \times \cos\frac{1}{\hbar}\left(\int_R^r p - \int_{R_0}^r p_0\right).
\end{aligned} \tag{13}$$

If $1 \ll R_0 \ll R$ then we have

$$\begin{aligned}
(13) &\sim \frac{1}{\hbar}\exp\left(\frac{1}{\hbar}\int_a^R |p|\right) \\
&\quad \times \left[\exp\left(\frac{1}{\hbar}\int_a^{R_0} |p_0|\right)\sin\frac{1}{\hbar}\left(\int_R^r p - \int_{R_0}^r p_0\right)\right. \\
&\quad + \frac{1}{2}\exp\left(-\frac{1}{\hbar}\int_a^{R_0} |p_0|\right) \\
&\quad \left. \times \cos\frac{1}{\hbar}\left(\int_R^r p - \int_{R_0}^r p_0\right)\right] \\
&= A\sin\left\{\frac{1}{\hbar}\left(\int_R^r p\,dr - \int_{R_0}^r p_0\,dr\right) + \gamma\right\},
\end{aligned}$$

where $\tan\gamma = \frac{1}{2}\exp[-(2/\hbar)\int_a^{R_0}|p_0|dr]$ and the constant A is independent of r. Therefore if we define the function $n(E)$ by

$$n(E) = \frac{1}{\pi\hbar}\lim_{r\to\infty}\left(\int_R^r p\,dr - \int_{R_0}^r p_0\,dr\right) + \frac{\gamma}{\pi} \quad [E = V(R)],$$

then

$$\lim_{r\to\infty} (\hat{f}_1(r,E)\hat{f}_1'(r,E_0) - \hat{f}_1'(r,E)\hat{f}_1(r,E_0)) = A\sin\{n(E)\pi\} .$$

Hence we conclude that an E is an eigenvalue of $H(\pi/2,\theta)$ if and only if $n(E)$ is an integer. By the same method as in case (i) we can see that

$$T_E = 2\pi\hbar n'(E) . \tag{14}$$

V. EXAMPLES

(I) Let $V(r) = -(\hbar^2/2m)e^{2r}$ $(-\infty < r < \infty)$, then this potential satisfies our assumptions (a1) and (a2). Furthermore solutions of $Tf = \lambda f$ are $J_{is}(e^r), J_{-is}(e^r)$, where J_ν is the Bessel function of order ν and $s = \sqrt{\lambda}$. If $\operatorname{Im}\lambda > 0$, only the latter is square integrable over $(-\infty,0)$. It is therefore case (i).

On the other hand, when θ is a certain value θ_0, we can calculate the exact eigenvalues of the operator $H(\theta_0)$. Eigenvalues are

$$E = -4(\hbar^2/2m)n^2 \quad (n = 1,2,\ldots)$$

(see Ref. 5, 4.14).

Now we have

$$\begin{aligned}
T_E &= 2m\int_R^\infty \frac{dr}{\sqrt{2m(E - V(r))}} = \frac{2m}{\hbar}\int_R^\infty \frac{dr}{\sqrt{e^{2r} - e^{2R}}} \\
&= (m\pi/\hbar)e^{-R} = \pi(m/2)^{1/2}(-E)^{-1/2} .
\end{aligned}$$

Hence solving Eq. (10) we have

$$n(E) = -(1/2\hbar)(2m)^{1/2}(-E)^{1/2} + C ,$$

where C is the constant of integration. Set $E_0 = -4(\hbar^2/2m)$. Determining the initial value $n(E) = 1$ at $E = E_0$, we have $n(E) = -(1/2\hbar)(2m)^{1/2}(-E)^{1/2}$. According to the results of Sec. IV, E is an eigenvalue of $H(\theta_0)$ if and only if

$$(1/2\hbar)(2m)^{1/2}(-E)^{1/2} = n \quad (n = 1,2,\ldots),$$

that is, $E = -4(\hbar^2/2m)n^2$ $(n = 1,2,\ldots)$. Thus the formula (10) yields exact values of all eigenvalues of $H(\theta_0)$.

Here we must indicate that the condition (8) is fulfilled in the vicinity of $r = \pm\infty$ but the conditions (*) and (**) are not fulfilled for large R.

(II) Let $V(r) = (\hbar^2/2m)(\alpha/r^2 - \beta r^\delta)$ $(0 < r < \infty, \alpha > 3/4, \beta > 0, \delta > 2)$, then our assumptions (a1) and (a2) are fulfilled. The roots of the indicial polynomial of the equation $Tf = \lambda f$ are $(1 + \sqrt{1 + 4\alpha})/2$ and $(1 - \sqrt{1 + 4\alpha})/2$. If $\alpha > 3/4$, only the latter is smaller than $-\frac{1}{2}$. It is therefore case (i). If $\alpha \gg 1$ then the condition (8) is fulfilled in the vicinity of $r = 0, \infty$. Moreover the requirement that the conditions (*) and (**) are fulfilled for sufficiently large R gives that

$$\delta < 4, \quad \text{otherwise } \delta = 4 \text{ and } \beta \ll 1.$$

Now if $R \gg 1$, we have

$$\begin{aligned}
T_E &= 2m\int_R^\infty \frac{dr}{\sqrt{2m(E - V)}} = \frac{2m}{\hbar}\beta^{-1/2}\int_R^\infty \frac{dr}{\sqrt{r^\delta - R^\delta}} \\
&= (2m/\delta\hbar)\beta^{-1/2}B(\tfrac{1}{2} - 1/\delta, \tfrac{1}{2})R^{1-\delta/2} \\
&= A(\beta,\delta)(-E)^{1/\delta - 1/2},
\end{aligned}$$

where

$$A(\beta,\delta) = \delta^{-1}(\beta\hbar^2)^{-1/\delta}(2m)^{1/\delta+1/2}B(\tfrac{1}{2} - 1/\delta, \tfrac{1}{2}).$$

Therefore solving Eq. (10) we have

$$n(E) = A'(\beta,\delta)(-E)^{1/\delta+1/2}/2\pi\hbar + \text{const}, \tag{15}$$

where $A'(\beta,\delta) = -(2\delta/(\delta+2))A(\beta,\delta)$.

Using (15), we can ascertain the nature of the distribution of eigenvalues of the operator $H(\theta)$. Let ΔE be the distance between two neighboring eigenvalues, i.e., eigenvalues whose quantum numbers n differ by unity. Then we can write, from (15),

$$(-E)^{1/\delta+1/2} - (-E+\Delta E)^{1/\delta+1/2} = 2\pi\hbar/A'(\beta,\delta).$$

Hence we have

$$\Delta E = (2\pi\hbar/A(\beta,\delta))(-E)^{1/2-1/\delta} = 2\pi\hbar/T_E.$$

(III) Let $V(r) = -(\hbar^2/2m)\beta r^{\delta}$ $(0<r<\infty, \beta>0, \delta>2)$. Then we have case (ii). Condition (8) is fulfilled in the vicinity of $r = 0, \infty$. The requirement that conditions (*) and (**) are fulfilled for sufficiently large R gives

$$\delta < 4, \quad \text{otherwise } \delta = 4 \quad \text{and } \beta \ll 1.$$

By the same method as in example (II), we have

$$\Delta E = 2\pi\hbar/T_E,$$

where ΔE is the distance between two neighboring eigenvalues of the operator $H(\pi/2,\theta)$.

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Quasiresonance of long life

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Schrödinger's equation for two-body scattering is analyzed in the tunneling range of energy for arbitrary, analytic potentials with one barrier. An exact scattering representation is given which furnishes a rigorous and efficient basis for the determination of all the eigenvalues of very long life and the associated linewidths and resonant responses. The approach is direct and simple enough to avoid computation or estimation of wave functions and asymptotic or perturbation expansions.

I. INTRODUCTION

In central scattering with potential barrier, bound states cannot exist in the tunneling range of energy, but some of the sharpest resonances arise in just that range. Such quasiresonances have been studied widely[1–16] and the key features are well understood, but different approaches to the phenomenon have led to proposals for different approximations and a considerable effort has been spent on their comparative testing.[3–6] In this connection, an exact treatment of Schrödinger's equation may be of interest because it provides an absolutely reliable basis and standard for the assessment and improvement of quantitative approximations. Such a treatment will be given here for two-body scattering with central singularity of Coulomb type because this simple and definite example can best serve an initial illumination of the issues and the method of their resolution, which covers most other cores as well.

Even though the narrow quasiresonances below the barrier top are the least controversial, the quantitative issues raised by them are particularly severe.[15,16] A definitive treatment of barrier-top phenomena, moreover, depends on clarification of the main set of quasiresonances. The following therefore focuses on them by a choice of exact representations of particular usefulness for quasiresonance of very long life.

The understanding of quasiresonance has been enhanced by the realization that the observed phenomena can be regarded as a manifestation at real energy of complex, but near-real, eigenvalues. This opens a mathematical approach of simplicity and clarity, which recognizes the *quasibound states as a natural extension of the set of bound states* (Sec. VI). Unfortunately, the quasibound eigenfunctions do not fit into conventional Hilbert spaces, and this has generated much interest in the coordinate-rotation method.[6,17–19] which constructs special Hilbert spaces to accommodate them. A much more direct approach, however, is from the *non-self-adjoint* eigenvalue problem of *quasistationary states*,[20] which can be formulated in a few lines (Sec. III) in a physically elementary way.

It leads immediately to a semiexplicit representation of the eigenrelation (Sec. III) which pinpoints the information really needed for the prediction of lives, levels, linewidths, etc. The mathematical theory begins here to be of numerical value because it shows that the expensive computation or delicate estimate of wave functions[3–6,16,19] is dispensable. The eigenvalues depend only on certain scattering coefficients, and accurate information on quasiresonance can be deduced quickly (Sec. VI) when adequate information is made available (Secs. IV and V) on the dependence of the scattering coefficients upon the energy. This is promoted by the familiar realization that quasiresonance of long life has an essentially quasiclassical character (and the transparency of the mathematical approach adopted permits a rigorous confirmation of this fact in Sec. III). Adequacy of information, however, turns out to make severe demands. The levels of long life have a linewidth so narrow that standard, mathematical WKB theory[21] cannot determine them; its power must be increased quite substantially (Secs. IV and V and Appendix C).

The first approximation to the eigenvalues, responses, and linewidths (Sec. VI) is not novel, of course. The way in which it is established (Appendix B), however, points in directions different from earlier numerical approaches[3–6] because it splits the problem of quantitative refinement between, on the one hand, efficient root finding within tiny complex disks (Sec. VI) and on the other hand, evaluation of the familiar bound-state quantization rule by whatever be the investigator's own method of preference. The proof relates both parts to connection properties (Secs. IV and V) of the Schrödinger equation, for which successive approximations with error bounds are known.[21,22] Estimates of the errors from various sources and levels of approximation can be assembled from these, but it is not obvious how fruitful such a discussion could be outside the framework of tolerances of a specific experiment. The main objective here will be to offer a definitive guide (Sec. VI) to all the sources of approximation error, including those not suspected by the familiar forms of the theory.

II. FORMULATION

In central scattering according to Schrödinger's equation,

$$(\hbar^2/2m)\nabla^2\Psi + [E - U(r)]\Psi = 0,$$

for a wave function $\Psi \exp(-iEt/\hbar)$ in a spherically symmetric potential $U(r)$, it is traditional[15] to split off the angular momentum with the help of spherical harmonics Y_{lm} so that $\Psi = r^{-1}\psi(r)Y_{lm}$ and $\psi(r)$ satisfies a radial Schrödinger equation

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dr^2} + [E - U_l(r)]\psi = 0, \quad U_l = U(r) + \frac{\hbar^2 l(l+1)}{2mr^2}. \tag{1}$$

The following concerns potentials of the type indicated in

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Fig. 1: smooth, with precisely one maximum (say, $U = U_m$ at $r = r_m$), tending as $r \to \infty$ to a limit (which will be taken as $U = 0$) and with a central singularity of Coulomb type,[23]

$$rU(r) \to -U_* < 0, \quad \text{as } r \to 0. \tag{2}$$

This type of core is chosen here in deference to Kramers[23] and because it is both singular and also involves characteristic difficulties at low angular momentum. A large class of potentials, including hard-core, multiparticle potentials, is free of those difficulties and hence is also covered by the analysis (Sec. V) for the case of large angular momentum (if spherical symmetry of the potential be an acceptable assumption). Another class involves difficulties similar to those arising for the Coulomb core and can be treated by relatively direct modification of the analysis (Sec. V) for the case of low angular momentum. A point to note is that the scattering-part proper (Sec. IV) of the Schrödinger problem is independent of the nature of the core, while the core-reflection part of the problem (Sec. V) may depend on the nature of the singularity and also on the angular momentum, as exemplified by the Coulomb case.

Such potentials with a single well and a single barrier (Fig. 1) possess a nondimensional wave number scale

$$K = (2mU_m)^{1/2} r_m/\hbar \tag{3}$$

describing a gross feature of the barrier, and if the potential is normalized by choosing the well radius r_m, barrier height U_m, and $\hbar/U_m$ as the respective units of length, energy, and time, the Schrödinger equation takes the nondimensional form

$$\psi'' + K^2(E - U_l)\psi(r) = 0, \quad U_l = U(r) + l(l+1)/(Kr)^2. \tag{4}$$

Attention will be restricted to angular momenta for which

$$\frac{2l(l+1)}{K^2} < \max \frac{r^3\, dU}{dr}, \tag{5}$$

so that the effective potential $U_l(r)$ also possesses a well, and to positive energies below the maximal potential, $0 < E < U_M$ $= \max U_l(r)$, because these two conditions are necessary for the occurrence of strict quasiresonance.

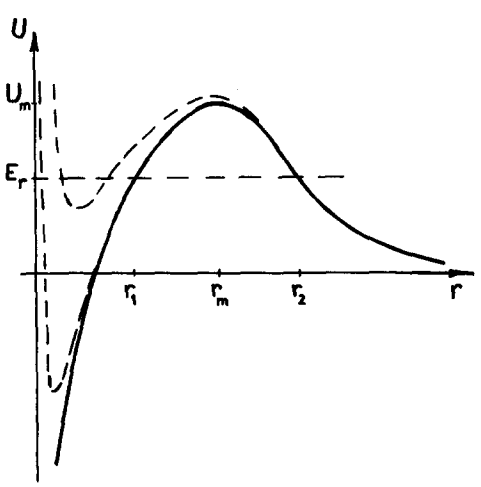

FIG. 1. The barrier potential. The full line represents the typical shape of $U(r)$ for real r; the broken lines indicate that of the effective, centrifugally corrected potential $U_l(r)$ for rather small l (lower curve) and relatively large l (upper curve).

Under such circumstances, the tunneling effect precludes bound states and implies time decay for quasistationary wave function (so that the energy range envisaged is really not $0 < E < U_M$, but $0 < \mathrm{Re}\, E < U_M$). On the other hand, such potentials are associated with states of long "life"[20]

$$T = -\hbar/(2U_m \,\mathrm{Im}\, E), \tag{6}$$

of primary physical interest because they possess a resonant character. Their study must of necessity involve the asymptotic notion $T \gg 1$. A question, of course, is how that notion relates to a given potential, and it will be shown that it must be largely interpretable in terms of the notion $K \gg 1$. That has long been recognized to be plausible, since excitation by tunneling is more effective with wider barriers, and "wide" can have an intrinsic interpretation only in terms of wavelengths. The plausibility stops a little short, however, when it is recalled that there are no wavelengths in a barrier and that the formal scale K may not be representative of the wave numbers in all important parts of the field. All the same, (3) is a natural, large scale associated with the problem and the cautionary implication is mainly that uniform applicability of quasiclassical approximations is not thereby assured.

Since the time decay resulting from tunneling must be associated with complex values of the energy, the roots of $E - U_l(r)$, which are the turning points marking the boundary of the potential barrier, must also be complex. Their central role in the structure of the Schrödinger equation makes it logical to give consideration also to complex values of the radius. The point emerging therefrom is that a rational and direct theory of quasiresonance of long life must necessarily involve analysis in two complex variables E and r, in addition to asymptotics with respect to a real parameter such as T or K.

The potential $U(r)$ then needs extension into the complex plane of r, and the simplest expedient is to envisage an analytic potential. Of two grounds on which that appears justified, one is that the observational evidence is unlikely to distinguish between a smooth potential in C^∞ and a sufficiently close, analytic approximation to it. The other is that related work on adiabatic invariance[24,25] indicates approximation by analytic functions to furnish the most effective approach to a theory of precision scattering for general potentials in C^∞. In short, the analytic case is central, and also the most illuminating case.

On the other hand, the complex extension needed below is notably economical; $U(r)$ will be assumed analytic on a neighborhood of $(0, \infty)$, however narrow, beyond which it is left undefined. A sectorial character[6,17,18] of the domain will not be required, and conditions on the rate at which $U(r) \to 0$ as $r \to \infty$ do not arise in the analysis which follows.

III. EIGENVALUE PROBLEM

The analysis of quasistationary states is best related to certain wave functions of clear-cut physical character. Figure 2 shows the structure of the complex r plane. For real energy in the tunneling range, $E - U_l(r)$ in (4) has three real roots r_0, r_1, and r_2, and by (6), those roots $r_s(E)$ remain close

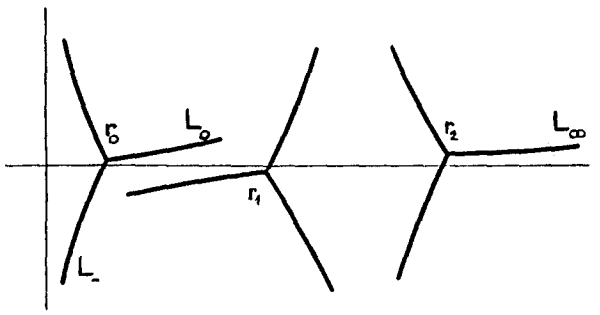

FIG. 2. The complex plane of the radius with turning points and Stokes lines for near-real energy.

to the real r axis for decaying states of long life. The figure also shows the "Stokes lines" (or "anti-Stokes lines") of (4) definable by

$$\mathrm{Re}\int_{r_s}^{r}[E-U_l(r')]^{1/2}\,dr'=0,\quad s=0,1,\text{ or }2.$$

Their physical relevance stems from the alternative definition[21] that to each Stokes line L_i (and only to such a line) corresponds a fundamental solution pair $u_i(r)$, $v_i(r)$ of (4) which approach on L_i, with increasing distance from the origin r_s of the Stokes line, the character of progressive waves, undamped and unamplified with distance from r_s. For definiteness u_i will denote the wave outgoing from r_s along L_i and v_i, the wave incident towards r_s. Both are exact solutions of (4) on the whole domain of $U(r)$, but they do not possess the undamped, progressive character on L_j for $j\neq i$.

The fundamental pairs of physical interest are u_0, v_0 and u_∞, v_∞, the respective progressive waves on the central Stokes line L_0 and the farfield Stokes line L_∞ (Fig. 2), because these lines coincide, for real energy, with segments (r_0, r_1) and (r_2, ∞) of the real r axis, where then $E-U_l(r)>0$. For long life (6), they depart only little from the real axis and the simple wave character of the respective fundamental pairs on L_0 and L_∞ remains symptomatic of the main features of their more complicated character on the real-axis segments nearby (Sec. IV). This indicates the correct formulation of the radiation condition of quasistationary states[20] (p. 134) that the wave function represents an outgoing wave in the farfield: the representation

$$\psi(r)=A_\infty u_\infty(r)+B_\infty v_\infty(r) \tag{7}$$

of the (reduced) wave function as a linear combination of u_∞, v_∞ must satisfy

$$B_\infty=0,\quad A_\infty\neq 0. \tag{8}$$

As a result of this radiation condition, the wave functions cannot be relied upon[20] (pp. 33–34, 134) to be square integrable in the farfield (Sec. IV) (and the language of Hilbert space loses some of its customary usefulness). The reflection process in the inner well (Fig. 1), however, is subject to the less global condition[20] (p. 103) that the total probability within the well region be finite, so that $\psi(r)\in L^2(0,r_m)$. The wave effect of this regularity condition is best described in terms of the central representation

$$\psi(r)=A_0u_0(r)+B_0v_0(r), \tag{9}$$

in which this condition will determine (Sec. V) the ratio

$$A_0/B_0=R, \tag{10}$$

naturally interpretable as the (amplitude) reflection coefficient at the inner barrier set up by the "centrifugal" effect of the angular momentum in (4).

Since the fundamental pairs are exact solutions of (4) on the whole domain of $U(r)$, they must be linearly related,

$$\begin{pmatrix}u_0(r)\\ v_0(r)\end{pmatrix}=S^T\begin{pmatrix}u_\infty(r)\\ v_\infty(r)\end{pmatrix},$$

with constant matrix S^T related to the F matrix.[13] Since (7) and (9) represent the same wave function $\psi(r)$, it follows that the amplitude coefficients are also linearly related,

$$\begin{pmatrix}A_\infty\\ B_\infty\end{pmatrix}=S\begin{pmatrix}A_0\\ B_0\end{pmatrix},$$

with a "scattering matrix" $S(E,K)=(\!(S_{ij})\!)$. The exact eigencondition for quasistationary states can therefore be written quite simply as

$$0=B_\infty/B_0=S_{22}+S_{21}A_0/B_0=S_{22}+S_{21}R. \tag{11}$$

It may help to sketch briefly the connection of this quasistationary eigenvalue problem with the time-delay approach to quasiresonance, which asks essentially the question: what stationary states could occur in the laboratory, which operates at real E and r? The fundamental pairs u_0, v_0 and u_∞, v_∞ then describe pure progressive waves along the real r axis, and as a solution of (4), the reduced wave function $\psi^s(r)$ of a stationary state must again be a linear combination

$$\psi^s(r)=A^s_0u_0(r)+B^s_0v_0(r)=A^s_\infty u_\infty(r)+B^s_\infty v_\infty(r).$$

If the wave pairs are normalized appropriately, $|A^s_i|^2$ and $|B^s_i|^2$ represent the outward and inward probability-flux densities,[20] respectively. To set up such a stationary state, the radiation damping due to outward tunneling must be compensated by incident radiation from "infinity", so that $B^s_\infty\neq 0$. Comparison of the fluxes $|B^s_\infty|^2$ and $|B^s_0|^2$ will then yield a measure

$$|\rho(E,K)|^2=|B^s_0/B^s_\infty|^2$$

of the probability level in the well for unit intensity of incident radiation in the farfield. It is a standard measure of the response to excitation (even if only a conservative upper bound, because it presumes long action of a spherically symmetrical, incident radiation).

Since the wave pairs are related by the matrix S^T, the stationary-state amplitudes must again be related by the scattering matrix $S(E,K)$, and by (11), the amplitude amplification is

$$\rho(E,K)=B^s_0/B^s_\infty=(S_{22}+S_{21}R)^{-1}. \tag{12}$$

For most real E, $|\rho|$ is very small (Sec. VI), but exceptions arise near any near-real roots E_n of (11), where $|\rho|\propto|E-E_n|^{-1}$. Quasistationary eigenvalues E_n of long life therefore predict strong, narrow spectral lines of quasiresonance, and the response is related closely to the eigenfunction lifetime.

The search for those eigenvalues, on the other hand, is seen from (11) to involve, not the question of approximation of wave functions, but only the "connection" question, how

fundamental wave pairs are related to each other. The only way that Schrödinger's equation enters into the quasiresonance problem is through the three coefficients in (11) and (12), and the concern of the following must be with adequate approximation of their dependence on E. Since $|\rho|$ is so conservative a bound, moreover, effective quasiresonance requires very large $|\rho|$, and accordingly requires eigenvalues of very long life, and hence, of very small $|\mathrm{Im}\, E|$, and this narrows the enquiry down further.

For a given potential $U(r)$ and *fixed* K and l, the characteristic form

$$S_{22} + S_{21}R = \Delta(E)$$

depends only on E. On the one hand, the coefficient of Schrödinger's equation is clearly analytic in E, and so are therefore its fundamental solution pairs on their common domain of definition D_E [which includes any neighborhood of the real E axis on which the turning points remain in the domain of $U(r)$]. It follows that the entries of S^T linking the wave pairs are analytic in E on D_E, and so are the scattering coefficients S_{22}, S_{21}, R and the function $\Delta(E)$. On the other hand, it is well known why conservation of probability precludes real eigenvalues E in the tunneling range, and $\Delta(E)$ has therefore no positive real roots. For any $\epsilon > 0$, there is therefore a lower bound $b(\epsilon) > 0$ for $|\mathrm{Im}\, E|$ at any root of $\Delta(E)$ with $\epsilon \leqslant \mathrm{Re}\, E \leqslant 1/\epsilon$: Roots of very long life can arise only from extremes of the other parameters l and K.

Unless (5) holds, however, the effective potential $U_l(r)$ in (1) has no well or barrier and has then only one real turning point at real E, so that $(u_0, v_0) = (u_\infty, v_\infty)$ and $R = A_\infty / B_\infty$. Since the regularity condition makes $|R| = 1$ at real E (Sec. V), the analyticity of R on D_E then precludes nontrivial wave functions satisfying the radiation condition (8). That narrows the scope for eigenvalues of very long life down to either $K \gg 1$, or possibly $l = 0$, $K \ll 1$.

However, K is an artificial parameter introduced for the mere sake of notation which can be eliminated from (4) by, for instance, measuring energy in units of $\hbar^2/(2mr_m)$, rather than of U_m. Accordingly, $K^2 \to 0$ amounts to the limit of zero barrier height, in which there cannot be a quasistationary state with $\mathrm{Re}\, E \geqslant \epsilon > 0$. It follows that eigenvalues of very long life are possible only for $K^2 \gg 1$ in (4), if the potential is normalized as indicated there. Of course, this only spells out in rigorous terms the long understanding that a large barrier, in an appropriate sense, is necessary for quasistationary states of long life and lends them a degree of quasiclassical character.

The necessary and sufficient concern of the following is therefore with the dependence of the three coefficients in the eigenrelation (11) upon E and $U(r)$ when K is large and fixed, and the next two sections are devoted to a description of that dependence. In that description and later, the word "exact" will continue to be used in the sense of the dictionary to characterize conclusions following from the definition of the eigenvalue problem in Secs. II and III *without any kind of approximation* or asymptotic expansion whatsoever.

IV. PRECISION SCATTERING

The computation of the asymptotic expansions of scattering coefficients in powers of K^{-1} is precisely the objective of turning-point connection theory,[21,26] and its application leads quite rigorously to the expansions

$$\gamma_0 S_{21} \sim i + \sum_1^\infty c_s(E) K^{-s},$$
$$\gamma_0 S_{22} \sim \exp[-2K\xi_w(E)] \left\{ 1 + \sum_1^\infty d_s(E) K^{-s} \right\}, \tag{13}$$

as $K \to \infty$, where ξ_w denotes a familiar WKB wave distance specified in (16) below and the common factor $\gamma_0 \neq 0$ is irrelevant to the eigencondition (11). It will emerge, however, that such a result fails to yield any information at all on the life T, and this theory cannot therefore offer a basis for reliable approximations to quasiresonant response and linewidth.

To remedy this, Lozano and Meyer[27] recalculated S_{21} and S_{22} and showed that, if the question of computing the quantitative content of the symbols be postponed, then these coefficients can be represented by

$$\gamma_0 S_{21} = i \exp\{i\Sigma_1(E,K)/K\} - (1+i)\{1 + \Omega(E,K)/K\} e^{-2K\xi_b}, \tag{14}$$

$$\gamma_0 S_{22} = e^{-2K\xi_w} \exp\{i\Sigma_2(E,K)/K\}, \tag{15}$$

where Σ_1, Σ_2 represent the functions expanded in (13), Ω denotes a similarly expandable function, and ξ_b another wave distance specified in (17) below. The second term on the right-hand side of (14) had not been given before because $\mathrm{Re}\, \xi_b > 0$, so that this term is meaningless in the conventional sense (13) of mathematical asymptotics. The coefficient $E - U_l(r)$ of (4), however, is clearly an analytic function of E and, according to the principle of conservation of probability,[20] is real when E and r are real. It follows[27] that some of the wave solutions u_i, v_i can be defined with a complex-conjugate symmetry in the r and E planes, which is inherited by some of their functionals. By reorganizing the turning-point connection calculations so that these properties of analyticity and complex E symmetry can be traced through them, Lozano and Meyer proved[27] the following.

Precision Scattering Theorem: For the three-turning-point problem defined in Secs. II and III the scattering coefficients S_{21} and S_{22} in (11) can be represented exactly in the form (14), (15) with

$$\xi_w(E,K) = \int_{r_0}^{r_1} [F_0(r)]^{1/2}\, dr, \tag{16}$$
$$F = U_l(r) - E,$$

$$\xi_b(E,K) = -\int_{r_1}^{r_2} [F_1(r)]^{1/2}\, dr, \tag{17}$$

where $r_s = r_s(E,K)$ and the subscripts on F denote a consistent determination of branches of the root. The functions $\Sigma_j(E,K)$ and $\Omega(E,K)$, moreover, have the properties that $\Sigma_j(E,K)$ is real for real E and, for large enough K, Σ_j and Ω are bounded and analytic in E on a K-independent neighborhood D_E of the real interval $(\min_{r\in\mathbf{R}} U_l(r), \max_{r\in\mathbf{R}} U_l(r))$.

This theorem is a deliberate compromise between the pure existence results for scattering coefficients sought by functional analysis and the computational approximations to them sought by WKB applications. Instead, the theorem concentrates on those exact, qualitative features of their

structure which have decisive, quantitative implications, especially when the wave number scale K is not too small. It also removes the need for estimates of eigenfunctions.[16,19]

As a corollary, the first term on the right-hand side of (14) is seen to be of exactly unit magnitude when E is real, so that the "very small," second term then describes the whole deviation of $|\gamma_0 S_{21}|$ from unity, regardless of any "much larger" uncertainties about $\arg(\gamma_0 S_{21})$. One thrust of the theorem is therefore that analyticity in E, and the principle of conservation of probability, permit us to filter certain *exponentially small scattering contributions* reliably out of the (algebraic) asymptotic expansions (13). Since just these contributions will turn out to determine the life T, the standard, technical meaning of asymptotically larger and smaller is seen to be misleading in regard to quasiresonance.

Such considerations reduce the importance of the asymptotic excpansions (13) for scattering, and instead, direct attention to the WKB integrals (16) and (17). A consistent scheme of branches has been described[27] in detail for an equation analogous to (4) and details of the functions Σ_j and Ω are there given. The main issue is that an analytic continuation of the fundamental wave pairs must be established along a chain of overlapping domains on each of which those functions have a coherent approximation. The procedure of Lozano and Meyer[27] was to construct such a chain below the turning points r_1, r_2 in the r plane (Fig. 2), and determinations of (16) and (17) consistent with the theorem were thus shown to be $\arg F_0 = \pi$ and $\arg F_1 = 2\pi$ at real energy, with extension by continuity to slightly complex energy. At real energy, therefore, $K\xi_w \exp(-i\pi/2) > 0$ and may be interpreted in the familiar way as the width of the potential well of U_l at the level $\mathrm{Re}\, E$ in units of local, radial wavelengths. Similarly, $K\xi_b > 0$ at real energy and—if the potential barrier were not just the place where there are no waves—should be interpreted as the barrier width of U_l in such units.

The scattering analysis also provides a check on the radiation condition (8). The WKB approximation to u_∞ is

$$u_\infty(r) \sim c_\infty F_\infty^{-1} \exp\{K\xi_\infty(r)\}, \quad \xi_\infty(r) = \int_{r_2}^{r} [F_\infty(s)]^{1/2}\, ds,$$

where c_∞ denotes a normalization factor and $F_\infty(r)$ the branch of the function F in (16) and (17) appropriate to the farfield. The determination consistent with those just mentioned is[27] $\arg F_\infty = \pi$ on L_∞, and as $r \to \infty$ along the real axis, where $U_l(r) \to 0$, this gives $\xi_\infty \sim E^{1/2} r \exp(i\pi/2)$. The phase of the full, farfield wave function $A_\infty r^{-1} u_\infty Y_{lm} \exp(-iEt)$ is therefore

$$\mathrm{Im}\{K\xi_\infty - iEt\} \sim Kr\, \mathrm{Re}\, E^{1/2} - t\, \mathrm{Re}\, E,$$

as $r \to \infty$ along the real axis, and this describes an outgoing wave for $\mathrm{Re}\, E > 0$, as it must be in the tunneling range. The radiation condition (8) therefore implies the intended wave character in the farfield even if L_∞ should leave the domain. However,

$$\mathrm{Re}\{K\xi_\infty - iEt\} \sim t\, \mathrm{Im}\, E - Kr\, \mathrm{Im}\, E^{1/2},$$

as $r \to \infty$ along the real axis and for positive life [as it will be seen in Sec. VI to be predicted by (11)], the wave function decays both at fixed position and at fixed phase, but at fixed time, it *grows* with increasing r. While this mathematical growth is exponential and precludes convergence of $\int |\psi|^2\, dr$, the magnitude of $K\, \mathrm{Im}\, E^{1/2}$ will emerge in Sec. VI to be so small, that the growth is postponed to very large distances.

V. REFLECTION

The regularity condition $\psi(r) \in L^2(0, r_m)$ (Sec. II) identifies a particular solution of Schrödinger's equation (4) as admissible. Its representation in terms of the central wave pair (u_0, v_0) (Sec. III) requires an analytic continuation through the inner barrier of $U_l(r)$, which is detailed in Appendix A for potentials of Coulomb type.

For angular momenta large enough to regard $l(l+1)/K^2$ as bounded from zero, but not too large to satisfy (5), this is done by an extension of WKB theory[23,28] analogous to that used[27] in the proof of the Precision Scattering Theorem: asymptotic estimates for large K are first used for a tentative identification of the analytic continuation of the reduced wave function around the inner turning point r_0 (Fig. 2), and analyticity and conservation of probability are then used to make that identification exact. This covers also singular, multiparticle potentials for $l \geqslant 0$, if they are spherically symmetrical.

For small angular momentum, the inner turning point lies within a distance of order K^{-2} of the Coulomb singularity at $r = 0$, and both these singularities must then be treated simultaneously. This is also done in Appendix A by an extension of Kramers'[23] analysis of achieve estimates of the necessary precision and uniformity.

The result is an exact representation of the reflection coefficient as

$$R = e^{-i\pi(1/2 + 2\sigma)} \exp[iK^{-1}\Sigma_0(E,K)], \tag{18}$$

with Σ_0 again analytic in E on D_E, bounded for large K, and real for real E, and with angular-momentum correction

$$\sigma(l) = l + \tfrac{1}{2} - [l(l+1)]^{1/2} \tag{19}$$

(which is one of those proposed by Kramers[23]).

While this result is established both for small and large angular momentum [such that $\sigma = O(K^{-1})$], the proof (Appendix A) leaves a gap for $1 \ll l \ll K$. The correction σ, however, is massive only for $l = 0$ and decreases so rapidly with increasing angular momentum [e.g., $\sigma(4) = 0.028$ only] that the difference, if any, between (19) and the exact correction at intermediate l should be rarely significant.

VI. EIGENVALUES

For states of long life, it is advantageous to split the characteristic form of (11) into two parts

$$S_{22} + S_{21}R = i\gamma_0^{-1} R\, \{\Delta_0(E,K) + \Delta_1(E,K)\},$$

with

$$\Delta_0 = \exp[-2K\xi_w + 2\pi i\sigma + i\Sigma_2/K - i\Sigma_0/K] + \exp(i\Sigma_1/K),$$

$$\Delta_1 = (i-1)(1 + \Omega/K)\exp(-2K\xi_b),$$

by (14), (15), and (18) because Δ_0 has a set of *real* roots E_r given exactly by

$$K|\xi_w(E_r,K)| + (\Sigma_1 - \Sigma_2 + \Sigma_0)/(2K) = (n + \tfrac{1}{2} + \sigma)\pi, \tag{20}$$

with non-negative integer n. In dimensional notation, that is the familiar quantization rule with first approximation

$$(2m)^{1/2}\int_{r_0}^{r_1} |E_r - U_l(r)|^{1/2}\,dr = \left(n + \frac{1}{2} + \sigma\right)\pi\hbar[1 + O(K^{-2})], \tag{21}$$
$$U_l(r_0) = U_l(r_1) = E_r,$$

where U_l is given by (1) and (r_0,r_1) is the U_l-well interval of the radius at the level E_r.

Since $U(r)$ is monotone increasing on $(0,r_m)$ (Fig. 1), the exact rule (20) is known to determine a unique, real $E_r(n)$ for all n such that still

$$E_r(n) < \max_{r\in\mathbf{R}} U_l(r) = U_M.$$

With the zero level of energy adopted here (Fig. 1), the negative roots $E_r(n)$ are the bound levels, because $\Delta_1 = 0$ for $\mathrm{Re}\,E \leqslant 0$. The positive roots are not eigenvalues, but it has long been understood[20] that eigenvalues of long life should be close to them. The results of Secs. IV and V support a mathematical proof (Appendix B) that precisely one, simple eigenvalue E_n exists very close to each $E_r(n) < U_m - a$ with any fixed $a > 0$, and also that there are no other eigenvalues E of long life with $\mathrm{Re}\,E < U_m - a$.

The proof is of some interest because it uses the degree principle to establish a rigorous computational basis for the efficient determination of the eigenvalues by complex root-finding procedures restricted to only very small disks (Appendix B). As a starting point for such computations, moreover, it provides a first approximation

$$E_n - E_r(n) \sim -\tfrac{1}{2}(1+i)[K|\xi_w'(E_r,K)|]^{-1} \times \exp[-2K\xi_b(E_r,K)]\{1 + O(K^{-1})\}, \tag{22}$$

where a prime denotes differentiation with respect to E. The corresponding approximation for the life is

$$T_n = \hbar/(2U_m\,\mathrm{Im}\,E_n) \sim (\hbar K/U_m)|\xi_w'(E_r(n),K)|\exp[2K\xi_b(E_r(n),K)] \sim (2m/U_m)^{1/2} r_m |\xi_w'(E_r(n),K)|\exp[(8mU_m)^{1/2} \times r_m\xi_b(E_r(n),K)/\hbar],$$

with $E_r(n)$, ξ_w', and ξ_b given by (20), (B2), and (17). This is novel only in that it is half the life predicted by the corresponding approximation of Connor and Smith[4–6] and an even smaller fraction of Child's.[7] Appendix C explains why this is merely an appearance of discrepancy arising from the unreliability of customary approximation procedures in the non-self-adjoint quantum mechanics of processes with radiation damping weak enough to call for exponential precision; the interpretation of "approximation" then becomes almost totally dependent on the fine print (Appendix C). With just the right interpretation, on the other hand, such approximations may have remarkable quantitative value far beyond the range for which they were constructed.[6]

Since the exponential proximity of the eigenvalues to the real energy axis makes the linewidth so narrow, quantitative questions of practical interest may often concern less the closer computation of the lives than that of the resonant levels of approximations to the functions Σ_j in the quantization rule (20). In this respect, the proof indicates the corrections arising from central reflection to be potentially as important as those arising from scattering, and for small angular momentum, where the former pose more of a challenge, the uniform analysis of Appendix A may be of help. Unless the wave-number scale is extremely large, moreover, the exponential level corrections indicated by the real part of (22) may compete in quantitative significance with those arising from the functions Σ_j in the conventional quantization rule (20).

It is not clear whether a quantitative assessment of these corrections for the very general class of potentials here covered (Sec. II) could be a profitable undertaking. The present account limits itself to showing how the analysis of Appendix A and that underlying[27] Sec. IV construct all those corrections from connection relations for which successive approximations with meticulous and realistic error bounds are known.[21,22]

For a more theoretical point of view, it may be of some interest to note the representations obtained for the *quasistationary extension of the exact, bound-state quantization rule* (20). They are (11) and $\Delta_0 + \Delta_1 = 0$, of course, and in more longhand notation,

$$K\xi_w = (n + \tfrac{1}{2} + \sigma)\pi i + i(\Sigma_2 - \Sigma_0)/(2K) - \tfrac{1}{2}\log\{e^{i\Sigma_1/K} + (i-1)(1 + \Omega/K)e^{-2K\xi_b}\}, \tag{23}$$

with K, ξ_w, and ξ_b given, respectively, by (3), (16), and (17), with Σ_j and Ω defined implicitly in Sec. IV and Appendix A and represented explicitly in Ref. 27, and with the principal branch of the logarithm, for definiteness of the quantum number n. In all the function symbols in (23), the argument of the function is understood to be (E_n,K,l).

The response $\rho(E,K) = (S_{22} + S_{21}R)^{-1}$ to excitation at real energy requires consideration also of the factor γ_0 in (14) and (15), which is[27] $\exp[-K(\xi_b + \xi_w)]\{1 + O(K^{-1})\}$. Thus $|\rho|^2$ has an exponentially large maximum

$$|\rho|^2_{\max} = \exp[2K\xi_b(E_r(n),K)]\{1 + O(K^{-1})\}$$

at each quasiresonant energy level given by (20) and (22), but the width of the energy band over which this response exceeds half its peak value is only

$$2\,\mathrm{Re}(E_r - E_n) = -2\,\mathrm{Im}\,E_n = \Gamma_n = [K|\xi_w'|\exp(2K\xi_b)]^{-1}\{1 + O(K^{-1})\},$$

and over nearly the whole interval between successive such levels, the response is only of the exponentially small order of its minimum,

$$|\rho|^2_{\min} \sim \tfrac{1}{4}\exp[-2K\xi_b].$$

These are again first approximations to quantities of exponential order and are therefore (Appendix C) dependent on the exact interpretation of (20); other interpretations[2–12] can give quite different formulas of equal validity.

This extreme character of quasiresonance moderates as the energy level increases because $\mathrm{Re}\,\xi_b$ decreases. Life and response decrease accordingly, and the bandwidth increases

in inverse proportion to the life. There are indications that the results of this section may extend to energy levels approaching the barrier top to within $O(K^{-1})$, but then the life and response cease to be large, the bandwidth broadens to almost $O(K^{-1})$, and different scattering representations are more suited to the study of barrier-top phenomena.

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APPENDIX A: ANALYSIS OF REFLECTION

In the computation of the reflection coefficient (10), a distinction between large and small angular momenta arises in the Coulomb case, and it is convenient to begin with the case of quantum numbers l so large that

$$l(l+1)/K^2 = \lambda^2$$

can be regarded as a parameter independent of K. Then U_l in (4) is independent of K and only a more precise version of quasiclassical analysis[23,28] is required. As long as (5) holds, $U_l(r)$ still possesses a well and quasiresonance may occur at energies of real part between min U_l and max U_l, to which attention will therefore be restricted. All three roots r_0, r_1, r_2 of $F(r) = U_l(r) - E$ are now independent of K. The branches chosen for (16) and (17) are based on $\arg F_0'(r_0) = \pi$ for real E and are consistently extended by $\arg(r - r_0) = -\pi$ for real $r \in (0, r_0)$ (Fig. 2) to match the analytic continuation of Sec. IV passing below the turning points in the r plane. The domains of validity of simple asymptotic approximations to solutions of (4) are restricted by conditions[29] that prevent the domain D_0 containing the Stokes line L_0 (Fig. 2) from reaching points in $(0, r_0)$, where the regularity condition can be plainly interpreted. To reach them, the domain D_- of L_- (Fig. 2) is needed, which lies below r_0 and overlaps with D_0. The branch F_- of F appropriate for L_- has $\arg F_-'(r_0) = 3\pi$ for real energy, and the corresponding wave variables

$$\xi_-(r) = \int_{r_0}^{r} [F_-(t)]^{1/2}\, dt \quad \text{on } D_-,$$
$$\xi_0(r) = \int_{r_0}^{r} [F_0(t)]^{1/2}\, dt \quad \text{on } D_0 \tag{A1}$$

are therefore related by

$$\xi_-(r) = \xi_0(r) e^{i\pi} \quad \text{on } D_- \cap D_0, \tag{A2}$$

even at nonreal energy. [The function $\xi_w(E,K)$ of Secs. IV and VI is thus seen to be $\xi_0(r_1(E,K))$ in the notation of this appendix.]

Langer's transformation[21] of (4) near r_0 is

$$\xi_- = \frac{2}{3}\zeta^{3/2}, \quad \psi(r) = \left(\frac{d\zeta}{dr}\right)^{-1/2} W(\zeta),$$

and casts (4) into the form

$$\frac{d^2W}{d\zeta^2} = (K^2\zeta + \phi_-)W,$$

with a function ϕ_- satisfying the hypotheses of Olver's[21] Theorem 9.1 (p. 417). Accordingly, (4) has a fundamental solution pair ψ_r, ψ_s with first approximations

$$\psi_r(r) \sim \left(\frac{d\zeta}{dr}\right)^{-1/2} \mathrm{Ai}(K^{2/3}\zeta),$$
$$\psi_s(r) \sim \left(\frac{d\zeta}{dr}\right)^{-1/2} \mathrm{Bi}(K^{2/3}\zeta), \tag{A3}$$

in terms of standard Airy functions Ai, Bi as $K \to \infty$, uniformly for bounded $|\zeta|$. In $(0, r_0)$, $\arg \xi_-$ is near zero for near-real energy and the same holds for $\arg \zeta$. Therefore, $\psi_s(r)$ does not yield a wave function square integrable in the well and only multiples of $\psi_r(r)$ are admissible.

To translate this into exact information on the central reflection coefficient R requires the representation of $\psi_r(r)$ in terms of the wave pair (u_0, v_0) of L_0 (Fig. 2) which has WKB approximation

$$u_0(r) \sim c_0 F_0^{-1/4} e^{K\xi_0(r)}[1 + O(K^{-1})],$$
$$v_0(r) \sim c_0 F_0^{-1/4} e^{-K\xi_0(r)}[1 + O(K^{-1})], \tag{A4}$$

for $|\xi_0|$ bounded from 0. That representation can be obtained from the asymptotic approximation[21]

$$-\mathrm{Ai}[K^{2/3}\zeta] \sim \tfrac{1}{2}\pi^{-1/2} K^{-1/6} \zeta^{-1/4} e^{-\pi i/2} \{ e^{K\xi} [1 + O(K^{-1})] + e^{-\pi i/2} e^{-K\xi} [1 + O(K^{-1})] \}$$

on L_0, where $\arg \xi = \pi$ and, accordingly,

$$\psi_r(r) \sim \tfrac{1}{2}\pi^{-1/2} K^{-1/6} F_-^{-1/4} \{ e^{K\xi_0(r)} [1 + O(K^{-1})] + e^{\pi i/2} e^{-K\xi_0(r)} [1 + O(K^{-1})] \}. \tag{A5}$$

Comparison with (9) and (A4) now shows

$$R = A_0/B_0 = e^{-i\pi/2} + O(K^{-1})$$

in (10).

This is the result of standard, quasiclassical[23,28] theory and is again inadequate for information on the life T because its degree of accuracy destroys the chance of using the new information of the Precision Scattering Theorem in the eigencondition (11). Nor would the asymptotic expansion of R help in that respect. However, the key to the proof[27] of the Precision Scattering Theorem (Sec. IV) lies in the observation that qualitative information on the errors may suffice for turning an asymptotic approximation to wave identification, such as (A5), into an exact identification. By their appeal to conservation of probability, Lozano and Meyer[27] showed that u_0, v_0 can be normalized so that the error terms in (A4) are complex conjugates of each other for real E. As a wave function of (4), $\psi_r(r)$ is similarly normalized to be real for real E and r, and the error terms in (A5) are then also complex conjugates when E is real. It now follows from the comparison of (9), (A4), and (A5) that $|R| = 1$ exactly for real E. Furthermore, since the solutions of (4) depend analytically on E, so does the functional R, and its exact form must be

$$R = e^{-i\pi/2}\exp[iK^{-1}\Sigma_0(E,K)], \tag{A6}$$

with Σ_0 again analytic in E on D_E, bounded as $K\to\infty$, and real for real E.

It may be noted that the analysis just sketched makes no reference to the specific nature of the singularity of $U(r)$ at $r=0$; it covers all cores for which the inner turning point is well separated from the central singularity.

As the angular momentum decreases, however, the turning point r_0 of the Coulomb case moves closer to the singular point $r=0$ of the potential, and standard, quasi-classical analysis begins to fail because more careful account must be taken[23] of the central singularity. For small $|r_0|$, the Langer transformation for (4) is[21] to variables

$$\zeta^{1/2} = \int_0^r [f_0(t)]^{1/2}\,dt, \quad W(\zeta) = \left(\frac{d\zeta}{dr}\right)^{1/2}\psi(r),$$

where $f_0(r)$ is a branch of $U(r)-E$. The Schrödinger equation (4) then takes the form[21]

$$\frac{d^2W}{d\zeta^2} = \left[\frac{K^2}{4\zeta} + \frac{l(l+1)}{\zeta^2} + \frac{\phi_0}{\zeta}\right]W,$$

where

$$\frac{\phi_0}{\zeta} = l(l+1)\left[r^{-2}\left(\frac{dr}{d\zeta}\right)^2 - \zeta^{-2}\right] + \left(\frac{dr}{d\zeta}\right)^{1/2}\frac{d^2}{d\zeta^2}\left(\frac{d\zeta}{dr}\right)^{1/2}$$

satisfies the hypotheses of Olver's[21] Theorem 9.1 (p. 458). Accordingly, (4) possesses a pair of exact solutions ψ_r, ψ_s with approximations in terms of modified Bessel functions I_m, K_m,

$$\begin{aligned}\psi_r &\sim [\zeta/(4f_0)]^{1/4}\{I_{2l+1}(K\zeta^{1/2})[1+O(K^{-2})] \\ &\quad + (B_0\zeta^{1/2}/K)I_{2l+2}(K\zeta^{1/2})[1+O(K^{-2})]\}, \qquad \text{(A7)}\\ \psi_s &\sim [\zeta/(4f_0)]^{1/4}\{K_{2l+1}(K\zeta^{1/2}) + O(|\zeta^{1/2}/K|)\},\end{aligned}$$

as $K\to\infty$ for fixed l, uniformly in a domain including the Stokes line L_0 (Fig. 2), if $f_0^{1/4}$ is that branch of $[E-U(r)]^{1/4}$ on which $[rf_0\exp(-i\pi)]^{1/4}\to U_*^{1/4}>0$ as $r\to 0$, by (2). From the properties of the Bessel functions,[21]

$$K^{-2l-1}r^{-l-1}\psi_r \quad \text{and} \quad K^{2l+1}r^l\psi_s$$

are seen to approach nonzero limits as $r\to 0$ for fixed K and l.

For angular momentum $l\geqslant 1$, ψ_s thus fails to be square integrable in the well and cannot contribute to the wave functions. The case $l=0$ will be considered at the end of this appendix.

To obtain the exponential precision needed for information on the life T, it will again suffice to combine the exact results quoted with a first approximation to ψ_r on a suitable segment of the Stokes line L_0 (Fig. 2) and to this end, a more precise version of Kramer's analysis[23] is needed: The function $rf_0^{1/2}e^{-i\pi/2} = z(r)$ is analytic on a neighborhood of the real interval of the radius r extending from 0 to near $\mathrm{Re}\, r_1$ and

$$\frac{r}{z}\frac{dz}{dr} \to \frac{1}{2} \quad \text{as } r\to 0. \tag{A8}$$

[In other words, z^2 may be thought of as a measure of the radius more directly related to the Schrödinger equation (4).] While dz/dr has a root on the domain of $z(r)$, (A8) still assures a K-independent domain Λ including the origin on which the inverse $r=r(z)$ is analytic, and for $z\in\Lambda$, the functions

$$\frac{z}{r}\frac{dr}{dz} = g(z^2) \quad \text{and} \quad \frac{1}{g(z^2)}$$

are also analytic. For fixed angular momentum l, the root r_0 of $U_l(\mathrm{r}) - \mathrm{E}$ is

$$r_0 = \frac{l(l+1)}{K^2U_*}\left[1+O\left(\frac{l(l+1)}{K^2}\right)\right],$$

by (2) and (4), and Λ therefore contains $z(r_0)$ and the image of a segment of the Stokes line L_0 (Fig. 2), and so does a subdomain $\Lambda_0\subset\Lambda$ on which $|g|$ is bounded. As $z\to 0$ in Λ, moreover,

$$z^{-2}(2g^{-1}-1) = h(z^2) \to \lim_{r\to 0}[E-U(r)-r^{-1}U_*]/U_*,$$

so that $h(z^2)$ is also analytic for $z\in\Lambda$ and $|h|$ and $|h'|$ are bounded for $z\in\Lambda_0$. Furthermore,

$$\zeta^{1/2}e^{-i\pi/2} = \int_0^z g(t^2)dt = \eta(z),$$

and from (A7),

$$\begin{aligned}\psi_r &\sim (\pi K)^{-1/2}f_0^{-1/4}e^{(l+3/4)\pi i} \\ &\quad \times\cos[K\eta - (l+\tfrac{3}{4})\pi + O(|K\eta|^{-1})] \qquad \text{(A9)}\end{aligned}$$

on a neighborhood of L_0 within Λ_0.

While (A9) looks like a wave representation of ψ_r, it is important[23] that η differs slightly from the natural wave variable ξ_0 of (4) defined by (A1). If

$$r^2e^{-i\pi}F_0(r) = y^2$$

[so that y^2 may be thought of as a measure of $r-r_0$ more directly related to the Schrödinger equation (4)], then

$$z^2 = y^2 + \lambda^2, \quad \text{with } \lambda^2 = l(l+1)/K^2 = \text{const.}$$

and from (A1),

$$e^{-i\pi/2}\frac{d\xi_0}{dr} = \frac{y}{r},$$

$$e^{-i\pi/2}\frac{d\xi_0}{dy} = \frac{y^2g(z^2)}{z^2} = g(z^2)\left[1-\left(\frac{\lambda}{z}\right)^2\right],$$

and if $2\lambda^2/z^2 = d\psi/dy$, then

$$\psi(y) - \psi(0) = \pi\lambda - 2\lambda\,\mathrm{arccot}(y/\lambda)$$

and

$$e^{-i\pi/2}\frac{d\xi_0}{dy} + \frac{d\psi}{dy} = g(z^2)[1+\lambda^2h(z^2)].$$

Therefore,

$$\begin{aligned}&e^{-i\pi/2}\xi_0(r(y)) + \psi(y) - \psi(0) - \eta(y) \\ &\quad = \int_0^y \{g(t^2+\lambda^2)[1+\lambda^2h(t^2+\lambda^2)] - g(t^2)\}dt \\ &\quad = \lambda^2\int_0^y g(t^2)\left\{h(t^2) + \frac{g'}{g} + O(\lambda^2)\right\}dt.\end{aligned}$$

Since $g'(t^2)/g(t^2) = -tg(t^2)(h+\frac{1}{2}th')$ is also bounded for $t\in\Lambda_0$,

$$\begin{aligned}&e^{i\pi/2}\xi_0(r) + \psi(y(r)) - \psi(0) = \eta(y(r)) + O(\lambda^2|\eta(y)|) \\ &\quad \text{as } \lambda^2 = l(l+1)/K^2\to 0, \qquad \text{(A10)}\end{aligned}$$

for $z = r^{1/2}[E-U(r)]^{1/4}\in\Lambda_0$. Note that this estimate holds uniformly on K-independent domains of the radius r that

contain the origin and on which $g = (z/r)dr/dz$, $h(z^2)$ and h' are analytic and bounded. By contrast, estimates restricting attention to small $|r|$ leave larger error-order terms in the quantization rule.

The approximation (A4) describes the wave pair (u_0, v_0) on a neighborhood of L_0-segments on which $|\xi_0|$ has positive lower bounds, and there $f_0(r)/F_0(r) = 1 + \lambda^2/y^2 = 1 + O(K^{-2})$ and $\eta(y(r)) = \eta(z(r)) + O(\lambda^2)$ so that (A9) and (A10) show the approximate ξ_0-wave representation of ψ_r to be there

$$\psi_r \sim (\pi K)^{-1/2} F_0^{-1/4} e^{(l+3/4)\pi i} \times \cos[K\xi_0 e^{-\pi i/2} - \pi/4 - \pi\sigma(l) + O(|K\xi_0|^{-1})], \tag{A11}$$

with

$$\sigma(l) = l + \tfrac{1}{2} - [l(l+1)]^{1/2}. \tag{A12}$$

Comparison with (10) and (A4) now shows

$$R = e^{-i\pi(1/2+2\sigma)} + O(K^{-1}).$$

This result is again insufficient for any information on the life T, but since the wave function ψ_r is again normalizable to be real for real E and r, it follows again that $|R| = 1$ exactly for real E and therefore

$$R = e^{-i\pi(1/2+2\sigma)} \exp[iK^{-1}\Sigma_0(E,K)], \tag{A13}$$

with Σ_0 still analytic in E on D_E, bounded as $K \to \infty$ and real for real E.

For $l = O(K)$, this result contains (A6) and it appears a plausible conjecture that (A13) holds for all angular momenta because the root r_0 of $U_l - E$ moves with increasing l close to the point where order and argument of the Bessel function in (A7) are equal, and for large order $2l + 1$, that is a turning point where the Bessel function has an Airy representation[21] corresponding to that encountered in (A3). A unified representation of the wave function ψ_r for all angular momenta might therefore exist, and would yield a further clarification of the quantization rules.

Since a uniform approximation of ψ_r up to the central singularity $r = 0$ of the potential (which is not mapped on any ξ_0) is obtainable only in terms of $\zeta^{1/2} = i\eta$, this is the variable used in the mathematical theory[21]; besides, ξ_0 differs from η only by correction terms tending to zero in the wave region as $K \to \infty$, and mathematical usage favors simple variables uncontaminated by correction terms. That can be shortsighted, for in terms of η, the wave representation of ψ_r is given already by (A9), but the corresponding reflection coefficient

$$R_\eta = e^{-3\pi i/2} \exp[iK^{-1}\Sigma_\eta(E,K)]$$

is quite different from (A6) and agrees with (A13) only for $l = 0$. Its use in the eigencondition would lead to an integer quantization rule, unless proper account, after all, is taken of the difference between ξ_0 and η.

The case of zero angular momentum $l = 0$ is exceptional in that a treatment of reflection on the basis of (1) is dependent on the premise that (1) can be regraded as valid uniformly for $r > 0$. If that is accepted and if the usual[20] (p. 103) condition $\psi(0) = 0$ is applied, the case $l = 0$ will be seen to be included in the analysis just given. For $l \geq 1$, the premise is only that (1) can be extended into the core to radii $\ll K^{-2}$.

APPENDIX B: PROOF OF EIGENVALUES

A useful approach to the determination of the eigenvalues may be based on the analytic dependence of the scattering structure on the energy E, which follows directly from Schrödinger's equation (4). To this end, the dependence on E of the characteristic form of (11) will now be considered for fixed quantum numbers n, l and for a *fixed*, large wave-number scale K such that $\min_{r\in\mathbb{R}} U_l(r) = U_{\min}$ has a negative upper bound and $-a < E_r(n) + a < \max_{r\in\mathbb{R}} U_l(r) = U_M$ for some fixed, small $a > 0$.

As connection functionals, Ω and Σ_j for $j = 0,1,2$ are analytic in E on the intersection D_E of the domains on which the turning points $r_s(E)$ and their derivatives dr_s/dE are defined for $s = 0$, 1, and 2 by

$$U_l(r_s(E)) = E.$$

Since the domain of $U(r)$ is assumed (Sec. II) to include $(0, \infty)$ and the r_s are real positive for real $E \in (U_{\min}, U_M)$, D_E contains a neighborhood of that real E interval. Admittedly, r_0 may be within distance $O(K^{-2})$ of the singular point $r = 0$ of $U(r)$, but then $dr_0/dE = O(K^{-4})$ only, so that no severe restriction on D_E arises therefrom. Accordingly,

$$D_E \supset \{0 < \mathrm{Re}\, E < U_M - a,\ |I_m E| < \delta_s\} = S, \tag{B1}$$

for some $\delta_s > 0$ and independent of K. A close, lower bound for the width $2\delta_s$ of the strip S (Fig. 3) of analyticity of the connection functionals would be pleasing, but must depend on closer specification of the potential $U(r)$ within the very general class admitted in Sec. II.

From (16), since $F = U_l(r) - E = 0$ at $r = r_s(E)$,

$$\xi'_w(E) = \frac{1}{2}\int_{r_0(E)}^{r_1(E)} [F_0(r)]^{-1/2} \frac{\partial F_0}{\partial E}\, dr$$

also exists on D_E, and for real E_r,

$$\xi'_w(E_r, K) = \frac{1}{2} e^{i\pi/2} \int_{r_0}^{r_1} |E_r - U_l(r)|^{-1/2}\, dr \neq 0. \tag{B2}$$

The phase integral (17) is similarly analytic on the strip S; admittedly, it has a singular point at $E = 0$, but this singularity has no adverse effect on the following and places no additional restriction on δ_s.

The reflection coefficient R is also analytic on S, by (18), and it cannot have a root in S. The common factor γ_0 in (14) and (15) is[27] $\exp[-K(\xi_b + \xi_w)]\{1 + O(K^{-1})\}$, and since ξ_b and ξ_w are analytic, γ_0^{-1} cannot vanish either in S. Ac-

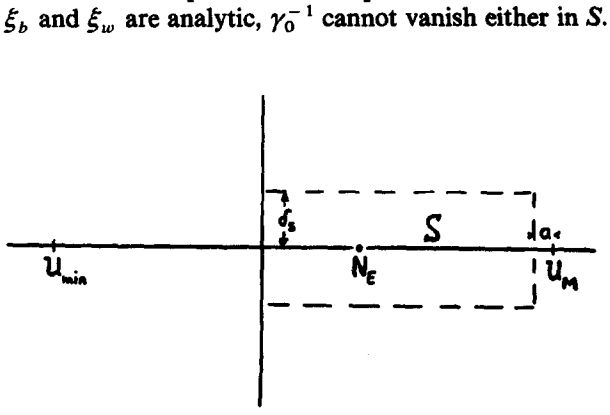

FIG. 3. The strip S in the complex E plane, and a disk N_E.

cordingly, Δ_0 and Δ_1 (Sec. VI) are also analytic on S and any eigenvalue of life $T > \hbar(2\delta_s U_m)$ must be a root of $\Delta_0 + \Delta_1$ in S (unless Re E differs from U_M by less than the arbitrarily small $a > 0$) and conversely, any root of $\Delta_0 + \Delta_1$ in S is an eigenvalue.

The quantization rule (20) assures precisely one real root E_r of Δ_0 in S for the given n and by (B2), it is a simple root. Since Δ_0 is effectively a function of KE, rather than E, there is a $\delta > 0$ and independent of K such that the function $\Delta_0(E)$ maps any disk N_E about E_r of radius $< \delta/K$ one-to-one onto an image N_Δ with simply connected boundary ∂N_Δ. A choice of the disk radius as small as

$$|K\xi'_w(E_r)|^{-1} \exp[-K\xi_b(E_r)] = \delta_E$$

suffices to assure $|\Delta_1/\Delta_0| < 1$ on ∂N_Δ and, since $\xi_b(E_r) > 0$, even moderately large K will make $\delta_E < \delta_s$ and $< \delta/K$. By Rouché's theorem, accordingly, $\Delta_0 + \Delta_1$ must have precisely one, simple root E_n in the small disk N_E of radius δ_E about E_r.

Conversely, ξ'_w is pure imaginary and ξ'_b, real, at real E, so that a positive $\delta_1 \leqslant K\delta_s$ and independent of K assures $|\Delta_0| > 0$ and Re $\xi_b \geqslant \alpha > 0$ in S for $0 < |\text{Im } E| \leqslant \delta_1/K$. If an eigenvalue E_* of multiplicity p can be found in S (Fig. 3), then any disk about E_* of radius d_1/K (with d_1 independent of K) must have a perimeter on which $\Delta(E)$ winds p times around the origin and on which $|\Delta_1/(\Delta_0 + \Delta_1)| < 1$, provided d_1 is small enough, but exceeds a sufficient multiple of $\exp(-2K\alpha/p)$. By Rouché's theorem, such a disk must contain a root of $\Delta_0(E)$. For large K, a choice making $d_1 < \delta_1/2$ can assure all this and hence, if E_* is not one of the eigenvalues E_n, then $d_1/K + |\text{Im } E_*| > \delta_1/K$, so that E_* has relatively short life

$$T < \hbar K/(\delta_1 U_M) \approx r_m \delta_1^{-1}(2m/U_m)^{1/2}$$

(Fig. 1).

The condition Re $E < U_M - a$ with fixed $a > 0$ is sufficient for these proofs, but unlikely to be necessary, because Re $\xi_b \geqslant 0$ for real $E \leqslant U_M$, while $|\xi'_w| \to \infty$ as $E \to U_M$, so that the conjecture is plausible that a could be replaced by a/K to carry the preceding arguments even closer to the potential-barrier top. A proof of this extension, however, would require a closer analysis of the functions Σ_j and Ω than appears profitable, since a different representation of the scattering coefficients is more effective for the study of barrier-top phenomena.

APPENDIX C: EIGENVALUE APPROXIMATIONS

The full, quasistationary quantization rule (23) has the exact representation

$$\exp[-2K\xi_w(E_n) + (2n + 1 + 2\sigma)\pi i - i\Sigma(E_n)/K + \nu e^{-K\xi_b(E_n)} - \nu e^{-K\xi_b(E_n)}] = 1 + (i-1)\exp(-2K\xi_b(E_n) + i\omega(E_n)/K), \quad \text{(C1)}$$

where $\Sigma = \Sigma_0 + \Sigma_1 - \Sigma_2$, $\omega = -\Sigma_1 - iK \log(1 + \Omega/K)$, and for the sake of clarity of structure, the notation suppresses the residual dependence of ξ_w, ξ_b, Σ, and ω upon K, since the main K dependence has, for large enough K, already been made explicit. In the redundant terms, ν is a number independent of E and K. The following addresses the situation in which K is large enough and the energy level is kept sufficiently below the barrier top for $|\xi_b(E)|$ not to be small.

A procedure adequate for the proof of Appendix B was to define an $E_r(n)$ by a direct extension

$$2K\xi_w(E_r) = (2n + 1 + 2\sigma)\pi i - i\Sigma(E_r)/K \quad \text{(C2)}$$

of the bound-state quantization rule to quantum numbers n and energies E_r beyond those at which bound levels can exist. If now $\Sigma(E_r)$ is to be determined quantitatively, e.g., by its complete asymptotic expansion with respect to K, then

$$2K\xi_w(E_r) = (2n + 1 + 2\sigma)\pi i - i\Sigma(E_r)/K + \nu e^{-K\xi_b(E_r)} \quad \text{(C3)}$$

is entirely equivalent to (C2) in the standard mathematical sense of asymptotics. If (C3) determines E_r, then (C1) becomes

$$\exp[2K\{\xi_w(E_r) - \xi_w(E_n)\} + iK^{-1}\{\Sigma(E_r) - \Sigma(E_n)\} - \nu e^{-2K\xi_b}] = 1 + (i-1)\exp(-2K\xi_b(E_n) + i\omega(E_n)/K), \quad \text{(C4)}$$

and since ξ_w and Σ are analytic, $|E_n - E_r|$ must be very small and an obvious, close approximation to exp[ ] in (C4) is 1 + [ ], while a consistent approximation to the braces is that linear in $(E_n - E_r)$, so that

$$2K(E_r - E_n)\xi'_w(E_r)\{1 + i\Sigma'(E_r)/(2K^2\xi'_w)\} - \nu e^{-2K\xi_b} \sim (i-1)e^{-2K\xi_b}\{1 + O(K^{-1})\},$$

with primes denoting again d/dE. From (B2), $\xi'_w = i|\xi'_w|$, and to the same order of approximation,

$$E_n - E_r \sim -\frac{1 + (1-\nu)i}{2K|\xi'_w|} e^{-2K\xi_b(E_r)}\{1 + O(K^{-1})\}, \quad \text{(C5)}$$

instead of (22). Of course, the rough steps from (C4) to (C5) could be improved to match the accuracy of those from (C1) to (C4) by working out the full asymptotic expansion

$$\left\{1 + \sum_1^\infty c_n K^{-n}\right\}$$

of the brace in (C5), but this would not change the factors in front of the brace.

The choice $\nu = 1/2$ gives Connor and Smith's[4-6] first approximation for life and linewidth, but of course, the standard mathematical sense of approximation in terms of expansions or series admits any other number ν equally well!

Mild objections to an arbitrary choice of ν arise when it is observed that (C3) does not determine a strictly real $E_r(n)$, unless ν is purely imaginary. A desire to preserve the complex-conjugate symmetry structure in the energy plane created by conservation of probability suggests that only such ν should, perhaps, be used. In that case, ν influences only Re$(E_n - E_r)$ in (C5), and all that we have done by the introduction of the redundant terms into (C1) and their subsequent use in (C3) and (C5) was to shift a correction term from the first step (C3) of approximation to the second step (C5) or vice versa. Indeed, $\nu = -i$ is an attractive choice annihilating Re$(E_n - E_r)$ to first order, and if the procedure is executed a little more systematically, it permits us to deter-

mine $E_r(n)$ from a modification of (C3) so that $E_r(n) = \mathrm{Re}\, E_n$, exactly. Whether that be the most rational guideline for the organization of the approximation procedure, must depend largely on taste or special cases. The choice $\nu = 0$ in Sec. VI served only the purpose of easing the reader's task by writing the first step (20) as a literal extension of the familiar quantization rule.

The point to be noted is how, in a context demanding exponential precision, whether by rigor or *defacto*, the customary approximation rules, proven universally reliable over many generations and proven "mathematically correct," can become unreliable to an unsettling degree. Similarly disturbing issues arise in the application of numerical analysis in such a context.

It may be appropriate to add here that the apparent discrepancy between (21) and the formula[4–6] of Connor and Smith has prompted careful checks on the calculations reported here and earlier,[27] which have shown (21) to be not misprinted; with the exact interpretation of (20), it is the correct first approximation for long life. Connor and Smith,[6] on the other hand, have demonstrated numerically that just the right use of their different formula can produce results of remarkable, quantitative excellence. The present study does not go far enough to indicate more than a glimmer of the reason for that; the exact result (23) holds the key.

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Charged particles with a short-range force: Perturbation theory with respect to the range and to additional effects

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Previously derived Blatt–Jackson type formulas for Coulomb corrected scattering lengths are generalized to include the effect of an additional strong interaction potential in first Born approximation. It is shown that the strong model dependence on the hadronic interaction is considerably reduced as soon as the finite extent of the charge is taken into account.

I. INTRODUCTION

From the point of view of experiment, charged particles are particularly suited for the investigation of the interaction between hadrons. On the theoretical side, however, this raises the problem of combining (resp. disentangling) the proper short-range hadronic forces from the electromagnetic ones. Here it is important[1] to take into account not only the Coulomb force but also other effects such as vaccum polarization and electromagnetic orbit–orbit interactions.

The theoretical questions raised by this superposition of forces are characterized by the fact that the effective expansion parameter e^2/k of the Coulomb interaction becomes large at small energies. The Coulomb effect at low energies eludes a perturbative treatment. This is particularly significant in the discussion of hadronic interactions in the low-energy limit; see, e.g., the Landau–Smorodinski version for charged particles of the effective range expansion for the scattering phase shift. To deal with this situation it is helpful that one can treat in closed form the superposition of the Coulomb force with part of the short-range interaction in the zero-range limit. This treatment[2–4] not only gives approximate formulas for scattering amplitudes, scattering lengths, level shifts in mesonic atoms, etc., but also a systematic expansion for the corrections due to finite range of the hadronic forces. To make the approach—of expansions around zero range—into a practical tool for the discussion of charged few-body systems it is desirable to further include other "small" but not necessarily short-range effects such as the non-Coulomb electromagnetic forces in a systematic way. Earlier studies of the scattering length in particular models have indicated that such effects should be significant, e.g., in discussion of the charge symmetry of the nucleon–nucleon system. In the present paper we present a consistent theoretical method for their inclusion as perturbations of the zero-range-plus-Coulomb model and exemplify this method for the scattering length.

Based on appropriate scaling techniques (following the low-energy expansion in Ref. 5) we generalize previously derived Blatt–Jackson type formulas for Coulomb corrected scattering lengths by including the effect of an additional strong interaction potential in first Born approximation. Our main results show that under the assumption of charge symmetry the strong model dependence on the hadronic interaction inherent in Blatt–Jackson type formulas if point charges are considered is strongly reduced as soon as the finite extent of the charge (described by a suitable charge form factor) is taken into account.

In Sec. II we first treat strongly interacting particles and extend some of the results in Refs. 2 and 5 concerning the short-range (ϵ-) expansion of neutral scattering lengths. The inclusion of an additional hadronic interaction potential in first Born approximation (based on the Gell-Mann–Goldberger formula) is discussed at the end of Sec. II. Strongly interacting pointlike charged particles are considered in Sec. III. The results of Ref. 2 concerning the short-range expansion of Coulomb modified scattering lengths are extended and again an additional strongly interacting potential is treated in first Born approximation. A comparison of Coulomb modified scattering lengths and their neutral counterparts exhibits a strong model dependence on the hadronic interaction due to the pointlike character of the charges. In Sec. IV we remove the pointlike nature of the charge and explicitly introduce a charge form factor to describe the finite extent. As described above this results in a considerable reduction of the model dependence when comparing charged and neutral scattering lengths under the assumption of charge symmetry. Our final formula [cf. Eq. (4.49)] provides an extremely simple and handy tool for the comparison of the $^1S_0$ proton–proton and neutron–neutron scattering lengths. Strongly singular interactions are briefly treated in Sec. V.

II. ZERO-RANGE DISTORTED BORN APPROXIMATION

Throughout this section we assume the potential V_1 to be a real-valued measurable function on $(0,\infty)$ obeying

$$\int_0^R dr|rV_1(r)| < \infty, \quad \int_R^\infty dr\, r^2|V_1(r)| < \infty, \quad \text{for some } R > 0. \tag{2.1}$$

Given condition (2.1), the following self-adjoint Hamiltonians (defined as form sums[6]) are introduced in the Hilbert space $L^2((0,\infty))$:

$$h_0 = -\frac{d^2}{dr^2}, \quad \mathscr{D}(h_0) = H_0^{2,2}((0,\infty)) \quad \text{(Ref. 7)}, \tag{2.2}$$

$$h_1 = h_0 + V_1, \tag{2.3}$$

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$$h_1(\epsilon) = h_0 + (1 + \lambda_1\epsilon)V_1, \quad \lambda_1 \in \mathcal{R}\setminus\{0\}, \quad \epsilon > 0, \tag{2.4}$$

$$h_{1,\epsilon} = \epsilon^{-2} U_\epsilon h_1(\epsilon) U_\epsilon^{-1} = h_0 + (1 + \lambda_1\epsilon)\epsilon^{-2} V_{1,\epsilon},$$
$$\epsilon > 0, \quad V_{1,\epsilon}(r) = V_1(r/\epsilon), \tag{2.5}$$

where U_ϵ,

$$(U_\epsilon f)(r) = \epsilon^{-1/2} f(r/\epsilon), \quad \epsilon > 0, \quad f \in L^2((0,\infty)), \tag{2.6}$$

denotes the unitary scaling operator in $L^2((0,\infty))$. Of special interest are the regular $F_1(r)$, $F_1(\epsilon,r)$, $F_{1,\epsilon}(r)$ and irregular $G_1(r)$, $G_1(\epsilon,r)$, $G_{1,\epsilon}(r)$ solutions associated with (2.3)–(2.5). From now on, to avoid complex expressions, we mainly discuss the quantities associated with $h_1(\epsilon)$ [from which the one corresponding to h_1 can be obtained by taking the limit $\epsilon \to 0_+$ and those for $h_{1,\epsilon}$ are given by scaling arguments, cf. Eq. (2.5)]. As discussed in Appendix A, regular and irregular solutions associated with $h_1(\epsilon)$ uniquely fulfill the integral equations

$$F_1(\epsilon,r) = r - \int_0^r dr'(r' - r)(1 + \lambda_1\epsilon)V_1(r')F_1(\epsilon,r'), \tag{2.7}$$

$$F_1(\epsilon,r) = \mathcal{F}_1(\epsilon)r - \int_0^\infty dr'\, \hat{g}_0(r,r')(1 + \lambda_1\epsilon)V_1(r')F_1(\epsilon,r'), \tag{2.8}$$

$$G_1(\epsilon,r) = 1 + \int_r^\infty dr'(r' - r)(1 + \lambda_1\epsilon)V_1(r')G_1(\epsilon,r'), \tag{2.9}$$

where

$$\hat{g}_0(r,r') = \begin{cases} r', & r' \leqslant r, \\ r, & r' \geqslant r, \end{cases} \tag{2.10}$$

denotes the "unperturbed" Fredholm Green's function associated with h_0 and $\mathcal{F}_1(\epsilon)$ is the Jost function corresponding to $h_1(\epsilon)$, i.e.,

$$\mathcal{F}_1(\epsilon) = 1 + \int_0^\infty dr(1 + \lambda_1\epsilon)V_1(r)F_1(\epsilon,r)$$
$$= W(G_1(\epsilon),F_1(\epsilon)), \tag{2.11}$$

where

$$W(G,F) = G\frac{\partial F}{\partial r} - F\frac{\partial G}{\partial r} \tag{2.12}$$

denotes the Wronskian of G and F. If $\mathcal{F}_1 \equiv \mathcal{F}_1(0) = W(G_1,F_1)$ represents the Jost function associated with h_1 we have to distinguish[5] the following.

Case I: $\mathcal{F}_1 \neq 0$. That is, h_1 has no zero-energy resonance [and hence $F_1(r)$ and $G_1(r)$ are linearly independent].

Case II: $\mathcal{F}_1 = 0$. That is, h_1 has a zero-energy resonance.[4,8–10]

In the latter case (which turns out to be the important one for applications[5]), F_1 and G_1 are multiples of each other. Therefore, in case II we introduce the irregular solution $\tilde{G}_1$ for h_1 as the unique solution of

$$\tilde{G}_1(r) = \left[\int_0^\infty dr'\, r' V_1(r')F_1(r')\right]^{-1} r$$
$$+ \int_r^\infty dr'(r' - r)V_1(r')\tilde{G}_1(r'). \tag{2.13}$$

Note that $\tilde{G}_1(r)$ fulfills $W(\tilde{G}_1,F_1) = 1$ (cf. Appendix A). In connection with Eq. (2.13) it is important that one can prove

$$\int_0^\infty dr'\, r' V_1(r')F_1(r') \neq 0 \quad \text{if} \quad \mathcal{F}_1 = 0 \tag{2.14}$$

(cf. Appendix A). This solves a problem raised in Ref. 8 (cf. also Appendix C in Ref. 10).

The importance of case II, i.e., of $\mathcal{F}_1 = 0$, for certain kinds of applications has been discussed in great detail in Ref. 5. Here it suffices to note in case II, $h_{1,\epsilon}$ describes a Hamiltonian with effective range parameter of order $O(\epsilon)$ which converges to the point-interaction Hamiltonian in $L^2((0,\infty))$ in norm resolvent sense as $\epsilon \to 0_+$ (in case I, $h_{1,\epsilon}$ converges to h_0 as $\epsilon \to 0_+$). More precisely, if r_1 denotes the effective range parameter corresponding to h_1 then as $\epsilon \to 0_+$ the effective range $r_{1,\epsilon}$ of $h_{1,\epsilon}$ obeys $r_{1,\epsilon} \underset{\epsilon \to 0_+}{=} \epsilon r_1 + O(\epsilon^2)$. As a consequence, $h_{1,\epsilon}$ is able to model hadronic interactions by choosing ϵ small enough. From now on we always assume case II ($\mathcal{F}_1 = 0$).

Next we study the low ϵ behavior of $\mathcal{F}_1(\epsilon)$. For this purpose we first note that (in case II) $\mathcal{F}_1(\epsilon,r)$ [in addition to Eq. (2.7)] also uniquely satisfies

$$F_1(\epsilon,r) = F_1(r) - \lambda_1\epsilon\int_0^r dr'\, \tilde{g}_1(r,r')V_1(r')F_1(\epsilon,r'), \tag{2.15}$$

where

$$\tilde{g}_1(r,r') = \tilde{G}_1(r)F_1(r') - \tilde{G}_1(r')F_1(r) \tag{2.16}$$

denotes the Green's function associated with h_1. Iteration of Eq. (2.15) yields

$$F_1(\epsilon,r) \underset{\epsilon \to 0_+}{=} F_1(r) - \lambda_1\epsilon\left[\int_0^r dr'\, F_1^2(r')V_1(r')\right]\tilde{G}_1(r) + \lambda_1\epsilon\left[\int_0^r dr'\, \tilde{G}_1(r')V_1(r')F_1(r')\right]F_1(r)$$
$$+ \lambda_1^2\epsilon^2\left[\int_0^r dr'\, F_1(r')V_1(r')\tilde{G}_1(r')\int_0^r dr''\, F_1^2(r'')V_1(r'')\right]\tilde{G}_1(r) - \lambda_1^2\epsilon^2\left[\int_0^r dr'\, F_1^2(r')V_1(r')\right.$$
$$\left.\times\int_0^r dr''\, F_1(r'')V_1(r'')\tilde{G}_1(r'')\right]\tilde{G}_1(r) - \lambda_1^2\epsilon^2\left[\int_0^r dr'\, \tilde{G}_1^2(r')V_1(r')\int_0^r dr''\, F_1^2(r'')V_1(r'')\right]F_1(r)$$
$$+ \lambda_1^2\epsilon^2\left[\int_0^r dr'\, F_1(r')V_1(r')\tilde{G}_1(r')\int_0^r dr''\, F_1(r'')V_1(r'')\tilde{G}_1(r'')\right]F_1(r) + O(\epsilon^3), \tag{2.17}$$

where by the relations analogous to those of (A4)–(A15) in Appendix A, $(1 + r)^{-1}O(\epsilon^3)$ is uniformly bounded with respect to $r \geqslant 0$. Obviously $F_1(\epsilon,r)$ is entire in ϵ,r. Inserting expansion (2.17) into Eq. (2.11), observing $\mathcal{F}_1 = 0$, (2.1) and Lebesgue's dominated convergence theorem after some integrations by parts yield

$$\mathscr{F}_1(\epsilon) \underset{\epsilon\to 0_+}{=} -\lambda_1\epsilon\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^{-1}\int_0^\infty dr\, F_1^2(r)V_1(r) + \lambda_1^2\epsilon^2\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^{-1}$$
$$\times\left\{\int_0^\infty dr\, F_1'(r)\tilde{G}_1'(r)\int_0^r dr'\,[F_1'(r')]^2 - \int_0^\infty dr\,[F_1'(r)]^2\int_0^r dr'\, F_1'(r')\tilde{G}_1'(r')\right\} + O(\epsilon^3). \tag{2.18}$$

Clearly $\mathscr{F}_1(\epsilon)$ is entire with respect to ϵ.

By scaling arguments, Eqs. (2.7) and (2.11) imply

$$F_{1,\epsilon}(\epsilon r) = \epsilon F_1(\epsilon,r), \tag{2.19}$$

$$\mathscr{F}_{1,\epsilon} = \mathscr{F}_1(\epsilon), \tag{2.20}$$

$$G_{1,\epsilon}(\epsilon r) = G_1(\epsilon,r), \tag{2.21}$$

where the left-hand sides of Eqs. (2.19)–(2.21) correspond to $h_{1,\epsilon}$.

Moreover, introducing the scattering length $a_1(\epsilon)$ associated with $h_1(\epsilon)$ (cf. Appendix C) we get for ϵ small enough

$$a_1(\epsilon) = [\mathscr{F}_1(\epsilon)]^{-1}(1+\lambda_1\epsilon)\int_0^\infty dr\, rV_1(r)F_1(\epsilon,r). \tag{2.22}$$

Equations (2.19) and (2.20) imply

$$a_{1,\epsilon} = \epsilon a_1(\epsilon), \tag{2.23}$$

where $a_{1,\epsilon}$ denotes the scattering length corresponding to $h_{1,\epsilon}$. In particular, Eqs. (2.17), (2.18), (2.22), and (2.23) finally yield

$$a_{1,\epsilon} \underset{\epsilon\to 0_+}{=} \left[-\lambda_1\int_0^\infty dr\, F_1^2(r)V_1(r)\right]^{-1}\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^2 - \epsilon\left[\int_0^\infty dr\, F_1^2(r)V_1(r)\right]^{-1}\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^2$$
$$+\epsilon\left[\int_0^\infty dr\, F_1^2(r)V_1(r)\right]^{-1}\int_0^\infty dr\, rV_1(r)F_1(r)\left\{\int_0^\infty dr\, rV_1(r)\tilde{G}_1(r)\int_0^r dr'\, F_1^2(r')V_1(r') - \int_0^\infty dr\, rV_1(r)F_1(r)\int_0^r dr'\right.$$
$$\left.\times\tilde{G}_1(r')V_1(r')F_1(r')\right\} - \epsilon\left[\int_0^\infty dr\, F_1^2(r)V_1(r)\right]^{-2}\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^2\left\{\int_0^\infty dr\, F_1'(r)\tilde{G}_1'(r)\int_0^r dr'\,[F_1'(r')]^2\right.$$
$$\left.-\int_0^\infty dr\,[F_1'(r)]^2\int_0^r dr'\, F_1'(r')\tilde{G}_1'(r')\right\} + O(\epsilon^2) \underset{\epsilon\to 0_+}{\equiv} a_1^{(0)} + \epsilon a_1^{(1)} + O(\epsilon^2). \tag{2.24}$$

As has been discussed in Ref. 5, $a_1^{(0)}$ represents the scattering length of the point interaction Hamiltonian mentioned above. For the generalization of the result (2.24) to non-spherically symmetric interactions cf. Refs. 2 and 5. At this point we note that $a_{1,\epsilon}$ would be of order $O(\epsilon)$ as $\epsilon\to 0_+$ if one considers case I ($\mathscr{F}_1 \neq 0$) instead of case II ($\mathscr{F}_1 = 0$).

In order to take into account leading-order effects of an additional potential gV_2, $g\in\mathscr{R}$, we assume V_2 to be a real measurable function obeying

$$\int_0^R dr|V_2(r)| < \infty, \quad \int_R^\infty dr\, r^2|V_2(r)| < \infty$$
$$\text{for some } R > 0. \tag{2.25}$$

We define the form sum in $L^2((0,\infty))$

$$h_\epsilon(g) = h_{1,\epsilon} + gV_2, \tag{2.26}$$

and note that the regular solution associated with $h_\epsilon(g)$ fulfills

$$F_\epsilon(g,r) = F_{1,\epsilon}(r) - g\int_0^r dr'\, g_{1,\epsilon}(r,r')V_2(r')F_\epsilon(g,r'), \tag{2.27}$$

where

$$g_{1,\epsilon}(r,r') = G_{1,\epsilon}(r)F_{1,\epsilon}(r') - G_{1,\epsilon}(r')F_{1,\epsilon}(r). \tag{2.28}$$

By the Gell-Mann–Goldberger formula (cf. Appendix C), $a_\epsilon(g)$, the scattering length associated with $h_\epsilon(g)$ for ϵ and $|g|$ small enough, is given by

$$a_\epsilon(g) = a_{1,\epsilon} + a_{12,\epsilon}(g), \tag{2.29}$$

where

$$a_{12,\epsilon}(g) = g\int_0^\infty dr\,\frac{F_{1,\epsilon}(r)}{\mathscr{F}_{1,\epsilon}}V_2(r)\frac{F_\epsilon(g,r)}{\mathscr{F}_{12,\epsilon}(g)} \tag{2.30}$$

and

$$\mathscr{F}_{12,\epsilon}(g) = W(G_\epsilon(g),F_\epsilon(g))$$
$$= \mathscr{F}_{1,\epsilon} + g\int_0^\infty dr\, G_{1,\epsilon}(r)V_2(r)F_\epsilon(g,r). \tag{2.31}$$

Clearly, $F_\epsilon(g,r)$ as well as $\mathscr{F}_{12,\epsilon}(g)$ are entire in g (applying, e.g., Poincare's theorem[11] and dominated convergence) and thus for ϵ small enough, $a_{12,\epsilon}(g)$ is analytic in g around $g=0$. The leading contribution is given by the so-called Born term $a_{12,\epsilon}^{\mathrm{B}}(g)$

$$a_{12,\epsilon}^{\mathrm{B}}(g) = g\int_0^\infty dr\left[\frac{F_{1,\epsilon}(r)}{\mathscr{F}_1(\epsilon)}\right]^2 V_2(r). \tag{2.32}$$

Equation (2.8) and (2.18)–(2.20) then imply ($r' = \epsilon r''$)

$$\frac{F_{1,\epsilon}(r)}{\mathscr{F}_{1,\epsilon}} = r - (1+\lambda_1\epsilon)\int_0^{r/\epsilon} dr''\, r''V_1(r'')\frac{\epsilon F_1(\epsilon,r'')}{\mathscr{F}_{1,\epsilon}}$$
$$-(1+\lambda_1\epsilon)r\int_{r/\epsilon}^\infty dr''\, V_1(r'')\frac{F_1(\epsilon,r'')}{\mathscr{F}_{1,\epsilon}}$$
$$\underset{\epsilon\to 0_+}{=} r + \left[\lambda_1\int_0^\infty dr\, F_1^2(r)V_1(r)\right]^{-1}$$
$$\times\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^2$$
$$-(1+\lambda_1\epsilon)r\int_{r/\epsilon}^\infty dr'\, V_1(r')\frac{F_1(\epsilon,r')}{\mathscr{F}_1(\epsilon)} + O(\epsilon), \tag{2.33}$$

where $O(\epsilon)$ is uniformly bounded with respect to $r \geqslant 0$ by the remark following expansion (2.17) and by condition (2.1).

Since

$$\left|(1+\lambda_1\epsilon)r\int_{r/\epsilon}^{\infty} dr'\, V_1(r')\frac{F_1(\epsilon,r')}{\mathscr{F}_1(\epsilon)}\right| < \text{const}\left(\frac{r}{\epsilon}\right)\left[1+\left(\frac{r}{\epsilon}\right)\right]^{-1}\int_{r/\epsilon}^{\infty} dr'\, r'(1+r')|V_1(r')|, \tag{2.34}$$

we obtain

$$\frac{F_{1,\epsilon}(r)}{\mathscr{F}_{1,\epsilon}} \underset{\epsilon\to 0_+}{=} r + \left[\lambda_1\int_0^{\infty} dr\, F_1^2(r)V_1(r)\right]^{-1} \times\left[\int_0^{\infty} dr\, rV_1(r)F_1(r)\right]^2 + o(1) \underset{\epsilon\to 0_+}{=} r - a_1^{(0)} + o(1), \tag{2.35}$$

where $o(1)$ is uniformly bounded with respect to $r \geqslant 0$. Applying Lebesgue's dominated convergence theorem finally proves

$$a_{12}^{\mathrm{B}}(g) = g\int_0^{\infty} dr\,[r - a_1^{(0)}]^2 V_2(r) + go(1) \tag{2.36}$$

and thus

$$a_\epsilon(g) \underset{\substack{\epsilon\to 0_+\\ g\to 0}}{=} a_1^{(0)} + \epsilon a_1^{(1)} + g\int_0^{\infty} dr\,[r - a_1^{(0)}]^2 V_2(r) + O(\epsilon^2) + go(1) + O(g^2), \tag{2.37}$$

where $a_1^{(j)}$, $j = 0,1$ are defined in Eq. (2.24).

In case V_2 is nonlocal and/or contains a velocity depending part[1], $a_{12,\epsilon}^{\mathrm{B}}(g)$ in Eqs. (2.36) and (2.37) has to be rewritten in the form

$$a_{12,\epsilon}^{\mathrm{B}}(g) = g\int_0^{\infty} r^2\, dr\, \psi(r)(V_2\psi)(r), \tag{2.38}$$

with

$$\psi(r) = 1 - a_1^{(0)} r^{-1}. \tag{2.39}$$

In particular, if V_2 is local but nonspherically symmetric, Eq. (2.36) can be generalized to

$$a_{12,\epsilon}^{\mathrm{B}}(g) = g(4\pi)^{-1}\int_{\mathscr{R}^3} d^3x\, \psi^2(|\mathbf{x}|)V_2(\mathbf{x}), \tag{2.40}$$

under suitable conditions on V_2.

III. COULOMB-PLUS-ZERO-RANGE DISTORTED BORN APPROXIMATION AND POINT CHARGES

In this section the real-valued potential V_1 is assumed to fulfill

$$\int_0^R dr\, r|V_1(r)| < \infty, \quad \int_R^{\infty} dr\, e^{br}|V_1(r)| < \infty, \quad \text{for some } b, R > 0. \tag{3.1}$$

Analogously to Sec. II we introduce in $L^2(0,\infty))$ the Hamiltonians (form sums)

$$h_\gamma = h_0 + \gamma r^{-1}, \quad \mathscr{D}(h_\gamma) = H_0^{2,2}((0,\infty)), \quad \gamma > 0, \tag{3.2}$$

$$h_{1,\epsilon\gamma}(\epsilon) = h_0 + \epsilon\gamma r^{-1} + \lambda_\gamma(\epsilon)V_1, \quad \epsilon > 0,$$

$$\lambda_\gamma(\epsilon) = 1 + \lambda_{10}\epsilon + \lambda_{01}\gamma\epsilon\ln\epsilon, \quad \lambda_{10}, \lambda_{01} \in \mathscr{R}, \tag{3.3}$$

$$h_{1,\gamma,\epsilon} = \epsilon^{-2}U_\epsilon h_{1,\epsilon\gamma}(\epsilon)U_\epsilon^{-1} = h_0 + \gamma r^{-1} + \lambda_\gamma(\epsilon)\epsilon^{-2}V_{1,\epsilon}, \quad \epsilon > 0, \quad V_{1,\epsilon}(r) = V_1(r/\epsilon). \tag{3.4}$$

If $F_\gamma(r)(G_\gamma(r))$ denote the (ir)regular zero-energy solutions corresponding to h_γ

$$F_\gamma(r) = \gamma^{-1/2}r^{1/2}I_1((4\gamma r)^{1/2}), \tag{3.5}$$

$$G_\gamma(r) = (4\gamma r)^{1/2}K_1((4\gamma r)^{1/2}) \tag{3.6}$$

[$I_1(z)$, $K_1(z)$ the modified Bessel functions of order one[12]], then $F_{1,\epsilon\gamma}(\epsilon,r)(G_{1,\epsilon\gamma}(\epsilon,r))$, the (ir)regular zero-energy solutions associated with $h_{1,\epsilon\gamma}(\epsilon)$, uniquely fulfill

$$F_{1,\epsilon\gamma}(\epsilon,r) = r - \int_0^r dr'(r'-r)[\lambda_\gamma(\epsilon)V_1(r') + \epsilon\gamma(r')^{-1}]F_{1,\epsilon\gamma}(\epsilon,r') \tag{3.7}$$

as well as

$$F_{1,\epsilon\gamma}(\epsilon,r) = F_1(r) - \int_0^r dr'\,\tilde{g}_1(r,r')\{[\lambda_\gamma(\epsilon)-1]V_1(r') + \epsilon\gamma(r')^{-1}\}F_{1,\epsilon\gamma}(\epsilon,r') \tag{3.8}$$

and

$$G_{1,\epsilon\gamma}(\epsilon,r) = G_{\epsilon\gamma}(r) + \lambda_\gamma(\epsilon)\int_r^{\infty} dr'\, g_{\epsilon\gamma}(r,r')V_1(r') \times G_{1,\epsilon\gamma}(\epsilon,r'), \tag{3.9}$$

$$g_{\epsilon\gamma}(r,r') = G_{\epsilon\gamma}(r)F_{\epsilon\gamma}(r') - G_{\epsilon\gamma}(r')F_{\epsilon\gamma}(r) \tag{3.10}$$

[$\tilde{g}_1(r,r')$ defined in Eq. (2.16)]. Similarly the Jost function $\mathscr{F}_{1,\epsilon\gamma}(\epsilon)$ corresponding to $h_{1,\epsilon\gamma}(\epsilon)$ reads

$$\mathscr{F}_{1,\epsilon\gamma}(\epsilon) = 1 + \lambda_\gamma(\epsilon)\int_0^{\infty} dr\, G_{\epsilon\gamma}(r)V_1(r)F_{1,\epsilon\gamma}(\epsilon,r), \tag{3.11}$$

and the Coulomb modified scattering length $a_{1,\epsilon\gamma}(\epsilon)$ is given by

$$a_{1,\epsilon\gamma}(\epsilon) = [\mathscr{F}_{1,\epsilon\gamma}(\epsilon)]^{-1}\lambda_\gamma(\epsilon)\int_0^{\infty} dr\, F_{\epsilon\gamma}(r)V_1(r)F_{1,\epsilon\gamma}(\epsilon,r), \tag{3.12}$$

as long as $\mathscr{F}_{1,\epsilon\gamma}(\epsilon) \neq 0$. By the scaling property in Eq. (3.4), by Eq. (3.7), and from

$$F_\gamma(\epsilon r) = \epsilon F_{\epsilon\gamma}(r) \underset{\epsilon\to 0_+}{=} \epsilon r + \tfrac{1}{2}\gamma(\epsilon r)^2 + O(\epsilon^3), \tag{3.13}$$

$$G_\gamma(\epsilon,r) = G_{\epsilon\gamma}(r) \underset{\epsilon\to 0_+}{=} 1 + \epsilon\gamma r\ln(\epsilon\gamma r) + [2\mathscr{C} - 1]\epsilon\gamma r + O(\epsilon^2\ln\epsilon), \tag{3.14}$$

where $\mathscr{C}$ denotes Euler's constant,[12] we get

$$F_{1,\gamma,\epsilon}(\epsilon r) = \epsilon F_{1,\epsilon\gamma}(\epsilon,r), \tag{3.15}$$

$$\mathscr{F}_{1,\gamma,\epsilon} = \mathscr{F}_{1,\epsilon\gamma}(\epsilon), \tag{3.16}$$

$$G_{1,\gamma,\epsilon}(\epsilon r) = G_{1,\epsilon\gamma}(\epsilon,r), \tag{3.17}$$

$$a_{1,\gamma,\epsilon} = \epsilon a_{1,\epsilon\gamma}(\epsilon), \tag{3.18}$$

where the quantities on the left-hand side of Eqs. (3.15)–(3.18) refer to $h_{1,\gamma,\epsilon}$.

Similar to Sec. II, $h_{1,\gamma,\epsilon}$ has a Coulomb modified effective range parameter of order $r_{1,\gamma,\epsilon} \underset{\epsilon\to 0_+}{=} \epsilon r_0 + o(\epsilon)$ as $\epsilon \to 0_+$ and hence is able to model hadronic interactions of charged particles if one considers again case II, i.e., $\mathscr{F}_1 = 0$. A care-

ful analysis shows that this is still insufficient to get nontrivial results for $a_{1,\gamma,\epsilon}$ as $\epsilon \to 0_+$.[2] In fact, the considerations following Eq. (3.21) imply that the assumption

$$\mathscr{F}_1 = 0$$

and

$$\lambda_{01} = \left[\int_0^\infty dr\, F_1^2(r) V_1(r)\right]^{-1} \int_0^\infty dr\, r V_1(r) F_1(r) \tag{3.19}$$

is needed. It turns out that if and only if both conditions in assumption (3.19) are fulfilled, $h_{1,\gamma,\epsilon}$ converges in norm resolvent sense to the Coulomb plus point interaction Hamiltonian as $\epsilon \to 0_+$. If at least one condition in (3.19) is not fulfilled, $h_{1,\gamma,\epsilon}$ simply converges to h_γ as $\epsilon \to 0_+$.[2]

Adopting conditions (3.19) for the rest of this section we now study $\mathscr{F}_{1,\gamma,\epsilon}$ as $\epsilon \to 0_+$. Iterating Eq. (3.8), one obtains

$$\begin{aligned} F_{1,\epsilon\gamma}(\epsilon,r) \underset{\epsilon\to 0_+}{=} & F_1(r) - \tilde{G}_1(r)\int_0^r dr'\, F_1^2(r')\{[\lambda_\gamma(\epsilon)-1]V_1(r') + \epsilon\gamma(r')^{-1}\} + F_1(r)\int_0^r dr'\, F_1(r')\tilde{G}_1(r') \\ & \times\{[\lambda_\gamma(\epsilon)-1]V_1(r') + \epsilon\gamma(r')^{-1}\} + \lambda_{01}^2\gamma^2\epsilon^2\ln^2\epsilon\Big\{\tilde{G}_1(r)\int_0^r dr'\, F_1(r')V_1(r')\tilde{G}_1(r')\int_0^r dr''\, F_1^2(r'')V_1(r'') \\ & - \tilde{G}_1(r)\int_0^r dr'\, F_1^2(r')V_1(r')\int_0^r dr''\, F_1(r'')\tilde{G}_1(r'')V_1(r'') - F_1(r)\int_0^r dr'\, \tilde{G}_1^2(r')V_1(r')\int_0^r dr''\, F_1^2(r'')V_1(r'') \\ & + F_1(r)\int_0^r dr'\, \tilde{G}_1(r')F_1(r')V_1(r')\int_0^r dr''\, F_1(r'')\tilde{G}_1(r'')V_1(r'')\Big\} + O(\epsilon^2\ln\epsilon), \end{aligned} \tag{3.20}$$

where $e^{-br}\,O(\epsilon^2\ln\epsilon)$ is uniformily bounded in $r>0$ for all $b>0$ by the estimates (B1) and (B2) of Appendix B. Inserting expansion (3.20) into (3.11), observing Eqs. (3.15), (3.19) and $\mathscr{F}_1 = 0$ yields by (3.1) and dominated convergence after various integrations by parts

$$\begin{aligned} \mathscr{F}_{1,\gamma,\epsilon} \underset{\epsilon\to 0_+}{=} & \gamma\epsilon[2\mathscr{C}-1]\int_0^\infty dr\, r V_1(r)F_1(r) - \lambda_{10}\epsilon\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^{-1}\int_0^\infty dr\, V_1(r)F_1^2(r) + \gamma\epsilon\ln(\gamma) \\ & \times\int_0^\infty dr\, r V_1(r)F_1(r) + \gamma\epsilon\int_0^\infty dr\, r V_1(r)F_1(r) + 2\gamma\epsilon\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^{-1}\int_0^\infty dr\, F_1(r)F_1'(r)\ln(r) \\ & + \gamma^2\epsilon^2\ln\epsilon\Big[\int_0^\infty dr\, r V_1(r)F_1^2(r)\Big]^{-2}\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^3\Big\{-\int_0^\infty dr[F_1'(r)]^2\int_0^r dr'\, F_1'(r')\tilde{G}_1'(r') \\ & + \int_0^\infty dr\, F_1'(r)\tilde{G}_1'(r)\int_0^r dr'[F_1'(r')]^2 - \int_0^\infty dr\, r V_1(r)F_1(r) + \int_0^\infty dr\, F_1^2(r)V_1(r)\Big\} + O(\epsilon^2\ln\epsilon). \end{aligned} \tag{3.21}$$

Equations (3.11), (3.12), (3.15), (3.18), and (3.21) finally imply

$$\begin{aligned} a_{1,\gamma,\epsilon} \underset{\epsilon\to 0_+}{=} & \int_0^\infty dr\, r V_1(r)F_1(r)\Big\{2\gamma\mathscr{C}\int_0^\infty dr\, r V_1(r)F_1(r) - \lambda_{10}\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^{-1}\int_0^\infty dr\, V_1(r)F_1^2(r) \\ & + \gamma\ln(\gamma)\int_0^\infty dr\, r V_1(r)F_1(r) + 2\gamma\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^{-1}\int_0^\infty dr\, F_1(r)F_1'(r)\ln(r)\Big\}^{-1} \\ & - \gamma^2\epsilon\ln^2\epsilon\Big[\int_0^\infty dr\, V_1(r)F_1^2(r)\Big]^{-2}\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^4\Big\{-\int_0^\infty dr[F_1'(r)]^2\int_0^r dr'\, F_1'(r')\tilde{G}_1'(r') \\ & + \int_0^\infty dr\, F_1'(r)\tilde{G}_1'(r)\int_0^r dr'[F_1'(r')]^2 - \int_0^\infty dr\, r V_1(r)F_1(r) + \int_0^\infty dr\, F_1^2(r)V_1(r)\Big\}\Big\{2\gamma\mathscr{C}\int_0^\infty dr\, r V_1(r)F_1(r) \\ & - \lambda_{10}\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^{-1}\int_0^\infty dr\, V_1(r)F_1^2(r) + \gamma\ln(\gamma)\int_0^\infty dr\, r V_1(r)F_1(r) + 2\gamma\Big[\int_0^\infty dr\, r V_1(r)F_1(r)\Big]^{-1} \\ & \times\int_0^\infty dr\, F_1(r)F_1'(r)\ln(r)\Big\}^{-2} + O(\epsilon\ln\epsilon) \\ \underset{\epsilon\to 0_+}{\equiv} & a_{1,\gamma}^{(0)} + (\epsilon\ln^2\epsilon)a_{1,\gamma}^{(1)} + O(\epsilon\ln\epsilon). \end{aligned} \tag{3.22}$$

A comparison with Ref. 2 (where also nonspherically symmetric interactions V_1 are discussed) shows that $a_{1,\gamma}^{(0)}$ represents the Coulomb modified scattering length of the Coulomb plus point interaction Hamiltonian. Again we are interested to take into account in leading order of the coupling constant g the effect of an additional (real-valued) potential gV_2, $g\in\mathscr{R}$. Assuming

$$\int_0^R dr|V_2(r)| < \infty, \quad \int_R^\infty dr\, e^{br}|V_2(r)| < \infty, \quad \text{for some } b,R>0, \tag{3.23}$$

we introduce in $L^2((0,\infty))$ the form sum

$$h_{\gamma,\epsilon}(g) = h_{1,\gamma,\epsilon} + gV_2. \tag{3.24}$$

The regular zero-energy solution associated with $h_{\gamma,\epsilon}(g)$ fulfills

$$F_{\gamma,\epsilon}(g,r) = F_{1,\gamma,\epsilon}(r) - g\int_0^r dr'\, g_{1,\gamma,\epsilon}(r,r')V_2(r')F_{\gamma,\epsilon}(g,r'), \tag{3.25}$$

where

$$g_{1,\gamma,\epsilon}(r,r') = G_{1,\gamma,\epsilon}(r)F_{1,\gamma,\epsilon}(r') - G_{1,\gamma,\epsilon}(r')F_{1,\gamma,\epsilon}(r). \tag{3.26}$$

As discussed at the end of Appendix C the Gell-Mann–Goldberger formula for $a_{\gamma,\epsilon}(g)$, the Coulomb modified scattering length associated with $h_{\gamma,\epsilon}(g)$, reads for ϵ and $|g|$ small enough

$$a_{\gamma,\epsilon}(g) = a_{1,\gamma,\epsilon} + a_{12,\gamma,\epsilon}(g), \tag{3.27}$$

where

$$a_{12,\gamma,\epsilon}(g) = g\int_0^\infty dr \frac{F_{1,\gamma,\epsilon}(r)}{\mathscr{F}_{1,\gamma,\epsilon}} V_2(r) \frac{F_{\gamma,\epsilon}(g,r)}{\mathscr{F}_{12,\gamma,\epsilon}(g)} \tag{3.28}$$

and

$$\mathscr{F}_{12,\gamma,\epsilon}(g) = \mathscr{F}_{1,\gamma,\epsilon} + g\int_0^\infty dr\, G_{1,\gamma,\epsilon}(r)V_2(r)F_{\gamma,\epsilon}(g,r). \tag{3.29}$$

Again by Poincaré's theorem,[11] $F_{\gamma,\epsilon}(g,r)$ and $\mathscr{F}_{12,\gamma,\epsilon}(g)$ are entire with respect to g. Since $\mathscr{F}_{12,\gamma,\epsilon}(g)$ and $\mathscr{F}_{1,\gamma,\epsilon}$ are nonzero for ϵ small enough, $a_{12,\gamma,\epsilon}(g)$ is analytic in g around $g=0$ and we introduce the Born term $a^{\mathrm{B}}_{12,\gamma,\epsilon}(g)$

$$a^{\mathrm{B}}_{12,\gamma,\epsilon}(g) = g\int_0^\infty dr \left[\frac{F_{1,\gamma,\epsilon}(r)}{\mathscr{F}_{1,\gamma,\epsilon}}\right]^2 V_2(r). \tag{3.30}$$

With the help of the Fredholm integral equation for $F_{1,\gamma,\epsilon}(r)$ we obtain by Eqs. (3.13)–(3.16) and (3.21) (cf. Sec. II)

$$\begin{aligned} F_{1,\gamma,\epsilon}(r)/\mathscr{F}_{1,\gamma,\epsilon} &\underset{\epsilon\to 0_+}{=} F_\gamma(r) - G_\gamma(r)\{A\}^{-1}\int_0^\infty dr'\, r'V_1(r')F_1(r') + o(1) \\ &\quad + \lambda_\gamma(\epsilon)F_\gamma(r)\int_{r/\epsilon}^\infty dr'\, G_{\epsilon\gamma}(r')V_1(r')\frac{F_{1,\epsilon\gamma}(\epsilon,r')}{\mathscr{F}_{1,\epsilon\gamma}(\epsilon)}, \end{aligned} \tag{3.31}$$

where $o(1)$ is uniformily bounded with respect to $r\geqslant 0$ and $\{A\}$ is defined by

$$\begin{aligned} \{A\} &= \gamma[2\mathscr{C} - 1]\int_0^\infty dr\, rV_1(r)F_1(r) - \lambda_{10} \\ &\quad \times\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^{-1}\int_0^\infty dr\, V_1(r)F_1^2(r) + \gamma\ln(\gamma) \\ &\quad \times\int_0^\infty dr\, rV_1(r)F_1(r) + \gamma\int_0^\infty dr\, rV_1(r)F_1(r) \\ &\quad + 2\gamma\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^{-1}\int_0^\infty dr\, F_1(r)F_1'(r)\ln(r). \end{aligned} \tag{3.32}$$

From

$$\begin{aligned} &\left|\lambda_\gamma(\epsilon)F_\gamma(r)\int_{r/\epsilon}^\infty dr'\, G_{\epsilon\gamma}(r')V_1(r')\frac{F_{1,\epsilon\gamma}(\epsilon,r')}{\mathscr{F}_{1,\epsilon\gamma}(\epsilon)}\right| \\ &\quad < \mathrm{const}\, r^{-1}F_\gamma(r)|\{A\}|^{-1}(r/\epsilon)[1+(r/\epsilon)]^{-1} \\ &\quad\quad \times\int_{r/\epsilon}^\infty dr'\, r'(1+r')|V_1(r')| = o(1), \quad \text{as } \epsilon\to 0_+, \end{aligned} \tag{3.33}$$

we finally get as in Eq. (2.35)

$$F_{1,\gamma,\epsilon}(r)/F_{1,\gamma,\epsilon} \underset{\epsilon\to 0_+}{=} F_\gamma(r) - a^{(0)}_{1,\gamma}G_\gamma(r) + o(1), \tag{3.34}$$

where by Eqs. (3.33) and (B1), $e^{-br}o(1)$ is bounded uniformily in $r\geqslant 0$ for all $b>0$. An application of Lebesgue's dominated convergence theorem then yields

$$a^{\mathrm{B}}_{12,\gamma,\epsilon}(g) \underset{\epsilon\to 0_+}{=} g\int_0^\infty dr[F_\gamma(r) - a^{(0)}_{1,\gamma}G_\gamma(r)]^2V_2(r) + go(1), \tag{3.35}$$

and hence

$$\begin{aligned} a_{\gamma,\epsilon}(g) &\underset{\epsilon\to 0_+}{=} a^{(0)}_{1,\gamma} + (\epsilon\ln^2\epsilon)a^{(1)}_{1,\gamma} + g\int_0^\infty dr[F_\gamma(r) \\ &\quad - a^{(0)}_{1,\gamma}G_\gamma(r)]^2V_2(r) + O(\epsilon\ln\epsilon) + go(1) + O(g^2), \end{aligned} \tag{3.36}$$

where $a^{(j)}_{1,\gamma}$, $j=0,1$ were introduced in Eq. (3.22).

If V_2 contains nonlocal and/or velocity-dependent parts[1] or if V_2 is local but nonspherically symmetric, Eqs. (3.35) and (3.36) can be generalized according to Eqs. (2.38)–(2.40)

Finally, we discuss an application of Secs. II and III concerning the comparison of charged and neutral scattering lengths.

Assuming charge symmetry, i.e.,

$$(1+\lambda_1\epsilon_0)V_1(r) = [1+\lambda_{10}\epsilon_0 + \lambda_{01}\gamma\epsilon_0\ln\epsilon_0]V_1(r), \tag{3.37}$$

where λ_{01} is given by (3.19) and $\epsilon_0 = r_0/r_1$ with r_0 the numerical value of the range of the nuclear force (r_1 the effective range parameter of h_1), and taking $|\lambda_1\epsilon_0| = |1-\lambda_\gamma(\epsilon_0)| \ll |g| \ll 1$, one obtains from Eqs. (2.36) and (3.36) the approximations

$$[a_{\epsilon_0}(g)]^{-1} \approx [a^{(0)}_1]^{-1} - g\int_0^\infty dr\{[a^{(0)}_1]^{-1}r - 1\}^2V_2(r) \tag{3.38}$$

and

$$\begin{aligned} [a_{\gamma,\epsilon_0}(g)]^{-1} &\approx [a^{(0)}_{1,\gamma}]^{-1} - g\int_0^\infty dr\{[a^{(0)}_{1,\gamma}]^{-1}F_\gamma(r) \\ &\quad - G_\gamma(r)\}^2V_2(r), \end{aligned} \tag{3.39}$$

and hence by Eqs. (3.37) and (3.22)

$$\begin{aligned} [a_{\gamma,\epsilon_0}(g)]^{-1} &\approx [a_{\epsilon_0}(g)]^{-1} \\ &\quad + \gamma\left[2\mathscr{C} + 2\int_0^\infty dr\,\phi_1(r)\phi_1'(r)\ln\frac{\gamma r_0 r}{r_1}\right], \end{aligned} \tag{3.40}$$

where terms of order $O(g\gamma^2\ln^2\gamma)$ have been neglected and where

$$\begin{aligned} \phi_1(r) &= -\left[\int_0^\infty dr\, rV_1(r)F_1(r)\right]^{-1}F_1(r), \\ &\left[\left(-\frac{d^2}{dr^2} + V_1\right)\phi_1\right](r) = 0 \end{aligned} \tag{3.41}$$

denotes the zero-energy resonance function of h_1 normalized to $\phi_1(r) \underset{r\to\infty}{=} 1 + o(1)$. In the special case $g=0$, Eq. (3.40) has been derived in Refs. 2 and 3 and independently in Ref. 4. In particular, approximation (3.40) exhibits a strong model dependence of this Blatt–Jackson type formula expressed by

the presence of the zero-energy wave function $\phi_1(r)$ as discussed in details in Ref. 2. For original references as well as the literature related to Eq. (3.40) we refer to Refs. 13–15 and the literature in Refs. 2–4.

IV. EXTENDED CHARGES

In this section we extend our previous considerations and include a description of extended charges in terms of form factors.[16]

Let $\Phi^c: (0,\infty)\to\mathscr{R}$ be a locally absolutely continuous function with

$$\int_R^\infty dr\, e^{br}|\Phi^c(r)-1|<\infty, \quad \text{for some } b,R>0 \tag{4.1}$$

In addition we assume that

$$|\Phi^c(r)-\Phi^c_{(0)}r^\nu|\leqslant \text{const}\, r^{\nu+\mu}, \quad \text{for some } \Phi^{(0)}_c\in\mathscr{R} \text{ and for some } \mu,\nu>0. \tag{4.2}$$

Next we introduce in $L^2((0,\infty))$

$$h^c_{\epsilon\gamma}(\epsilon)=h_0+\epsilon\gamma\Phi^c(\epsilon r)r^{-1}, \tag{4.3}$$

$$\mathscr{D}(h^c_{\epsilon\gamma}(\epsilon))=H^{2,2}_0((0,\infty)), \quad \epsilon,\gamma>0,$$

$$h^c_\gamma=\epsilon^{-2}U_\epsilon h^c_{\epsilon\gamma}(\epsilon)U_\epsilon^{-1}=h_0+\gamma\Phi^c(r)r^{-1}, \tag{4.4}$$

$$\mathscr{D}(h^c_\gamma)=H^{2,2}_0((0,\infty)),$$

$$h^c_{1,\epsilon\gamma}(\epsilon)=h^c_{\epsilon\gamma}(\epsilon)+(1+\lambda_1\epsilon)V_1, \quad \epsilon>0, \quad \lambda_1\in\mathscr{R}, \tag{4.5}$$

$$h^c_{1,\gamma,\epsilon}=\epsilon^{-2}U_\epsilon h^c_{1,\epsilon\gamma}(\epsilon)U_\epsilon^{-1}=h^c_\gamma+(1+\lambda_1\epsilon)\epsilon^{-2}V_{1,\epsilon}, \quad \epsilon>0, \quad V_{1,\epsilon}(r)=V_1(r/\epsilon), \tag{4.6}$$

where V_1 is real valued and obeys condition (3.1). For reasons analogous to those in Sec. II we assume case II, i.e., $\mathscr{F}_1=0$ throughout this section. The (ir)regular solutions $F^c_{1,\epsilon\gamma}(\epsilon,r)$ $[G^c_{1,\epsilon\gamma}(\epsilon.r)]$ associated with $h^c_{1,\epsilon\gamma}(\epsilon)$ uniquely obey

$$F^c_{1,\epsilon\gamma}(\epsilon,r)=r-\int_0^r dr'(r'-r)[(1+\lambda_1\epsilon)V_1(r')+\epsilon\gamma\Phi^c(\epsilon r')(r')^{-1}]F^c_{1,\epsilon\gamma}(\epsilon,r'), \tag{4.7}$$

$$F^c_{1,\epsilon\gamma}(\epsilon,r)=F_1(r)-\int_0^r dr'\,\tilde g_1(r,r')[\lambda_1\epsilon V_1(r')+\epsilon\gamma\Phi^c(\epsilon r')(r')^{-1}]F^c_{1,\epsilon\gamma}(\epsilon,r'), \tag{4.8}$$

$$F^c_{1,\epsilon\gamma}(\epsilon,r)=F^c_{\epsilon\gamma}(\epsilon,r)-\int_0^r dr'\,g^c_{\epsilon\gamma}(\epsilon,r,r')(1+\lambda_1\epsilon)\times V_1(r')F^c_{1,\epsilon\gamma}(\epsilon,r'), \tag{4.9}$$

$$G^c_{1,\epsilon\gamma}(\epsilon,r)=G^c_{\epsilon\gamma}(\epsilon,r)+\int_r^\infty dr'\,g^c_{\epsilon\gamma}(\epsilon,r,r')(1+\lambda_1\epsilon)\times V_1(r')G^c_{1,\epsilon\gamma}(\epsilon,r'), \tag{4.10}$$

where $\tilde g_1(r,r')$ has been defined in Eq. (2.16)

$$g^c_{\epsilon\gamma}(\epsilon,r,r')=[\mathscr{F}^c_{\epsilon\gamma}(\epsilon)]^{-1}[G^c_{\epsilon\gamma}(\epsilon,r)F^c_{\epsilon\gamma}(\epsilon,r')-G^c_{\epsilon\gamma}(\epsilon,r')F^c_{\epsilon\gamma}(\epsilon,r)], \tag{4.11}$$

$$\mathscr{F}^c_{\epsilon\gamma}(\epsilon)=W(G^c_{\epsilon\gamma}(\epsilon),F^c_{\epsilon\gamma}(\epsilon)). \tag{4.12}$$

Here $F^c_{\epsilon\gamma}(\epsilon,r)[G^c_{\epsilon\gamma}(\epsilon,r)]$, the (ir)regular solutions corresponding to $h^c_{\epsilon\gamma}(\epsilon)$, uniquely fulfill

$$F^c_{\epsilon\gamma}(\epsilon,r)=F_{\epsilon\gamma}(r)-\epsilon\gamma\int_0^r dr'\,g_{\epsilon\gamma}(r,r')[\Phi^c(\epsilon r')-1]\times(r')^{-1}F^c_{\epsilon\gamma}(\epsilon,r'), \tag{4.13}$$

$$G^c_{\epsilon\gamma}(\epsilon,r)=G_{\epsilon\gamma}(r)+\epsilon\gamma\int_r^\infty dr'g_{\epsilon\gamma}(r,r')[\Phi^c(\epsilon r')-1]\times(r')^{-1}G^c_{\epsilon\gamma}(\epsilon,r') \tag{4.14}$$

[F_γ, G_γ, g_γ were introduced in Eqs. (3.5), (3.6), and (3.10)]. For ϵ small enough the Coulomb modified scattering length associated with $h^c_{1,\epsilon\gamma}(\epsilon)$ is given by

$$a^c_{1,\epsilon\gamma}(\epsilon)=[\mathscr{F}^c_{1,\epsilon\gamma}(\epsilon)]^{-1}(1+\lambda_1\epsilon)\int_0^\infty dr\,F^c_{\epsilon\gamma}(\epsilon,r)\times V_1(r)F^c_{1,\epsilon\gamma}(\epsilon,r), \tag{4.15}$$

$$\mathscr{F}^c_{1,\epsilon\gamma}(\epsilon)=W(G^c_{1,\epsilon\gamma}(\epsilon),F^c_{1,\epsilon\gamma}(\epsilon))=1+[\mathscr{F}^c_{\epsilon\gamma}(\epsilon)]^{-1}(1+\lambda_1\epsilon)\int_0^\infty dr\,G^c_{\epsilon\gamma}(\epsilon,r)\times V_1(r)F^c_{1,\epsilon\gamma}(\epsilon,r). \tag{4.16}$$

Scaling properties of $F_\gamma(r)$, $G_\gamma(r)$ [cf. Eqs. (3.13) and (3.14)] and Eqs. (4.7) and (4.10) imply

$$F^c_\gamma(\epsilon r)=\epsilon F^c_{\epsilon\gamma}(\epsilon,r), \tag{4.17}$$

$$G^c_\gamma(\epsilon r)=G^c_{\epsilon\gamma}(\epsilon,r), \tag{4.18}$$

$$\mathscr{F}^c_\gamma=\mathscr{F}^c_{\epsilon\gamma}(\epsilon)=1+\gamma\int_0^\infty dr\,G_\gamma(r)[\Phi^c(r)-1]r^{-1}F^c_\gamma(r), \tag{4.19}$$

$$F^c_{1,\gamma,\epsilon}(\epsilon r)=\epsilon F^c_{1,\epsilon\gamma}(\epsilon,r), \tag{4.20}$$

$$G^c_{1,\gamma,\epsilon}(\epsilon r)=G^c_{1,\epsilon\gamma}(\epsilon,r), \tag{4.21}$$

$$\mathscr{F}^c_{1,\gamma,\epsilon}=\mathscr{F}^c_{1,\epsilon\gamma}(\epsilon), \tag{4.22}$$

$$a^c_{1,\gamma,\epsilon}=\epsilon a^c_{1,\epsilon\gamma}(\epsilon). \tag{4.23}$$

As in Secs. II, and III, the quantities on the left-hand side of Eqs. (4.20)–(4.23) belong to $h^c_{1,\gamma,\epsilon}$.

Following our strategy in Sec. II and III, we again concentrate on the small ϵ behavior of $\mathscr{F}^c_{1,\epsilon\gamma}(\epsilon)$. Iterating Eq. (4.8), we obtain

$$\begin{aligned}F^c_{1,\epsilon\gamma}(\epsilon,r)\underset{\epsilon\to0_+}{=}{}&F_1(r)-\lambda_1\epsilon\tilde G_1(r)\int_0^r dr'\,F_1^2(r')V_1(r')\\&+\lambda_1\epsilon F_1(r)\int_0^r dr'\,\tilde G_1(r')F_1(r')V_1(r')\\&-\epsilon^{1+\nu}\gamma\Phi^c_{(0)}\tilde G_1(r)\int_0^r dr'\,F_1^2(r')(r')^{\nu-1}\\&+\epsilon^{1+\nu}\gamma\Phi^c_{(0)}F_1(r)\int_0^r dr'\,F_1(r')\tilde G_1(r')(r')^{\nu+1}\\&+\begin{cases}O(\epsilon^{1+\nu+\mu}, & \text{if } \nu+\mu<1,\\ O(\epsilon^2), & \text{if } \nu+\mu\geqslant1,\end{cases}\end{aligned} \tag{4.24}$$

with $\mu,\nu>0$, $\nu<1$. Here $e^{-br}O(\epsilon^{1+\nu+\mu})$ if $\nu+\mu<1$ [resp. $e^{-br}O(\epsilon^2)$ if $\nu+\mu\geqslant1$] is uniformly bounded with respect to $r\geqslant0$ for all $b>0$ by estimates of the type (B1).

Next we have to expand $G^c_{\epsilon\gamma}(\epsilon,r)$. Taking $\epsilon r'=r''$ in Eq. (4.14) leads to

$$G^c_{\epsilon\gamma}(\epsilon,r)=G_{\epsilon\gamma}(\epsilon r)+\epsilon\gamma\int_{\epsilon r}^\infty dr''\,g_{\epsilon\gamma}(r,r''/\epsilon)[\Phi^c(r'')-1]\times(r'')^{-1}G^c_\gamma(r''). \tag{4.25}$$

Using

$$g_{\epsilon\gamma}(r,r''/\epsilon)=\epsilon^{-1}g_{\epsilon\gamma}(\epsilon r,r''), \tag{4.26}$$

Eq. (4.19), and several integrations by parts one infers after a

straightforward but lengthy calculation that

$$[\mathscr{F}_\gamma^c]^{-1}G_{\epsilon\gamma}^c(\epsilon,r)$$

$$\underset{\epsilon\to 0_+}{=} 1+\epsilon\gamma r\ln(\gamma)+2\mathscr{C}\epsilon\gamma r+[\mathscr{F}_\gamma^c]^{-1}$$

$$\times\epsilon\gamma r\int_0^\infty dr'\ln(r')\frac{d}{dr'}\{G_\gamma(r')G_\gamma^c(r')[\Phi^c(r')-1]\}$$

$$-\epsilon^{1+\nu}\frac{(r)^{1+\nu}}{1+\nu}\gamma\Phi_{(0)}^c+\begin{cases}O(\epsilon^{1+\nu+\mu}), & \mu+\nu<1,\\ O(\epsilon^2), & \mu+\nu\geqslant 1,\end{cases}$$

$$\mu>0,\quad 0<\nu<1, \tag{4.27}$$

where $O(\epsilon^{1+\nu+\mu})$ if $\mu+\nu<1$ [resp. $O(\epsilon^2)$ if $\mu+\nu\geqslant 1$] is uniformly bounded with respect to $r\geqslant 0$. Insertion of Eqs. (4.24) and (4.27) into (4.16), observing $\mathscr{F}_1=0$, and several integrations by parts finally lead to

$$\mathscr{F}_{1,\epsilon\gamma}^c(\epsilon)\underset{\epsilon\to 0_+}{=}\epsilon\gamma\ln(\gamma)\int_0^\infty dr\,rV_1(r)F_1(r)-\lambda_1\epsilon\left[\int_0^\infty dr\,rV_1(r)F_1(r)\right]^{-1}\int_0^\infty dr\,F_1^2(r)V_1(r)+\epsilon\gamma 2\mathscr{C}\int_0^\infty dr\,rV_1(r)F_1(r)$$

$$+[\mathscr{F}_\gamma^c]^{-1}\epsilon\gamma\int_0^\infty dr\,rV_1(r)F_1(r)\int_0^\infty dr'\ln(r')\frac{d}{dr'}\{G_\gamma(r')G_\gamma^c(r')[\Phi_c(r')-1]\}-\epsilon^{1+\nu}\gamma\Phi_{(0)}^c$$

$$\times\left[\int_0^\infty dr\,rV_1(r)F_1(r)\right]^{-1}\int_0^\infty dr\,F_1^2(r)r^{\nu-1}-\epsilon^{1+\nu}\gamma\Phi_{(0)}^c\int_0^\infty dr\,F_1(r)(r')^{\nu-1}+\epsilon^{1+\nu}(1+\nu)^{-1}\gamma\Phi_{(0)}^c$$

$$\times\int_0^\infty dr\,r^{1+\nu}V_1(r)F_1(r)+\begin{cases}O(\epsilon^{1+\nu+\mu}), & \nu+\mu<1,\\ O(\epsilon^2), & \nu+\mu\geqslant 1,\end{cases}\qquad \mu,\nu>0,\quad \nu<1. \tag{4.28}$$

In the special case $\nu=1$ the corresponding expansion of $\mathscr{F}_{1,\epsilon\gamma}(\epsilon)$ can be easily obtained. Since the result involves considerably long expressions we omit the details. Next we note that Eq. (4.2), together with

$$F_{\epsilon\gamma}^c(\epsilon,r)=r-\epsilon\gamma\int_0^r dr'(r'-r)\Phi^c(\epsilon r')(r')^{-1}F_{\epsilon\gamma}^c(\epsilon,r') \tag{4.29}$$

immediately imply

$$F_{\epsilon\gamma}^c(\epsilon,r)\underset{\epsilon\to 0_+}{=}r+O(\epsilon^{1+\nu}), \tag{4.30}$$

where $e^{-br}O(\epsilon^{1+\nu})$ is uniformly bounded in $r\geqslant 0$ for all $b>0$ [cf. the estimate (B1)]. Consequently Eqs. (4.15), (4.23), (4.28), and (4.30) imply

$$a_{1,\gamma,\epsilon}^c\underset{\epsilon\to 0_+}{=}\int_0^\infty dr\,rV_1(r)F_1(r)\Big\{\gamma\ln(\gamma)\int_0^\infty dr\,rV_1(r)F_1(r)-\lambda_1\left[\int_0^\infty dr\,rV_1(r)F_1(r)\right]^{-1}\int_0^\infty dr\,F_1^2(r)V_1(r)$$

$$+2\gamma\mathscr{C}\int_0^\infty dr\,rV_1(r)F_1(r)+\gamma[\mathscr{F}_\gamma^c]^{-1}\int_0^\infty dr\,rV_1(r)F_1(r)\int_0^\infty dr'\ln(r')\frac{d}{dr'}\{G_\gamma(r')G_\gamma^c(r')[\Phi^c(r')-1]\}\Big\}^{-1}$$

$$+\epsilon^\nu\gamma\Phi_{(0)}^c\int_0^\infty dr\,rV_1(r)F_1(r)\Big\{\int_0^\infty dr\,F_1(r)r^{\nu-1}-\frac{1}{1+\nu}\int_0^\infty dr\,r^{1+\nu}V_1(r)F_1(r)+\left[\int_0^\infty dr\,rV_1(r)F_1(r)\right]^{-1}$$

$$\times\int_0^\infty dr\,F_1^2(r)r^{\nu-1}\Big\}\Big\{\gamma\ln(\gamma)\int_0^\infty dr\,rV_1(r)F_1(r)-\lambda_1\left[\int_0^\infty dr\,rV_1(r)F_1(r)\right]^{-1}\int_0^\infty dr\,F_1^2(r)V_1(r)$$

$$+2\gamma\mathscr{C}\int_0^\infty dr\,rV_1(r)F_1(r)+\gamma[\mathscr{F}_\gamma^c]^{-1}\int_0^\infty dr\,rV_1(r)F_1(r)\int_0^\infty dr'\ln(r')\frac{d}{dr'}\{G_\gamma(r')G_\gamma^c(r')[\Phi^c(r')-1]\}\Big\}^{-2}$$

$$+\begin{cases}O(\epsilon^{\nu+\mu}), & \mu+\nu<1,\\ O(\epsilon), & \mu+\nu\geqslant 1,\end{cases}\qquad \mu,\nu>0,\quad \nu<1$$

$$\underset{\epsilon\to 0_+}{\equiv}a_{1,\gamma}^{c(0)}+\epsilon^\nu a_{1,\gamma}^{c(1)}+\begin{cases}O(\epsilon^{\nu+\mu}), & \mu+\nu<1,\\ O(\epsilon), & \mu+\nu\geqslant 1,\end{cases}\qquad \mu>0,\quad 0<\nu<1. \tag{4.31}$$

For $\nu\geqslant 1$ the corresponding expansion reads

$$a_{1,\gamma,\epsilon}^c=\epsilon a_{1,\epsilon\gamma}^c(\epsilon)\underset{\epsilon\to 0_+}{=}a_{1,\gamma}^{c(0)}+O(\epsilon), \tag{4.32}$$

where the $O(\epsilon)$ term can be written down explicitly. In order to avoid too lengthy expressions we omit further details.

As in Secs. II and III we finally introduce an additional interaction gV_2, $g\in\mathscr{R}$. Assuming $V_2:(0,\infty)\to\mathscr{R}$ to be measurable and

$$\int_0^R dr|V_2(r)|<\infty,\quad \int_R^\infty dr\,e^{br}|V_2(r)|<\infty,$$

$$\text{for some } b,R>0, \tag{4.33}$$

we define in $L^2((0,\infty))$

$$h_{\gamma,\epsilon}^c(g)=h_{1,\gamma,\epsilon}^c+gV_2. \tag{4.34}$$

The corresponding regular function uniquely fulfills

$$F^c_{\gamma,\epsilon}(g,r) = F^c_{1,\gamma,\epsilon}(r) - g\int_0^r dr'\, g^c_{1,\gamma,\epsilon}(r,r') \times V_2(r')F^c_{\gamma,\epsilon}(g,r'), \tag{4.35}$$

$$g^c_{1,\gamma,\epsilon}(r,r') = [\mathscr{F}^c_{1,\gamma,\epsilon}]^{-1}[G^c_{1,\gamma,\epsilon}(r)F^c_{1,\gamma,\epsilon}(r') - G^c_{1,\gamma,\epsilon}(r')F^c_{1,\gamma,\epsilon}(r)]. \tag{4.36}$$

For ϵ small enough the two-potential formula (cf. Appendix C) then implies for $a^c_{\gamma,\epsilon}(g)$ the Coulomb modified scattering length of $h^c_{\gamma,\epsilon}(g)$

$$a^c_{\gamma,\epsilon}(g) = a^c_{1,\gamma,\epsilon} + a^c_{12,\gamma,\epsilon}(g), \tag{4.37}$$

where

$$a^c_{12}(g) = g\int_0^\infty dr\, \frac{F^c_{1,\gamma}(r)}{\mathscr{F}^c_{1,\gamma,\epsilon}}\, V_2(r)\, \frac{F^c_{\gamma,\epsilon}(g,r)}{\mathscr{F}^c_{12,\gamma,\epsilon}(g)} \tag{4.38}$$

and

$$\mathscr{F}^c_{12,\gamma,\epsilon}(g) = \mathscr{F}^c_{1,\gamma,\epsilon} + g\int_0^\infty dr\, G^c_{1,\gamma,\epsilon}(r)V_2(r)F^c_{\gamma,\epsilon}(g,r). \tag{4.39}$$

Similar to Secs. II and III, Poincare's theorem[11] implies that $F_{\gamma,\epsilon}(g,r)$ and $\mathscr{F}^c_{12,\gamma,\epsilon}(g)$ are entire with respect to g. Consequently, for ϵ small enough, $a^c_{12,\gamma,\epsilon}(g)$ is analytic in g around $g=0$. As usual, the Born term is defined by

$$a^{c,B}_{12,\gamma,\epsilon}(g) = g\int_0^\infty dr\left[\frac{F^c_{1,\gamma,\epsilon}(r)}{\mathscr{F}^c_{1,\gamma,\epsilon}}\right]^2 V_2(r). \tag{4.40}$$

In order to expand (4.40) with respect to ϵ around $\epsilon=0$ we again introduce the Fredholm integral equation corresponding to $F^c_{1,\gamma,\epsilon}(r)$ and obtain (cf. Sec. II)

$$F^c_{1,\gamma,\epsilon}(r)/\mathscr{F}^c_{1,\gamma,\epsilon} \underset{\epsilon\to 0_+}{=} F^c_\gamma(r) - G^c_\gamma(r)\{B\}^{-1}\int_0^\infty dr'\, r'V_1(r')F_1(r') + o(1) + (1+\lambda_1\epsilon)F^c_\gamma(r)\int_{r/\epsilon}^\infty dr'\, G^c_\gamma(\epsilon r')V_1(r')\frac{F^c_{1,\epsilon\gamma}(\epsilon,r')}{\mathscr{F}^c_{1,\epsilon\gamma}(\epsilon)}, \tag{4.41}$$

where $o(1)$ is uniformly bounded in $r\geqslant 0$ and $\{B\}$ is defined by

$$\{B\} = \gamma\ln(\gamma)\int_0^\infty dr\, rV_1(r)F_1(r) - \lambda_1\Big[\int_0^\infty dr\, r \times V_1(r)F_1(r)\Big]^{-1}\int_0^\infty dr\, F_1^2(r)V_1(r) + 2\gamma\mathscr{C}\int_0^\infty dr\, rV_1(r)F_1(r) + \gamma[\mathscr{F}^c_\gamma]^{-1}\int_0^\infty dr\, rV_1(r)F_1(r)\int_0^\infty dr'\ln(r')\frac{d}{dr'} \times\{G_\gamma(r')G^c_\gamma(r')[\Phi^c(r')-1]\}. \tag{4.42}$$

From

$$\left|(1+\lambda_1\epsilon)F^c_\gamma(r)\int_{r/\epsilon}^\infty dr'\, G^c_\gamma(\epsilon r')V_1(r')\frac{F^c_{1,\epsilon\gamma}(\epsilon,r')}{\mathscr{F}^c_{1,\epsilon\gamma}(\epsilon)}\right| \leqslant \text{const}\, r^{-1}F^c_\gamma(r)|\{B\}^{-1}|(r/\epsilon)[1+(r/\epsilon)]^{-1} \times\int_{r/\epsilon}^\infty dr'\, r'(1+r')|V_1(r')| \underset{\epsilon\to 0_+}{=} o(1), \tag{4.43}$$

we finally infer

$$\frac{F^c_{1,\gamma,\epsilon}(r)}{\mathscr{F}^c_{1,\gamma,\epsilon}} \underset{\epsilon\to 0_+}{=} F^c_\gamma(r) - a^{c(0)}_{1,\gamma}[\mathscr{F}^c_\gamma]^{-1}G^c_\gamma(r) + o(1), \tag{4.44}$$

where, by Eqs. (4.43) and (B1), $e^{-br}o(1)$ is bounded uniformly in $r\geqslant 0$ for all $b>0$. Lebesgue's dominated convergence theorem then yields

$$a^{c,B}_{12,\gamma,\epsilon}(g) \underset{\epsilon\to 0_+}{=} g\int_0^\infty dr\{F^c_\gamma(r) - a^{c(0)}_{1,\gamma}[\mathscr{F}^c_\gamma]^{-1}G^c_\gamma(r)\}^2V_2(r) + go(1), \tag{4.45}$$

and thus

$$a^c_{\gamma,\epsilon}(g) = a^{c(0)}_{1,\gamma} + \epsilon^\nu a^{c(1)}_{1,\gamma} + g\int_0^\infty dr\{F^c_\gamma(r) - a^{c(0)}_{1,\gamma}[\mathscr{F}^c_\gamma]^{-1}G^c_\gamma(r)\}^2V_2(r) + \begin{cases} O(\epsilon^{\nu+\mu}), & \nu+\mu<1 \\ O(\epsilon), & \nu+\mu\geqslant 1\end{cases} + go(1) + O(g^2), \quad \mu>0,\ 0<\nu<1, \tag{4.46}$$

where $a^{c(j)}_{1,\gamma}, j=0,1$, were defined in Eq. (4.31). If $\nu\geqslant 1$ we have

$$a^c_{\gamma,\epsilon}(g) = a^{c(0)}_{1,\gamma} + g\int_0^\infty dr\{F^c_\gamma(r) - a^{c(0)}_{1,\gamma}[\mathscr{F}^c_\gamma]^{-1}G^c_\gamma(r)\}^2V_2(r) + O(\epsilon) + go(1) + O(g^2). \tag{4.47}$$

At the end we again discuss the application of Sec. III, i.e., we compare charged and neutral scattering lengths taking explicitly into account the finite extent of the charge [described by $\Phi^c(r)$]. To include realistic interactions we take $\nu=1$ for the rest and again suppose $|\lambda_1\epsilon_0| \ll |g| \ll 1$ ($\epsilon_0 = r_0/r_1$ as in Sec. III). Assuming charge symmetry we obtain from Eq. (4.47) the approximation

$$[a^c_{\gamma,\epsilon_0}(g)]^{-1} \approx [a^{c(0)}_{1,\gamma}]^{-1} - g\int_0^\infty dr\{[a^{c(0)}_{1,\gamma}]^{-1}F^c_\gamma(r) - [\mathscr{F}^c_\gamma]^{-1}G^c_\gamma(r)\}^2V_2(r). \tag{4.48}$$

Equation (4.48) together with Eq. (3.38) [cf. Eq. (4.32)] and an expansion for small values of γ finally yields

$$[a^c_{\gamma,\epsilon_0}(g)]^{-1} \approx [a_{\epsilon_0}(g)]^{-1} + \gamma\Big\{2\mathscr{C} + \int_0^\infty dr\ln(\gamma r)\frac{d}{dr}[\Phi^c(r)]\Big\}, \tag{4.49}$$

where terms of $O(\gamma^2\ln^2\gamma)$ have been neglected.

A comparison of the results (3.40) and (4.49) shows that the strong model dependence exhibited in the point Coulomb case is reduced to higher-order effects [i.e., the zero energy solution $\phi_1(r)$ appears in higher orders only] as soon as the finite extent of the charge (i.e., $\Phi^c \not\equiv 1$) is taken into account. Equation (4.49) offers a handy tool for the comparison of charged and neutral scattering lengths by identifying $a^c_{\gamma,\epsilon_0}(g)$ with the $^1S_0$ proton–proton scattering length and $a_{\epsilon_0}(g)$ with the $^1S_0$ neutron–neutron scattering length.

V. STRONGLY SINGULAR PERTURBATIONS

Finally, we discuss strongly singular interactions of the type $\beta r^{-2} + \gamma r^{-1}$, $-\frac{1}{4} < \beta < \frac{3}{4}$, $\gamma\geqslant 0$. In contrast to Secs. II–IV we now confine ourselves to the short-range limit $\epsilon\to 0_+$ and hence directly implement an additional zero-range in-

teraction by choosing appropriate boundary conditions at $r=0$ [instead of considering $\lambda_\gamma(\epsilon)\epsilon^{-2}\,V_{1,\epsilon}(r)$ and taking $\epsilon\to 0_+$]. Under suitable conditions on the additional hadronic interaction potential gV_2 we again study the associated scattering length in first Born approximation.

Let $h_{\beta,\gamma}$ denote the closure of the minimal differential operator $\dot{h}_{\beta,\gamma}$ in $L^2((0,\infty))$

$$\dot{h}_{\beta,\gamma} = -\frac{d^2}{dr^2} + \beta r^{-2} + \gamma r^{-1}, \quad -\tfrac{1}{4} < \beta < \tfrac{3}{4}, \quad \gamma \geqslant 0,$$
$$\mathscr{D}(\dot{h}_{\beta,\gamma}) = C_0^\infty((0,\infty)). \tag{5.1}$$

Then, as is well known, $h_{\beta,\gamma}$ has deficiency indices one and all self-adjoint extensions $h_{\alpha,\beta,\gamma}$ may be parametrized by[17–19]

$$h_{\alpha,\beta,\gamma} = -\frac{d^2}{dr^2} + \beta r^{-2} + \gamma r^{-1}, \quad -\infty < \alpha \leqslant +\infty, \ -\tfrac{1}{4} < \beta < \tfrac{3}{4}, \quad \gamma \geqslant 0,$$
$$\mathscr{D}(h_{\alpha,\beta,\gamma}) = \{ f \in L^2((0,\infty)) \mid f, f' \in AC_{\rm loc}((0,\infty)); \ -4\pi\alpha f_0 + f_1 = 0; \ -f'' + \beta r^{-2} f + \gamma r^{-1} f \in L^2((0,\infty)) \}, \tag{5.2}$$

where $AC_{\rm loc}((0,\infty))$ denotes the set of locally absolutely continuous functions on $(0,\infty)$. Here f_0 and f_1 are defined by

$$f_0 = \lim_{r\to 0_+} r^{\tilde{\beta}-1/2} f(r), \quad \tilde{\beta} = (\beta + \tfrac{1}{4})^{1/2},$$
$$f_1 = \lim_{r\to 0_+} r^{-\tilde{\beta}-1/2}\{ f(r) - f_0 [r^{-\tilde{\beta}+1/2} + \gamma^{2\tilde{\beta}} \times (\Gamma(-2\tilde{\beta})/\Gamma(2\tilde{\beta}) + 1 - 2\mathscr{C}) r^{\tilde{\beta}+1/2} - \gamma(2\tilde{\beta}-1)^{-1} r^{-\tilde{\beta}+3/2}] \}, \quad \text{if } \beta \neq 0 \tag{5.3}$$

[$\Gamma(z)$ being the gamma function[12]] and by

$$f_0 = f(0_+),$$
$$f_1 = \lim_{r\to 0_+} r^{-1}\{ f(r) - f(0_+)[1 + \gamma r \ln(\gamma r)] \}, \quad \text{if } \beta = 0. \tag{5.4}$$

We note that the boundary conditions (5.3) are continuous at $\beta = 0$ and indeed converge to those in (5.4) as $\beta \to 0$. If $\beta \geqslant \frac{3}{4}$, $h_{\beta,\gamma}$ is self adjoint and hence no additional point (zero-range) interaction exists. If $\beta < -\frac{1}{4}$, $h_{\beta,\gamma}$ is unbounded from below and thus not suitable for our purpose [if $\beta = -\frac{1}{4}$ the boundary conditions (5.3) can be modified to apply again[17–19]]. As mentioned in the beginning, $h_{\alpha,\beta,\gamma}$ describes a $\beta r^{-2} + \gamma r^{-1}$ plus zero-range interaction (if $|\alpha| < \infty$).

Next we introduce (ir)regular zero-energy solutions $F_{\beta,\gamma}(r)$ [$G_{\beta,\gamma}(r)$] associated with $h_{\beta,\gamma}$

$$F_{\beta,\gamma}(r) = \gamma^{-\tilde{\beta}}\Gamma(1+2\tilde{\beta}) r^{1/2} I_{2\tilde{\beta}}((4\gamma r)^{1/2}), \tag{5.5}$$
$$G_{\beta,\gamma}(r) = 2\gamma^{\tilde{\beta}}\Gamma(1+2\tilde{\beta})^{-1} r^{1/2} K_{2\tilde{\beta}}((4\gamma r)^{1/2}), \tag{5.6}$$

such that $W(G_{\beta,\gamma}, F_{\beta,\gamma}) = 1$. Defining

$$F_{\alpha,\beta,\gamma}(r) = F_{\beta,\gamma}(r) - a_{\alpha,\beta,\gamma} G_{\beta,\gamma}(r), \tag{5.7}$$

where

$$a_{\alpha,\beta,\gamma} = -2\tilde{\beta}\,[4\pi\alpha - \gamma^{2\tilde{\beta}}(2\mathscr{C} - 1)]^{-1}, \quad -\infty < \alpha < +\infty, \tag{5.8}$$

then by Eq. (5.3), $F_{\alpha,\beta,\gamma}$ and $a_{\alpha,\beta,\gamma}$ are easily seen to be the zero-energy scattering wave function, respectively, the scattering length (induced by the additional contact interaction) associated with $h_{\alpha,\beta,\gamma}$. In particular, taking $\beta = 0$, $\gamma = 0$, $a_{\alpha,0,0}$ corresponds to $a_1^{(0)}$ of Eq. (2.24) and taking $\beta = 0$, $a_{\alpha,0,\gamma}$ corresponds to $a_{1,\gamma}^{(0)}$ of Eq. (3.22) if the boundary condition parameter α is chosen appropriately (cf. Refs. 2 and 5). The special case $\gamma = 0$ in (5.3) has been discussed in detail in Ref. 20.

Finally, following Secs. II–IV, we again consider the effect of an additional (real-valued) potential gV_2, $g \in \mathscr{R}$ to first order in g. Assuming

$$\int_0^R dr\, r^{1-2\tilde{\beta}} |V_2(r)| < \infty,$$
$$\int_R^\infty dr\, r^{1+2\tilde{\beta}} |V_2(r)| < \infty, \quad \text{if } \gamma = 0,$$
$$\int_R^\infty dr\, e^{br} |V_2(r)| < \infty, \quad \text{if } \gamma > 0, \tag{5.9}$$
$$\text{for suitable } b, R > 0,$$

we define in $L^2((0,\infty))$

$$h_{\alpha,\beta,\gamma}(g) = h_{\alpha,\beta,\gamma} + gV_2. \tag{5.10}$$

Then the regular solution $F_{\alpha,\beta,\gamma}(g,r)$ associated with $h_{\alpha,\beta,\gamma}(g)$ uniquely fulfills

$$F_{\alpha,\beta,\gamma}(g,r) = F_{\alpha,\beta,\gamma}(r) - g\int_0^r dr'\, g_{\beta,\gamma}(r,r') \times V_2(r') F_{\alpha,\beta,\gamma}(g,r'), \tag{5.11}$$

where

$$g_{\beta,\gamma}(r,r') = G_{\beta,\gamma}(r) F_{\beta,\gamma}(r') - G_{\beta,\gamma}(r') F_{\beta,\gamma}(r). \tag{5.12}$$

Using $(C_M, C'_M$ appropriate constants possibly depending on $\alpha,\beta,\gamma)$

$$|F_{\alpha,\beta,\gamma}(r)| \leqslant C_M r^{1/2-\tilde{\beta}}, \quad r \leqslant M \tag{5.13}$$

and

$$|g_{\beta,\gamma}(r,r')| \leqslant C'_M (r')^{-\tilde{\beta}+1/2} r^{\tilde{\beta}+1/2}, \quad r' \leqslant r \leqslant M, \tag{5.14}$$

which follows from monotonic increase of $F_{\beta,\gamma}(r)/G_{\beta,\gamma}(r)$ [$(F_{\beta,\gamma}/G_{\beta,\gamma})'(r) = G_{\beta,\gamma}^{-2}(r) > 0$], and standard estimates on $F_{\beta,\gamma}(r)$ and $G_{\beta,\gamma}$ (cf. Refs. 12 and 21), iteration of Eq. (5.11) proves that $F_{\alpha,\beta,\gamma}(g,r)$ is entire with respect to g (a fact which could also be derived from Poincare's theorem[11]). Similar to Secs. II–IV, the scattering length $a_{\alpha,\beta,\gamma}(g)$ corresponding to $h_{\alpha,\beta,\gamma}(g)$ splits up into

$$a_{\alpha,\beta,\gamma}(g) = a_{\alpha,\beta,\gamma} + a_{12,\alpha,\beta,\gamma}(g), \tag{5.15}$$

where

$$a_{12,\alpha,\beta,\gamma}(g) = g\int_0^g dr\, F_{\alpha,\beta,\gamma}(r) V_2(r) \frac{F_{\alpha,\beta,\gamma}(g,r)}{\mathscr{F}_{12,\alpha,\beta,\gamma}(g)} \tag{5.16}$$

is analytic in g near $g = 0$ and

$$\mathscr{F}_{12,\alpha,\beta,\gamma}(g) = 1 + g\int_0^\infty dr\, G_{\beta,\gamma}(r) V_2(r) F_{\alpha,\beta,\gamma}(g,r). \tag{5.17}$$

As a result we immediately obtain for the first Born approximation

$$a^{\rm B}_{12,\alpha,\beta,\gamma}(g) = \int_0^\infty dr\, F^2_{\alpha,\beta,\gamma}(r) V_2(r), \tag{5.18}$$

and hence

$$a_{\alpha,\beta,\gamma}(g) = a_{\alpha,\beta,\gamma} + g\int_0^\infty dr\, F^2_{\alpha,\beta,\gamma}(r)V_2(r) + O(g^2), \tag{5.19}$$

with $a_{\alpha,\beta,\gamma}$ and $F_{\alpha,\beta,\gamma}(r)$ defined in Eqs. (5.7) and (5.8). The result (5.19) represents a generalization of the approach of Secs. II and III (if the zero-range limit is taken throughout) in the sense that an additional strongly singular potential βr^{-2} has been included.

Obviously the above treatment extends to the case $\gamma < 0$ and to cases where the potential looks like $\beta r^{-2} + \gamma r^{-1}$, $-\frac{1}{4} < \beta < \frac{3}{4}$, $\gamma \in \mathscr{R}$ in an interval $(0, r_0]$, $r_0 > 0$ and is smooth (e.g., continuous) in $[r_0, \infty]$. Instead of repeating the above arguments we end up with the following illustration.

Example: Let

$$\phi(r) = \begin{cases} C(r + gr^2/2) + 1 + gr\ln(r) \\ \quad r \leqslant R, \\ \text{const}(1 - r/a_g), \quad r \geqslant R, \quad R > 0,' \\ \quad C \in \mathscr{R}\setminus\{0\}, \quad g \in \mathscr{R} \end{cases} \tag{5.20}$$

assuming ϕ, ϕ' to be continuous at $r = R$, and define the potential V to be

$$V(r) = \phi''(r)/\phi(r). \tag{5.21}$$

Note that gV approximates a screened Coulomb potential $gr^{-1}\Theta(R - r)$ if R is small enough. Calculating the scattering length a_g yields

$$a_g = (-1 + gR + gCR^2/2)/(C + gCR + g + g\ln(R)). \tag{5.22}$$

Hence

$$a_g = a^0 + ga^1 + O(g^2), \quad a^0 = -1/C,$$
$$a^1 = (a^0)^2[\ln(R) + 1] - 2a^0R + R^2/2, \tag{5.23}$$

and in particular a^1 coincides with the "renormalized expression" [cf. Eq. (2.36)]

$$a^1 = \lim_{\delta \to 0_+}\left\{\int_\delta^\infty dr[r - a^0]^2V(r) + (a^0)^2[\ln(\delta) + 1]\right\}. \tag{5.24}$$

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APPENDIX A: ASYMPTOTIC RELATIONS

Based on standard techniques (cf., e.g., Ref. 22), we derive asymptotic formulas for (ir)regular solutions associated with h_1 and prove the claim in Eq. (2.14) assuming condition (2.1).

Introducing $F_1(r)$, $G_1(r)$, and $H_1(r)$ as the unique solutions of the integral equations

$$F_1(r) = r - \int_0^r dr'(r' - r)V_1(r')F_1(r'), \tag{A1}$$

$$G_1(r) = 1 + \int_r^\infty dr'(r' - r)V_1(r')G_1(r'), \tag{A2}$$

$$H_1(r) = r + \int_r^\infty dr'(r' - r)V_1(r')H_1(r'), \tag{A3}$$

one obtains

$$F_1(r) \underset{r\to 0_+}{=} r + o(r), \tag{A4}$$

$$F_1'(r) \underset{r\to 0_+}{=} 1 + o(1), \tag{A5}$$

$$G_1(r) \underset{r\to 0_+}{=} 1 + \int_0^\infty dr'\, r'V_1(r')G_1(r') - r\int_0^\infty dr'\, V_1(r')G_1(r') + o(r), \tag{A6}$$

$$G_1'(r) \underset{r\to 0_+}{=} -\int_0^\infty dr'\, V_1(r')G_1(r') + o(1), \tag{A7}$$

$$H_1(r) \underset{r\to 0_+}{=} \int_0^\infty dr'\, r'V_1(r')H_1(r') + r - r\int_0^\infty dr'\, V_1(r')H_1(r') + o(r), \tag{A8}$$

$$H_1'(r) \underset{r\to 0_+}{=} 1 - \int_0^\infty dr'\, V_1(r')H_1(r') + o(1), \tag{A9}$$

$$F_1(r) \underset{r\to \infty}{=} r + r\int_0^\infty dr'\, V_1(r')F_1(r') - \int_0^\infty dr'\, r'V_1(r')F_1(r') + o(1), \tag{A10}$$

$$F_1'(r) \underset{r\to \infty}{=} 1 + \int_0^\infty dr'\, V_1(r')F_1(r') + o(r^{-1}), \tag{A11}$$

$$G(r) \underset{r\to \infty}{=} 1 + o(r^{-1}), \tag{A12}$$

$$G'(r) \underset{r\to \infty}{=} o(r^{-2}), \tag{A13}$$

$$H(r) \underset{r\to \infty}{=} r + o(1), \tag{A14}$$

$$H'(r) \underset{r\to \infty}{=} 1 + o(r^{-1}). \tag{A15}$$

Consequently, calculating Wronskians at $r = 0$ and $r \to \infty$ yields

$$W(G_1,F_1) = 1 + \int_0^\infty dr\, V_1(r)F_1(r) = 1 + \int_0^\infty dr\, rV_1(r)G_1(r) \equiv \mathscr{F}_1, \tag{A16}$$

$$W(G_1,H_1) = \mathscr{F}_1\left[1 - \int_0^\infty dr\, V_1(r)H_1(r)\right] + \int_0^\infty dr\, r \times V_1(r)H_1(r)\int_0^\infty dr'\, V_1(r')G_1(r') = 1, \tag{A17}$$

$$W(H_1,F_1) = \int_0^\infty dr\, rV_1(r)H_1(r) = \int_0^\infty dr\, rV_1(r)F_1(r). \tag{A18}$$

Now we specialize to case II, i.e., to $\mathscr{F}_1 = 0$. Then (A16)–(A18) imply

$$1 = W(G_1,H_1) = \int_0^\infty dr\, rV_1(r)H_1(r)\int_0^\infty dr'\, V_1(r')G_1(r') = \int_0^\infty dr\, rV_1(r)F_1(r)\int_0^\infty dr'\, V_1(r')G_1(r'), \tag{A19}$$

and therefore Eq. (2.14) follows. Obviously we have

$$\tilde{G}_1(r) = \left[\int_0^\infty dr\, r V_1(r) F_1(r)\right]^{-1} H_1(r). \tag{A20}$$

APPENDIX B: ESTIMATES FOR COULOMB-TYPE SOLUTIONS

Here we recall the estimates of (ir) regular solutions $F_{1,\gamma}(r)$ $[G_{1,\gamma}(r)]$ associated with $h_{1,\gamma} = h_\gamma + V_1$, $\gamma > 0$, where V_1 obeys the integrability conditions (3.1). Iterating the corresponding Volterra integral equations (cf. Refs. 20) one obtains

$$|F_{1,\gamma}(r)| \leqslant \text{const}\, r^{1/4}[r/(1+r)]^{3/4} e^{(4\gamma r)^{1/2}}, \quad \gamma > 0, \tag{B1}$$

$$|G_{1,\gamma}(r)| \leqslant \text{const}\, r^{1/4}[r/(1+r)]^{-1/4} e^{-(4\gamma r)^{1/2}}, \quad \gamma > 0. \tag{B2}$$

APPENDIX C: THE GELL-MANN–GOLDBERGER FORMULA FOR SCATTERING LENGTHS

We indicate a proof of the Gell-Mann–Goldberger relation for scattering lengths.

Assuming $V_j : (0,\infty) \to \mathscr{R}$, $j = 1,2$ to be measurable and

$$\int_0^R dr\, r|V_j(r)| < \infty, \quad \int_R^\infty dr\, r^2 |V_j(r)| < \infty,$$
$$\text{for some } R > 0 \tag{C1}$$

we define the form sums in $L^2((0,\infty))$

$$h_1(\lambda_1) = h_0 + \lambda_1 V_1, \tag{C2}$$

$$h(\lambda_1,\lambda_2) = h_0 + \lambda_1 V_1 + \lambda_2 V_2, \quad \lambda_j \in \mathscr{R}, \quad j = 1,2. \tag{C3}$$

According to Eq. (A10), $F_1(\lambda_1,r)$, the regular solution associated with $h(\lambda_1)$ fulfills

$$F_1(\lambda_1,r) = r - \lambda_1 \int_0^r dr'(r'-r) V_1(r') F_1(\lambda_1,r') \tag{C4}$$

and thus

$$F_1(\lambda_1,r) \underset{r\to\infty}{\sim} \left[1 + \lambda_1 \int_0^\infty dr'\, V_1(r') F_1(\lambda_1,r')\right] r - \lambda_1 \int_0^\infty dr'\, r' V_1(r') F_1(\lambda_1,r') + o(1), \tag{C5}$$

implying

$$a_1(\lambda_1) = \left[1 + \lambda_1 \int_0^\infty dr'\, V_1(r') F_1(\lambda_1,r')\right]^{-1} \lambda_1 \times \int_0^\infty dr\, r V_1(r) F_1(\lambda_1,r), \tag{C6}$$

where $a_1(\lambda_1)$ represents the scattering length of $h_1(\lambda_1)$ and we assume that $h_1(\lambda_1)$ has no zero-energy resonance, i.e., that

$$1 + \lambda_1 \int_0^\infty dr\, V_1(r) F_1(\lambda_1,r) \neq 0. \tag{C7}$$

Similarly, the regular solution $F(\lambda_1,\lambda_2,r)$ corresponding to $h(\lambda_1,\lambda_2)$ fulfills

$$F(\lambda_1,\lambda_2,r) = r - \int_0^r dr'(r'-r)[\lambda_1 V_1(r') + \lambda_2 V_2(r')] \times F(\lambda_1,\lambda_2,r'), \tag{C8}$$

as well as

$$F(\lambda_1,\lambda_2,r) = F_1(\lambda_1,r) - \lambda_2 \int_0^r dr'\, g_1(\lambda_1,r,r') \times V_2(r') F(\lambda_1,\lambda_2,r'), \tag{C9}$$

$$g_1(\lambda_1,r,r') = [W(\lambda_1)]^{-1}[G_1(\lambda_1,r)F_1(\lambda_1,r') - G_1(\lambda_1,r')F_1(\lambda_1,r)], \tag{C10}$$

where $G_1(\lambda_1,r)$, the irregular solution of $h_1(\lambda_1)$, obeys

$$G_1(\lambda_1,r) = 1 + \lambda_1 \int_r^\infty dr'(r'-r) V_1(r') G_1(\lambda_1,r') \tag{C11}$$

and

$$W(\lambda_1) = W(G_1(\lambda_1), F_1(\lambda_1)) = 1 + \lambda_1 \int_0^\infty dr\, V_1(r) F_1(\lambda_1,r). \tag{C12}$$

Equations (C8) and (C9) imply

$$F_1(\lambda_1,\lambda_2,r) \underset{r\to\infty}{\sim} 1 + \int_0^\infty dr'[\lambda_1 V_1(r') + \lambda_2 V_2(r')] F(\lambda_1,\lambda_2,r') - \int_0^\infty dr'\, r'[\lambda_1 V_1(r') + \lambda_2 V_2(r')] F(\lambda_1,\lambda_2,r') + o(1), \tag{C13}$$

as well as

$$F(\lambda_1,\lambda_2,r) \underset{r\to\infty}{\sim} \left[1 + \lambda_2 \int_0^\infty dr' \frac{G_1(\lambda_1,r')}{W(\lambda_1)} V_2(r') F(\lambda_1,\lambda_2,r')\right] \times F_1(\lambda_1,r) - \left[\lambda_2 \int_0^\infty dr'\, F_1(\lambda_1,r') V_2(r') \times F(\lambda_1,\lambda_2,r')\right] \frac{G_1(\lambda_1,r)}{W(\lambda_1)} + o(1). \tag{C14}$$

Assuming that $h(\lambda_1,\lambda_2)$ has no zero-energy resonance, i.e., that

$$1 + \int_0^\infty dr[\lambda_1 V_1(r) + \lambda_2 V_2(r)] F(\lambda_1,\lambda_2,r) \neq 0, \tag{C15}$$

the scattering length $a(\lambda_1,\lambda_2)$ associated with $h(\lambda_1,\lambda_2)$ is defined by [cf. Eq. (C13)]

$$a(\lambda_1,\lambda_2) = \left\{1 + \int_0^\infty dr[\lambda_1 V_1(r) + \lambda_2 V_2(r)] \times F(\lambda_1,\lambda_2,r)\right\}^{-1} \int_0^\infty dr\, r[\lambda_1 V_1(r) + \lambda_2 V_2(r)] F(\lambda_1,\lambda_2,r). \tag{C16}$$

Inserting Eq. (C5) into (C14), a comparison with (C13) finally implies the Gell-Mann–Goldberger relation (two-potential formula)

$$a(\lambda_1,\lambda_2) = a_1(\lambda_1) + \lambda_2 \int_0^\infty dr \frac{F_1(\lambda_1,r)}{W(\lambda_1)} V_2(r) \times \frac{F(\lambda_1,\lambda_2,r)}{W(\lambda_1) + \lambda_2 \int_0^\infty dr'\, G_1(\lambda_1,r') V_2(r') F(\lambda_1,\lambda_2,r')}. \tag{C17}$$

Equation (C17) is derived for short-range potentials V_j, $j = 1,2$. If h_0 in Eqs. (C2) and (C3) is replaced by h_γ, $\gamma > 0$ and V_j, $j = 1,2$, obey

$$\int_0^R dr\, r|V_j(r)| < \infty, \quad \int_R^\infty dr\, e^{br}|V_j(r)| < \infty, \quad j = 1,2, \quad \text{for some } b,R > 0 \tag{C18}$$

[instead of (C1)], then Eq. (C17) also holds for the Coulomb modified scattering lengths associated with

$$h_{1,\gamma}(\lambda_1) = h_\gamma + \lambda_1 V_1, \tag{C19}$$

$$h_\gamma(\lambda_1,\lambda_2) = h_\gamma + \lambda_1 V_1 + \lambda_2 V_2, \quad \gamma > 0. \tag{C20}$$

For the proof one simply replaces the "free" (ir)regular functions $r(1)$ by the Coulomb (ir)regular functions $F_\gamma(r)$ $[G_\gamma(r)]$ [cf. Eqs. (3.5) and (3.6)] and observes the estimates in Appendix B.

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Fluid sources for Bianchi I and III space-times

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Four analytic solutions to the Einstein field equations are presented. The solutions are parametrized to have either Bianchi I or Bianchi III symmetry. The associated fluid parameters are given and some of them are discussed in detail.

I. INTRODUCTION

Space-times admitting a three-parameter group of automorphisms are important in discussing cosmological models. The case where the group is simply transitive over the three-dimensional, constant-time subspace is particularly useful for two reasons. First, Bianchi[1] has shown there are only nine distinct sets of structure constants for groups of this type so that the algebra may be easily used to classify homogeneous space-times. The second reason for the importance of the Bianchi spaces is the simplicity of the field equations. The relative ease of solution has made these space-times useful in constructing models of spatially homogeneous cosmologies. There is a large literature concerning specific Bianchi spaces which contain fluids with specified equations of state. A partial list is given in the bibliography.[2–17]

In this paper we present and discuss some solutions which can belong to either Bianchi type I or III. These solutions have a special interest as they allow one to investigate fluid behavior across two Bianchi types. The solutions we find are also locally rotationally symmetric and fit into type II of the classification scheme given by Stewart and Ellis.[18]

II. FIELD EQUATIONS AND THEIR SOLUTIONS

The metric we consider is

$$ds^2 = -dt^2 + \gamma_1(t)dx^2 + \gamma_2(t)e^{-2ax}dy^2 + \gamma_3(t)dz^2, \tag{2.1}$$

where $a=0$ gives Bianchi I and $a=1$ gives Bianchi III space-times. The field equations are $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = 8\pi T_{\mu\nu}$.

The Einstein tensors $G_{\mu\nu}$ for our metric are

$$G_{00} = \frac{\dot\gamma_3\dot\gamma_1}{4\gamma_1\gamma_3} + \frac{\dot\gamma_3\dot\gamma_2}{4\gamma_3\gamma_2} + \frac{\dot\gamma_1\dot\gamma_2}{4\gamma_1\gamma_2} - \frac{a^2}{\gamma_1}, \tag{2.2}$$

$$G_1^1 = -\frac{\ddot\gamma_2}{2\gamma_2} - \frac{\ddot\gamma_3}{2\gamma_3} - \frac{\dot\gamma_3\dot\gamma_2}{4\gamma_3\gamma_2} + \frac{\dot\gamma_2^2}{4\gamma_2^2} + \frac{\dot\gamma_3^2}{4\gamma_3^2}, \tag{2.3}$$

$$G_2^2 = -\frac{\ddot\gamma_1}{2\gamma_1} - \frac{\ddot\gamma_3}{2\gamma_3} - \frac{\dot\gamma_3\dot\gamma_1}{4\gamma_1\gamma_3} + \frac{\dot\gamma_1^2}{4\gamma_1^2} + \frac{\dot\gamma_3^2}{4\gamma_3^2}, \tag{2.4}$$

$$G_3^3 = -\frac{\ddot\gamma_1}{2\gamma_1} - \frac{\ddot\gamma_2}{2\gamma_2} - \frac{\dot\gamma_1\dot\gamma_2}{4\gamma_1\gamma_2} + \frac{\dot\gamma_2^2}{4\gamma_1^2} + \frac{\dot\gamma_2^2}{4\gamma_2^2} + \frac{a^2}{\gamma_1}, \tag{2.5}$$

$$R_{01} = +\frac{a}{2}\frac{\dot\gamma_1}{\gamma_1} - \frac{a}{2}\frac{\dot\gamma_2}{\gamma_2}. \tag{2.6}$$

To find analytic solutions with Bianchi I and III symmetry we consider locally rotationally symmetric metrics, with $\gamma_1 = \gamma_2$. This metric falls into type II of the classification scheme given by Stewart and Ellis.[18] For this choice of γ, G_1^1 is identically equal to G_2^2, and the isotropic pressure requirement for perfect fluid sources gives

$$\frac{\ddot\gamma_3}{2\gamma_3} - \frac{\ddot\gamma_1}{2\gamma_1} + \frac{\dot\gamma_3\dot\gamma_1}{4\gamma_1\gamma_3} - \frac{\dot\gamma_3^2}{4\gamma_3^2} + \frac{a^2}{\gamma_1} = 0. \tag{2.7}$$

The method we shall use to generate solutions to (2.7) is to assume a solution for $\gamma_1(t)$ [or $\gamma_3(t)$] and then solve for $\gamma_3(t)$ [or $\gamma_1(t)$]. At this stage the only criteria we use is the integrability of the field equations. We then will evaluate some of the physical parameters and discuss them.[19]

Solution 1: Assume $\gamma_3(t) = C_1\tilde t$. Then

$$\gamma_1(t) = -(1/C_0)[A_1\tilde t + A_2 e^{-(1/2)\tilde t} + 8a^2], \tag{2.8}$$

with[20] $\tilde t = \sqrt{C_0/2}\,t$. The pressure and density are

$$\begin{aligned} 8\pi p(t) &= -\frac{C_0}{8} + \frac{3}{8}\frac{A_1\tilde t}{\gamma_1} \\ &\quad + \frac{1}{8\gamma_1^2 C_0}\left(A_1\tilde t - \frac{1}{2}A_2 e^{-(1/2)\tilde t}\right)^2 + \Lambda, \\ 8\pi\epsilon(t) &= -\frac{a^2}{\gamma_1} - \frac{1}{4\gamma_1}\left(A_1\tilde t - \frac{1}{2}A_2 e^{-(1/2)\tilde t}\right) \\ &\quad + \frac{(A_1\tilde t - \frac{1}{2}Be^{-(1/2)\tilde t})^2}{8\gamma_1^2 C_0} - \Lambda. \end{aligned} \tag{2.9}$$

We have included the cosmological constant in Eq. (2.9) for generality. Its inclusion does not alter (2.7). As $t\to 0$

$$\begin{aligned} 8\pi p(0) &= -\frac{C_0}{8}\frac{(4A_1 + 8A_2 + 8a^2)}{(A_1 + A_2 + 8a^2)} \\ &\quad + \frac{C_0}{8}\frac{(A_1 - A_2/2)^2}{(A_1 + A_2 + 8a^2)^2} + \Lambda, \\ 8\pi\epsilon(0) &= \frac{C_0}{8}\frac{(2A_1 - A_2 + 8a^2)}{(A_1 + A_2 + 8a^2)} \\ &\quad + \frac{C_0}{8}\frac{(A_1 - A_2/2)^2}{(A_1 + A_2 + 8a^2)^2} - \Lambda. \end{aligned} \tag{2.10}$$

At $t\to\infty$, using $\gamma_1(t)$ we find

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$$8\pi p(\infty) = \Lambda - \tfrac{3}{8}C_0, \quad 8\pi\epsilon(\infty) = \tfrac{3}{8}C_0 - \Lambda. \tag{2.11}$$

Choosing $\Lambda = \frac{3}{8}C_0$, one can generate in a Bianchi III spacetime, a variety of initial perfect fluids which expand at large times to a very dilute, essentially empty space solution.

For example, choosing $A_2 = 0$ and $A_1 < 0$, we have, with $\Lambda = \frac{3}{8}C_0$,

$$\begin{aligned} 8\pi p(0) &= C_0 a^2(-|A_1| + 16a^2)/(-|A_1| + 8a^2)^2, \\ 8\pi\epsilon(0) &= C_0 a^2(3|A_1| - 16a^2)/(-|A_1| + 8a^2)^2. \end{aligned} \tag{2.12}$$

Physical solutions correspond to $8 < |A_1|/a^2 \leqslant 16$.

The Bianchi I solution is a vacuum. In Bianchi III the solution is a fluid which can have an equation of state of the form $p = \alpha\epsilon$ with $0 \leqslant \alpha < 1$ at $t = 0$.

Solution 2: Assume $\gamma_3(t) = C_1 \cos^2 \tilde{t}$. Then one finds

$$\gamma_1(t) = (1/C_0)(\bar{\gamma}_1(t) + 2a^2), \quad C_0 > 0, \tag{2.13}$$

with $\tilde{t} = \sqrt{(C_0/2)}\,(t - C_2)$ and

$$\bar{\gamma}_1(t) = \cos^2(\tilde{t})\left[A_1 - A_2 \tan\tilde{t} \sec\tilde{t} - A_2 \ln\left|\frac{1 + \sin\tilde{t}}{\cos\tilde{t}}\right|\right].$$

The pressure and density are

$$\begin{aligned} 8\pi p(t) &= C_0 - \frac{a^2}{\gamma_1} - \frac{C_0 \tan^2\tilde{t}}{2} \\ &\quad + \frac{(2a^2 \tan\tilde{t} - A_2 \sec\tilde{t})^2}{2C_0\gamma_1^2} + \Lambda, \\ 8\pi\epsilon(t) &= \frac{3}{2}C_0 \tan^2\tilde{t} - \frac{4a^2 \tan^2\tilde{t}}{\gamma_1} \\ &\quad + \frac{2A_2 \sec\tilde{t} \tan\tilde{t}}{\gamma_1} - \frac{a^2}{\gamma_1} \\ &\quad + (1/2C_0\gamma_1^2)[2a^2 \tan\tilde{t} - A_2 \sec\tilde{t}\,]^2 - \Lambda. \end{aligned} \tag{2.14}$$

This solution could be valid over a range of time.

Solution 3:

(a) Assume $\gamma_3(t) = \tilde{t}^{\,2}$, where $\tilde{t} = C_1 t + C_2$, then one obtains

$$\gamma_1(t) = A_1\tilde{t}^{\,2} + a^2\tilde{t}^{\,2}(\ln(A_2\tilde{t}) - \tfrac{1}{2})/C_1^2. \tag{2.15}$$

The pressure and density distributions are

$$\begin{aligned} 8\pi p(t) &= -\frac{C_1^2}{\tilde{t}^{\,2}} - \frac{a^2}{\gamma_1} + \frac{\tilde{t}^{\,2}a^4}{4\gamma_1^2 C_1^2} + \Lambda, \\ 8\pi\epsilon(t) &= \frac{3C_1^2}{\tilde{t}^{\,2}} + \frac{a^2}{\gamma_1} + \frac{\tilde{t}^{\,2}a^4}{4C_1^2\gamma_1^2} - \Lambda. \end{aligned} \tag{2.16}$$

As $t \to \infty$, $p(\infty) = \Lambda$ and $\epsilon(\infty) = -\Lambda$, so $\Lambda = 0$ would give a large time an essentially empty universe. As t approaches zero we have

$$\begin{aligned} 8\pi p(0) &= -\frac{C_1^2}{C_2^2} + a^2\frac{a^2C_2^2}{4\gamma_1^2C_1^2} - \frac{1}{\gamma_1}, \\ 8\pi\epsilon(0) &= \frac{3C_1^2}{C_2^2} + a^2\frac{a^2C_2^2}{4\gamma_1^2C_1^2} - \frac{1}{\gamma_1}. \end{aligned} \tag{2.17}$$

For Bianchi I, a positive pressure is not possible with $\Lambda = 0$. For Bianchi III, a proper choice of constants will produce a range of physical solutions.

For example, take C_1 and C_2 as input, $a^2 = 1$. Choose $A_2 = 1/C_2$. This choice sets a limit on A_1

$$A_1 > 1/2C_1^2, \quad C_1 \neq 0, \tag{2.18}$$

or

$$A_1 = n/2C_1^2, \quad n > 1.$$

This is required to keep $\gamma_1 > 0$ and maintain the signature. Here, n parametrizes A_1. The pressure and density are

$$\begin{aligned} \frac{8\pi p(t)\tilde{t}^{\,2}}{C_1^2} &= -1 - \frac{2}{n-1} + \frac{1}{(n-1)^2}, \\ \frac{8\pi\epsilon(t)\tilde{t}^{\,2}}{C_1^2} &= 3 + \frac{2}{n-1} + \frac{1}{(n-1)^2}. \end{aligned} \tag{2.19}$$

Positive pressure requires $n^2 < 2$ so range of n is

$$1 < n^2 < 2.$$

The equation of state of this fluid can be written as $p = \alpha\epsilon$, with

$$\frac{1}{\alpha} = \frac{3(n-1)^2 + 2(n-1) + 1}{2 - n^2}. \tag{2.20}$$

The positive pressure condition allows any $\alpha > 0$. A radiation equation of state $\alpha = \frac{1}{3}$ corresponds to $n = 1.22$, and $\alpha = 1$ is forbidden by the signature requirement $n > 1$. The allowed equation of states have any $\alpha < 1$.

(b) There are two additional solutions which we provide for completeness.

(1): Given

$$\gamma_3(t) = C_2, \tag{2.21}$$

one finds $\gamma_1(t) = a^2t^{\,2} + A_1t + A_2$. The pressure and density are

$$\begin{aligned} 8\pi p &= -\frac{a^2}{\gamma_1} + \frac{(2a^2t + A_1)^2}{4\gamma_1^2} + \Lambda, \\ 8\pi\epsilon &= -\frac{a^2}{\gamma_1} + \frac{(2a^2t + A_1)^2}{4\gamma_1^2} - \Lambda. \end{aligned} \tag{2.22}$$

For zero Λ, these describe an empty universe at large time.

(2): Given

$$\gamma_1 = C_0(C_1t + C_2)^m \text{ and } a = 0, \tag{2.23}$$

one finds $\gamma_3 = (C_1t + C_2)^n$, with

$$2n(n-1) - 2m(m-1) + nm - n^2 = 0. \tag{2.24}$$

The fluid parameters are

$$\begin{aligned} 8\pi p &= \frac{C_1^2}{(C_1t + C_2)^2}\left[\frac{m^2}{4} - m(m-1)\right], \\ 8\pi\epsilon &= \frac{C_1^2}{(C_1t + C_2)^2}\left(\frac{nm}{2} + \frac{m^2}{4}\right). \end{aligned} \tag{2.25}$$

These fluid parameters go to zero at large time. Vacuum corresponds to $m = 0$ and to $m = \frac{4}{3}$, $n = -\frac{2}{3}$, the latter a Kasner solution.[21] This fluid can have an equation of state $p = \alpha\epsilon$, with

$$\alpha = (4 - 3m)/(m + 2n). \tag{2.26}$$

Equation (2.24) has two possible solutions, $n = 2(1 - m)$ and $n = m$. This allows an easy classification of possible fluids.

(i) $\alpha \neq 1$:

$$m = n = \tfrac{1}{3}(1+\alpha),$$

$$8\pi p = 8\pi\alpha\epsilon = 4C_1^2\alpha/3(1+\alpha)^2(C_1 t + C_2)^2. \tag{2.27}$$

For example, a radiation fluid corresponds to $m = n = 1$.

(ii) $\alpha = 1$: All m with $n = 2(1-m)$. There is an infinite set of solutions for the stiff fluid. We find

$$8\pi p = 8\pi\epsilon = C_1^2(4m - 3m^2)/4(C_1 t + C_2)^2. \tag{2.28}$$

Only those solutions with $m^2 < \frac{4}{3} m$ will correspond to physical fluids. An infinite sequence of hard universes has been noted before by Jacobs[22] and Gröbner and Hofreiter.[23] We believe our results are a simple case of their solutions. A recent method[24] using metrically valid but unphysical fluid solutions to generate physical fluids makes these simple solutions valuable.

Solution 4: Given $\gamma_1(t) = a^2 t^2 + C_0 t + C_1$, one obtains

$$\gamma_3(t) = A_0 + \frac{A_1}{a}\ln|2a(a^2t^2 + C_0 t + C_1)^{1/2} + 2a^2 t + C_0|. \tag{2.29}$$

The pressure and energy density are

$$\begin{aligned} 8\pi p &= \frac{C_0^2 - 4a^2 C_1}{4\gamma_1^2} + \Lambda, \\ 8\pi\epsilon &= \frac{C_0^2 - 4a^2 C_1}{4\gamma_1^2} + \frac{A_1(2a^2 t + C_0)}{\gamma_1^{3/2}\gamma_3^{1/2}} - \Lambda. \end{aligned} \tag{2.30}$$

Choosing $C_0 = 0$, $A_1 = 0$, and $C_1 < 0$ gives a solution

$$\begin{aligned} 8\pi p &= \frac{4a^2|C_1|}{4\gamma_1^2}, \\ 8\pi\epsilon &= \frac{4a^2|C_1|}{4\gamma_1^2} + \frac{A_1 2a^2 t}{\gamma_1^{3/2}\gamma_3^{1/2}}. \end{aligned} \tag{2.31}$$

This is a vacuum Bianchi I. In Bianchi III, a more complex fluid is obtained. For $A_1 = 0$, there is a stiff fluid equation of state.[12]

III. DISCUSSION

We have seen that the metric solution can generate very different fluid pressure and densities in the two Bianchi types. A convenient indicator of other possible differences are the velocity paremeters: expansion, vorticity, acceleration, and shear. For the metric we have discussed, all of the fluids are acceleration and rotation free, but they do have expansion θ and shear $\sqrt{\sigma^2}$ given by[25]

$$\begin{aligned} \theta &= \dot{\gamma}_3/2\gamma_3 + \dot{\gamma}_1/\gamma_1, \\ \sigma^2 &= \tfrac{1}{6}(\dot{\gamma}_1/\gamma_1 - \dot{\gamma}_3/\gamma_3)^2. \end{aligned} \tag{3.1}$$

We find the shear can be very type dependent for our solutions. For example, in Solution 1, the effect of Bianchi type is largest at small times. For small times we find

$$\sigma^2 \cong \frac{C_0}{12}\left(\frac{1.5A_2 + 8a^2}{A_1 + A_2 + 8a^2}\right)^2. \tag{3.2}$$

The model we gave, $A_2 = 0$, gives a shear-free vacuum in Bianchi I and a nonzero shear in Bianchi III. It is clear that choosing $A_2 = -16a^2/3$ would reverse this. Solution 3 shows similar effects for large times.

In conclusion, we have presented four combined fluid solutions to Bianchi I and III space-times. The behavior of the fluid is type dependent and can be physically reasonable. Using metric solutions parametrized over several Bianchi types is a useful tool in constructing and studying fluid cosmologies.

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$$\frac{1}{\gamma_1\gamma_2}\frac{d}{dt}(\gamma_1\dot{\gamma}_2) - \frac{1}{2}\frac{d}{dt}\left(\frac{\dot{\gamma}_1}{\gamma_1}\ln\gamma_1\gamma_2^3\right) + \frac{d}{dt}\left(\frac{\dot{\gamma}_1}{\gamma_1}\right)\left[-1 + \frac{1}{2}\ln\gamma_1\gamma_2^3\right] = 0.$$

This is analogous to the Tolman equation given for the relativistic fluid sphere field equation.

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Petrov type *D* perfect-fluid solutions in generalized Kerr–Schild form

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Generalized Kerr–Schild space-times for a perfect-fluid source are investigated. New Petrov type *D* perfect fluid solutions are obtained starting from conformally flat perfect-fluid metrics.

I. INTRODUCTION

This work is concerned with perfect-fluid solutions of Einstein's equations for a metric in generalized Kerr–Schild form. Since the original Kerr–Schild paper,[1] a lot of generalizations of the Kerr–Schild ansatz have appeared.[2] Bilge and Gürses[3] have shown how the Newman–Penrose spin coefficients, trace-free Ricci, Ricci scalar, and Weyl spinors transform under the most general Kerr–Schild transformation. In this paper we treat generalized Kerr–Schild metrics of the form

$$\tilde{g}_{\alpha\beta} = g_{\alpha\beta} + 2Hl_\alpha\, l_\beta, \tag{1.1}$$

where $g_{\alpha\beta}$ is the metric of any space-time, l_α is a null, geodesic vector field for the metric $g_{\alpha\beta}$, and H is a scalar field.

As far as we know, no perfect-fluid solution of the Kerr–Schild type is known. All the solutions we obtain are of Petrov type *D*, and most of these are new since the velocity of the fluid does not lie in the two-space defined by the principal null directions of the Weyl tensor.[4]

In Sec. II we obtain the Riemann, Ricci, and Weyl tensors of the metric $\tilde{g}$ as functions of the Riemann, Ricci, and Weyl tensors of the metric g and the spin coefficients defined by a null tetrad associated with l_α. Our notation and calculations are quite close to those of Taub (Ref. 2). Section III is devoted to writing down the equations in the case where g is a conformally flat solution of Einstein's equations for a perfect fluid. It is shown easily that the geodesic (shear-free) null vector fields in a conformally flat space-time are the geodesic (shear-free) null vector fields in flat space-time. Since the most general vector field of this kind is already known,[5] one has great freedom in choosing the vector field l_α. Two cases appear depending on whether l_α is shear-free or not. They are studied in Secs. IV and V. Finally, in Sec. VI we give some examples of how the method works and some explicit solutions.

II. THE RIEMANN, RICCI, AND WEYL TENSORS OF GENERALIZED KERR–SCHILD METRICS

It is easily shown that[6]

$$\tilde{g}^{\alpha\beta} = g^{\alpha\beta} - 2Hl^\alpha l^\beta, \tag{2.1}$$

$$\tilde{l}^\alpha = l^\alpha, \quad \tilde{l}^\alpha \tilde{l}_\alpha = 0. \tag{2.2}$$

Then, we obtain for the Christoffel symbols

$$\tilde{\Gamma}^\alpha_{\beta\lambda} = \Gamma^\alpha_{\beta\lambda} + A^\alpha_{\beta\lambda} + 2Hl^\alpha l_\beta\, l_\lambda\, l^\mu \nabla_\mu H, \tag{2.3}$$

where the $\Gamma^\alpha_{\beta\lambda}$ are the Christoffel symbols for the metric g and

$$A^\alpha_{\beta\lambda} \equiv \nabla_\beta(Hl^\alpha l_\lambda) + \nabla_\lambda(Hl^\alpha l_\beta) - \nabla^\alpha(Hl_\beta\, l_\lambda) \tag{2.4}$$

or

$$A^\alpha_{\beta\lambda} = Hl^\alpha S_{\beta\lambda} + l_\beta(l^\alpha \nabla_\lambda H + HA_\lambda{}^\alpha) + l_\lambda(l^\alpha \nabla_\beta H + HA_\beta{}^\alpha) - l_\beta\, l_\lambda\, \nabla^\alpha H, \tag{2.5}$$

with

$$S_{\alpha\beta} \equiv \nabla_\alpha l_\beta + \nabla_\beta l_\alpha, \quad A_{\alpha\beta} \equiv \nabla_\alpha l_\beta - \nabla_\beta l_\alpha. \tag{2.6}$$

Next, we compute the Riemann tensor from the expression (2.3) and we find the following:

$$\tilde{R}^\alpha_{\beta\lambda\mu} = R^\alpha_{\beta\lambda\mu} + \nabla_\lambda A^\alpha_{\beta\mu} - \nabla_\mu A^\alpha_{\beta\lambda} + \nabla_\lambda [2Hl^\alpha l_\beta\, l_\mu\, l^\rho \nabla_\rho H] - \nabla_\mu [2Hl^\alpha l_\beta\, l_\lambda\, l^\rho \nabla_\rho H] + A^\alpha_{\rho\lambda} A^\rho_{\beta\mu} - A^\alpha_{\rho\mu} A^\rho_{\beta\lambda}, \tag{2.7}$$

where $R^\alpha_{\beta\lambda\mu}$ is the Riemann tensor for the metric g. Then, for the Ricci tensor we obtain

$$\tilde{R}_{\beta\mu} = R_{\beta\mu} + \nabla_\lambda A^\lambda_{\beta\mu} + 2Hl_\beta\, l^\rho \nabla_\lambda A^\lambda_{\rho\mu}, \tag{2.8}$$

where $R_{\beta\mu}$ is the Ricci tensor for the metric g. After a long calculation it may be shown that

$$\nabla_\rho A^\rho_{\beta\lambda} = Nl_\beta\, l_\lambda - l^\rho \Phi_\rho(l_\beta\, k_\lambda + l_\lambda\, k_\beta) + \bar{\Sigma}(l_\beta\, m_\lambda + l_\lambda\, m_\beta) + \bar{\Omega} m_\beta\, m_\lambda + \Sigma(l_\beta\, \bar{m}_\lambda + l_\lambda\, \bar{m}_\beta) + \Omega \bar{m}_\beta\, \bar{m}_\lambda + \Gamma(m_\beta\, \bar{m}_\lambda + m_\lambda\, \bar{m}_\beta), \tag{2.9}$$

where we have chosen a null tetrad $(l, k, m, \bar{m})$ for the metric g and[7]

$$\Gamma \equiv (\rho + \bar{\rho})\nabla_\alpha(Hl^\alpha) - 2H(\rho\bar{\rho} + \sigma\bar{\sigma} + \phi_{00}), \tag{2.10}$$

$$\Omega \equiv 2\sigma\nabla_\alpha(Hl^\alpha) - 2H(\psi_0 + 2\rho\sigma), \tag{2.11}$$

$$\Sigma \equiv m^\alpha \Phi_\alpha - (\beta + \bar{\alpha} + \tau)\nabla_\alpha(Hl^\alpha) - 2H[\psi_1 - \rho(\beta + \bar{\alpha}) - \sigma(\bar{\beta} + \alpha) - \phi_{01}], \tag{2.12}$$

$$\Phi_\beta \equiv \nabla_\beta \nabla_\alpha(Hl^\alpha) - H\nabla^\rho \nabla_\rho l_\beta - 2(\nabla^\rho l_\beta)\nabla_\rho H + Hl^\rho R_{\rho\beta}, \tag{2.13}$$

$$N \equiv -g^{\rho\sigma}\nabla_\rho \nabla_\sigma H + 2(\gamma + \bar{\gamma})\nabla_\alpha(Hl^\alpha) - 2H(k^\beta \nabla_\rho l_\beta)(k^\lambda \nabla^\rho l_\lambda) - 2k^\alpha \Phi_\alpha - 2H[\psi_2 + \bar{\psi}_2 + k^\rho l^\sigma R_{\rho\sigma} + 4\Lambda]. \tag{2.14}$$

Therefore, if the metric g is given, the Einstein equations

$$\tilde{R}_{\beta\mu} = \chi(\tilde{T}_{\beta\mu} - \tfrac{1}{2}\tilde{g}_{\beta\mu}\tilde{T}) \tag{2.15}$$

are defined by (2.8) and (2.9). In particular, from (2.8), (2.9),

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and (2.15) we obtain the interesting relation

$$\chi l^\alpha \tilde{T}_{\alpha\mu} = l^\alpha R_{\alpha\mu} + l_\mu (l^\rho \Phi_\rho + (\chi/2)\tilde{T}). \tag{2.16}$$

We distinguish two cases.

(1) $l^\alpha R_{\alpha\mu} = a l_\mu$. In this case l_α is an eigenvector of $\tilde{T}_{\alpha\beta}$ and then perfect-fluid solutions cannot exist.

(2) $l^\alpha R_{\alpha\mu} \neq a l_\mu$. In this case $\tilde{T}_{\alpha\beta}$ can be the energy-momentum tensor of a perfect fluid. It is the purpose of this paper to study this case when both $\tilde{T}_{\alpha\beta}$ and $T_{\alpha\beta}$ are perfect-fluid energy-momentum tensors.

Let $(l^\alpha, k^\alpha, m^\alpha, \bar{m}^\alpha)$ be a null tetrad for the metric g. Then

$$\tilde{l}^\alpha = l^\alpha, \quad \tilde{k}^\alpha = k^\alpha + H l^\alpha, \quad \tilde{m}^\alpha = m^\alpha, \quad \tilde{\bar{m}}^\alpha = \bar{m}^\alpha$$

is a null tetrad for the metric $\tilde{g}$. By using this null tetrad we compute the Weyl tensor and we finally obtain

$$\tilde{\psi}_0 = \psi_0, \quad \tilde{\psi}_1 = \psi_1, \tag{2.17}$$

$$3\tilde{\psi}_2 = 3\psi_2 - 2H\phi_{00} - \tfrac{1}{2}\nabla_\lambda [l^\lambda \nabla_\alpha (H l^\alpha)] + 3\rho[DH - H(\rho - \bar{\rho})], \tag{2.18}$$

$$\tilde{\psi}_3 = \psi_3 - H\tilde{\psi}_1 + \tfrac{1}{2}\bar{\Sigma} - 2H\phi_{10} - (\bar{\tau} - \bar{\beta} - \alpha)(DH - 2H\rho) - \bar{\delta}DH + \rho\bar{\delta}H - H\bar{\tau}(\rho - \bar{\rho}) + 2H\bar{\sigma}(\tau - \beta - \bar{\alpha}) + \bar{\sigma}\delta H, \tag{2.19}$$

$$\tilde{\psi}_4 = \psi_4 + H^2\bar{\psi}_0 - 2H\Delta\bar{\sigma} - \bar{\sigma}\Delta H + 2H\bar{\sigma}\bar{\mu} + 4H\bar{\sigma}(\gamma - \bar{\gamma}) - 2H^2\bar{\sigma}(\rho - \bar{\rho}) - \bar{\delta}[\bar{\delta}H - 2H(\bar{\beta} + \alpha)] - \lambda(DH - 2H\rho) + (\bar{\beta} + 3\alpha - 2\bar{\tau})(\bar{\delta}H - 2H(\bar{\beta} + \alpha)). \tag{2.20}$$

III. THE EINSTEIN EQUATIONS FOR A CONFORMALLY FLAT PERFECT-FLUID METRIC $g_{\alpha\beta}$

Henceforth, we choose the metric g to be conformally flat; that is,

$$\psi_0 = \psi_1 = \psi_2 = \psi_3 = \psi_4 = 0 \Leftrightarrow g_{\alpha\beta} = \phi^2 \eta_{\alpha\beta}, \tag{3.1}$$

where ϕ^2 is a positive function of the coordinates and $\eta_{\alpha\beta}$ is the metric of flat space-time. Moreover, we assume that $g_{\alpha\beta}$ is a solution of Einstein's equations for a perfect-fluid energy-momentum tensor; that is to say

$$R_{\alpha\beta} = \chi(T_{\alpha\beta} - \tfrac{1}{2} g_{\alpha\beta} T), \tag{3.2}$$

$$T_{\alpha\beta} = (q + p)u_\alpha u_\beta + p g_{\alpha\beta}, \quad g^{\alpha\beta} u_\alpha u_\beta = -1. \tag{3.3}$$

All metrics of this kind are known: they are either generalized interior Schwarzschild solutions or generalized Friedmann solutions (Ref. 4).

It may easily be verified that if $g_{\alpha\beta}$ is a conformally flat space-time, and if l_α is a null geodesic (shear-free) vector field for $g_{\alpha\beta}$ then it is also a null geodesic (shear-free) vector field for flat space-time. But the general solution for vector fields of this kind in flat space-time is known and is given by[5]

$$l = du + \bar{Y}\, d\zeta + Y\, d\bar{\zeta} + Y\bar{Y}\, dv, \tag{3.4}$$

where Y is a complex function of the coordinates $\{u, v, \zeta, \bar{\zeta}\}$ verifying

$$Y\frac{\partial Y}{\partial \zeta} + \bar{Y}\frac{\partial Y}{\partial \zeta} - \frac{\partial Y}{\partial v} - Y\bar{Y}\frac{\partial Y}{\partial u} = 0. \tag{3.5}$$

When l_α is also shear-free, Y is defined implicitly by

$$F(Y, \bar{\zeta}Y + u, v, Y + \zeta) = 0, \tag{3.6}$$

where F is an arbitrary analytic function of three complex variables. The coordinates $\{u, v, \zeta, \bar{\zeta}\}$ are related with the usual coordinates of the Minkowski space-time by

$$\sqrt{2}\, u = t - z, \quad \sqrt{2}\, v = t + z, \quad \sqrt{2}\, \zeta = x + iy, \tag{3.7}$$

and the metric $g_{\alpha\beta}$ may be written in these coordinates as

$$g_{\alpha\beta}\, dx^\alpha\, dx^\beta = 2\phi^2[-du\, dv + d\zeta\, d\bar{\zeta}]. \tag{3.8}$$

Now, we choose the null tetrad associated with l_α as follows:

$$l, \quad k = \phi^2\, dv, \quad m = \phi(d\zeta + Y\, dv). \tag{3.9}$$

Then, after a straightforward calculation, we obtain the spin coefficients

$$\pi = -\alpha = -\phi^{-1}\bar{m}^\alpha \nabla_\alpha \phi, \quad \gamma = -\mu = \phi^{-1} k^\alpha \nabla_\alpha \phi,$$
$$\rho = \phi^{-2}[\rho_M + \phi\, l^\alpha \nabla_\alpha \phi], \quad \rho_M = \frac{\partial Y}{\partial \zeta} - \bar{Y}\frac{\partial Y}{\partial u},$$
$$\tau = \phi^{-1}\tau_M + \bar{\alpha}, \quad \tau_M = -\frac{\partial Y}{\partial u}, \tag{3.10}$$
$$\sigma = \phi^{-2}\sigma_M, \quad \sigma_M = \frac{\partial Y}{\partial \bar{\zeta}} - Y\frac{\partial Y}{\partial u},$$
$$\kappa = \epsilon = \lambda = \beta = \nu = 0.$$

Moreover, it is well known that the null tetrad is defined up to a transformation of the form

$$l' = l, \quad m' = e^{iC}(m + \bar{Z}l), \tag{3.11}$$
$$k' = k + Zm + \bar{Z}\bar{m} + Z\bar{Z}l.$$

We make such a transformation choosing

$$\bar{Z} = -m^\alpha u_\alpha / l^\alpha u_\alpha \tag{3.12}$$

so that

$$m'^\alpha u_\alpha = 0. \tag{3.13}$$

After this change of null tetrad, the new spin coefficients are[8]

$$\pi' = \pi - DZ, \quad \kappa' = \epsilon' = 0, \quad \rho' = \rho,$$
$$\sigma' = \sigma, \quad \beta' = Z\sigma, \quad \alpha' = \alpha + Z\rho,$$
$$\mu' = \mu + \bar{Z}\pi + Z^2\sigma - \delta' Z, \quad \tau' = \tau + Z\sigma + \bar{Z}\rho,$$
$$\lambda' = Z\pi + 2Z\alpha + Z^2\rho - \bar{\delta}' Z, \tag{3.14}$$
$$\gamma' = \gamma + Z\tau + Z^2\sigma + Z\bar{Z}\rho + \bar{Z}\alpha,$$
$$\nu' = Z\mu + Z\bar{Z}\pi + Z^2\tau + Z^3\sigma + Z^2\bar{Z}\rho + 2Z\gamma + 2Z\bar{Z}\alpha - \Delta' Z.$$

Hereafter, we shall drop the primes.

We search for solutions $\tilde{g}_{\alpha\beta}$ of Einstein's equations for a perfect-fluid energy-momentum tensor

$$\tilde{T}_{\alpha\beta} = (\tilde{q} + \tilde{p})\tilde{u}_\alpha \tilde{u}_\beta + \tilde{p}\tilde{g}_{\alpha\beta}, \tag{3.15}$$

$$\tilde{g}^{\alpha\beta}\tilde{u}_\alpha \tilde{u}_\beta = -1. \tag{3.16}$$

Taking into account all previous assumptions and results, the Einstein equations (2.15), (2.8), and (2.9)—once they are projected onto the null tetrad—lead us to the following set of equations:

$$m^\alpha \tilde{u}_\alpha = 0, \tag{3.17}$$

$$\Omega = 0, \tag{3.18}$$

$$(\tilde{q}+\tilde{p})(l^\alpha \tilde{u}_\alpha)^2 = (q+p)(l^\alpha u_\alpha)^2, \tag{3.19}$$

$$\nabla_\lambda\,[l^\lambda \nabla_\mu (H l^\mu)] = \chi[\tfrac{1}{2}(\tilde{q}-3\tilde{p}) - \tfrac{1}{2}(q-3p) + H(q+p)(l^\alpha u_\alpha)^2], \tag{3.20}$$

$$\Gamma = (\chi/2)[\tilde{q}-\tilde{p}-q+p], \tag{3.21}$$

$$N = \chi\left[\frac{\tilde{q}+\tilde{p}}{4(l^\alpha \tilde{u}_\alpha)^2} - \frac{q+p}{4(l^\alpha u_\alpha)^2} - H^2(q+p)(l^\alpha u_\alpha)^2 - 2Hp\right], \tag{3.22}$$

$$\Sigma = 0. \tag{3.23}$$

Starting from (2.11), Eq. (3.18) becomes

$$\sigma[DH - H(\rho-\bar{\rho})] = 0. \tag{3.18'}$$

We can consider two cases.

(A) $\sigma \neq 0$. Then Eq. (3.18') implies that we must have

$$\rho = \bar{\rho}, \quad DH = 0. \tag{3.24}$$

This case is studied in the following section.

(B) $\sigma = 0$. Then (3.18') is automatically satisfied. This case is studied in Sec. V.

IV. THE CASE $\sigma \neq 0$

In this section we try to solve Eqs. (3.17)–(3.23) with the assumption $\sigma \neq 0$.

Throughout this and the next sections we shall use repeatedly (but not explicitly) the Bianchi identities and the Newman–Penrose equations for the metric $g_{\alpha\beta}$ (the Bianchi identities are given in the Appendix). Whenever we make some assumption or specialization we must restrict these equations in the appropriate fashion. The details are omitted.

First of all, from (3.20), (3.21), and (3.24) we obtain $\tilde{q}$ and $\tilde{p}$ as functions of q, p, and H,

$$\chi\tilde{p} = \chi p + 2H\phi_{00}, \tag{4.1}$$

$$\chi\tilde{q} = \chi q + 4H(\rho^2 - \sigma\bar{\sigma}) - 2H\phi_{00}. \tag{4.2}$$

Furthermore, from (3.19), (3.17), and (3.16), we get $\tilde{u}_\alpha$:

$$(l^\alpha \tilde{u}_\alpha)^2 = \chi(q+p)(l^\alpha u_\alpha)^2[\chi(q+p) + 4H(\rho^2-\sigma\bar{\sigma})]^{-1},$$

$$m^\alpha \tilde{u}_\alpha = 0. \tag{4.3}$$

Then, we only must solve Eqs. (3.22) and (3.23).

Starting from (2.12) and (2.13), making use of (3.24), and after some standard calculations, we obtain for (3.23)

$$\bar{\delta}H = 2H(\alpha+\bar{\beta}) - H\bar{\tau} - H\rho(\tau/\sigma). \tag{4.4}$$

In the same way, it follows from (2.14), (3.24), and (4.1)–(4.4) that Eq. (3.22) becomes

$$\rho\Delta H = H\{\rho(\mu+\gamma+\bar{\gamma}) + \sigma\lambda + \delta(\rho(\tau/\sigma)) + \rho(\tau/\sigma)(\bar{\alpha}-\beta) - \Delta\rho - \rho^2(\tau\bar{\tau}/\sigma\bar{\sigma}) - 4(\phi_{11}/\phi_{00})(\rho^2-\sigma\bar{\sigma}) - 2\Lambda\} - (H^2/\phi_{00})[(\rho^2-\sigma\bar{\sigma})^2 - \phi_{00}^2]. \tag{4.5}$$

From (2.18) and (2.19) with (3.24), (4.5), and (4.4) we get[9] (for the sake of brevity $\tilde{\psi}_4$ is not written here)

$$\tilde{\psi}_0 = 0, \quad 3\tilde{\psi}_2 = H(\sigma\bar{\sigma} - \rho^2 - \phi_{00}),$$
$$\tilde{\psi}_1 = 0, \quad \tilde{\psi}_3 = H(\tau/\sigma)(\sigma\bar{\sigma} - \rho^2). \tag{4.6}$$

The question now is the following: Are Eqs. (3.24), (4.4), and (4.5) compatible? Since Eqs. (3.24) and (4.4) are linear in H, their compatibility with (4.5) (which is nonlinear in H) gives us an expression for H which is not, in general, a solution of Eqs. (3.24), (4.4), and (4.5). In order to proceed we assume

$$\rho^2 - \sigma\bar{\sigma} = \phi_{00}, \tag{4.7}$$

so that Eq. (4.5) becomes linear as well.

Keeping this in mind, the compatibility condition of (3.24) and (4.4) is simply

$$\pi = 0 \tag{4.8}$$

and the compatibility condition of (4.4) with its complex conjugate is the reality condition

$$\bar{\sigma}(\delta\tau + \tau(\beta-\bar{\alpha})) = \sigma(\bar{\delta}\bar{\tau} + \bar{\tau}(\bar{\beta}-\alpha)). \tag{4.9}$$

Furthermore, Eq. (4.5) now becomes

$$\Delta H = H\left\{2(\mu+\gamma+\bar{\gamma}) - 2\rho\frac{\bar{\lambda}}{\sigma} - \frac{1}{2}\left(\frac{\tau^2}{\sigma} + \frac{\bar{\tau}^2}{\bar{\sigma}}\right) - \rho\frac{\tau\bar{\tau}}{\sigma\bar{\sigma}}\right\}, \tag{4.10}$$

which is compatible with (3.24). Finally, a new integrability condition arises from (4.4) and (4.10):

$$\Delta\tau + 3\bar{\lambda}\bar{\tau} + \tau(\mu+\gamma-\bar{\gamma}) + \tau(\bar{\tau}^2/\bar{\sigma}) + 2\rho\bar{\nu} = 0. \tag{4.11}$$

It is easily shown that this condition is compatible with the Newman–Penrose equations.

We can summarize our results as follows: Let us choose the conformally flat perfect-fluid metric $g_{\alpha\beta}$ and the null geodesic vector field l_α such that they verify $\rho = \bar{\rho}$, (4.7), (4.8), (4.9), and (4.11). Then, let us solve the integrable system of equations for H given by (3.24), (4.4), and (4.10). The new Kerr–Schild metric $\tilde{g}_{\alpha\beta}$ is a solution of Einstein's equations for a perfect-fluid energy-momentum tensor (3.15), where $\tilde{q}$, $\tilde{p}$, and $\tilde{u}_\alpha$ are given by (4.1), (4.2), and (4.3). The Weyl tensor of these new solutions is (τ never vanishes)

$$\tilde{\psi}_0 = \tilde{\psi}_1 = 0, \quad 3\tilde{\psi}_2 = -2H\phi_{00},$$
$$\tilde{\psi}_3 = -H(\tau/\sigma)\phi_{00}, \quad \tilde{\psi}_4 = -H(\tau^2/\sigma^2)\phi_{00},$$

so that we have $3\tilde{\psi}_2\tilde{\psi}_4 = 2\tilde{\psi}_3^2$, and therefore they are of Petrov type D. Since $\tilde{\psi}_3$ and $\tilde{\psi}_4$ do not vanish, the vector field $\tilde{k}^\alpha$ is not a multiple null eigenvector of the Weyl tensor, but l^α certainly is. From (4.4) we have

$$\tilde{u}^\alpha = a l^\alpha + b\tilde{k}^\alpha$$

and then $\tilde{u}^\alpha$ does not lie in the preferred two-space spanned by the two multiple null eigenvectors of the Weyl tensor. Excepting the Wahlquist solution, no solutions of this kind were known up to now.

V. THE CASE $\sigma = 0$

Now, we assume $\sigma = 0$ so that the function Y of (3.4) is defined by (3.6) and also we have

$$\beta = \lambda = 0. \tag{5.1}$$

We define in this section

$$U \equiv \delta H - 2H\bar{\alpha}, \quad V \equiv DH - 2H\rho. \tag{5.2}$$

From (3.20), (3.21), (3.19), (3.17), and using the same procedure of the previous section we get

$$\chi\tilde{p}=\chi p-DV-V(3\rho+\bar{\rho})-3H\rho^2-4H\rho\bar{\rho}+H\bar{\rho}^2+4H\phi_{00}, \tag{5.3}$$

$$\chi\tilde{q}=\chi q+V(\bar{\rho}-\rho)-DV+3H(\rho^2+\bar{\rho}^2), \tag{5.4}$$

$$(l^\alpha\tilde{u}_\alpha)^2=2\phi_{00}\{\chi(q+p)+4H\phi_{00}-2[DV+2V\rho+2H\bar{\rho}(\rho-\bar{\rho})]\}^{-1}. \tag{5.5}$$

Equations (3.23) and (3.22) become, respectively,

$$\delta V+(\rho+\bar{\rho})U+(\tau-\bar{\alpha})V+H[\bar{\rho}\bar{\alpha}+\delta\bar{\rho}+2\tau(\bar{\rho}-\rho)]=0, \tag{5.6}$$

$$\rho\Delta H=-H\Delta(\rho+\bar{\rho})-\delta\bar{U}+\bar{\alpha}\bar{U}-\bar{\tau}U-\tau\bar{U}-\mu V-4H\phi_{11}+H(\gamma+\bar{\gamma})(\rho-\bar{\rho})-(1/4\phi_{00})\times[DV+2V\rho+2H\bar{\rho}(\rho-\bar{\rho})]\times[DV+2V\rho+2H\bar{\rho}(\rho-\bar{\rho})-4H\phi_{00}-8\phi_{11}]. \tag{5.7}$$

In order to make compatible U and V we must have

$$DU+(2\bar{\rho}-\rho)U+(\tau+\bar{\pi})V+H[\bar{\rho}\bar{\alpha}+\delta\bar{\rho}+2\bar{\pi}(\rho-\bar{\rho})]=0. \tag{5.8}$$

Also, U must verify the reality condition

$$\bar{\delta}U+\bar{\rho}\Delta H+\bar{\mu}\bar{V}-U\alpha+2H\rho(\gamma+\bar{\gamma})=\text{c.c.} \tag{5.9}$$

Now, the Weyl tensor is given by

$$\tilde{\psi}_0=\tilde{\psi}_1=0,\quad -6\tilde{\psi}_2=[D-2(\rho-\bar{\rho})]V,$$
$$\tilde{\psi}_3=H[\rho\alpha+\bar{\delta}\rho+\bar{\tau}(\rho-\bar{\rho})]+(2\rho-\bar{\rho})\bar{U}, \tag{5.10}$$
$$\tilde{\psi}_4=-[\bar{\delta}-(3\alpha-2\bar{\tau})]\bar{U}.$$

In this paper, we only solve these equations under the assumptions

$$\rho=\bar{\rho},\quad V=-2H\rho, \tag{5.11}$$

and so we have

$$DH=0. \tag{5.12}$$

Then, Equations (5.6), (5.7), (5.8), and (5.9) become, respectively,

$$\tau=0, \tag{5.13}$$

$$\rho\Delta H=H[-2\Delta\rho+2\mu\rho-4\rho^2(\phi_{11}/\phi_{00})]-\delta\bar{U}+\bar{\alpha}\bar{U}-(H^2/\phi_{00})(\rho^2+\phi_{00})(\rho^2-\phi_{00}), \tag{5.14}$$

$$DU+\rho U=0, \tag{5.15}$$

$$\bar{\delta}U-\alpha U=\delta\bar{U}-\bar{\alpha}\bar{U}. \tag{5.16}$$

As in the previous section, in order to avoid nonlinear terms in H we assume

$$\rho^2=\phi_{00}, \tag{5.17}$$

so that Eq. (5.14) may be written

$$\rho\Delta H=2H[\rho(\gamma+\bar{\gamma})-2(\phi_{11}+\Lambda)]-\delta\bar{U}+\bar{\alpha}\bar{U}. \tag{5.18}$$

The compatibility of this equation with (5.12) leads us to

$$\mu\rho+\phi_{11}+\Lambda=0. \tag{5.19}$$

This condition eliminates many candidates for $g_{\alpha\beta}$ (i.e., all generalized Schwarzschild metrics).[10] Now, the integrability condition of (5.18) with U is

$$\rho\Delta U+\bar{\delta}\delta U-2\bar{\alpha}\bar{\delta}U-2\alpha\delta U+U[3\alpha\bar{\alpha}-\rho(5\mu+3\bar{\gamma}+\gamma)]=0. \tag{5.20}$$

For the Weyl tensor we have

$$3\tilde{\psi}_2=-2H\rho^2,\quad \tilde{\psi}_3=\rho\bar{U},\quad \tilde{\psi}_4=-[\bar{\delta}-3\alpha]\bar{U}. \tag{5.21}$$

Consequently, if we want to obtain Petrov type D solutions, that is to say

$$3\tilde{\psi}_2\tilde{\psi}_4=2\tilde{\psi}_3^2,$$

we must have

$$\delta U=3\bar{\alpha}U+U^2/H. \tag{5.22}$$

We put

$$f\equiv U/H \tag{5.23}$$

and then Eqs. (5.15), (5.16), and (5.22) are written as follows:

$$Df=-\rho f, \tag{5.24}$$

$$\bar{\delta}f+f(\alpha+\bar{f})=\delta\bar{f}+\bar{f}(\bar{\alpha}+f), \tag{5.25}$$

$$\delta f=\bar{\alpha}f. \tag{5.26}$$

On the other hand, bearing Eqs. (5.23)–(5.26) in mind, Eq. (5.20) becomes

$$\rho\Delta f-\rho f(\mu+\bar{\gamma}-\gamma)+f(\bar{\alpha}\bar{f}-\alpha f-4\alpha\bar{\alpha})+(\bar{\alpha}+f)\bar{\delta}f=0. \tag{5.27}$$

Equations (5.24)–(5.27) are satisfied by choosing

$$f=A\bar{\alpha},$$

where A is an arbitrary real constant, and where two supplementary conditions remain:

$$\delta\bar{\alpha}=\bar{\alpha}^2,\quad \Delta\bar{\alpha}=\bar{\alpha}[\mu+\bar{\gamma}-\gamma+(\alpha\bar{\alpha}/\rho)(5+A)]. \tag{5.28}$$

These conditions are compatible with the Newman–Penrose equations.

Now, we summarize our results in this section: Let us choose the conformally flat perfect-fluid metric $g_{\alpha\beta}$ and the shear-free geodesic null vector field l_α verifying $\rho=\bar{\rho}$, (5.13), (5.17), (5.19), and (5.28). Then we set $U=AH\bar{\alpha}$ and we solve Eqs. (5.12), (5.18), and $\delta H=(2+A)H\bar{\alpha}$. These equations always have solutions. The new generalized Kerr–Schild metric $\tilde{g}_{\alpha\beta}$ is a solution of the Einstein equations for a perfect-fluid energy-momentum tensor (3.15), where $\tilde{q}$, $\tilde{p}$, and $\tilde{u}_\alpha$ are given by (5.3)–(5.5) (when they are conveniently restricted to the case we have studied). The Weyl tensor of the new metrics is Petrov type D. Unless we have $A=0$ or $\alpha=0$, reasoning similar to that in the previous section leads us to solutions previously unknown, as $\tilde{u}_\alpha$ does not lie in the preferred two-space spanned by the two multiple null eigenvectors of the Weyl tensor. In the cases $A=0$ or $\alpha=0$ the solutions may belong to the family given by Wainwright.[11]

Obviously, we only have solved a very particular case in this section. Other more general cases remain for a subsequent paper.

VI. EXPLICIT EXAMPLES

In this section we give some examples of how the equations may be solved explicitly. We can assume two different forms for the metric $g_{\alpha\beta}$: the form manifestly conformally

flat as given in (3.8) and other forms in which the spin coefficients of the null tetrad are adapted to the conditions obtained in Secs. IV and V, even though we do not know the conformal factor explicitly. In the first case the conditions on the spin coefficients become equations for the function Y of (3.4). Once we have obtained the function Y, we can solve the integrable equations for H. In the second case, we have the advantage that we do not need the conformal factor, which is unknown in many metrics. Next, we give some examples for both cases.

(1) In this example, we choose the conformally flat metric given by Oleson[12] in coordinates $\{x^0, x^1, x^2, x^3\} = \{u,t, x, y\}$ in the following form:

$$g_{\alpha\beta}\,dx^\alpha\,dx^\beta = t^{3/2}(dx - (2/\sqrt{t})\,G_{,x}\,du)^2 + \sqrt{t}\,(dy + 2\sqrt{t}\,G_{,y}\,du)^2 - 2G\,dt\,du + 2G^2M\,du^2,$$

$$_{,x} \equiv \frac{\partial}{\partial x}, \quad M(t) = 2\sqrt{t}\,(a^2 + b^2 t), \quad a, b = \text{const},$$

$$G(x, y, u) = g(x, u)h(y,u), \quad g_{,xx} + a^2 g = 0,$$

$$h_{,yy} + b^2 h = 0, \quad p = (3/4t^{3/2})(a^2 - 7b^2 t),$$

$$q = p + \frac{12b^2}{\sqrt{t}}, \quad \mathbf{l} = \frac{\partial}{\partial t},$$

$$\mathbf{m} = \frac{1}{\sqrt{2t}}\left(t^{-1/4}\frac{\partial}{\partial x} + it^{1/4}\frac{\partial}{\partial y}\right),$$

$$\mathbf{k} = G^{-1}\left(\frac{\partial}{\partial u} + GM\frac{\partial}{\partial t} + \frac{2}{\sqrt{t}}G_{,x}\frac{\partial}{\partial x} - 2\sqrt{t}\,G_{,y}\frac{\partial}{\partial y}\right),$$

$$\rho = \bar{\rho} = \frac{1}{2t}, \quad \sigma = \bar{\sigma} = \frac{1}{4t}, \quad (l^\alpha u_\alpha)^2 = \frac{1}{2M}.$$

This metric verifies

$$\phi_{00} = 3\sigma\bar{\sigma}, \quad \rho^2 = 4\sigma\bar{\sigma}, \quad \pi = 0,$$

so that the conditions (4.7) and (4.8) are satisfied. Then, a straightforward calculation leads us to

$$\tau = (1/\sqrt{2t}\,G)(t^{-1/4}G_{,x} + it^{1/4}G_{,y}), \quad \alpha = 0.$$

Now, it may easily be verified that

$$\delta\tau = \bar{\delta}\,\bar{\tau}.$$

Therefore, condition (4.9) is also automatically satisfied. Next, we obtain

$$\mu = -2b^2\sqrt{t}, \quad \gamma - \bar{\gamma} = 2iG^{-2}G_{,x}\,G_{,y},$$

and after a little computation the condition (4.11) becomes

$$G_{,xu} - G^{-1}G_{,x}\,G_{,u} = 0, \quad G_{,yu} - G^{-1}G_{,y}\,G_{,u} = 0.$$

Consequently, we must restrict the metric $g_{\alpha\beta}$ to the case in which

$$G(x, y, u) = g(x)h(y)n(u),$$

where $n(u)$ is an arbitrary function of the variable u. Once this restriction is imposed we know that the equations for H are compatible. The integration of these equations [(3.24), (4.4), and (4.10)] is standard and we finally obtain

$$H = ch(y)/g^3(x), \quad c = \text{const}.$$

From (4.1)–(4.3) we have

$$(l^\alpha \tilde{u}_\alpha)^2 = [2(M + H)]^{-1}, \quad m^\alpha \tilde{u}_\alpha = 0,$$

$$\chi\tilde{p} = \chi p + 3H/8t^2, \quad \chi\tilde{q} = \chi(\tilde{p} + 12b^2/\sqrt{t}).$$

The final form for the metric $\tilde{g}_{\alpha\beta}$ is the following:

$$\tilde{g}_{\alpha\beta}\,dx^\alpha\,dx^\beta = g_{\alpha\beta}\,dx^\alpha\,dx^\beta + 2h(y)g^{-3}(x)G^2\,du^2,$$

$$G(x, y, u) = g(x)h(y)n(u), \quad g_{,xx} + a^2 g = 0,$$

$$h_{,yy} + b^2 h = 0, \quad a, b = \text{const}.$$

(2) The most simple metric $g_{\alpha\beta}$ we can choose is the "flat" Robertson–Walker metric, that is to say

$$g_{\alpha\beta}\,dx^\alpha\,dx^\beta = 2R^2(-du\,dv + d\zeta\,d\bar{\zeta}),$$

$$R = R(u + v), \quad q = q(u + v), \quad p = p(u + v),$$

$$\dot{q} = -3(q + p)\frac{\dot{R}}{R}, \quad \dot{R}^2 = \frac{\chi}{3}qR^4, \quad \equiv\frac{\partial}{\partial t},$$

$$t \equiv (1/\sqrt{2})(u + v), \quad l_\alpha\,dx^\alpha = du + \bar{Y}\,d\zeta + Y\,d\bar{\zeta} + Y\bar{Y}\,dv,$$

$$u_\alpha\,dx^\alpha = -(R/\sqrt{2})(du + dv).$$

Now, the function Z of (3.12) is given by

$$Z = -\bar{Y}R/(1 + Y\bar{Y}),$$

so that Eqs. (3.11) and (3.14) provide the null tetrad and the spin coefficients, respectively. The function Y is defined by (3.6).

To satisfy Eqs. (5.13) and (5.19) it is necessary that

$$Y = 0.$$

Then (5.28) is automatically verified. Finally, the condition (5.17) leads us to[13]

$$p = -\tfrac{1}{3}q,$$

and therefore we must restrict the Robertson–Walker metric such that

$$q = A^2/R^2, \quad R = Be^{\pm Ct}, \quad C \equiv \sqrt{\chi/3}\,A, \quad A, B = \text{const}.$$

Solving the integrable system of equations for H we easily obtain

$$H = \text{const}.$$

Consequently, we obtain the following solution:

$$\tilde{g}_{\alpha\beta}\,dx^\alpha\,dx^\beta = g_{\alpha\beta}\,dx^\alpha\,dx^\beta + 2H\,du^2,$$

$$R = Be^{\pm Ct}, \quad \tilde{q} = \frac{A^2}{R^2}\left(1 + \frac{1}{3R^2}\right), \quad \tilde{p} = \frac{A^2}{R^2}\left(\frac{1}{3R^2} - 3\right),$$

$$(l^\alpha \tilde{u}_\alpha)^2 = 1/2(H + R^2), \quad m^\alpha \tilde{u}_\alpha = 0, \quad A, B, H = \text{const}.$$

APPENDIX: BIANCHI IDENTITIES

Next, we list the Bianchi identities for a conformally flat perfect-fluid metric. We choose the null tetrad (3.11) such that

$$\phi_{01} = \phi_{02} = \phi_{12} = \kappa = \epsilon = \rho - \bar{\rho} = 0,$$

$$\Lambda = (\chi/24)(q - 3p), \quad \phi_{00} = (\chi/2)(q + p)(l^\alpha u_\alpha)^2,$$

$$\phi_{11} = (\chi/8)(q + p), \quad \phi_{00}\phi_{22} = 4\phi_{11}^2,$$

and then we have

$$\phi_{00}\lambda = 2\phi_{11}\bar{\sigma}, \quad \phi_{00}\bar{\nu} = 2\phi_{11}(\tau + \bar{\pi}),$$
$$\delta(\phi_{11} + \Lambda) = 0, \quad \delta\phi_{11} = \bar{\pi}\phi_{11}, \quad \mu = \bar{\mu},$$
$$D(\phi_{11} + \Lambda) = \mu\phi_{00} - 2\rho\phi_{11},$$
$$\Delta(\phi_{11} + \Lambda) = 2\mu\phi_{11} - \rho\phi_{22},$$
$$\delta\phi_{00} = (\bar{\pi} - 2\bar{\alpha} - 2\beta)\phi_{00},$$
$$2\Delta\phi_{11} - D\phi_{22} + \rho\phi_{22} - 2\mu\phi_{11} = 0,$$
$$\Delta\phi_{00} - 2D\phi_{11} - 2\rho\phi_{11} + \phi_{00}(\mu + 2\gamma + 2\bar{\gamma}) = 0.$$

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[6]In this paper there are three kinds of objects related to the metrics $\tilde{g}_{\alpha\beta}$, $g_{\alpha\beta}$, or $\eta_{\alpha\beta}$. We denote these, respectively, by a tilde (i.e., $\tilde{\psi}_0$, $\tilde{k}^{\alpha}$, etc.), no label (i.e., k_α, σ, ρ, etc.), and by M (i.e., σ_M, ρ_M, etc.). Consequently, we raise and lower indices of the tensors with $\tilde{g}_{\alpha\beta}$, $g_{\alpha\beta}$, or $\eta_{\alpha\beta}$, respectively.

[7]We use standard notation in Newman–Penrose formalism. Our conventions coincide with those of Kramer *et al.*[4] except for the spin coefficients where the sign is changed. The signature of the metric is $(-, +, +, +)$.

[8]B. Aronson and E. T. Newman, J. Math. Phys. **13**, 1847 (1972).

[9]It is a consequence of the expression (4.6) for the Weyl tensor that solutions of Petrov type N cannot be obtained. This may be seen as follows. Oleson[12] has shown that perfect-fluid solutions of Petrov type N with a geodesic principal null vector must satisfy $\tilde{\sigma} \neq 0$ and $\tilde{\phi}_{00} = 3\sigma\bar{\sigma}$. It is easily shown that $\tilde{\sigma} = \sigma$ and $\tilde{\phi}_{00} = \phi_{00}$, therefore we must have $\sigma \neq 0$ and $\phi_{00} = 3\sigma\bar{\sigma}$. Since $\tilde{\psi}_0 = \tilde{\psi}_1 = 0$, in order to obtain solutions of Petrov type N, it is necessary to satisfy $\tilde{\psi}_2 = 0$. But then, we have $-\rho^2 - 2\sigma\bar{\sigma} = 0$ which is not possible.

[10]Generalized Schwarzschild interior metrics verify $\phi_{11} + \Lambda = \text{const} > 0$ and $\rho = 2(l^{\alpha}u_{\alpha})^2\mu$. Therefore $\mu\rho > 0$ and Eq. (5.19) is not possible.

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[13]Although $p = -\frac{1}{3}q$ is not physically admissible we allow it since we can obtain an energy density $\tilde{q}$ and a pressure $\tilde{p}$ that are physically reasonable.

Fluid spheres of uniform density in general relativity

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A number of exact solutions for spherically symmetric nonstatic fluids of uniform density, surrounded by empty space, are derived and investigated. Solutions that represent expanding and contracting spheres, which tend asymptotically to static configurations described by the Schwarzschild interior solution ($\rho = \text{const}$), are obtained In some cases the motion of contraction or expansion is reversed, while in other cases there is no bouncing at all. Oscillating solutions are presented.

I. INTRODUCTION

In general relativity the first model of a perfect fluid sphere with uniform density was the well-known Schwarzschild interior solution. It is customary to give this solution in the form[1]

$$ds^2 = [A - B(1 - a^2R^2)^{1/2}]^2\,dT^2 - (1 - a^2R^2)^{-1}\,dR^2 - R^2\,d\Omega^2, \tag{1}$$

where $d\Omega^2 = (d\theta^2 + \sin^2\theta\,d\phi^2)$.

The pressure p of the fluid is

$$p = \rho[(2A/3)/(A - B(1 - a^2R^2)^{1/2}) - 1], \tag{2}$$

where $\rho = (3a^2/8\pi)$ is the mass-energy density of the fluid, and A, B, and a are constants to be determined from the boundary conditions.

The generalization of Schwarzschild's homogeneous fluid sphere problem to the case where the density ρ is a function of the time coordinate t has been studied by several authors. Pulsating models have been examined by Gupta[2] and Bonnor and Faulkes.[3] Different aspects of the motion of uniform-density spheres have been investigated by Thompson and Whitrow,[4] Bondi,[5] Taub,[6] Nariai,[7] Banerjee,[8] and McVittie and Stabell.[9] More recently Glass[10] and Knutsen[11] have discussed the apparent horizons. Other interesting features of uniform-density models have been examined by Wyman,[2] Gürses and Gürsey,[13] Krishna Rao,[14] and Cook.[15] However, as far as the author knows, exact solutions corresponding to nonstatic spheres asymptotically tending to a static configuration described by the Schwarzschild interior solution [Eqs. (1) and (2)] have never been derived. It is the object of this paper to obtain this kind of solution. As a by-product of the investigation we find a family of oscillating solutions.

The paper is organized as follows. The field equations as well as the conventions used are described in Sec. II. In Sec. III, we display the solutions. The discussion of the results and conclusions are given in Sec. IV. Finally, some details of calculations are included in the Appendix.

II. THE FIELD EQUATIONS AND CONVENTIONS

Let us consider a nonstatic distribution of matter represented by a perfect fluid and which is spherically symmetric.

In comoving coordinates the line element may be written as (see the Appendix)

$$ds^2 = e^{\nu}\,dt^2 - e^{\alpha}\,dr^2 - R^2\,d\Omega^2, \tag{3}$$

where ν, α, and R are functions of t and r, and

$$d\Omega^2 = (d\theta^2 + \sin^2\theta\,d\phi^2), \quad x^{0,1,2,3} \equiv t, r, \theta, \phi.$$

The energy momentum tensor is

$$T_{\mu\nu} = (\rho + p)U_\mu U_\nu - pg_{\mu\nu}, \tag{4}$$

where U^μ is the unit four-velocity of matter, ρ is the energy density, and p is the isotropic pressure. Also, since we are in a comoving frame,

$$U^\mu = \delta^\mu_0 e^{-\nu/2}. \tag{5}$$

The conservation equations $T^{\mu\nu}{}_{;\nu} = 0$ in the comoving coordinate system yield

$$\nu' = -2p'/(\rho + p), \tag{6}$$

$$\dot{\alpha} + 4(\dot{R}/R) = -2\dot{\rho}/(\rho + p), \tag{7}$$

where dots and primes denote differentiation with respect to t and r, respectively.

The Einstein field equations relate the mass-energy $m(r, t)$ within the sphere passing the point (t, r, θ, ϕ) to the density $\rho(r, t)$ and pressure $p(r, t)$; viz,

$$2m(r, t) = R\,[1 + e^{-\nu}\dot{R}^2 - e^{-\alpha}R'^2], \tag{8}$$

$$m' = 4\pi\rho R^2 R', \tag{9}$$

$$\dot{m} = -4\pi p R^2 \dot{R}. \tag{10}$$

There are five equations (6)–(10) and six unknowns; namely, m, ρ, p, ν, α, and R. The problem becomes determinate if we consider a perfect fluid with spatially uniform density [$\rho'(r, t) = 0$]. With this condition we integrate Eq. (9) to obtain

$$m(r, t) = (4\pi/3)\rho(t)R^3 + f(t),$$

where $f(t)$ is an arbitrary function. For interior solutions we require the vanishing of R and m at the center of the symmetry $r = 0$. Then $f(t) = 0$ and

$$m(r, t) = (4\pi/3)\rho(t)R^3. \tag{11}$$

Differentiating Eq. (11) with respect to t and employing Eqs. (7) and (10), we obtain

$$\dot{\alpha} = 2\dot{R}/R, \tag{12}$$

which has the integral

$$\alpha = 2\ln R + F(r), \tag{13}$$

where F is an arbitrary function of r.

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When choosing the line element in the form given by Eq. (3), we have the freedom to perform the coordinate transformation

$$t = t(\bar{t}), \quad r = r(\bar{r}), \tag{14}$$

which leaves the comoving nature of coordinate system unchanged.[16] Thus, introducing a new radial coordinate $\bar{r}$, defined by

$$e^{F(r)/2}\, dr = d\bar{r}/\bar{r},$$

and using (13), the line element (3) becomes

$$ds^2 = e^{\nu(\bar{r},\, t)}\, dt^2 - e^{\mu(\bar{r},\, t)}(d\bar{r}^2 + \bar{r}^2\, d\Omega^2), \tag{15}$$

where $e^{\mu/2} = R/\bar{r}$.

The new mass function will be given by

$$\frac{2m(\bar{r},\, t)}{\bar{r}e^{\mu/2}} = 1 + e^{-\nu}\left[\frac{\partial}{\partial t}(\bar{r}e^{\mu/2})\right]^2 - e^{-\mu}\left[\frac{\partial}{\partial \bar{r}}(\bar{r}e^{\mu/2})\right]^2. \tag{16}$$

In what follows we shall use the line element in the form given by Eq. (15) and suppress the bar over r.

The Einstein field equations for the line element (15) read[17]

$$8\pi p = e^{-\mu}\left(\frac{\mu'^2}{4} + \frac{\mu'\nu'}{2} + \frac{\mu' + \nu'}{r}\right) - e^{-\nu}\left(\ddot{\mu} + \frac{3}{4}\dot{\mu}^2 - \frac{\dot{\mu}\dot{\nu}}{2}\right), \tag{17}$$

$$8\pi p = e^{-\mu}\left(\frac{\mu'' + \nu''}{2} + \frac{\nu'^2}{4} + \frac{\mu' + \nu'}{2r}\right) - e^{-\nu}\left(\ddot{\mu} + \frac{3}{4}\dot{\mu}^2 - \frac{\dot{\mu}\dot{\nu}}{2}\right), \tag{18}$$

$$8\pi\rho = -e^{-\mu}\left(\mu'' + \frac{\mu'^2}{4} + 2\frac{\mu'}{r}\right) + \frac{3}{4}e^{-\nu}\dot{\mu}^2, \tag{19}$$

$$0 = 2\dot{\mu}' - \dot{\mu}\nu'. \tag{20}$$

The last equation is easily integrated, with the result

$$\nu = 2\ln\dot{\mu} + A(t), \tag{21}$$

where $A(t)$ is an arbitrary function of t.

The pressure isotropy yields the equation[18]

$$e^{\mu/2}(\mu'' - \mu'^2/2 - \mu'/r) = \Psi(r), \tag{22}$$

where Ψ is an arbitrary function of r.

Substituting the mass function (16) and Eq. (22) into Eq. (19), we get

$$m = \frac{4\pi}{3}\rho R^3 + \frac{r^3\Psi(r)}{6}. \tag{23}$$

From Eqs. (11) and (23) we obtain

$$\Psi(r) = 0. \tag{24}$$

Thus, the solutions with uniform density that satisfy the regularity condition $R(0, t) = 0$ and $m(0, t) = 0$ correspond to the choice $\Psi(r) = 0$.

Next, we shall assume that the fluid is bounded by empty space. Then the exterior metric, in curvature coordinates, is

$$ds^2 = (1 - 2M/R)\, dT^2 - (1 - 2M/R)^{-1}\, dR^2 - R^2\, d\Omega^2. \tag{25}$$

To match the interior metric (15) with the Schwarzschild line element (25) the Einstein equations must be solved subject to the boundary condition

$$m(r_0, t) = M, \quad r_0 = \text{const}, \tag{26}$$

where r_0 defines the outer boundary of the matter distribution. The Eq. (26) implies that the pressure vanishes at the interface $r = r_0$, i.e.,

$$p(r_0, t) = 0. \tag{27}$$

Finally, the time dependence of the boundary is given by

$$R_b(t) = r_0 e^{\mu(r_0,\, t)/2}, \tag{28}$$

where subscript b means evaluation at the boundary.

III. THE SOLUTIONS

In this section we obtain some solutions for uniform density matter.

Setting $Z = e^{-\mu/2}$ and $\Psi(r) = 0$ in Eq. (22) we have

$$Z'' - Z'/r = 0.$$

Integrating this equation, we obtain

$$Z = e^{-\mu/2} = \tfrac{1}{2}g(t)r^2 + h(t), \tag{29}$$

where $g(t)$ and $h(t)$ are arbitrary functions of t.

Substituting Eq. (29) into (21) we get

$$\nu = \mu + \ln[r^2 + 2\dot{h}(t)/\dot{g}(t)]^2 + A(t) + \ln\dot{g}^2(t). \tag{30}$$

As was pointed out before, we still have the freedom to perform the coordinate transformation $t = t(\bar{t})$. Thus, defining a new comoving time $\bar{t}$ by

$$d\bar{t} = \dot{g}(t)e^{A(t)/2}\, dt,$$

and using (29), the line element (15) becomes

$$ds^2 = \frac{[r^2 + 2\dot{h}(\bar{t})/\dot{g}(\bar{t})]^2}{[\frac{1}{2}g(\bar{t})r^2 + h(\bar{t})]^2} \times\left[d\bar{t}^2 - \frac{1}{[r^2 + 2\dot{h}(\bar{t})/\dot{g}(\bar{t})]^2}(dr^2 + r^2\, d\Omega^2)\right]. \tag{31}$$

Henceforth, $\bar{t}$ will be used as the time coordinate and the bar will be suppressed.

Using the field equations (17)–(19), we obtain

$$8\pi\rho = 6h(t)g(t) + \tfrac{3}{4}\dot{g}^2(t), \tag{32}$$

$$p = \dot{\rho}(t)\frac{[g(t)r^2 + 2h(t)]}{3\dot{g}(t)[r^2 + 2\dot{h}(t)/\dot{g}(t)]} - \rho(t). \tag{33}$$

The mass function is given by Eq. (16); viz.,

$$m(r, t) = r^3 e^{3\mu/2}[\dot{g}^2(t)/8 + g(t)h(t)]. \tag{34}$$

The boundary condition $m(r_0, t) = M$ yields

$$[\dot{g}^2(t)/8 + g(t)h(t)] = M[\tfrac{1}{2}g(t) + h(t)]^3. \tag{35}$$

Here, we have used the fact that no generality is lost if the boundary is given by[19]

$$r_0 = 1.$$

Equation (35) relates the functions $h(t)$ and $g(t)$. Thus, Eqs. (32)–(35) give the uniform-density solutions in terms of one arbitrary function [$g(t)$ or $h(t)$].

We will not attempt to analyze all possible functions which satisfy Eq. (35). Instead we work out the specimen solutions, which are obtained under the assumption

$$h(t) = (\alpha/2)g(t) + \beta, \tag{36}$$

where α and β are constants.

Then Eqs. (32) and (33) yield

$$\rho(t) = (3M/4\pi)[1/R_b^3(t)], \tag{37}$$

$$p = \rho(t)R_b(t)\beta[(1+\alpha)/(r^2+\alpha) - 1], \tag{38}$$

where $R_b(t)$ is, according to Eq. (28), given by

$$R_b(t) = [\tfrac{1}{2}g(t)(1+\alpha) + \beta]^{-1}. \tag{39}$$

Substituting Eqs. (36) and (39) into (35), we obtain the equation which governs the evolution of the boundary; viz.,

$$\dot{R}_b^2 = 2MR_b(\alpha+1)^2 - 4\alpha R_b^2 + 4\beta(\alpha-1)R_b^3 + 4\beta^2 R_b^4. \tag{40}$$

The integration of this equation is not, in general, possible in terms of elementary functions. Thus, in general, numerical integration would be needed. Nevertheless, there exist a number of elementary particular integrals for some specific choices of α and β.

(i) First consider the case $\alpha \neq 0, \beta = 0$. We integrate Eq. (40) to obtain

$$R_b(t) = [M(\alpha+1)^2/2\alpha]\cos^2\sqrt{\alpha}(t-t_0). \tag{41}$$

Equation (37) yields the energy density, and from Eq. (38) we get $p = 0$. Thus, the solutions with $\beta = 0$ represent oscillating dust spheres whose radius R_b lies in the interval $[0, M(\alpha+1)^2/2\alpha]$. In particular when $\alpha = 2$ we have $g(t) = h(t)$ and $R_b \in [0, 9M/4]$.

(ii) Let us take $h(t) = 0$, i.e., we put $\alpha = \beta = 0$ in Eq. (36). Integrating Eq. (40), we get

$$2\sqrt{R_b(t)} = \pm\sqrt{2M}\,t + 2C. \tag{42}$$

The constant of integration C may be expressed in terms of R_b at the time $t = 0$ as $C = \sqrt{R_b(0)}$. Then Eq. (42) yields the following cases:

$$R_b^{(1)}(t) = [(\sqrt{2M}/2)t - \sqrt{R_b(0)}]^2, \tag{43}$$

$$R_b^{(2)}(t) = [(\sqrt{2M}/2)t + \sqrt{R_b(0)}]^2. \tag{44}$$

The solution given by Eq. (43) represents a dust sphere which starts to contract from the initial value $R_b(0)$, reaching the origin at the time $\tau = 2\sqrt{R_b(0)/2M}$. Afterwards, for $t > \tau$, the boundary is expanding. The second case given by Eq. (44) has only expansion.

The line element (31), in terms of the new radial variable

$$u = 1/r,$$

becomes

$$ds^2 = [R_b^{(i)}]^2[dt^2 - (du^2 + u^2\,d\Omega^2)], \tag{45}$$

where $R_b^{(i)}$ means $R_b^{(1)}$ and $R_b^{(2)}$ as given by Eqs. (43) and (44), respectively.

(iii) Now consider $h(t) = \text{const}$. Putting $\alpha = 0$ in Eq. (36), we have $h(t) = \beta \neq 0$. The energy density and the pressure are given by Eqs. (37) and (38). Using (31) and (39) we may write the line element in the form

$$ds^2 = \frac{r^4 R_b^2(t)}{[r^2 + \beta(1-r^2)R_b(t)]^2}\left\{dt^2 - \frac{1}{r^4}(dr^2 + r^2\,d\Omega^2)\right\}. \tag{46}$$

Equation (40) becomes

$$\dot{R}_b^2 = 2MR_b - 4\beta R_b^3 + 4\beta^2 R_b^4. \tag{47}$$

Some features of the solutions of this equation may be exhibited by introducing the function

$$V = 4\beta/R_b - 2M/R_b^3, \tag{48}$$

in terms of which Eq. (47) reads

$$\dot{R}_b^2 = R_b^4[4\beta^2 - V(R_b)]. \tag{49}$$

Thus, the region of allowed values of R_b is given by the inequality

$$V(R_b) \leqslant 4\beta^2, \quad \beta \neq 0. \tag{50}$$

Figure 1 shows that for values of β in the interval $(0, 8/27M)$ there are two kinds of solutions. Solutions of region I represent spheres oscillating between zero and some value of R_b in the interval $(\sqrt{M/2\beta}, \sqrt{3M/2\beta})$. In region II we have contraction with subsequent bounce for some value of R_b (which depends on β). In region III, for $\beta > 8/27M$, R_b may change in the interval $(0, \infty)$ and there is no bouncing at all. Finally, for $\beta = 8/27M$, we integrate Eq. (47) to obtain

$$R_b^{(1)}(t) = 9M/\{12\coth^2[\sqrt{\tfrac{3}{4}}(t-t_0)] - 8\}, \tag{51}$$

$$R_b^{(2)}(t) = 9M/\{12\tanh^2[\sqrt{\tfrac{3}{4}}(t-t_0)] - 8\}. \tag{52}$$

The first solution, given by (51), represents an expanding boundary surface which asymptotically tends to a sphere with radius $R_b = 2.25M$ as $t \to \infty$. Furthermore, we see that if we choose $t_0 = 0$, then the sphere is concentrated at the origin at the initial time $t = 0$. The boundary surface crosses the horizon ($R_b = 2M$) at the comoving time

$$t_g = \sqrt{\tfrac{3}{2}}\coth^{-1}(5/\sqrt{24}). \tag{53}$$

The second solution, given by (52), represents a contracting boundary surface which also tends to a sphere of radius $R_b = 2.25M$ as $t \to \infty$. To exclude negative values of R_b in the interval $t \in (0, \infty)$ we choose $t_0 = \sqrt{\tfrac{3}{2}}\tanh^{-1}\sqrt{\tfrac{2}{3}}$ so that $R_b^{(2)}(0) = \infty$.

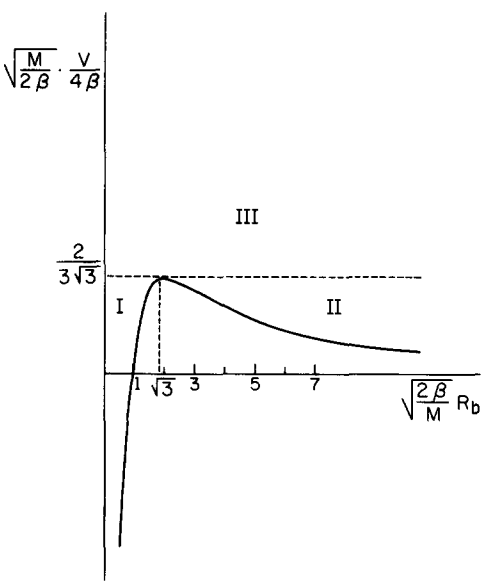

FIG. 1. When β is such that $0 < 4\beta^2 < V_{max}$ we have $0 < \beta < 8/27M$ and the boundary of the sphere may vary in region I or in region II. If $4\beta^2 = V_{max}$ we have solutions asymptotically tending to a static sphere with radius $R_b = 9M/4$. The region III corresponds to an unlimited contraction (expansion) of the fluid.

Substituting Eqs. (51) and (52) into (46), we obtain the line element for expanding and contracting solutions, respectively. Both solutions have the same final (asymptotic) configuration described by the line element

$$ds^2 = \frac{(27M)^2 r^4}{16[r^2+2]^2}\left\{dt^2 - \frac{1}{r^4}(dr^2 + r^2\, d\Omega^2)\right\}. \tag{54}$$

The pressure and the energy density are given by

$$p = \tfrac{2}{3}\rho\{1/r^2 - 1\}, \tag{55}$$

$$\rho = 3M/4\pi R_b^3, \quad R_b = \tfrac{9}{4}M. \tag{56}$$

Transforming (54)–(56) to Schwarzschild-like coordinates

$$t = \frac{4}{27M}T, \quad r = \frac{4R}{3R_b\left[1+\sqrt{1-8R^2/9R_b^2}\right]}, \tag{57}$$

we get

$$ds^2 = \left(\frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{8}{9}\frac{R^2}{R_b^2}}\right)^2 dT^2 - \left(1 - \frac{8}{9}\frac{R^2}{R_b^2}\right)^{-1} dR^2 - R^2\, d\Omega^2, \tag{58}$$

$$p = \rho\left[\frac{2}{3(1-\sqrt{1-8R^2/9R_b^2})} - 1\right]. \tag{59}$$

Thus, we have obtained the Schwarzschild interior solution [Eqs. (1) and (2)] with $A = B = \frac{1}{2}$ and $a^2 = 8/9R_b^2$. We notice that at the center of the distribution the pressure becomes infinity.

(iv) From Eq. (38) we see that the pressure for all configurations with $\alpha > 0$ is finite and non-negative everywhere within the sphere. For the sake of simplicity we shall analyze the case $\alpha = 1$. From Eqs. (31) and (39) we obtain the line element

$$ds^2 = \frac{4[r^2+1]^2 R_b^2(t)}{[(r^2+1)+\beta R_b(t)(1-r^2)]^2} \times [dt^2 - (1/(r^2+1)^2)(dr^2 + r^2\, d\Omega^2)]. \tag{60}$$

The time history of the boundary is given by the equation

$$\dot{R}_b^2 = 8MR_b - 4R_b^2 + 4\beta^2 R_b^4. \tag{61}$$

The region of allowed values of R_b is given by

$$W(R_b) < \beta^2,$$

where

$$W(R_b) = 1/R_b^2 - 2M/R_b^3.$$

In the case $\alpha = 1$ different pictures may be obtained by specializing the choice of β. For $\beta = 0$ (see Fig. 2) we recover the solution given by Eq. (41) with $\alpha = 1$. If we take $\beta^2 \in (0, 1/27M^2)$ there will be, in general, oscillating and bouncing spheres in regions I and II, respectively. According to Fig. 2 the radius of the oscillating spheres changes between zero and some value of $R_b \in (2M, 3M)$.

The value of R_b for bouncing is larger than $3M$. Furthermore, for $\beta^2 > 1/27M^2$ the radius of the sphere changes in the interval $(0, \infty)$. Finally for $\beta^2 = 1/27M^2$, Eq. (61) is easily integrated to obtain

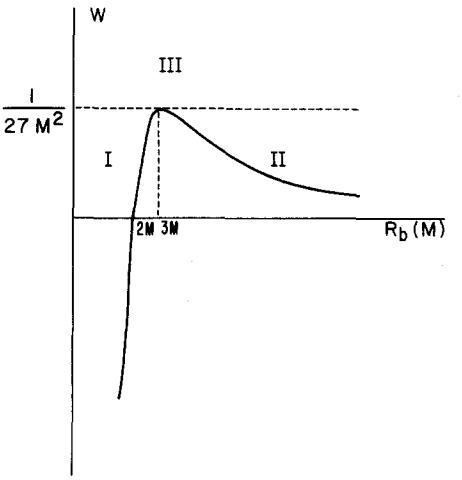

FIG. 2. W as a function of R_b. The maximum of W corresponds to the asymptotic static configuration with radius $R_b = 3M$. The regions I and II are separated from the region III by the line $W = 1/27M^2$.

$$R_b^{(1)}(t) = 6M/[3\coth^2(t - t_0) - 1], \tag{62}$$

$$R_b^{(2)}(t) = 6M/[3\tanh^2(t - t_0) - 1]. \tag{63}$$

Equations (62) and (63) have the same physical interpretation as Eqs. (51) and (52) in the previous case. Solution (62), with $t_0 = 0$, represents an expanding sphere, which, at the initial time $t = 0$, is concentrated at the origin and crosses the horizon at

$$t_g = \coth^{-1} 2/\sqrt{3}.$$

The radius of the sphere, as $t \to \infty$, tends asymptotically to the value $R_b^{(1)} = 3M$.

The second solution given by (63) with $t_0 = \coth^{-1} 1/\sqrt{3}$, is interpreted as a sphere contracting from infinity, which tends asymptotically to a static sphere with radius $R_b^{(2)} = 3M$.

The final configuration for both solutions is

$$ds^2 = \frac{36M^2(r^2+1)^2}{(br^2+a)^2}\left[dt^2 - \frac{1}{(r^2+1)^2}(dr^2 + r^2\, d\Omega^2)\right], \tag{64}$$

where $a = 1 + 1/\sqrt{3}$ and $b = 1 - 1/\sqrt{3}$, $ab = \frac{2}{3}$,

$$8\pi\rho = 2/9M^2, \tag{65}$$

$$p = (\rho/\sqrt{3})[2/(r^2+1) - 1]. \tag{66}$$

With the aid of the transformation

$$t = T/6M\sqrt{3}, \tag{67}$$

$$r = aR/3M(1 + \sqrt{1 - 2R^2/3R_b^2}), \quad R_b = 3M,$$

the static solution (64)–(66) becomes

$$ds^2 = \left[\frac{\sqrt{3}}{2} - \frac{1}{2}\sqrt{1 - \frac{2R^2}{3R_b^2}}\right]^2 dT^2 - \left(1 - \frac{2R^2}{3R_b^2}\right)^{-1} dR^2 - R^2\, d\Omega^2, \tag{68}$$

$$8\pi p = \frac{2}{9M^2}\left[\frac{2}{3 - \sqrt{3}\sqrt{1 - 2R^2/3R_b^2}} - 1\right]. \tag{69}$$

This is the Schwarzschild interior solution with $A=\sqrt{3}/2$ and $B=\frac{1}{2}$. The radius of the sphere is $R_b=3M$, and the pressure is finite throughout the matter.

Finally, we would like to discuss further the motion of the sphere in the "system of the outside observer" defined by Eq. (25).

The differential equation which describes the evolution of the boundary in terms of time T of a distant observer can be easily obtained by comparing the metric induced upon the boundary surface derived from Eq. (31) and the metric induced upon the same surface derived from Eq. (25), and using Eqs. (36) and (40). We find

$$\left(\frac{dR_b}{dT}\right)^2=\frac{[2M(\alpha+1)^2-4\alpha R_b+4\beta(\alpha-1)R_b^2+4\beta^2R_b^3]}{R_b^3}\left[\frac{R_b-2M}{2\beta R_b+\alpha-1}\right]^2. \tag{70}$$

Solving this equation we obtain the motion of the sphere as seen by an external observer. In the remainder of this section we analyze in detail the solution (i) and (ii) given above. First we analyze the oscillating solutions given by Eq. (41). Taking $\beta=0$, $\alpha\neq 0$ we integrate Eq. (70) and give the solution in the form

$$e^{-|T-T_0|/2M}=\frac{(ky-1)e^{I(y)}}{1+y(k-2)+2\sqrt{k-1}\sqrt{y-y^2}}, \tag{71}$$

where T_0 is a constant of integration and

$$I(y)=-\sqrt{k-1}\left[k\sqrt{y-y^2}+\frac{k+2}{2}\cos^{-1}(2y-1)\right], \tag{72}$$

$$k=(\alpha+1)^2/4\alpha, \quad k>0, \quad R_b=2Mky.$$

From Eqs. (71) and (72) we find that $y\leqslant 1$, which implies that $R_b\leqslant M(\alpha+1)^2/2\alpha$. Moreover, these equations indicate that the approach to the gravitational radius (which occurs within a finite interval of comoving time t) takes an infinite time T of a distant observer, as one would expect. On the other hand, taking derivative in (71) and using (72) we find the equation

$$\frac{dR_b}{dT}=-\frac{(T-T_0)}{|T-T_0|}\frac{\sqrt{2M(\alpha+1)^2-4\alpha R_b}}{|\alpha-1|\sqrt{R_b}}\left(1-\frac{2M}{R_b}\right). \tag{73}$$

It shows, in particular, that for $T<T_0$ the sphere is expanding and for $T>T_0$ the sphere is contracting. Thus, the solution under consideration ($\alpha\neq 0$, $\beta=0$) represents a sphere which emerges into the exterior Schwarzschild space-time at $T=-\infty$, reaching its largest radius $R_b=M(\alpha+1)^2/2\alpha$ at the time $T=T_0$, after which the sphere begins to contract tending asymptotically as $T\to+\infty$ again to radius $R_b=2M$.

Now we proceed to analyze the solution (ii). We integrate Eq. (70) with $\alpha=\beta=0$ and find

$$\frac{dR}{dT}=\pm\sqrt{\frac{2M}{R_b}}\left(1-\frac{2M}{R_b}\right), \tag{74}$$

$$A^2e^{\pm T/2M}=\left[(\sqrt{R_b}-\sqrt{2M})/(\sqrt{R_b}+\sqrt{2M})\right]e^{G(R_b)}, \tag{75}$$

where A^2 is a constant of integration, and

$$G(R_b)=\tfrac{2}{3}\sqrt{R_b/2M}\,(3+R_b/2M).$$

First choosing the upper sign in (74) and (75) we obtain an expanding sphere which emerges into the exterior Schwarzschild space time at $T=-\infty$. Similarly, choosing the lower sign we have a sphere which continually contracts to form a black hole. These both cases correspond to the solutions given, in a comoving frame, by Eqs. (43) and (44).

IV. CONCLUSIONS

In this work we have examined spherically symmetric distributions of uniform-density perfect fluid in the comoving frame. Imposing the requirement of regularity at the center, and exploiting the freedom to specify the coordinate system, we are able to give the uniform-density solutions in terms of one arbitrary function of t [Eqs. (32)–(35)]. Choosing this function in different ways, we gave some explicit examples of the motion of uniform-density spheres; viz., the following.

(a) Expanding solutions representing spheres growing out of a singularity, crossing the horizon, and tending asymptotically to static spheres. Thus, we have here obtained examples of white holes.

(b) Contracting solutions, which represent spheres shrinking from an initial highly diffuse state, towards static spheres. These solutions describe the collapse of spheres whose final states are close to that of a black hole, but are still outside the horizon.

(c) Oscillating solutions, representing spheres whose boundary oscillates between the center and some value of R_b which depends upon a parameter α [see Eq. (41)]. If this parameter is not larger than unity, then the sphere is always inside the Schwarzschild surface and a comoving observer is not able to send signals to the Schwarzschild external observer. For the values of α larger than unity the sphere crosses periodically (as seen by an observer comoving with the matter) the Schwarzschild surface. Since the approach to the gravitational radius takes an infinite time T of a distant observer, it follows that the oscillating solution under consideration [see Eq. (41)] can only be joined to a specific Schwarzschild exterior metric (with coordinate ranges $R>R_b$, $-\infty<T<+\infty$) for certain values of the comoving coordinate t. According to Eqs. (71)–(73) the matter emerges into the exterior space-time at $T=-\infty$ and goes back only at $T=+\infty$. Having reached the gravitational radius (as seen by a comoving observer) the sphere will continue to contract arriving at the center within a finite comoving time t, after which the matter will expand approaching the Scharzschild sphere from inside and emerging into another distinct exterior space time, and so on.

(d) Bouncing solutions representing spheres contracting from an initial value $R_b(0)$ and reaching the center at the

finite time τ [see Eq. (43)], after which the spheres are expanding. The interpretation of these solutions in terms of an external observer is given by Eqs. (74) and (75).

Configuration of the kind (a), (b), and (c) have recently been found, in a different context, by Herrera and Ponce de Leon.[20,21]

Finally we would like to conclude with the following remarks.

(i) According to Bondi[22] the largest value of the ratio of mass to radius, for perfect fluid, is 4/9. This maximum value is asymptotically attained in the solutions given by (51) and (52) for a infinite central pressure.

(ii) We have analyzed only some solutions of the equation of the surface [Eq. (40)].

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APPENDIX: TRANSFORMATION TO THE COMOVING COORDINATE SYSTEM

The most general metric form for a spherically symmetric space-time in "spherical" space coordinates r, θ, ϕ, is

$$ds^2 = g_{00}(r,t)dt^2 + g_{11}(r,t)dr^2 + 2g_{01}(r,t)dr\,dt + g_{22}(r,t)d\Omega^2, \tag{A1}$$

where

$$d\Omega^2 = (d\theta^2 + \sin^2\theta\, d\phi^2), \quad x^{0,1,2,3} \equiv t, r, \theta, \phi.$$

The direct calculation of the Einstein's equations for the line element (A1) shows that $T_{02} = T_{03} = T_{12} = T_{13} = T_{23} = 0$. What this means is that the motion of the fluid is radial. Therefore the four-velocity in the reference system of (A1) is

$$U^\mu = (U^0(r,t), U^1(r,t), 0, 0). \tag{A2}$$

The arbitrariness in the choice of a reference system in general relativity allows us to subject the coordinates r, t to any transformation of the form[16]

$$r = r(r', t'), \quad t = t(r', t').$$

Let the coordinates r' and t' be defined as

$$dt' = A^{-1}(r,t)[U_1\,dr + U_0\,dt],$$
$$dr' = B^{-1}(r,t)[U^0\,dr - U^1\,dt], \tag{A3}$$

where $A(r,t)$ and $B(r,t)$ are factors defined to make the right-hand side of (A3) perfect differentials, and $U_\mu = g_{\mu\alpha}U^\alpha$.

In these coordinates the metric has the diagonal form; namely

$$ds^2 = A^2(dt')^2 + B^2[g_{00}g_{11} - (g_{01})^2](dr')^2 + g_{22}(r', t')d\Omega^2, \tag{A4}$$

where the coefficients of $(dt')^2$, $(dr')^2$, and $d\Omega^2$ must be expressed now as functions of t' and r'. The four-velocity becomes

$$U'^\mu = (A^{-1}, 0, 0, 0). \tag{A5}$$

Since the radial velocity vanishes at each point, it follows that the coordinates r' and t' are comoving with the matter. We denote the coefficients of $(dt')^2$, $(dr')^2$, and $d\Omega^2$ by e^ν, $-e^\alpha$, and $-R^2$, respectively. Then, dropping primes, the line element in such a comoving system is (we use $c = 1$)

$$ds^2 = e^\nu dt^2 - e^\alpha dr^2 - R^2 d\Omega^2, \tag{A6}$$

where ν, α, and R are functions of t and r. The four-velocity is

$$U^\mu = e^{-\nu/2}\delta^\mu_0. \tag{A7}$$

Thus, without loss of generality we can choose the coordinates r and t in such a way that, first, the metric has the diagonal form, and second, the coordinate system is comoving with the matter.

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Magnetized diagonal Weyl metrics

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A generalization of the diagonal Weyl metrics, which is obtained by a Harrison transformation over the Ernst potential ϵ, is presented. The Ernst potential is defined for a linear combination of the Killing vectors ∂_τ and ∂_σ. The cases which correspond to Kasner and Voorhees metrics are analyzed in some detail.

I. INTRODUCTION

Methods of generating new solutions of the Einstein–Maxwell equations, starting with any particular solution, have been known for a long time and employed to obtain a large number of solutions. However, although the techniques are well known, the outcoming solutions are, in general, fairly complicated and it is thus very difficult to understand their structure and physical relevance. Care must be taken in selecting a seed solution; it must have a simple structure and a physical interpretation. For instance, a convenient way to introduce a magnetic field in a given space-time is to apply a Harrison transformation[1]; its importance in astrophysical situations is well recognized. Wald,[2] Ernst,[3] and Ernst and Wild[4] employed a Harrison-type transformation to magnetize black holes. Recently Iyer and Vishveshwara[5] magnetized all cylindrically symmetric vacuum metrics and García Díaz[6] and García Díaz and Bretón Baez.[7] employed this technique to magnetize type D metrics. In this work, a simple family of vacuum metrics—the group of diagonal metrics[8] $S(a,b,c/m)$ that contain as particular cases several solutions of physical relevance such as the Voorhees–Zipoy metric,[9,10] the Kasner metric,[11] the Schwarzschild solution,[12] etc.,—are magnetized by applying a Harrison transformation to the Ernst potentials, which are determined for a linear combination of the Killing vectors ∂_τ and ∂_σ. Since the seed metrics $S(a,b,c/m)$ are multipole moment solutions, the magnetized $S(a,b,c/m)$ solutions will also be endowed with multipole gravitational moments.

In Sec. II, the new general solution, which has three additional parameters $\rho = E + iB$ and a_0/b_0, is presented. This metric structure is simple because the seed metric is vacuum type and diagonal. In general these metrics are twisted. In Sec. III the case when the combination of the Killing vectors ∂_τ and ∂_σ reduce to a single vector ∂_σ is discussed. This branch contains the known results of magnetic universe[13] (Melvin spaces), twisted magnetic universe,[1] Schwarzschild magnetic black holes,[2] and the new solutions corresponding to magnetized Kasner and Voorhees metrics. The general solution obtained in Sec. III with zero twist is again a diagonal metric. In Sec. IV, we discuss the case where the Killing vectors reduce to ∂_τ. A new magnetized flat space is obtained. A possible interpretation of the new solution is an X-Y charged plane moving along the Z axis with constant acceleration.

II. THE MAGNETIZATION OF $S(a,b,c/m)$ METRICS

In this section the $S(a,b,c/m)$ metrics are magnetized by applying a Harrison transformation to the Ernst potential ϵ, determined for a given linear combination of the Killing vectors ∂_τ and ∂_σ given by $\kappa^\mu = a_0\delta^\mu{}_\tau + b_0\delta^\mu{}_\sigma$. We employed the technique developed in Sec. V of Ref. 14. The seed metric $S(a,b,c/m)$ can be written as

$$S(a,b,c/m): \quad g_4 = f^{-1}[g_3 - \kappa^2], \tag{1}$$

where κ is the Killing form associated with a Killing vector κ_μ: $\kappa = \kappa_\mu\, dx^\mu = -a_0 C\, d\tau + b_0 B\, d\sigma$, whereas f is related to the Ernst potential ϵ via

$$\begin{aligned} &\tfrac{1}{2}(\epsilon + \bar{\epsilon}) = f := -\kappa^\mu\kappa_\mu = a_0^2 C - b_0^2 B, \\ &\tfrac{1}{2}\, d(\epsilon - \bar{\epsilon}) = -i*(\kappa \wedge d\kappa), \end{aligned} \tag{2}$$

from which one obtains

$$\epsilon = f - 2ia_0b_0m^2S + i\epsilon_0, \quad S := 2bp + 2cq - (1+2a)pq, \tag{3}$$

and g_3 is a three-dimensional metric that is not altered by the Harrison transformation (Kinnersley group in general) and is given by

$$g_3 = (a_0^2 C - b_0^2 B)Ag_2 + CB(b_0\, d\tau - a_0\, d\sigma)^2. \tag{4}$$

The expression for the bidimensional metric g_2 as well as for A, B, C, a, b, and c, which define the $S(a,b,c/m)$ metrics, can be found in Ref. 8. Here, ϵ_0 is an integration constant, and $*$ denotes the Hodge star.

To obtain the magnetized version we replaced the f and κ in Eq. (1) by f' and κ' defined by

$$\begin{aligned} &f' = f/|\psi|^2, \quad \psi = 1 - \rho\bar{\rho}\epsilon, \quad \rho := E + iB, \\ &\kappa' = |\psi|^{-2}[\kappa - wf], \end{aligned} \tag{5}$$

with w determined by

$$dw = -if^{-2}(\rho\bar{\rho})^2 * \{(\epsilon\bar{\epsilon} - 2f^2)\tfrac{1}{2}\, d(\epsilon - \bar{\epsilon}) + 2f\tfrac{1}{2}(\epsilon - \bar{\epsilon})\, df\}. \tag{6}$$

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The solution of Eq. (6) is

$$w = 2a_0b_0m^4(\rho\bar{\rho})^2\left\{\frac{a_0^2C+b_0^2B}{a_0^2C-b_0^2B}+2bq(1+p^2)+2cp(1+q^2)-\frac{1}{2}(1+2a)(p^2+q^2+p^2q^2)\right\}(b_0\,d\tau-a_0\,d\sigma)$$
$$+2\epsilon_0m^2(\rho\bar{\rho})^2\left\{pq+\frac{a_0^2C+b_0^2B}{a_0^2C-b_0^2B}S+\frac{1}{4}\frac{\epsilon_0}{a_0b_0}\right\}(b_0\,d\tau-a_0\,d\sigma), \tag{7}$$

with $a_0\neq 0\neq b_0$ and $S:=2bp+2cq-(1+2a)pq$. When a_0 or b_0 are equal to zero, Eq. (7) is still valid if we eliminate the ϵ_0/a_0b_0 term.

The electromagnetic field associated with the new solution of the Einstein–Maxwell equations is given by the two-form

$$\omega = f'^{-1}[\kappa'\wedge f'+{}^*\kappa'\wedge f'], \qquad \text{where } f':=d\phi',\ \phi':=\rho\epsilon/\psi. \tag{8}$$

These new metrics are in general twisted, where the twist potential is given by the imaginary part of the Ernst potential, Eq. (3).

III. MAGNETIZED SOLUTIONS WITH $a_0 = 0$

In this section we analyze some particularly interesting cases when the associated Killing vector κ^μ reduces to $\kappa^\mu=\delta^\mu{}_\sigma$. The magnetized $S(a,b,c/m)$ metric restricted in this way has the simple structure

$$g_4' = |\psi|^2[Ag_2 - C\,d\tau^2] + |\psi|^{-2}B\,[d\sigma+w]^2, \tag{9}$$

whereas ψ and w reduce to

$$w = 4\epsilon_0^2m^2(\rho\bar{\rho})^2\{-bp-cq+(1+a)pq\}\,d\tau,$$
$$|\psi|^2 = [1+(\rho\bar{\rho}B)]^2+(\rho\bar{\rho})^2\epsilon_0^2. \tag{10}$$

Notice that in this case the twist potential is the constant ϵ_0.

Furthermore if one takes $\epsilon_0=0$, the electromagnetic two-form ω is given by

$$\omega = \rho d\{-(B/\psi)\,d\sigma+2im^2[bp+cq+(1+a)pq]\,d\tau\}. \tag{11}$$

Equations (9) and (10) contain as particular solutions a magnetized Schwarzschild black hole,[3] a Melvin magnetic universe,[3,13] and a twisted Melvin magnetic universe. However, more general and interesting cases are the magnetized Kasner metrics and the magnetized Voorhees–Zipoy metrics. These metrics are also contained in Eqs. (9) and (10) and we analyze them in the remainder of this section.

A. Magnetized Kasner metric with $a_0 = 0$

Here, $S(a,b,c/m)=S(a,0,0/m)$ corresponds to the Kasner metric. This can be verified by applying the coordinate transformation

$$u:=[(q^2-1)(1-p^2)]^{1/2},\quad v:=qp, \tag{12}$$

with τ and σ unchanged.

In this coordinatization, and with $b=c=0$, Eqs. (9) and (10) take the form

$$g_4' = m^2|\psi|^2[u^{2a(a+1)}(du^2+dv^2)-u^{-2a}\,d\tau^2]$$
$$+m^2|\psi|^{-2}u^{2(a+1)}[d\sigma+w]^2,$$
$$w = 4\epsilon_0^2m^2(\rho\bar{\rho})^2(1+a)v\,d\tau, \tag{13}$$
$$|\psi|^2 = (1+\rho\bar{\rho}m^2u^{2(a+1)})^2+(\rho\bar{\rho})^2\epsilon_0^2.$$

When $a=1$, the twisted magnetized Kasner's Metric, Eq. (11), reduces to the twisted Melvin magnetic universe. On the other hand a magnetic universe is obtained when ϵ_0 is taken equal to zero (to get the expression in cylindrical coordinates, one must apply the coordinate transformation[8] $r:=mu$, $z:=mv$, $\phi:=\sigma$, and $t:=\tau$). When $b=0=c$ and $a=-1$, the corresponding germinal $S(a,b,c/m)$ metric is a Minkowskian space-time and the magnetized metric is also Minkowskian.

If the twist potential ϵ_0 vanishes the electromagnetic two-form ω associated with the magnetized Kasner's metric is given by

$$\omega = m^2\rho d\{(u^{2(a+1)}/\psi)\,d\sigma+2i(1+a)v\,d\tau\} \tag{14}$$

B. Magnetized Voorhees–Zipoy metric with $a_0 = 0$

When $S(a,b,c/m)=S(0,\delta,0/m)$ corresponds to the Voorhees–Zipoy metric, the twisted magnetized solution is given by Eqs. (9) and (10) with $a=0=c$ and $b=\delta$. For this case, the bidimensional metric g_2 and the structural functions A, B, and C are

$$g_2 = (q^2-p^2)^{1-\delta^2}\left[\frac{dq^2}{q^2-1}+\frac{dp^2}{1-p^2}\right],$$
$$A = m^2(q^2-1)^{\delta^2}((q+1)/(q-1))^\delta,$$
$$B = m^2(q^2-1)((q+1)/(q-1))^\delta(1-p^2), \tag{15}$$
$$C = m^2((q-1)/(q+1))^\delta.$$

If the distortion parameter δ is equal to 1, the Voorhees solution corresponds to the Schwarzschild black hole and the magnetized solution obtained is a twisted magnetized Schwarzschild solution.

This solution can be written in "spherical coordinates" by applying the coordinate transformation

$$r:=m(q+1),\quad t=m\tau,\quad \cos\theta:=p,\quad \text{and}\quad \phi=\sigma. \tag{16}$$

In these coordinates, the Eqs. (9) and (10) take the form

$$g_4' = |\psi|^2\left[\frac{dr^2}{1-2mr} + r^2\,d\theta^2 - \left(1-\frac{2m}{r}\right)dt^2\right]$$
$$+ |\psi|^{-2}\,r^2\sin^2\theta\left[d\phi + \psi\epsilon_0^2(\rho\bar{\rho})^2 r \times \cos\theta\left(1-\frac{2m}{r}\right)dt\right]^2, \quad (17)$$
$$|\psi|^2 = (1+(\rho\bar{\rho})\,r^2\sin^2\theta)^2 + (\rho\bar{\rho})^2\epsilon_0^2\,.$$

The magnetized Schwarzschild black hole devised by Ernst corresponds to the nontwisted $\epsilon_0 = 0$ solution [see Eq. (17)]. The associated electromagnetic form is

$$\omega = \rho d\{(-r^2\sin^2\theta/\psi)\,d\phi + 2ir\cos\theta\,d\tau\}\,. \quad (18)$$

To obtain the analog to the twisted magnetized Schwarzschild solution but with negative mass, we take $\delta = -1$ and apply the coordinate transformation

$$r = m(q-1)\,,\quad \cos\theta = p\,,\quad t = m\tau\,,\text{ and }\phi = \sigma\,. \quad (19)$$

The resulting magnetized metric is as (17) when we change m to $-m$.

IV. MAGNETIZED SOLUTIONS WITH $b_0 = 0$

In this section we analyze another simple particular case: when the Killing vector is ∂_τ, i.e., $\kappa^\mu = \delta^\mu_\tau$. Notice that this Killing vector is timelike. The resulting magnetized metric is

$$g_4' = |\psi|^2[Ag_2 + B\,d\sigma^2] - |\psi|^{-2}C\,[d\tau + w]^2\,, \quad (20)$$

whereas ψ and w reduce to

$$w = -4\epsilon_0^2 m^2(\rho\bar{\rho})^2(bp + cq - apq)\,d\sigma\,,$$
$$|\psi|^2 = (1-\rho\bar{\rho}\,C)^2 + (\rho\bar{\rho})^2\epsilon_0^2\,. \quad (21)$$

Notice that one can obtain Eq. (18) from Eq. (9) by changing $B\to -C$, $C\to -B$, $\sigma\to\tau$, $\tau\to\sigma$, and by changing w as given by Eq. (10) to w as given by Eq. (19). The twist potential is constant (ϵ_0) and if this vanishes the associated electromagnetic form is

$$\omega = \rho d\{(C/\psi)\,d\tau + 2im^2[bp + cp - apq]\,d\sigma\}\,. \quad (22)$$

As in Sec. III, the magnetized Kasner and Voorhees metric, now with $b_0 = 0$, are particularly interesting cases which we now analyze.

A. Magnetized Kasner metric with $b_0 = 0$

Taking $S(a,b,c/m) = S(a,0,0/m)$ and applying the coordinate transformation (11) in Eqs. (20) and (21) we arrive at the metric

$$g_4' = m^2|\psi|^2[u^{2a(a+1)}(du^2+dv^2) + u^{2(a+1)}\,d\sigma^2] - m^2|\psi|^{-2}u^{-2a}[d\tau + w]^2\,,$$
$$w = +4\epsilon_0^2(\rho\bar{\rho})av\,d\sigma\,, \quad (23)$$
$$|\psi|^2 = (1-m^2\rho\bar{\rho}u^{-2a})^2 + (\rho\bar{\rho})^2\epsilon_0^2\,.$$

If $a = 0$, the seed metric $S(0,0,0/m)$ is a Minkowskian space-time and the magnetized metric Eq. (22) is also Minkowskian. However, if the germinal metric is $S(-1,0,0/m)$, Eq. (22) gives a new magnetic universe. In fact, taking the twist $\epsilon_0 = 0$ and applying the transformation to "Cartesian coordinates"

$$x = mv\,,\quad y = m\sigma\,,\quad z = mu\cosh\tau\,,\quad t = mu\sinh\tau\,, \quad (24)$$

we obtain

$$g_4' = |\psi|^2\left[dx^2 + dy^2 + \frac{z\,dz - t\,dt}{z^2-t^2}\right] + |\psi|^{-2}\frac{(tdz - zdt)^2}{z^2-t^2}\,,$$
$$\psi = 1 - \rho\bar{\rho}(z^2-t^2)\,. \quad (25)$$

The associated electromagnetic form is given by

$$\omega = \rho d\{-(1/\psi)(t\,dz - z\,dt) + 2ix\,dy\}$$
$$= 2\rho\{(1/\psi^2)\,dz\wedge dt + i\,dx\wedge dy\}\,. \quad (26)$$

The electromagnetic field has a singularity defined by $\psi = 0$ which is a $Z = \text{const}$ plane moving with constant acceleration on z direction respect to Minkowskian space. Then, one can imagine this solution as generated by a $z = \text{const}$ charged plane moving with constant acceleration in the z direction. However a detailed interpretation is still lacking.

B. Magnetized Voorhees metric with $b_0 = 0$

Finally when the germinal metric is $S(a,b,c/m) = S(0,\delta,0/m)$, Eqs. (20) and (21) take the form

$$g_4' = |\psi|^2 m^2\left(\frac{q+1}{q-1}\right)^\delta[(q^2-p^2) \times \left(\frac{q^2-1}{q^2-p^2}\right)^\delta\frac{dq^2}{q^2-1} + \frac{dp^2}{1-p^2} + (q^2-1)(1-p^2)\,d\sigma^2] - |\psi|^{-2}m^2\left(\frac{q-1}{q+1}\right)^\delta \times [d\tau - 4\epsilon_0^2 m^2(\rho\bar{\rho})^2\delta p\,d\sigma]\,,$$
$$|\psi|^2 = \left[1-\rho\bar{\rho}\,m^2\left(\frac{q-1}{q+1}\right)^\delta\right]^2 + (\rho\bar{\rho})^2\epsilon_0^2\,. \quad (27)$$

In this case the corresponding Schwarzschild generalization can be obtained by taking $\delta = 1$ and applying the coordinate transformation (16). To obtain the Schwarzschild generalization with negative mass, one takes $\delta = -1$ and applies the coordinate transformation (19). In the first case, $\delta = 1$, with $\epsilon_0 = 0$, the metric and the electromagnetic forms are

$$g_4' = \psi^2\left[\frac{dr^2}{1-2m/r} + r^2(d\theta^2 + \sin^2\theta\,d\phi^2)\right] - \psi^{-2}\left(1-\frac{2m}{r}\right)dt^2\,, \quad (28)$$

$$\omega = m^2\rho d\left\{\frac{1}{\psi}\left(1-\frac{2m}{r}\right)dt + 2i\cos\theta\,d\phi\right\}$$
$$= 2m^2\rho\left\{\frac{m}{r^2\psi^2}\,dr\wedge dt - i\sin\theta\,d\theta\wedge d\phi\right\}, \quad (29)$$
$$\psi = 1 - \rho\bar{\rho}\,m^2\left(1-\frac{2m}{r}\right).$$

The electromagnetic field has a singularity over the sphere of radius

$$r = 2m^3 \rho\bar{\rho}/(\rho\bar{\rho}\, m^2 - 1), \quad \text{for} \quad \rho\bar{\rho}\, m^2 > 1,$$

thus, this solution can be interpreted as a mass surrounded by a spherical charged layer.

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Symmetries and conserved quantities in geodesic motion

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Recently obtained results linking several constants of motion to one (non-Noetherian) symmetry to the problem of geodesic motion in Riemannian space-times are applied. The construction of conserved quantities in geodesic motion as well as the deduction of geometrical statements about Riemannian space-times are achieved.

I. INTRODUCTION

One of the most important applications of the knowledge of symmetries in physics is the construction of quantities that remain constant during the evolution of physical systems. Noether's theorem[1] provides a strikingly simple way of testing whether a given infinitesimal transformation is a symmetry for a given Lagrangian system and associates a constant of motion to each (Noetherian) symmetry. On the other hand, the symmetries of the equations of motion constitute a larger set, which includes those (Noetherian) symmetries of the Lagrangian.[2] Nevertheless, there were no systematic ways of constructing constants of motion associated to non-Noetherian symmetries up to now. Recently, new kinds of Lagrangian symmetries could be defined in such a way that this new set (which includes Noetherian symmetries) would be equivalent to one of symmetries of the equations of motion.[2] Furthermore, a systematic way of constructing several constants of motion associated with each symmetry was provided.[2–6]

The purpose of this paper is to apply these new concepts and results to geodesic equations of motion in Riemannian space-times.

The paper is organized as follows: In Sec. II we review and present new results on Lagrangian symmetries and constants of motion for first-order differential systems. In Sec. III we translate these results for second-order systems. In Sec. IV we apply these concepts to geodesic motion in Riemannian space-times. Section V is conclusions and outlook.

II. SUMMARY OF RECENT RESULTS

In this and the next sections we briefly sketch the methods and summarize the main results of recent works[2–7] to be used here.

Consider a system of n second-order differential equations

$$\ddot{q}^i - F^i(q^j,\dot{q}^j,t) = 0, \quad i,j = 1,...,n. \tag{2.1}$$

It is convenient for our purposes to define

$$x^i = q^i, \quad x^{i+n} = \dot{q}^i, \quad f^i = x^{i+n}, \quad f^{i+n} = F^i(x^j,x^{j+n},t), \tag{2.2}$$

so that the first-order system of $2n$ equations

$$\dot{x}^a - f^a(x^b,t) = 0, \quad a,b = 1,...,2n, \tag{2.3}$$

is equivalent to (2.1). Even if no Lagrangian exists for the system (2.1), there are infinitely many Lagrangians for system (2.3) (see Refs. 4,6, and 7). In fact,

$$L = L(x^a,\dot{x}^a,t) = l_a(x^b,t)(\dot{x}^a - f^a) \tag{2.4}$$

is a Lagrangian for system (2.3) if l_a satisfies

$$\frac{\bar{d}}{dt} l_a + l_b \frac{\partial f^b}{\partial x^a} = 0 \tag{2.5}$$

and

$$\det \sigma_{ab} \neq 0, \tag{2.6}$$

where

$$\sigma_{ab} = \frac{\partial l_a}{\partial x^b} - \frac{\partial l_b}{\partial x^a} \tag{2.7}$$

and

$$\frac{\bar{d}}{dt} \equiv f^a \frac{\partial}{\partial x^a} + \frac{\partial}{\partial t}. \tag{2.8}$$

Equations (2.5) and (2.6) have infinitely many solutions.[4] The equations of motion for (2.4) are

$$E_a L = \sigma_{ab}(\dot{x}^b - f^b) = 0, \tag{2.9}$$

when Eqs. (2.5) are satisfied. We have used

$$E_a L \equiv \frac{d}{dt}\frac{\partial L}{\partial \dot{x}^a} - \frac{\partial L}{\partial x^a}. \tag{2.10}$$

Equations (2.9) are equivalent to (2.3) if (2.6) holds. It is straightforward to prove that σ obeys

$$\frac{\bar{d}}{dt}\sigma_{ab} + \sigma_{ac} f^c{}_{,b} + \sigma_{cb} f^c{}_{,a} = 0, \tag{2.11}$$

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on account of (2.5).

The infinitesimal transformation

$$x'^a = x^a + \epsilon\eta^a(x^b,t), \quad \delta t = 0, \tag{2.12}$$

is said to be a symmetry transformation for Eq. (2.3) if it maps any solution of (2.3) into another solution of (2.3), i.e., if η^a satisfies

$$\frac{\bar{d}}{dt}\eta^a - f^a{}_{,b}\eta^b = 0, \tag{2.13}$$

to within terms of order ϵ^2.

We consider local transformations ($\delta t = 0$) only. The results for $\delta t = \epsilon\eta^0$ can be reobtained by redefining a new local transformation $\epsilon\eta'^a = \epsilon(\eta^a - \dot{x}^a\eta^0)$.

For details see Refs. 2 and 8.

On the other hand, (Noetherian) Lagrangian symmetries may be defined as follows.

Consider the local infinitesimal transformation

$$x'^a = x^a - \delta x^a(x^b,t) \equiv x^a - \epsilon\gamma^a(x^b,t), \quad \delta t = 0. \tag{2.14}$$

The new Lagrangian L' is defined as usual:

$$L'(x'^a,\dot{x}'^a,t) = L(x^a,\dot{x}^a,t). \tag{2.15}$$

The functional change of the Lagrangian is

$$\delta L \equiv L'(x^a,\dot{x}^a,t) - L(x^a,\dot{x}^a,t). \tag{2.16}$$

A straightforward computation yields

$$\delta L = \frac{\partial L}{\partial x^a}\delta x^a + \frac{\partial L}{\partial \dot{x}^a}(\delta x^a)^{\cdot}. \tag{2.17}$$

The transformation (2.14) is said to be a (Noetherian) symmetry of the Lagrangian if

$$\delta L \equiv -\epsilon\frac{d\phi(x^a,t)}{dt}. \tag{2.18}$$

The conserved quantity K associated with transformation (2.14) is

$$K = \frac{\partial L}{\partial \dot{x}^a}\gamma^a + \phi = l_a\gamma^a + \phi. \tag{2.19}$$

Conditions (2.18) can be equivalently stated as

$$E_a\delta L \equiv 0. \tag{2.20}$$

Note that δL is a function of x^a, $\dot{x}^a$, and t only [see Eq. (2.21)].

It can be easily seen that all Noetherian symmetries satisfy (2.13) but the converse is not true.[2,7,9] As a matter of fact, δL can be identically rewritten as

$$\delta L = \epsilon[(l_a\gamma^a)^{\cdot} - \gamma^a\sigma_{ab}(\dot{x}^b - f^b)], \tag{2.21}$$

and it can be proved that if γ^a satisfies (2.13) then

$$E_a\delta L = \epsilon\Lambda_a{}^b E_b L, \tag{2.22}$$

where

$$\Lambda_a{}^b = \sigma^*{}_{ac}(\sigma^{-1})^{cb} \tag{2.23}$$

and

$$\sigma^*{}_{ab} = \frac{\partial l^*{}_a}{\partial x^b} - \frac{\partial l^*{}_b}{\partial x^a}, \quad l^*{}_a = \sigma_{ab}\gamma^b. \tag{2.24}$$

Equation (2.22) can be rewritten as

$$E_a\delta L\,|_{E_bL=0} = 0. \tag{2.25}$$

Lagrangian symmetries defined by Eqs. (2.22) and (2.25) are completely equivalent to the symmetries of equations of motion defined by Eq. (2.13). For higher-order differential equations new concepts need to be defined[2,9,10] in order to achieve equivalence between the two sets of symmetries.

The concept introduced by Eq. (2.22) is sometimes called S equivalence[2-7] and is related to the covariance of equations of motion under the symmetry transformation (rather than the invariance concept which defines Noetherian symmetries). It has been proved[2-6,9] that

$$\frac{\bar{d}}{dt}I_k = 0, \tag{2.26}$$

with

$$I_k = \operatorname{tr}\Lambda^k, \quad k = 1,2,..., \tag{2.27}$$

and

$$\frac{\bar{d}}{dt}J = 0, \tag{2.28}$$

with

$$J = l_a\gamma^a, \tag{2.29}$$

so that several conserved quantities I_k and J associated to one S equivalence symmetry transformation γ^a. These results can be easily reobtained using Eqs. (2.5), (2.11), and (2.13).

It is interesting to realize that the basic equations (2.5), (2.11), and (2.13) can be rewritten in a geometrical language[11] as

$$(\partial_t + \mathcal{L}_f)l_a \equiv \frac{\partial l_a}{\partial t} + l_{a,b}f^b + f^b{}_{,a}l_b = 0, \tag{2.30}$$

$$(\partial_t + \mathcal{L}_f)\eta^a \equiv \frac{\partial \eta^a}{\partial t} + \eta^a{}_{,b}f^b - f^a{}_{,b}\eta^b = 0, \tag{2.31}$$

$$(\partial_t + \mathcal{L}_f)\sigma_{ab} \equiv \frac{\partial \sigma_{ab}}{\partial t} + \sigma_{ab,c}f^c + \sigma_{ac}f^c{}_{,b} + \sigma_{cb}f^c{}_{,a} = 0, \tag{2.32}$$

where ∂_t denotes partial differentiation with respect to time and $\mathcal{L}_f$ stands for the Lie derivative along f^a. Note that l is a one-form, f and η are vector fields, and σ as defined by Eq. (2.7),

$$\sigma = dl, \tag{2.33}$$

is a two-form.

Equations (2.32) [or (2.13)] define the symmetries of the problem (both for the equations of motion and Lagrangians) and are associated with the constants of motion defined by Eqs. (2.19), (2.27), and (2.29). For brevity, we will say that any one-form l satisfying Eq. (2.30) is a Lagrangian and any vector field η, which is such that (2.32) holds, is a symmetry. Any two-form σ such that Eqs. (2.31) and (2.33) [or (2.34) below] are fulfilled is a symplectic form. Note that in view of (2.33),

$$d\sigma = 0. \tag{2.34}$$

If in addition,

$$\det\sigma \neq 0, \tag{2.35}$$

the symplectic form is said to be regular.

It is straightforward to prove that if η_1 and η_2 are sym-

metries, then a new symmetry η_3 may be defined by

$$\eta_3{}^a = \mathcal{L}_{\eta_1}\eta_2{}^a \equiv \eta_2{}^a{}_{,b}\eta_1{}^b - \eta_1{}^a{}_{,b}\eta_2{}^b. \tag{2.36}$$

Similarly, if l is a Lagrangian and η is a symmetry, $\bar{l}$ defined by

$$\bar{l}_a = \mathcal{L}_\eta l_a \equiv l_{a,b}\eta^b + l_b\eta^b{}_{,a} \tag{2.37}$$

is also a Lagrangian. Furthermore, if σ is a symplectic form then $\bar{\sigma}$, defined by

$$\bar{\sigma}_{ab} = \mathcal{L}_\eta \sigma_{ab} \equiv \sigma_{ab,c}\eta^c + \sigma_{ac}\eta^c{}_{,b} + \sigma_{cb}\eta^c{}_{,a}, \tag{2.38}$$

is also a symplectic form. Note that $\bar{\sigma}$ can also be written as

$$\bar{\sigma} = d\bar{l}, \tag{2.39}$$

with $\bar{l}$ defined by Eqs. (2.37).

Define

$$\bar{l}'_a = \sigma_{ab}\eta^b. \tag{2.40}$$

It is straightforward to see that

$$\bar{l}'_a = \bar{l}_a - (l_b\eta^b)_{,a}. \tag{2.41}$$

Define $\bar{\sigma}'_{ab}$ as

$$\bar{\sigma}'_{ab} = \frac{\partial \bar{l}'_a}{\partial x^b} - \frac{\partial \bar{l}'_b}{\partial x^a} \tag{2.42}$$

to get

$$\bar{\sigma}'_{ab} = \bar{\sigma}_{ab}. \tag{2.43}$$

In other words the new Lagrangians $\bar{l}$ and $\bar{l}'$ defined through Eqs. (2.37) and (2.40) are trivially equivalent in the same sense that they differ by dJ and give rise to exactly the same equations of motion or, equivalently, to the same symplectic form $\bar{\sigma}$ as Eqs. (2.41) and (2.43) show.

In summary, for any symmetry η, J is conserved. In addition, if η in non-Noetherian the quantities I_k are conserved, and if η is Noetherian, K is conserved.

Furthermore, in case two or more symmetries $\eta_i{}^a$ are known one can, in addition, construct the constants M_{ij} as

$$M_{ij} = \eta_i{}^a\sigma_{ab}\eta_j{}^b, \quad i \neq j, \tag{2.44}$$

for each nontrivial σ. The fact that the M_{ij} are constant follows from Eqs. (2.28), (2.29), (2.40), and (2.41).

III. SECOND-ORDER FORMALISM

In what follows we will make contact with the second-order formalism.[2]

The local infinitesimal transformation

$$q'^i = q^i + \epsilon\xi^i(q^j,\dot{q}^j,t), \quad \delta t = 0, \tag{3.1}$$

is said to be a symmetry transformation for Eqs. (2.1) if it satisfies[2]

$$\frac{\bar{d}}{dt}\frac{\bar{d}}{dt}\xi^i - \frac{\partial F^i}{\partial \dot{q}^j}\frac{\bar{d}}{dt}\xi^j - \frac{\partial F^i}{\partial q^j}\xi^j = 0 \tag{3.2}$$

to within terms of order ϵ^2, where

$$\frac{\bar{d}}{dt} \equiv F^i\frac{\partial}{\partial \dot{q}^i} + \dot{q}^i\frac{\partial}{\partial q^i} + \frac{\partial}{\partial t}. \tag{3.3}$$

Equation (3.2) will be called the symmetry equation. It is straightforward to prove that if ξ^i satisfies Eqs. (3.2), then η^a, defined by[2]

$$\eta^i = \xi^i, \quad \eta^{i+n} = \frac{\bar{d}}{dt}\xi^i, \tag{3.4}$$

satisfies Eqs. (2.13).

It has also been proved that if a Lagrangian $L(q^i,\dot{q}^i,t)$ exists for a second-order differential system like (3.1) then another Lagrangian $\tilde{L}(q^i,\dot{q}^i,\ddot{q}^i,t)$, which differs from L by a total time derivative, can always be written as a linear combination of the left-hand side of its own equations of motion,[7] that is,

$$\tilde{L}(q^i,\dot{q}^i,\ddot{q}^i,t) = \mu_i(q^j,\dot{q}^j,t)(\ddot{q}^i - F^i), \tag{3.5}$$

where

$$L(q^i,\dot{q}^i,t) = \tilde{L} + \frac{dg(q^i,\dot{q}^i,t)}{dt}. \tag{3.6}$$

The functions μ_i have to satisfy[7]

$$\frac{\partial \mu_i}{\partial \dot{q}^j} - \frac{\partial \mu_j}{\partial \dot{q}^i} = 0, \tag{3.7}$$

$$\frac{\bar{d}}{dt}\left(\frac{\bar{d}}{dt}\mu_i + \mu_k\frac{\partial F^k}{\partial \dot{q}^i}\right) - \mu_k\frac{\partial F^k}{\partial q^i} = 0, \tag{3.8}$$

$$\det A_{ij} \neq 0, \tag{3.9}$$

where

$$A_{ij} = \frac{\partial}{\partial \dot{q}^j}\left(\frac{\bar{d}}{dt}\mu_i + \mu_k\frac{\partial F^k}{\partial \dot{q}^i}\right) + \frac{\partial \mu_j}{\partial q^i}, \tag{3.10}$$

in order that

$$G_i\tilde{L} = 0 \tag{3.11}$$

be equivalent to Eqs. (2.1). The (acceleration-dependent) Euler–Lagrange operator G_i is defined by

$$G_i \equiv -\frac{d^2}{dt}\frac{\partial}{\partial \ddot{q}^i} + \frac{d}{dt}\frac{\partial}{\partial \dot{q}^i} - \frac{\partial}{\partial q^i}. \tag{3.12}$$

It is straightforward to prove that if μ_i satisfies Eqs. (3.7)–(3.9), then l_a, defined by

$$l_i = -\left(\frac{\bar{d}}{dt}\mu_i + \mu_k\frac{\partial F^k}{\partial \dot{q}_i}\right), \quad l_{i+n} = \mu_i, \tag{3.13}$$

satisfies Eqs. (2.5) and (2.6).

The matrix σ can be written as

$$\sigma = \begin{pmatrix} B & -A \\ A^T & C \end{pmatrix}, \tag{3.14}$$

with $A^T{}_{ij} \equiv A_{ji}$, where A is defined by Eq. (3.10), and B and C are defined as follows:

$$B_{ij} = -\frac{\partial}{\partial q^j}\left(\frac{\bar{d}}{dt}\mu_i + \mu_k\frac{\partial F^k}{\partial \dot{q}^i}\right) + (i \leftrightarrow j), \tag{3.15}$$

$$C_{ij} = \frac{\partial \mu_i}{\partial \dot{q}^j} - \frac{\partial \mu_j}{\partial \dot{q}^i}. \tag{3.16}$$

A Lagrangian $L(q^i, \dot{q}^i, t)$ for system (2.1) exists if and only if $C = 0$ and, in that case, A is symmetric.[2,7] For the acceleration-independent Lagrangian L one may define

$$W_{ij} = \frac{\partial^2 L}{\partial \dot{q}^i\,\partial \dot{q}^j} = W_{ji}, \tag{3.17}$$

$$T_{ij} = \frac{\partial^2 L}{\partial \dot{q}^i\,\partial q^j} - \frac{\partial^2 L}{\partial q^i\,\partial \dot{q}^j} = -T_{ji}, \tag{3.18}$$

and prove that

$$A = -W, \tag{3.19}$$

$$B = -T. \tag{3.20}$$

Let us consider the case when a Lagrangian $L(q^i,\dot{q}^i,t)$ for Eq. (2.1) exists. Define ΔL as

$$\Delta L \equiv \frac{1}{\epsilon}\delta L \equiv \left[\frac{\partial L}{\partial q^i}\xi^i + \frac{\partial L}{\partial \dot{q}^i}(\xi^i)^{\cdot}\right], \tag{3.21}$$

associated with transformation (3.1). It is straightforward to prove that[2]

$$\Delta L = \left[\left(\frac{\partial L}{\partial \dot{q}^i}\xi^i\right)^{\cdot} - \xi^i W_{ij}(\ddot{q}^j - F^j)\right], \tag{3.22}$$

i.e., ΔL has the structure (3.5) up to a total time derivative[2] and

$$-\bar{\mu}_i = -W_{ij}\xi^j \tag{3.23}$$

satisfies Eq. (3.8) if ξ^j solves Eq. (3.2).

For the case of S equivalence, i.e., when $\bar{C} = 0$ with

$$\bar{C}_{ij} = \frac{\partial \bar{\mu}_i}{\partial \dot{q}^j} - \frac{\partial \bar{\mu}_j}{\partial \dot{q}^i}, \tag{3.24}$$

it is easier to apply Theorem (2.26) because the I_k, given by Eq. (2.27), reduce to[2]

$$I_k = 2\,\mathrm{tr}(\bar{A}A^{-1}) = -2\,\mathrm{tr}(\bar{A}W^{-1}), \tag{3.25}$$

where

$$\bar{A}_{ij} = \frac{\partial}{\partial \dot{q}^j}\left(\frac{\bar{d}}{dt}\bar{\mu}_i + \bar{\mu}_k\frac{\partial F^k}{\partial \dot{q}^i}\right) + \frac{\partial \bar{\mu}_j}{\partial q^i}. \tag{3.26}$$

For $\bar{C} \neq 0$, Theorem (2.26) applies as it stands.

The dictionary provided to translate from a second-order to a first-order formalism allows us to construct the same conserved quantities described in Sec. II if the second-order equations do have a Lagrangian and their symmetries are known. If no Lagrangian for the second- (or any-) order set of differential equations exist, the first-order results of Sec. II may still be applied because first-order Lagrangians always exist.[4]

IV. GEODESIC MOTION

We will now apply the results summarized in Secs. II and III to the motion of a pointlike test particle moving in an arbitrary gravitational field, i.e., we study the conservation laws associated with the geodesic equation

$$\frac{d^2q^\alpha}{ds^2} + \Gamma_{\beta\gamma}^{\alpha}\frac{dq^\beta}{ds}\frac{dq^\gamma}{ds} = 0 \tag{4.1}$$

in an arbitrary Riemannian space-time with metric tensor $g_{\alpha\beta}(q^\gamma)$. The Christoffel symbols

$$\Gamma_{\alpha\beta}^{\gamma} = \tfrac{1}{2}g^{\gamma\delta}(-g_{\alpha\beta,\delta} + g_{\beta\delta,\alpha} + g_{\delta\alpha,\beta}) \tag{4.2}$$

are defined as usual. The independent variable s is the proper time (we are taking the velocity of light $c = 1$).

Equations (4.1) may be obtained from the acceleration-independent Lagrangian (M is the mass of the particle)

$$L = L(q^\alpha,\dot{q}^\alpha) = \tfrac{1}{2}Mg_{\alpha\beta}(q^\gamma)\frac{dq^\alpha}{ds}\frac{dq^\beta}{ds} \tag{4.3}$$

or the acceleration-dependent one

$$\tilde{L} = \tilde{L}(q^\alpha,\dot{q}^\alpha,\ddot{q}^\alpha,s) = -sMg_{\alpha\beta}\dot{q}^\alpha(\ddot{q}^\beta + \Gamma_{\gamma\delta}^{\beta}\dot{q}^\gamma\dot{q}^\delta), \tag{4.4}$$

where

$$\mu_\alpha = -sMg_{\alpha\beta}(g^\gamma)\dot{q}^\beta, \tag{4.5}$$

which satisfies Eqs. (3.7)–(3.9) with

$$A_{\lambda\rho} = -Mg_{\lambda\rho}. \tag{4.6}$$

A first-order Lagrangian for the (4.7), (4.8) set [equivalent to (4.1)],

$$M\frac{dq^\alpha}{ds} - P^\alpha = 0, \tag{4.7}$$

$$\frac{dP^\alpha}{ds} + \frac{1}{M}\Gamma_{\beta\gamma}^{\alpha}P^\beta P^\gamma = 0, \tag{4.8}$$

can be written as

$$L = l_a(\dot{x}^a - f^a), \quad a = 0,1,\ldots,7, \tag{4.9}$$

where

$$x^\alpha = q^\alpha, \quad x^{\alpha+4} = P^\alpha, \quad f^\alpha = P^\alpha/M,$$

$$f^{\alpha+4} = -\Gamma_{\beta\gamma}^{\alpha}P^\beta P^\gamma/M, \tag{4.10}$$

$$l_\alpha = -\left(\frac{\bar{d}}{dt}\mu_\alpha + \mu_\beta\frac{\partial f^{\beta+4}}{\partial P^\alpha}\right), \quad l_{\alpha+4} = \mu_\alpha. \tag{4.11}$$

The matrix σ is given by

$$B_{\alpha\beta} = (g_{\beta\gamma,\alpha} - g_{\alpha\gamma,\beta})P^\gamma, \tag{4.12}$$

$$C = 0, \tag{4.13}$$

and A defined by Eqs. (4.6).

In order to be able to apply the conservation laws described in the preceding sections to the problem of geodesic motion in Riemannian space-times, we write down the symmetry equation for geodesics as

$$\frac{\bar{D}}{Ds}\frac{\bar{D}}{Ds}\xi^\mu + \frac{1}{M^2}R^\mu{}_{\alpha\beta\gamma}P^\alpha P^\beta\xi^\gamma = 0, \tag{4.14}$$

where

$$\delta q^\mu \equiv \epsilon\xi^\mu(q^\alpha,P^\beta,s), \tag{4.15}$$

the Riemann tensor is

$$R^\mu{}_{\alpha\beta\gamma} \equiv \Gamma^\mu_{\alpha\beta,\gamma} - \Gamma^\mu_{\alpha\gamma,\beta} + \Gamma^\rho_{\alpha\beta}\Gamma^\mu_{\rho\gamma} - \Gamma^\rho_{\alpha\gamma}\Gamma^\mu_{\rho\beta}, \tag{4.16}$$

P^α is defined by (4.7), and the covariant derivative along the geodesic is

$$\frac{\bar{D}}{Ds}\xi^\mu \equiv \frac{\bar{d}}{ds}\xi^\mu + \frac{1}{M}\Gamma^\mu_{\alpha\beta}P^\alpha\xi^\beta, \tag{4.17}$$

with

$$\frac{\bar{d}}{ds}\xi^\mu = \frac{\partial\xi^\mu}{\partial q^\alpha}\frac{dq^\alpha}{ds} + \frac{\partial\xi^\mu}{\partial P^\alpha}\frac{\bar{d}P^\alpha}{ds} + \frac{\partial\xi^\mu}{\partial s}, \tag{4.18}$$

or

$$\frac{\bar{d}}{ds}\xi^\mu = \frac{1}{M}\left(\frac{\partial\xi^\mu}{\partial q^\alpha}P^\alpha - \frac{\partial\xi^\mu}{\partial P^\alpha}\Gamma_{\sigma\tau}^{\alpha}P^\sigma P^\tau\right) + \frac{\partial\xi^\mu}{\partial s}. \tag{4.19}$$

Equation (4.14) is a generalization of the equation of geodesic deviation, which is usually written for a vector ξ^μ depending on s only.[12]

The solutions to Eq. (4.14) give rise to conserved quantities according to Eqs. (2.19), (2.27), and (2.29).

In what follows we find a few particular solutions to Eq. (4.14).

(i) Consider the case ξ^μ parallel to P^μ,

$$\xi^\mu = \lambda(q,P,s)P^\mu. \tag{4.20}$$

It is easy to verify that, due to Eq. (4.8),

$$\lambda = C_1 s + C_2 \tag{4.21}$$

solves Eq. (4.14) in this case. Here C_1 and C_2 are arbitrary constants of motion of Eq. (4.1). In particular,

$$\xi_1^\mu = P^\mu, \tag{4.22}$$

and

$$\xi_2^\mu = sP^\mu \tag{4.23}$$

are solutions to Eq. (4.14) for *any* metric tensor.

(ii) Consider the case

$$\xi^\mu = \xi^\mu(q) \tag{4.24}$$

only.

In this case, Eq. (4.14) reduces to

$$(\xi^\mu{}_{;\alpha;\beta} + R^\mu{}_{\alpha\beta\gamma}\xi^\gamma)P^\alpha P^\beta = 0, \tag{4.25}$$

which is solved by affine collineations.[13] Therefore

$$\xi_3^\mu = \text{affine collineation} \tag{4.26}$$

is also a particular solution to Eq. (4.14). Affine collineations may be defined by

$$\mathcal{L}_{\xi_3}\Gamma_{\alpha\beta}^\gamma = 0 \tag{4.27}$$

and satisfy

$$\xi_3{}^\alpha{}_{;\beta;\gamma} + R^\alpha{}_{\beta\gamma\delta}\xi_3{}^\delta = 0 \tag{4.28}$$

or

$$\xi_{3(\alpha;\beta);\gamma} = 0. \tag{4.29}$$

Of course, Killing vectors (or motions), defined by

$$\mathcal{L}_\chi g_{\mu\nu} = 0 \tag{4.30}$$

and satisfying

$$\chi_{(\alpha;\beta)} = 0, \tag{4.31}$$

are special cases of affine collineations and are Noetherian symmetries of the Lagrangian (4.3).

(iii) Consider now ξ such that

$$R^\mu{}_{\alpha\beta\gamma}\xi^\gamma = 0. \tag{4.32}$$

Equation (4.14) reduces to

$$\frac{\bar{D}}{Ds}\frac{\bar{D}}{Ds}\xi^\mu = 0, \tag{4.33}$$

so that ξ^μ has to satisfy Eqs. (4.32) and (4.33) simultaneously. A particular solution to this problem is found in Ref. 14 for special metrics which admit constant vector fields. In fact, a constant vector field ξ_4^μ, which is a function of q only, is such that

$$\xi_4{}^\mu{}_{;\nu} = 0, \tag{4.34}$$

which implies (by repeated differentiation)

$$R^\mu{}_{\alpha\beta\gamma}\xi_4{}^\gamma = 0 \tag{4.35}$$

and

$$\frac{\bar{D}}{Ds}\xi_4{}^\mu = \xi_4{}^\mu{}_{;\nu}P^\nu = 0, \tag{4.36}$$

and therefore satisfies (4.32) and (4.33) simultaneously. Of course, it would be interesting to find more general solutions to the ansatz specified by Eqs. (4.32) and (4.33).

Now we will write down explicitly the constants of motion associated with the symmetries we have found.

Consider $\xi_1{}^\mu$ first. The only nontrivial constant of motion it yields is

$$K_1 = \tfrac{1}{2}P_\mu P^\mu = \tfrac{1}{2}M^2, \tag{4.37}$$

where

$$\phi = -\tfrac{1}{2}P_\mu P^\mu. \tag{4.38}$$

The constant J_1 is trivially related to K_1 in this case. In fact,

$$J_1 = P_\mu P^\mu. \tag{4.39}$$

Of course, the traces theorem [(2.26) and (2.27)] is not useful for the Noetherian symmetries, because it gives constants which vanish identically.

Let us now turn our attention to $\xi_2{}^\mu$. This is a vector which gives rise to s equivalence and, in this case, the traces theorem yields numerical constants. Furthermore,

$$J_2 \equiv 0. \tag{4.40}$$

These results are not surprising because $\xi_1{}^\mu$ and $\xi_2{}^\mu$ are symmetry transformations of geodesic motion for *any* metric and the associated constants should exist for any metric too, and they are therefore just functions of M^2.

Consider $\xi_3{}^\mu$ now. Affine collineations are s equivalence symmetries. In fact, $\bar{A}_{3\alpha\beta}$, defined by Eq. (3.26), is

$$\bar{A}_{3\alpha\beta} = -M(\xi_{3\alpha;\beta} + \xi_{3\beta;\alpha}) \equiv -Mh_{\alpha\beta}. \tag{4.41}$$

The conservation laws (3.25) state that the traces of the powers of $h_{\alpha\beta}$ are just numbers. These are not dynamical statements and constitute rather geometrical laws, which may, of course, be independently obtained from Eqs. (4.29), say. This is so because $h_{\alpha\beta}$ is a function of q^μ only, independent of P^μ. Therefore, these conservation laws can give rise either to dynamical or to geometrical statements. We will find other geometrical laws further down. The constant J_3 is

$$J_3 = P_\alpha \xi^\alpha{}_3 - (s/M)P_\alpha \xi^\alpha{}_{3;\beta}P^\beta. \tag{4.42}$$

Consider constant vector fields $\xi_4{}^\mu$. A constant vector field is a special kind of Killing vector and constitutes, therefore, a Noetherian symmetry. The constants J and K coincide and they are

$$J_4 = K_4 = P_\alpha \xi_4{}^\alpha. \tag{4.43}$$

Consider now the matrices σ defined by Eqs. (4.6), (4.12), and (4.13) and $\bar{\sigma}$:

$$\bar{\sigma} = \mathcal{L}_{\xi_3}\sigma. \tag{4.44}$$

We can now write down the constants M and $\bar{M}$ associated with different symmetries. Consider the eight-dimensional symmetry vector η_A^a associated with ξ_A^μ ($A = 1,2,3,4$) according to Eq. (3.4). The following are new constants of motion:

$$M_{13} = \eta_1^a \sigma_{ab}\eta_3^b = P^\alpha h_{\alpha\beta}P^\beta, \tag{4.45}$$

$$\bar{M}_{13} = \eta_1^a \bar{\sigma}_{ab}\eta_3^b = P^\alpha h_{\alpha\beta}\xi_{3;\gamma}^\beta P^\gamma, \tag{4.46}$$

$$\bar{M}_{23} = \eta_2^a \bar{\sigma}_{ab}\eta_3^b = (s/M)P^\alpha h_{\alpha\beta}\xi_{3;\gamma}^\beta P^\gamma - \xi_3^\alpha h_{\alpha\beta}P^\beta. \tag{4.47}$$

By reiterating the procedure one may prove that the whole series of dynamical quantities (in terms of powers of the matrix h)

$$N_{2j+1} = P^{\alpha}(h^{j})_{\alpha\beta}\xi^{\beta}_{3;\gamma}P^{\gamma}, \tag{4.48}$$

$$N_{2j+2} = (s/M)P^{\alpha}(h^{j})_{\alpha\beta}\xi^{\beta}_{3;\gamma}P^{\gamma} - \xi^{\alpha}_{3}(h^{j})_{\alpha\beta}P^{\beta} \tag{4.49}$$

are constants of motion.

Similarly, using Eq. (3.23) repeatedly and the fact that Eq. (4.14) defines symmetries of Lagrangians for geodesic motion, one may prove that

$$\theta^{\alpha} = h^{\alpha}{}_{\beta}\zeta^{\beta} \tag{4.50}$$

is an affine collineation if ζ^{β} is (which can also be proved by the usual techniques of differential geometry, but in a more involved fashion). We have thus obtained another geometrical result using dynamical statements.

Of course, one may continue combining these ideas to get new results, but we will leave these and concrete examples for a future publication.

V. CONCLUSIONS AND OUTLOOK

We have applied ideas recently developed about Lagrangian symmetries and constants of motion to geodesic equations and we have constructed several conserved quantities associated to symmetries. These new ideas allowed us to work with symmetries that are *not* point transformations, i.e., they may have an explicit dependence on the momentum (or the tangent vector) and have found with a unified formalism some constants that had been constructed using different techniques before. As far as we know the constants N are new. We have also found geometrical results using this dynamical idea.

It would be interesting in the future to present concrete examples for specific metric tensors with symmetries and include the study of projective collineations as well. We have left this part out to avoid making this paper unbearably long.

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Simplicial minisuperspace. II. Some classical solutions on simple triangulations

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The extrema of the Euclidean Regge gravitational action are investigated numerically for some closed, compact, four-dimensional simplicial manifolds with topologies S^4, CP^2, and $S^2\times S^2$.

I. INTRODUCTION

Sums over geometries such as occur in the Euclidean functional integral approach to quantum gravity may be given a practical meaning through simplicial approximation. In this approximation sums over smooth geometries are replaced by sums over simplicial geometries built up out of flat simplices by the methods of the Regge calculus.[1] Simplicial geometries are specified by the way the simplices are joined together and by the squared lengths of their edges. A sum over different topologies is approximated by a sum over different ways of putting simplices together. A sum over metrics on a given manifold is approximated by a multiple integral over the squared edge lengths of a collection of simplices which triangulate the manifold.

Simplicial approximations to sums over geometries were discussed in general in the first paper in this series[2] (Paper I) where some references to the extensive earlier literature may be found. The expectation value of some physical quantity A in the state of minimum excitation for closed cosmologies provides a typical example of such a sum. This might read

$$\langle A\rangle = \frac{\int_C d\Sigma_1\, A(s_i)\exp[-I(s_i)]}{\int_C d\Sigma_1 \exp[-I(s_i)]}, \tag{1.1}$$

where I is the Euclidean Regge gravitational action for a closed compact simplicial geometry. For simplicity we have illustrated only a sum over metrics on a fixed simplicial manifold. Both I and A are functions of the squared edge lengths s_i, $i=1,\ldots,n_1$. The integral is a multiple integral over the space of squared edge lengths along some appropriate contour C with some appropriate measure. As throughout we use units where $\hbar = c = 1$ and write the Planck length as $l=(16\pi G)^{1/2}$.

In suitable limits the integral (1.1) can be evaluated by the method of steepest descents. This is the semiclassical approximation. The value of the integral is dominated by the contribution near one or more stationary points through which the contour can be distorted to pass. At these,

$$\frac{\partial I}{\partial s_i} = 0\,. \tag{1.2}$$

These are the simplicial analogs of the Einstein field equations. Even when not quantitatively accurate the semiclassical approximation often yields qualitative insight into the behavior of the integral in a straightforward way.

The important quantities for constructing a simplicial sum over geometries and evaluating it in the semiclassical approximation are the Regge action and its stationary points. Methods for evaluating the action and the Regge equations (1.2) were reviewed in Paper I. In this paper we shall illustrate these methods by numerically evaluating the action and locating its stationary points for a few simple simplicial manifolds. We make no attempt to be exhaustive. We consider only the Regge gravitational action with positive cosmological constant. In the continuum limit this is the action of Einstein's theory. We shall confine attention to compact simplicial manifolds which have no boundary. These are the important nets for evaluating expectation values such as (1.1) (Paper I). We shall consider only real (Euclidean) edge lengths. Even if the contour of integration in (1.1) is complex, the real stationary points seem likely to play a significant role in any semiclassical evaluation of the integral.[3] Within this limited scope, however, we shall be able to illustrate how the Regge action approximates the continuum action, to display its values in a number of interesting cases, and to solve for the stationary points on simple manifolds with differing topologies.

To evaluate the action one must first have a simplicial manifold. That is, one must specify a set of vertices, edges, triangles, tetrahedra, and four-simplices which make up a manifold with the desired topology. The specification of a simplicial manifold is discussed in Sec. II. Quoting largely from the mathematical literature we shall exhibit simplicial manifolds which are triangulations of S^4, CP^2, $S^2\times S^2$, and $S^1\times S^3$.

In Sec. III we illustrate the evaluation of the action using families of geometries on S^4 and CP^2. We compare the action of the most symmetric simplicial geometries with that of the most symmetric continuum geometries on these manifolds. In less symmetric cases we illustrate the behavior of the action for homogeneous, anisotropic geometries and for geometries which are conformal deformations from the most symmetric cases. We shall recover features familiar from the continuum theory such as arbitrarily negative actions arising from conformal deformations.

Section IV is concerned with the solution of the Regge equations on S^4 and CP^2. Solutions are found by imposing symmetries. The eigenvalues of the matrix describing the second variation of the action at these stationary points is also calculated. A more systematic approach to solving the Regge equations is discussed in Sec. V and the difficulties for this method arising from the approximate diffeomorphism group of a simplicial geometry are illustrated.

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II. SOME SIMPLICIAL MANIFOLDS

A four-dimensional simplicial manifold is a collection of vertices, edges, triangles, tetrahedra, and four-simplices joined together such that a neighborhood of every point can be smoothly and invertibly mapped into a region of four-dimensional Euclidean space $\mathbb{R}^4$. In more mathematical terminology, a simplicial manifold is a simplicial complex which is a piecewise linear manifold.[4]

A complex may be described by labeling its simplices and specifying how they are contained in one another. (Here and from now on we shall omit the qualification "simplicial" from manifold, complexes, etc., it being understood that the objects of interest in this paper are constructed from simplices.) A complex which is a four-manifold is homogeneously four-dimensional. That is, every simplex of dimension $k<4$ is contained in some four-simplex. Homogeneously four-dimensional complexes may be specified by labeling their k-simplices by integers from 1 up to the total number n_k and then listing the vertices of the four-simplices. Such a list defines the vertex matrix $j_4(i,j)$ which gives the five vertices $j=1,\ldots,5$ of the ith four-simplex. From this the vertices of the edges, triangles, and tetrahedra of the complex can be computed and in particular the matrices $j_k(i,j)$ which give the vertices $j=1,\ldots,k+1$ of every k-simplex i.

An alternative way of specifying a complex is to give its incidence matrices. We assign numbers $1,\ldots,n_k$ to label the k-simplices of the complex. The incidence matrix[5] $i_k(i,j)$ for $j=1,2,\ldots$ gives the labels of the k-simplices contained in the $(k+1)$-simplex i. Clearly the incidence matrices can be computed from the vertex matrices and vice versa. Given the matrix $j_4(i,j)$ which specifies the vertices of the four-simplices of a complex we can compute all the other i_k and j_k. It is not true, however, that given the matrix $i_0(i,j)$, which specifies which vertices are connected by edges, one can compute the rest of the complex. For example, there might be a complex with $n_0>5$ vertices in which every vertex is connected to every other (we shall display some subsequently), so that $i_0(i,j)$ is always 1 for $i\neq j$. This i_0 is the same as the i_0 for the (n_0-1)-simplex. To be a four-dimensional complex the five-simplices, which *could* be constructed from the given edges, and the four-simplices in which they intersect must be left out and i_0 does not say which they are.

Not every matrix $j_4(i,j)$ which specifies a four-dimensional complex specifies a manifold. A complex is a manifold if every point (including the interior points of the simplices) has a neighborhood which is homeomorphic to a ball in $\mathbb{R}^4$. A necessary and sufficient condition for a complex to be a manifold may be stated in terms of the star and link of a simplex. The *star* of a simplex σ is the collection of all simplices which have σ as a face together with all of their faces. The *link* of a simplex σ consists of all simplices in its star which do not have σ as a face. (See Paper I for some illustrations.) A complex is a four-manifold if and only if the link of every k-simplex is a $(3-k)$-sphere.[6] This is not a condition which translates very straightforwardly (if at all) into an algorithm for deciding whether a complex is a manifold or not.[7] However, necessary conditions which are easy to test can be derived. For example, for the link of every tetrahedron to be a zero-sphere (two vertices), two four-simplices must intersect in exactly two tetrahedra or not at all. This is the analog of two triangles intersecting in exactly one edge in a two-manifold. In particular this implies that the total number of tetrahedra and four-simplices are related by

$$5n_4=2n_3\,. \tag{2.1}$$

Another condition on the total number of simplices may be derived[8] by fixing attention on a vertex σ and considering the collection of simplices $N(\sigma)$ which is the star of σ less its link and less the vertex σ itself. The Euler number of any homogeneously n-dimensional complex with m_k k-simplices is

$$\chi=\sum_{k=0}^{n}(-1)^k m_k\,. \tag{2.2}$$

Since the link of a vertex of a four-manifold is a sphere with $\chi=2$, and since the star of a vertex is a four-ball with $\chi=1$, the Euler number of $N(\sigma)$ vanishes. Summing this relation over all vertices of the manifold one finds

$$2n_1-3n_2+4n_3-5n_4=0\,. \tag{2.3}$$

This is an example of a Dehn–Sommerville relation.

Neither (2.1) nor (2.3) is sufficient to guarantee that a complex is a manifold. The absence of a straightforward combinatoric check of whether a complex is a manifold means that finding explicit simplicial manifolds with interesting topology is a challenging mathematical problem. In the literature (to quote a review of the three-dimensional problem[9]) "explicit triangulations of topologically nontrivial three-manifolds have been observed only very rarely" and their construction by and large has been by special techniques. Given this situation we cannot attempt a systematic survey of four-dimensional simplicial manifolds. Rather in this section, drawing almost entirely on the mathematical literature, we shall exhibit a few examples. We shall classify them by the customary name of their topological space. The specific complex is then said to be a specific *triangulation* of the space.

A. S^4

The surfaces of the tetrahedron, octohedron, and icosohedron are triangulations of the two-sphere. They are regular in the sense that no vertex or edge is distinguished from any other. The analog regular triangulations of S^4 are the surfaces of the regular solids in five dimensions, which are composed entirely of four-simplices. There are only two.[10] The first is the surface of the five-simplex α_5 obtained by joining each of six vertices in five-dimensional Euclidean space to every other vertex. Thus, $n_0=6$, $n_1=15$, $n_2=20$, $n_3=15$, and $n_4=6$. The second is the surface of the five-dimensional cross polytope β_5. This may be constructed by taking five orthogonal axes, locating two vertices on each axis on opposite sides of the origin, and connecting each vertex to every other except its opposite. For β_5, $n_0=10$, $n_1=40$, $n_2=80$, $n_3=80$, and $n_4=32$. The vertex matrices of α_5 and β_5 are given in Table I. The regular nature of the triangulations α_5 and β_5 can be expressed concretely by giving their symmetry groups expressed as operations on the vertices.[11] The symmetry group of α_5 is the permutation group on the six-vertices S_6. In the context of the construction described above the symmetry group of β_5 consists of

TABLE I. Four-simplices of α_5, β_5, and CP_9^2.

α_5 $n_0=6,\ n_4=6$	β_5 $n_0=10,\ n_4=3$	CP_9^2 $n_0=9,\ n_4=36$
1 2 3 4 5	1 2 3 4 5	1 2 4 5 6
1 2 3 4 6	1 2 3 4 6	2 3 5 6 4
1 2 3 5 6	1 2 3 5 7	3 1 6 4 5
1 2 4 5 6	1 2 3 6 7	1 2 4 5 9
1 3 4 5 6	1 2 4 5 8	2 3 5 6 7
2 3 4 5 6	1 2 4 6 8	3 1 6 4 8
	1 2 5 7 8	2 3 6 4 9
	1 2 6 7 8	3 1 4 5 7
	1 3 4 5 9	1 2 5 6 8
	1 3 4 6 9	3 1 5 6 9
	1 3 5 7 9	1 2 6 4 7
	1 3 6 7 9	2 3 4 5 8
	1 4 5 8 9	4 5 7 8 9
	1 4 6 8 9	5 6 8 9 7
	1 5 7 8 9	6 4 9 7 8
	1 6 7 8 9	4 5 7 8 3
	2 3 4 5 10	5 6 8 9 1
	2 3 4 6 10	6 4 9 7 2
	2 3 5 7 10	5 6 9 7 3
	2 3 6 7 10	6 4 7 8 1
	2 4 5 8 10	4 5 8 9 2
	2 4 6 8 10	6 4 8 9 3
	2 5 7 8 10	4 5 9 7 1
	2 6 7 8 10	5 6 7 8 2
	3 4 5 9 10	7 8 1 2 3
	3 4 6 9 10	8 9 2 3 1
	3 5 7 9 10	9 7 3 1 2
	3 6 7 9 10	7 8 1 2 6
	4 5 8 9 10	8 9 2 3 4
	4 6 8 9 10	9 7 3 1 5
	5 7 8 9 10	8 9 3 1 6
	6 7 8 9 10	9 7 1 2 4
		7 8 2 3 5
		9 7 2 3 6
		7 8 3 1 4
		8 9 1 2 5

permutations of the five orthogonal axes and the reflections in each. In more mathematical terminology[12] it is the wreath product of the permutation groups S_2 and S_5 written S_2 wr S_5. Less regular triangulations of S^4 could be obtained by subdividing α_5 or β_5 in a systematic fashion or by subdividing the faces of the only other regular solid in five dimensions—the cube.

B. CP^2

A highly symmetric triangulation of CP^2 has recently been given by Kühnel and Lassmann[13] and many of its beautiful properties explained in a lucid article by Kühnel and Banchoff.[14] Their triangulation, which they denote by CP_9^2, has $n_0=9$, $n_1=36$, $n_2=84$, $n_3=90$, and $n_4=36$, so that the Euler number is indeed 3. They found their triangulation by a series of arguments that suggested nine vertices and then a computer search to see how a known list of eight vertex triangulations of the sphere could serve as links of a nine vertex manifold. Their vertex matrix for CP_9^2 is given in Table II. There is an edge connecting every pair of vertices and a triangle filling in every triple of vertices. The symmetry group of CP_9^2 is of order 54 and is generated by the permutations

TABLE II. The action for equal-edged triangulation of S^4 and CP^2.

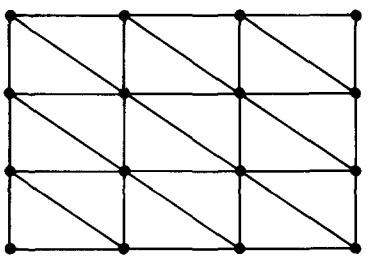
Manifold	Triangulation	a	HL_{ext}/l
S^4	α_5	107.9	4.90
	β_5	81.1	2.80
	round sphere	61.6	...
CP^2	CP_9^2	50.4	2.14
	Fubini–Study	37.7	...

$$\alpha=(123)(465),$$
$$\beta=(147)(258)(369), \tag{2.4}$$
$$\tau=(12)(45)(78).$$

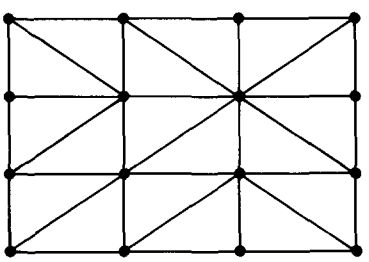
The authors of Ref. 14 denote this by H_{54}.

C. T^4

The most straightforward way to triangulate a two-torus is to represent it as a rectangle with opposite sides identified, divide the rectangle into a sufficient number of smaller rectangles, and triangulate each one. An example is given in Fig. 1(a). In four dimensions, an analogous triangulation of the four-torus T^4 may be constructed by joining together triangulated hypercubes. This construction has been given in detail by Rocek and Williams[15] and used by Hamber and Williams[16] in explicit calculations. The minimum number of hypercubes is 81. This triangulation has 81 vertices and 1944



(a)



(b)

FIG. 1. Two triangulations of a two-torus. The identification of the opposite sides of a rectangle without twist produces a two-dimensional torus T^2. Division of this rectangle into triangles such that the conditions for a simplicial complex are satisfied produces a triangulation of T^2. Two nine-vertex triangulations are shown. The triangulation (a) builds the torus out of standard squares and has two translation symmetries. Viewing the torus as $S^1\times S^1$ and applying the product construction described in the text to the product of two triangles produces the triangulation shown in (b). It is not as symmetric as (a).

four-simplices. The symmetry group clearly contains the symmetry group of the hypercubic lattice which makes T^4.

The straightforward triangulation of T^2 shown in Fig. 1(a) is not the one with the minimum number of vertices. The minimum number is 7. Similarly, triangulations of T^4 can be found with a smaller number of vertices than the hypercubic triangulation. Kühnel[17] has exhibited a 31 vertex triangulation of T^4. The vertex matrix for its four-simplices is generated by taking the four-simplices (0,1,3,7,15), (0,1,3,11,15), (0,1,5,13,15), and (0,4,5,13,15) and applying the group $x \to x+1$, $x \to -x$, $x \to 2x$ to all the entries considered as elements of Z_{31}. There results a triangulation with 704 four-simplices.

D. $S^2 \times S^2$

The product of two simplices is not another simplex but a cell. For example, the product of two edges is not a triangle but a quadrilateral. Cells, however, can always be divided up into simplices and furthermore in a way which does not introduce any new vertices.[18] In this way a triangulation of a product manifold can be generated from triangulations of its products. The simplest example is the construction of a triangulation of a two-torus $T^2 = S^1 \times S^1$ from the product of two "triangles," which are the simplest triangulations of S^1. The result is a nine vertex triangulation of the torus (e.g., Fig. 1).

The process of triangulating the cells can be systematized as follows[18,19]: Consider the cell $\sigma^m \times \sigma^n$ which is the product of an m-simplex with an n-simplex. Number the vertices of σ^m in some ordered fashion $i_0 < i_1 < \cdots < i_m$ and do similarly for σ^n, $j_0 < j_1 < \cdots < j_n$. The vertices of the cell $\sigma^m \times \sigma^n$ are the pairs (i_α, j_β). The ordering of the vertices establishes a partial ordering on the pairs. We say $(i,j) < (k,l)$ if $i \leqslant k$, $j < l$, or if $i < k$, $j \leqslant l$. A triangulation of the cell $\sigma^m \times \sigma^n$ is given by the k-simplices spanned by vertices $(i_0, j_0), \ldots, (i_k, j_k)$ such that

$$(i_0, j_0) < (i_1, j_1) < \cdots < (i_k, j_k) . \tag{2.5}$$

A triangulation of a product manifold may be obtained by triangulating the products of simplices in its factors in this manner. In the case of the torus described above this systematic procedure yields the rather unsymmetric triangulation shown in Fig. 1(b).

Applied to the product of two tetrahedra, the above procedure yields a triangulation of $S^2 \times S^2$. There are 16 vertices formed by the products (i,j) of the four vertices of each tetrahedron, $i = 0,\ldots,3; j = 0,\ldots,3$. The four-dimensional cells are the products of the form $\sigma^2 \times \sigma^2$. The k-simplices of the triangulation are spanned by all sequences of the form (2.5) in which not all four vertices occur either in the sequence $i_0,\ldots,i_k$ or in the sequence $j_0,\ldots,j_k$. This condition arises because the triangles in the factors of $\sigma^2 \times \sigma^2$ have three vertices so that no more than three different vertices occur in any cell. This triangulation of $S^2 \times S^2$ has $n_0 = 16$, $n_1 = 84$, $n_2 = 216$, $n_3 = 240$, and $n_4 = 96$. Like the triangulation of the torus exhibited in Fig. 1(b), it is not very symmetric. There are 25 independent edge lengths. It is an interesting question whether there are more symmetric triangulations of $S^2 \times S^2$.

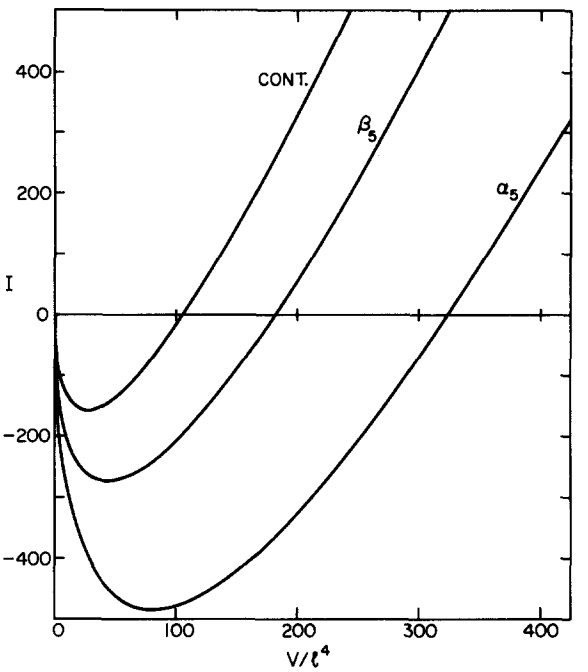


FIG. 2. The action for some homogeneous, isotropic, simplicial four-geometries on S^4. The figure shows the action for the four-geometries which are the boundaries of the five-simplex (α_5) and the five-dimensional cross polytope (β_5) (the five-dimensional generalization of the octohedron). In these triangulations no edge is distinguished from any other. The action for the geometries of highest symmetry with all edges equal is plotted against the total four-volume V for the value of the cosmological constant corresponding to $H^2 = 1$. Also plotted is the "continuum" action for the round four-sphere. The actions are negative for small V but become positive at large V due to the cosmological constant term in the action. At the minimum there is a solution of the Regge equations with all edges equal. The triangulation β_5 is more refined than α_5 and better approximates the continuum action.

E. $S^3 \times S^1$

An 11 vertex triangulation of $S^3 \times S^1$ has been constructed by Kühnel.[20] It is generated by taking the four-simplices (0,2,3,4,5), (0,1,3,4,5), (0,1,2,4,5), and (0,1,2,3,5) and applying the operation $x \to x+1$ to all vertices of each considered as elements of Z_{11}. There result 44 four-simplices.

III. EVALUATING THE ACTION

The Regge action for a simplicial manifold consisting of collections of k-simplices Σ_k, $k = 0,1,\ldots,4$, is

$$l^2 I = -2 \sum_{\sigma \in \Sigma_2} V_2(\sigma) \theta(\sigma) + \frac{6H^2}{l^2} \sum_{\tau \in \Sigma_4} V_4(\tau) . \tag{3.1}$$

Here, we have written $3H^2/l^2$ for the cosmological constant, V_k is the volume of a k-simplex, and $\theta(\sigma)$ is the deficit angle of triangle σ. This is defined by

$$\theta(\sigma) = 2\pi - \sum_{\tau \supset \sigma} \theta(\sigma,\tau) , \tag{3.2}$$

where the sum is over the four-simplices τ, which contain σ, and $\theta(\sigma,\tau)$ is the dihedral angle between the two tetrahedral faces of τ, which intersect in σ. The volumes V_k and dihedral angles $\theta(\sigma,\tau)$ may all be expressed in terms of the squared edge lengths of the geometry through standard flat space

formulas. (How to do this was reviewed in detail in Paper I, Sec. III.) In this way the action becomes a function of the squared edge lengths of the simplicial geometry.

For even the simple triangulations displayed in Sec. II the number of edge lengths is large enough that the functional form of the action can be readily displayed only on slices through the space of edge lengths. The symmetry of the triangulation often suggests suitable slices. In this section we display some numerical calculations of the Regge action on some obvious slices of the triangulations of S^4 and CP^2 described in Sec. II.

The edges of the triangulations α_5 and β_5 of S^4 are equivalent in the sense that any one edge is transformed into every other by the action of the symmetry group. It is therefore interesting to investigate the action of the triangulations when all their edge lengths are equal; this turns out to be an interesting case for CP_9^2 as well. Equivalently one can quote the action as a function of the total volume of the closed geometry since the total volume of n_4 four-simplices of equal squared edge lengths s is

$$V = n_4(\sqrt{5}/96)s^2 . \tag{3.3}$$

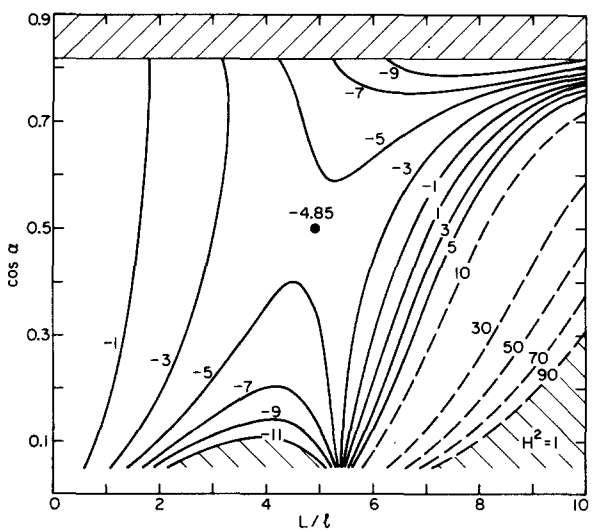


FIG. 3. The action for distorted five-simplices. The figure shows a contour map of the action (divided by 100) for a two-parameter family of five-simplices in which all the edges are of length L except for those emerging from one vertex which have the value $L/(2\cos\alpha)$. The cosmological constant has the value corresponding to $H^2 = 1$. As shown in Fig. 6, values of $\cos\alpha$ near zero correspond to long thin five-simplices while small values of α correspond to nearly flat five-simplices. The solid contour lines are spaced by units of 200 in I while the dotted ones are spaced by units of 2000. The contour lines become too closely spaced for clear display in the hatched areas at bottom and right. Contour lines are not shown for very small values of $\cos\alpha$ because the author's calculation was not very accurate there. There are no five-simplices with a value of $\cos\alpha$ greater than 0.81 because the four-simplex inequalities are not satisfied for larger values. The action is well behaved at this boundary of the space of edge lengths. The contour map shows the negative gravitational action associated with inhomogeneous conformal distortions. There is an extremum corresponding to all equal edges with a value of $4.9l$. This extremum is a saddle point not a maximum or minimum. The action generally becomes positive at large L because of the positive cosmological constant term. For large L and $\cos\alpha$ near 1, however, the action does not become positive but remains negative. These values correspond to large but nearly zero volume four-geometries. They are directions along which the sum over geometries evaluated along a real contour will not be exponentially damped.

On dimensional grounds the action at equal edge lengths must take the form

$$I = -a(V/l^4)^{1/2} + 6H^2V/l^4 . \tag{3.4}$$

Table II shows the dimensionless parameter a for the triangulations α_5 and β_5 of S^4 and the triangulation CP_9^2 of CP^2. For the case of α_5 and β_5 this parameter agrees with that calculated analytically by Hamber and Williams.[16] Its agreement is thus a check of the numerical algorithm.

Table II also shows the continuum value of the parameter a for the metrics of highest symmetry. This is the round sphere metric on S^4 and the Fubini–Study metric[21] on CP^2. The equal edged α_5, β_5, and CP_9^2 may be considered as approximations to these most symmetric continuum geometries. The simplicial actions lie below the continuum action for given V. In the case of S^4, as one proceeds from α_5 to the more refined triangulation β_5, the approximation to the continuum action improves, as is shown more graphically in Fig. 2. The actions are negative for small V as a consequence of the dominance of the curvature term and positive at large V because of the cosmological constant term. The minimum of the action corresponds to a solution of the Regge equations (1.2) as will be discussed in Sec. IV.

Figures 3, 4, and 5 show the Regge action for S^4 evaluated on some two-dimensional slices of the space of edge lengths. Figure 3 shows the action on a family of distorted five-simplices. All edges have the value L except for those emanating from one particular vertex which have the value $L/(2\cos\alpha)$. A two-dimensional analog is shown in Fig. 6. For fixed L, as $\cos\alpha$ increases from zero, the five-simplex ranges from "long and thin" to "short and squat." Beyond a value $\cos\alpha_e = (5/8)^{1/2}$, where it becomes degenerate, it is no longer possible to embed the five-simplex in five-dimension-

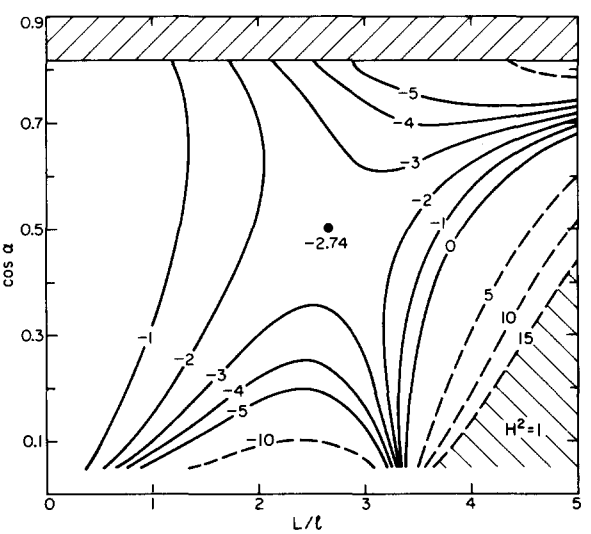


FIG. 4. The action for distorted β_5's. This figure shows the action (divided by 100) for a two-parameter family of geometries which are the surface of a five-cross polytope. All edges have the value L except those emerging from one vertex which have the value $L/(2\cos\alpha)$. The family of geometries is thus essentially the same as that displayed in Fig. 3 but with a more refined triangulation of S^4. The qualitative features of this map are essentially the same as those of Fig. 3 to whose caption the reader is referred for a description.

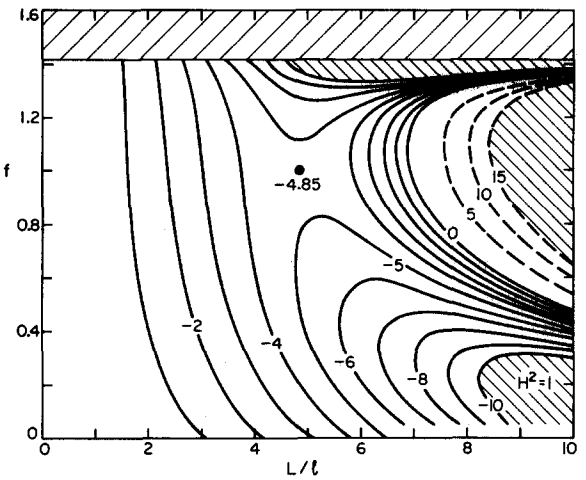


FIG. 5. The action for some homogeneous anisotropic five-simplices. If four of the five edges emerging from any one vertex of a five-simplex are assigned a value L and the remaining edge is assigned the value fL, there results a simplicial geometry which is homogeneous in the sense that any vertex is equivalent to any other, but anisotropic in the sense that not all directions at a given vertex are equivalent. A contour map of the action (divided by 100) for these geometries is shown here for the vlaue of the cosmological constant corresponding to $H^2 = 1$. Solid contour lines are spaced by intervals of 100 in action and dotted lines by 500. In the shaded regions the contours are too close together for clear display. The four-simplex inequalities are violated for sufficiently large f so that there is a boundary to the space of edge lengths. The action has a saddle point extremum at the isotropic (all edges equal) geometry previously shown in Fig. 2 and 3.

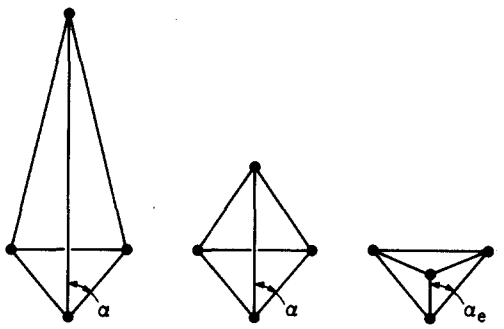


FIG. 6. A family of distorted three-simplices. The figure shows two-dimensional analogs of the distorted five-simplices whose action is displayed in Fig. 3. All the edges are equal except those emanating from the top vertex. The ratio of the two types of edges is controlled by the angle α. As α decreases from $\pi/2$ to 0 one moves from a long and thin three-simplex, through shorter and squatter ones. Eventually at a value α_e the three-simplex degenerates. For values of α smaller than α_e the geometry is no longer embeddable in flat three-dimensional space. It remains a well defined two-geometry, however, since the triangle inequalities are not violated until $\alpha = 0$.

al flat space even as it is impossible to embed the two-dimensional analog of Fig. 6 in three-dimensional flat space beyond $\cos\alpha_e = (3/4)^{1/2}$. Embedability in a higher-dimensional flat space, however, is not a physical requirement for a four-geometry. The physical range of α extends beyond α_e to the value α_{crit} where $\cos\alpha_{\text{crit}} = (2/3)^{1/2}$ at which the volume of the four-simplices vanishes and the four-simplex analog of the triangle inequalities are no longer satisfied.

One may think of the sequence of five-simplices generated by varying α as produced by a conformal deformation of the equal-edged five-simplex. Following Rocek and Williams,[16] a conformal transformation of a simplicial geometry may be defined by giving a function Ω_i on the vertices and then transforming the edge lengths as

$$s_{ij} = \Omega_i \Omega_j \tilde{s}_{ij} \,. \tag{3.5}$$

If we take $\tilde{s}_{ij} = L$, for all i and j and $\Omega_i = 1$, on all vertices but one where it equals $1/(2\cos\alpha)$, we recover the sequence of distorted five-simplices.

A contour map of the action for the two-parameter family $(L,\cos\alpha)$ of distorted five-simplices is shown[22] in Fig. 3. A similar family of distorted cross polytopes can be constructed by singling out the edges extending from a particular vertex. The contour map for this family is shown in Fig. 4. The two cases have essentially the same features: The action becomes positive for large L where the cosmological constant term dominates. There is one extremum which has all edges equal ($\cos\alpha = \frac{1}{2}$). It is not a minimum or a maximum but a saddle point. In the directions of conformal deformation away from the extremum the action becomes significantly negative. This is a simplicial example of the nonpositivity of the gravitational action in the continuum theory.[23]

The distorted α_5's and β_5's described above are inhomogeneous in the sense that one vertex is distinguished from among all others. A class of homogeneous but anisotropic simplicial geometries may be produced by treating all vertices equally but by allowing different length edges to emanate from each vertex. For example, we can consider the five-parameter family of surfaces of the five-simplex obtained by allowing the five edges meeting in each vertex to take on different values. A simple example is the two-parameter family in which four edges have equal values and the remaining edge a distinct value. The action for such a two-parameter family is shown in Fig. 5. The familiar saddle point extremum is seen again on this new slice.

While all the vertices of the triangulation CP^2_9 of the manifold CP^2 are equivalent, all the edge lengths are not. The edge lengths fall into two classes. For any pair of edges of a given class there is an element of the symmetry group H_{54} which carries one edge into the other. With the labeling of the vertices used in Table I, one class (class I) consists of the edges (12), (13), (23), (45), (46), (56), (78), (79), and (89), and the other (class II) consists of all the rest. It is therefore interesting to plot the action when all the edge lengths of class I have the value L_{I} and all those of class II the value L_{II}. Such a plot is shown in Fig. 7 for $H^2 = 1$. Again the familiar saddle point extrema of the action is observed at a point where $L_{\text{I}} = L_{\text{II}}$.

IV. SOLUTIONS FOR SIMPLICIAL GEOMETRIES WITH HIGH SYMMETRY

Two things are important for the exploration of the semiclassical approximation to a sum over geometries such as that of Eq. (1.1). First, one needs the extrema of the action, that is the solutions of the Regge equations

$$\frac{\partial I}{\partial s_i} = 0, \quad i = 1,\ldots,n_1. \tag{4.1}$$

Second, one needs the eigenvalues λ_i, $i = 1,\ldots,n_1$ of the second derivative matrix of the action

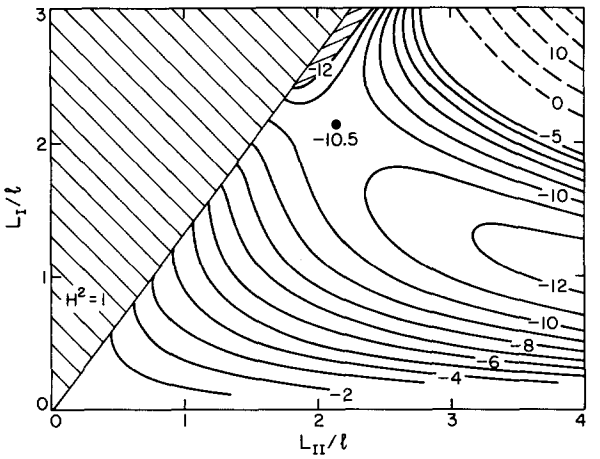


FIG. 7. The action for the triangulation CP_9^2 of the manifold CP^2 plotted as a function of the edge lengths of the two types of edges. Here CP_9^2 has two classes of edges which are carried into each other by the action of its symmetry group. The action (divided by 10) is plotted here for $H^2 = 1$ against the two values of the edge lengths L_I and L_{II}. Solid contour lines are spaced by units of 10 and dotted lines by units of 50. The simplicial inequalities are violated in the shaded region to the left. Contours become too dense for display in the shaded region at the upper left. There is a saddle point extremum when $L_I = L_{II} = 2.14$.

$$I_{ij}^{(2)} = \frac{\partial^2 I}{\partial s_i\, \partial s_j} \tag{4.2}$$

evaluated at the extrema. The extrema determine where the action is to be evaluated in constructing the semiclassical approximation. The determinant of $I_{ij}^{(2)}$ gives the contribution from the integration over quadratic fluctuations about the extremum [see, e.g., Eq. (4.1) of Paper I]. This determinant is the product of the eigenvalues λ_i.

For simplicial geometries in which the typical edge length is small compared to the curvature scale, there will be local regions containing many vertices in which the geometry is essentially flat. Variations in the edge lengths corresponding to those induced by motions of these vertices in flat space will leave the geometry and hence the action approximately unchanged. These variations are the analogs of the diffeomorphisms of the continuum theory.[2,15] Their presence is signaled by small eigenvalues λ_i, which may require special treatment to evaluate the semiclassical approximation accurately. The values of the individual λ_i are therefore of interest.

In constructing the semiclassical approximation, solutions of (4.1) with both real and imaginary s_i are of interest, but the real solutions are easiest to find. One would expect to find real solutions for triangulations of manifolds for which real solutions of Einstein's equation

$$R_{\alpha\beta} = (3H^2/l^2) g_{\alpha\beta} \tag{4.3}$$

exist in the continuum theory. There could also be "spurious" extrema of a simplicial action which do not correspond to continuum solutions; some have been reported.[24] The Euler number of a manifold for which there is a real solution of Eq. (4.3) must satisfy

$$\chi > 0. \tag{4.4}$$

Thus, for the catalog of simplicial manifolds described in Sec. II, we do not expect to find real solutions for triangulations of T^4 and $S^1 \times S^3$ whose Euler number vanishes. We do expect to find solutions for S^4, CP^2, and $S^2 \times S^2$ for which continuum solutions exist.

For simplicial manifolds of high enough symmetry that no edge is distinguished from any other, it is easy to find the solutions of (4.1) with all edges equal if they exist. With all equal edges, all the $\partial I/\partial s_i$ are equal and one can easily calculate this one number and see where it passes through zero. We have carried out such a procedure for the triangulations α_5 and β_5 of S^4. As described in Paper I, $\partial I/\partial s_i$ was computed from

$$f_i \equiv l^2 \frac{\partial I}{\partial s_i} = -2 \sum_{\sigma \in \Sigma_2} \theta(\sigma) \frac{\partial V_2}{\partial s_i} + \frac{6H^2}{l^2} \sum_{\tau \in \Sigma_4} \frac{\partial V_4(\tau)}{\partial s_i} = 0. \tag{4.5}$$

The value of the edge length L_{ext} for which the action is extremized is shown in Table II for α_5 and β_5. These correspond to the extrema located graphically in Sec. III.

Figure 7 suggests that the extrema for CP_9^2 is found when all the edge lengths of the simplicial geometry are equal. We have verified numerically that all the f_i are equal when all the edge lengths are equal by evaluating (4.5). The value of the edge length L_{ext}, which extremizes the action, is quoted in Table II.

The matrix $I_{ij}^{(2)}$ at the stationary point can be straightforwardly computed by numerical differentiation of Eq. (4.5) and its eigenvalues and eigenvectors can be computed by standard numerical methods. The resulting eigenvalues λ and their multiplicities ρ_λ are shown in Table III for α_5, β_5, and CP_9^2. These eigenvalues and eigenvectors are classifiable by the irreducible representations of the symmetry group of the triangulation. Not all irreducible representations will occur. Those that do occur and the corresponding multiplicities can be predicted as follows: The matrix $I_{ij}^{(2)}$ may be viewed as the matrix elements of a linear operation on an n_1-dimensional vector space in a basis in which there is a correspondence between the basis vectors and the edges in some standard order. We shall call this the edge vector space. A permutation of the vertices induces a permutation of the edges and thus a linear operation in the edge vector space. Since the symmetry group G of a simplicial complex is a subgroup of the permutation group on n_0 vertices S_{n_0}, its elements p can be represented as matrices on the edge vector

TABLE III. Eigenvalues and multiplicities of $\partial^2 I/\partial s_i\, \partial s_j$ at the stationary point.

α_5		β_5		CP_9^2	
$l^4 H^{-2}\lambda$	ρ_λ	$l^4 H^{-2}\lambda$	ρ_λ	$l^4 H^{-2}\lambda$	ρ_λ
−0.27	9	−0.39	4	−0.72	6
−0.11	5	−0.36	15	−0.67	2
+0.11	1	−0.34	5	−0.37	5
		−0.30	10	−0.25	6
		−0.15	5	−0.16	6
		+0.23	1	−0.048	2
				−0.047	2
				−0.012	6
				+0.29	1

space. These matrices give a representation of G which is reducible. The irreducible represenations that it contains are the irreducible representations that label the eigenvalues of $I^{(2)}_{ij}$ and the dimensions of these irreducible representations are the multiplicities with which the eigenvalues occur.

To find the irreducible representations of G, which are contained in the reducible representation on the edge vector space, one can analyze the characters of the reducible representation $\pi(p)$ into the characters of the irreducible representations $\chi^{(i)}$ (p) of G. That is, one forms

$$\langle \pi, \chi^{(i)} \rangle = \frac{1}{g} \sum_{p \in G} \pi(p) \chi^{(i)}(p), \tag{4.6}$$

where g is the order of G. An irreducible representation i occurs $\langle \pi, \chi^{(i)} \rangle$ times in π.

The characters $\pi(p)$ are easily seen to be

$$\pi(p) = (\text{number of edges left unchanged by } p). \tag{4.7}$$

The characters $\chi^{(i)}$ are determined by the group G. For α_5 the symmetry group is S_6. For β_5 it is S_2 wr S_5 as discussed in Sec. II. Character tables for these groups can be found in Ref. 12. A character table for the group H_{54} of CP^2_9 was very generously computed for the author by Dr. J. Saxl. The results of the above analysis are as follows: The 15-dimensional reducible representation of S_6 splits as $15 = 1 + 5 + 9$, where the factors are the dimensions of the irreducible representations. The 40-dimensional reducible representation of S_2 wr S_5 splits as $40 = 1 + 4 + 5 + 5 + 10 + 15$. The 36-dimensional reducible representation of H_{54} splits as $2(1 + 1 + 1) + 4{\cdot}6 + 2 + 2 + 2$ where multiplication indicates an irreducible representation which occurs more than once. The multiplicities of the eigenvalues calculated numerically shown in Table III are consistent with this analysis although there is an unaccounted for degeneracy among five of the eigenvalues for CP^2_9.

In each of the cases α_5, β_5, and CP^2_9, one of the eigenvalues is positive and all the rest are negative. The eigenvector of the positive eigenvalue shows that it corresponds to a uniform increase or decrease in the lengths of all edges. This reflects the fact that the stationary configuration is a minimum of (3.4). In all other principle directions the action is a maximum. Thus with these small number of vertices there are not enough degrees of freedom to represent the true physical degrees of freedom of the continuum theory.

V. ITERATIVE SOLUTIONS

Simplicial manifolds with a large number of vertices should not be expected to also possess high symmetry. Only for very special manifolds, therefore, can one expect to be able to use symmetry to find extrema of the action. In general one must simply solve the n_1 algebraic equations

$$f_i = l^2 \frac{\partial I}{\partial s_i} = 0 \tag{5.1}$$

for the sets of n_1 squared real or complex edge lengths which extremize the action.

The numerical problem of extremizing the action is a difficult one. One cannot use the familiar algorithms to search for maxima or minima because, as the examples in Sec. III show, the extrema are, in general, saddle points. There appears to be no better way of locating saddle points than solving Eqs. (5.1) directly.

The Newton–Raphson method is conceptually the simplest technique for solving a system of algebraic equations. Introducing vector notation in the edge vector space, one chooses an assignment of edge lengths $\mathbf{s}$ and attempts to solve for the displacement $\Delta\mathbf{s}$ to an assignment which will make $\mathbf{f}(\mathbf{s} + \Delta\mathbf{s}) = 0$. Expanding this requirement to first order in $\Delta\mathbf{s}$ one finds

$$\Delta\mathbf{s} = -[\mathsf{I}^{(2)}(\mathbf{s})]^{-1} \cdot \mathbf{f}(\mathbf{s}), \tag{5.2}$$

where $\mathsf{I}^{(2)}$ is the matrix of first derivatives of the field equations or second derivatives of the action

$$I^{(2)}_{ij} = \frac{\partial f_i}{\partial s_j} = \frac{\partial^2 I}{\partial s_i \, \partial s_j}. \tag{5.3}$$

In the usual Newton–Raphson method one picks intelligently a starting $\mathbf{s}$, iterates Eq. (5.2), and hopes to converge to a solution.

For simplicial manifolds with small numbers of vertices the Newton–Raphson method works well. For example, we have located the equal-edged extremum of α_5 by starting with significantly differing edge lengths and iterating Eq. (5.2) less than ten times.

For simplicial manifolds with larger number of vertices, the Newton–Raphson method is doomed to work poorly. It requires the inversion of the matrix $\mathsf{I}^{(2)}$. As has been discussed in Sec. IV, one expects the approximate diffeomorphisms of a manifold with a large number of vertices to mean that the matrix $\mathsf{I}^{(2)}$ will have near-zero eigenvalues corresponding to the directions along which the action is approximately constant. In the limit of large n_0 it is increasingly difficult to invert $\mathsf{I}^{(2)}$ and increasingly less likely to find a predicted $\Delta\mathbf{s}$ of reasonable size which does not violate the simplicial inequalities. We have verified this the hard way by attempting to solve the field equations for the 16 vertex triangulation of $S^2 \times S^2$ described in Sec. II. This triangulation has 25 inequivalent edges. Evaluated at a typical point, approximately four of the 25 eigenvalues were near zero. We were unable to locate an extremum in a short time.

Of course, there are many better algorithms for solving algebraic equations than the naive one (5.2) and some have been applied to the Regge calculus with success by Sorkin.[25] It would be of interest to apply them here.

The difficulty encountered in the Newton–Raphson method is generic. For large n_0, the extrema of the action lie in long "troughs" in the space edge lengths along which the action is nearly constant. There *is* an extremum, but it will be difficult to distinguish it from other configurations in the trough. This is no surprise and is in fact a familiar problem in general relativity. Einstein's equation does not possess a unique continuum metric for a solution but rather a family of metrics equivalent under diffeomorphisms. To pick out a unique solution one must specify a coordinate system or "fix the gauge." There are no exact diffeomorphisms of the general simplicial geometry but approximate diffeomorphisms produce an approximate ambiguity in the solution of the Regge equations in approximately the same way.

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Exterior differentiation in the Regge calculus

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Regge manifolds are piecewise continuous manifolds constructed from a finite number of basic building blocks. On such manifolds piecewise continuous forms can be defined in a way similar to differential forms on a differentiable manifold. Regge manifolds are used extensively in the construction of space-times in numerical general relativity. In this paper a definition of exterior differentiation suitable for use on piecewise continuous forms on a Regge manifold is presented. It is shown that this definition leads to a version of Stokes' theorem and also to the usual result that $d^2 = 0$. This is preceded by a discussion of certain geometrical properties of the Regge manifolds. It is shown that the version of Stokes' theorem presented here coincides with the usual definition when the Regge manifold is refined, by increasing the number of cells while keeping the total volume constant, to a smooth manifold.

I. INTRODUCTION

It is assumed that solutions of Regge's field equations[1–5], Regge space-times, are approximations, to a degree, of an Einstein space-time, this being a differentiable solution of Einstein's field equations. This assumption is based on two facts. First, the Regge and Einstein manifolds are equivalent under a homeomorphism. Second, both sets of field equations are derived from the same action principle. It is therefore not unreasonable to expect that there should exist a correspondence between certain properties of the Regge and Einstein space-times. In particular the operation of exterior differentiation on an Einstein manifold should lead to a related operation on a Regge manifold.

The main result to be presented here is an operation on forms built on Regge manifolds which mimics the usual operation of exterior differentiation. This result[6] is presented in Sec. IV. In Secs. II and III the basic notation and formulas are presented. Finally, in Sec. V, it is shown that this definition reduces to the version usually employed on smooth manifolds.

II. SIMPLEXES AND COMPLEXES

The fundamental building blocks for the manifolds to be considered here are known as n-simplexes. They may be defined in a recursive fashion as follows.

(i) A 0-simplex is a single point. This object is also called a vertex.

(ii) An $(n+1)$-simplex is constructed from a n-simplex by first introducing one new vertex and then joining this vertex to each of the $(n+1)$ vertices of the n-simplex, and second by demanding that any set of m vertices $(1<m<n+2)$ of the $(n+1)$-simplex is an $(m-1)$-simplex.

(iii) A Lorentzian n-simplex is obtained by imposing a flat Lorentzian metric throughout the n-simplex. Only those n-simplexes in which the induced metric on each of its m-simplexes $(0<m<n)$ is also flat will be considered. This has the effect of disallowing any n-simplexes with curved boundaries.

The obvious method of constructing an n-dimensional manifold is to glue together a collection of n-simplexes. The resulting object is referred to as an n-complex. To avoid certain pathological cases the following restrictions are imposed: (i) the region of the n-complex common to two or more adjacent n-simplexes is an m-simplex with $0<m<$ n, and (ii) any m-simplex of the complex is contained within at least one n-simplex of the n-complex.

The following notation is drawn, primarily, from Seifert and Threlfall.[7]

A typical n-simplex is denoted by $\sigma_n(i)$, with the index i being the label which distinguishes this simplex from all other n-simplexes. The set of all n-simplexes is represented by S_n. Each n-simplex contains exactly $(n+1)$ vertices and is represented as follows:

$$\sigma_n(i) = (i_0 i_1 i_2 \cdots i_n), \quad n = 0,1,2,\ldots, \tag{2.1}$$

where each of the i_j is unique and is the label of a vertex of $\sigma_n(i)$. The order in which the vertices are listed is unimportant unless the simplex is oriented. One of the two possible orientations to the simplex is defined by reading the vertices in (2.1) from left to right. The opposite sense of orientation is obtained if any two vertices in the sequence are swapped. This is indicated by writing

$$(i_0 \cdots i_j \cdots i_k \cdots i_n) = -(i_0 \cdots i_k \cdots i_j \cdots i_n), \tag{2.2}$$

provided that $j \neq k$ and $j, k = 0, 1, 2, \ldots, n$.

An n-complex is denoted by ρ_n and represented by the formal sum

$$\rho_n = \sum_i a_i \sigma_n(i), \tag{2.3}$$

with each $a_i = 0, -1,$ or $+1$. The coefficients a_i represent whether the associated n-simplex is present or not and what orientation it possesses in the complex. Complexes in which certain n-simplexes are absent are referred to as sub- or secondary complexes. The original complex, when required, is referred to as the primary complex.

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One particularly important subcomplex is the boundary of the primary complex. It is defined as follows. First suppose that $\sigma_n(i)$ is represented as in (2.1). Then define the operation

$$\sigma_n(i/i_j) = (i_0 i_1 \cdots i_n / i_j) = \begin{cases} (-1)^j (i_0 i_1 \cdots \hat{i}_j \cdots i_n), \\ 0, \quad \text{if } i_j \text{ is not in } i_0, i_1, \ldots, i_n. \end{cases} \tag{2.4}$$

The symbol $\hat{}$ over i_j indicates that the vertex i_j is excluded from the list. The boundary of an n-simplex $\sigma_n(i)$ is defined as

$$\partial \sigma_n(i) = \sum_{i_j} \sigma_n(i/i_j). \tag{2.5}$$

Similarly for an n-complex

$$\begin{aligned} \rho_n &= \sum_i a_i \sigma_n(i), \\ \partial \rho_n &= \sum_{i,j} a_i \sigma_n(i/j). \end{aligned} \tag{2.6}$$

Obviously $\sigma_n(i/j)$ is also a simplex and thus the operation (2.5) may be applied twice. However from (2.2) and (2.4) it is clear that

$$\sigma_n(i/j/k) = -\sigma_n(i/k/j). \tag{2.7}$$

This leads to the usual result[7]

$$\partial^2 \sigma_n(i) = 0. \tag{2.8}$$

III. THE METRIC FRAME OF A SIMPLEX

A. The natural frame

One of the easiest ways of ensuring that the metric of a simplex is flat is to demand that all of the metric coefficients are constant throughout the simplex. Of course there are other frames in which the coefficients are not constant and yet the metric is flat. For simplicity such frames will be ignored.

It will be convenient to distinguish between the terms "coordinate frame" and "metric frame." The term "coordinate frame" will be used to refer to a frame possessing coordinates but not a metric. In a "metric frame" there are both coordinates and a metric. A very useful metric frame, the natural frame, will now be described.

Choose one n-simplex, $\sigma_n(1)$, and label its vertices from 0 to n. Adopt the vertex (0) as the origin of the coordinate frame. The basis vectors for this n-simplex are chosen as the n vectors that join (0) to the remaining vertices, i.e., along those legs connected to the origin. The coordinate frame is chosen such that the coordinates of the vertices are

$$\begin{aligned} &\sigma_0(0) = (0) \quad : \quad (v_0^\mu) = (0,0, \ldots ,0), \\ &\sigma_0(1) = (1) \quad : \quad (v_1^\mu) = (1,0, \ldots ,0), \\ &\sigma_0(2) = (2) \quad : \quad (v_2^\mu) = (0,1, \ldots ,0), \\ &\qquad\qquad \vdots \\ &\sigma_0(n) = (n) \quad : \quad (v_n^\mu) = (0,0, \ldots ,1). \end{aligned}$$

In short

$$v_n^\mu = \begin{cases} 0, & \text{if } n = 0, \quad \mu = 1,2, \ldots ,n, \\ \delta_n^\mu, & \text{if } n > 0, \quad \mu = 1,2, \ldots ,n. \end{cases} \tag{3.1}$$

Denote the basis vectors by $\mathbf{e}_\mu$. Then any point P in the simplex is described by the vector

$$\mathbf{P} = x^\mu \mathbf{e}_\mu, \quad \text{with each } x^\mu \geqslant 0 \text{ and } \sum_\mu x^\mu \leqslant 1. \tag{3.2}$$

The requirement that $\Sigma_\mu x^\mu \leqslant 1$ ensures that the vector does not pass through the face opposite the origin. This completes the construction of a coordinate frame for this simplex. A metric frame will now be constructed by introducing the leg lengths L_{ij} and the metric components $g_{\mu\nu}$.

Denote the proper distance between the vertices (i) and (j) by L_{ij}. If all the $g_{\mu\nu}$ are known then, using (3.1), the L_{ij} would be computed as

$$\begin{aligned} &L_{0i}^2 = g_{ii}, && 1 \leqslant i \leqslant n, \\ &L_{ij}^2 = (g_{ii} - 2g_{ij} + g_{jj}), && 1 \leqslant i,j \leqslant n \text{ and } i \neq j. \end{aligned} \tag{3.3}$$

In this instance there is no summation over repeated indices. Solve these equations for the $g_{\mu\nu}$ to obtain

$$\begin{aligned} &g_{ii} = L_{01}^2, && 1 \leqslant i \leqslant n, \\ &g_{ij} = (L_{0i}^2 + L_{0j}^2 - L_{ij}^2)/2, && 1 \leqslant i,j \leqslant n \text{ and } i \neq j. \end{aligned} \tag{3.4}$$

So far nothing has been said about the signature of the metric. For a physically realistic space-time, in the sense of general relativity, the signature must be Lorentzian (i.e., $-+++$). Thus it is clear that not all of the leg lengths can be specified without restriction. However, this restriction is somewhat weak for it is possible, in all but a few exceptions, to make small arbitrary changes in the L_{ij} and yet not change the signature. Therefore assume that the signature is Lorentzian for each and every n-simplex of the primary complex. In a later paper a technique of constructing an n-simplex will be described by which the signature may be guaranteed to be Lorentzian.

A knowledge of the $g_{\mu\nu}$ also enables the computation of areas and volumes of n-simplexes. Define the measure of an n-simplex, σ_n, as the n-fold integral

$$M(\sigma_n) = \int_{n\text{-simplex}} ({}^n g)^{1/2} \, d^n x, \tag{3.5}$$

where ${}^n g$ is the determinant of the $g_{\mu\nu}$. The limits of integration are easily deduced from (3.1). For example, for a four-simplex, the four-dimensional measure is

$$M(\sigma_4) = ({}^4 g)^{1/2} \times \int_0^1 \int_0^{1-x^1} \int_0^{1-x^1-x^2} \int_0^{1-x^1-x^2-x^3} dx^4 \, dx^3 \, dx^2 \, dx^1,$$

since ${}^4 g$ is a constant. In this instance the repeated integral has the value $\frac{1}{4}!$, in the general case of (3.5) the value is $1/n!$. Since the signature of the metric may be indefinite it is possible to obtain an imaginary value for $M(\sigma_n)$. This is an unnecessary complication and will be avoided by using the absolute value of ${}^n g$ in (3.5). Thus the measure of an n-simplex, σ_n, is

$$M(\sigma_n) = (1/n!) \, (\text{abs}({}^n g))^{1/2}. \tag{3.6}$$

B. The general frame

On occasions it may be useful to employ a frame other than the natural frame. For example, if a study of the proper-

ties of a group of simplexes is to be made then it may be necessary to build a metric frame covering all simplexes of the group. Clearly the natural frame is inappropriate in this example. The construction of a general class of metric frames will now be discussed. Once again assume that the $g_{\mu\nu}$ are constant throughout each n-simplex and that the basis vectors are chosen as $\partial/\partial x^{\mu}$.

Consider a complex with one or more n-simplexes. To each vertex, $\sigma_0(i)$, of this complex, associate n coordinates, $x^{\mu}(i)$. Provided the topology of this complex is not too peculiar, it should be possible to choose these coordinates so that, for each and every n-simplex, the coordinates constitute a coordinate frame for that simplex. This condition simply ensures that locally (i.e., within one n-simplex) the coordinate frame is n-dimensional. Assume that such a choice can and has been made.

The components of the vector joining $\sigma_0(j)$ to $\sigma_0(i)$, denoted by $L^{\mu}(ij)$, have the values

$$L^{\mu}(ij) = x^{\mu}(i) - x^{\mu}(j). \tag{3.7}$$

The values of the $g_{\mu\nu}$ are obtained by solving the equation

$$L_{ij}^{2} = g_{\mu\nu}L^{\mu}(ij)L^{\nu}(ij). \tag{3.8}$$

Since there are $n(n+1)/2$ leg lengths in each n-simplex and a similar number of $g_{\mu\nu}$'s there may exist a unique solution of (3.8). That a unique solution does exist is guaranteed by the earlier requirement that the coordinate frame be everywhere n-dimensional.

Notice that the values of the $g_{\mu\nu}$ need not be the same in each n-simplex. Thus there may be discontinuous changes in the $g_{\mu\nu}$ across the interfaces between pairs of n-simplexes. Consequently there results a possible ambiguity in the process of raising and lowering indices. For example suppose the leg (ij) is common to two n-simplexes. Then the values of $L^{\mu}(ij)$ with the index lowered may depend upon the choice of simplex in which the computation was performed. There is of course no ambiguity in the $L^{\mu}(ij)$. It would therefore be inaccurate to write $L_{\mu}(ij)$ as the lowered version of $L^{\mu}(ij)$, however, in most applications it will be clear which n-simplex is intended.

Consider one m-simplex $\sigma_m = (i_0 i_1 \cdots i_m)$ in an $(m+1)$-complex and now define the following quantities

$$L_j^{\mu} = L^{\mu}(i_0 i_j), \quad \text{for } j = 1,2,\ldots,m,$$

$$L^{\mu_1\mu_2\cdots\mu_m}(\sigma_m) = e_{12\cdots m}^{\nu_1\nu_2\cdots\nu_m} L_{\nu_1}^{\mu_1} L_{\nu_2}^{\mu_2} \cdots L_{\nu_m}^{\mu_m}, \tag{3.9}$$

with $e_{ij\cdots k}^{\mu\nu\cdots\rho} = +1, -1, 0$ when $(\mu\nu\cdots\rho)$ is either an even, odd, or a nonpermutation of $(ij\cdots k)$, respectively. For example, for $m = 3$,

$$L^{\mu\nu\rho}(\sigma_3) = L_1^{\mu}L_2^{\nu}L_3^{\rho} - L_1^{\nu}L_2^{\mu}L_3^{\rho} + L_1^{\nu}L_2^{\rho}L_3^{\mu} - L_1^{\rho}L_2^{\nu}L_3^{\mu} + L_1^{\rho}L_2^{\mu}L_3^{\nu} - L_1^{\mu}L_2^{\rho}L_3^{\nu}.$$

The following expressions, shown only for $m = 3$ but easily generalized, are all derived from the definition (3.9):

$$L^{\mu\nu\rho}(\sigma_3) = e_{123}^{ijk} L_i^{\mu} L_j^{\nu} L_k^{\rho}, \tag{3.10a}$$

$$L^{\mu\nu\rho}(\sigma_3) = e_{123}^{ijk} N_i^{\mu} L_j^{\nu} L_k^{\rho}, \tag{3.10b}$$

$$L^{\mu\nu\rho}(\sigma_3) = e_{\alpha\beta\gamma}^{\mu\nu\rho} L^{\alpha}(\sigma_1) L^{\beta\gamma}(\sigma_2), \tag{3.10c}$$

$$L^{\mu\nu\rho}(\sigma_3) = e_{\alpha\beta\gamma}^{\mu\nu\rho} N^{\alpha}(\sigma_1) L^{\beta\gamma}(\sigma_2), \tag{3.10d}$$

with σ_2 = one face of σ_3, σ_1 = one leg of σ_3 but not of σ_2, $N^{\alpha}(\sigma_2)$ = the projection of $L^{\alpha}(\sigma_1)$ onto the normal to σ_2, and N_i^{α} = the projection of L_i^{α} onto the normal of its adjacent face.

Now let $L(\sigma_n)$ = the measure of the parallel n-cube formed from the n legs

$$(i_0 i_1),\ldots,(i_0 i_n) \text{ of } \sigma_n = (i_0 i_1 \cdots i_n).$$

It is well known that

$$n!L^{2}(\sigma_n) = L_{(\mu)}(\sigma_n)L^{(\mu)}(\sigma_n), \quad \text{with } (\mu) = (\mu_1\mu_2\cdots\mu_n). \tag{3.11}$$

Alternatively $L(\sigma_n)$ can be computed by an integration like that in (3.5). In this case the limits of integration must now be chosen to cover an n-cube rather than an n-simplex. The result of this integration is similar to (3.6) with the exclusion of the $n!$, thus

$$M(\sigma_n) = (1/n!)L(\sigma_n). \tag{3.12}$$

As the measure of any simplex must be a property of that simplex alone, it follows that any ambiguity in the computation of, for example, $L_{\mu\nu}(\sigma_2)$ must be resolved in the process of computing $L(\sigma_2)$. This circumstance is also evident from the fact that (3.11) is a scalar equation.

For the remaining part of this section it is assumed that the dimension of the complex is 3. After presenting and justifying the definition of exterior differentiation the result will be extended to higher dimensions.

Consider a typical three-simplex σ_3. Suppose that σ_3 has σ_2 as a base and that σ_1 is a leg of σ_3 but not of σ_2. Then from (3.10c)

$$L^{\rho\mu\nu}(\sigma_3) = L^{\rho}(\sigma_1)L^{\mu\nu}(\sigma_2) - L^{\mu}(\sigma_1)L^{\rho\nu}(\sigma_2) + L^{\nu}(\sigma_1)L^{\rho\mu}(\sigma_2). \tag{3.13}$$

Now suppose that $n_{\rho}(\sigma_2)$ is a unit vector normal to the base σ_2. Then a contraction of (3.13) with n_{ρ} results in

$$n_{\rho}(\sigma_2)L^{\rho\mu\nu}(\sigma_3) = n_{\rho}(\sigma_2)L^{\rho}(\sigma_1)L^{\mu\nu}(\sigma_2).$$

However, $n_{\rho}(\sigma_2)L^{\rho}(\sigma_1)$ is the projection of L^{ρ} in the direction of n_{ρ}, which is just the height of σ_1 above σ_2, which in turn is just $L(\sigma_3)/L(\sigma_2)$. This leads to

$$\frac{L^{\mu\nu}(\sigma_2)}{L(\sigma_2)} = n_{\rho}(\sigma_2)\frac{L^{\rho\mu\nu}(\sigma_3)}{L(\sigma_3)}. \tag{3.14}$$

This expression will be used to obtain a relation between a sum of a two-form over a two surface and a sum of a three-form over a three-surface. A similar relation, on a smooth manifold, will involve the exterior derivative of a two-form. The essence of our definition of exterior differentiation is that it is chosen so as to mimic the usual form of Stokes' theorem.

The expression (3.14) is easily generalized to complexes of dimension greater than 3. Suppose that σ_{m-1} is one face of σ_m and that σ_m is one m-simplex of an m-complex. If the unit inward normal to σ_{m-1} is $n_{\rho}(\sigma_{m-1})$ then

$$\frac{L^{\mu_1\mu_2\cdots\mu_{m-1}}(\sigma_{m-1})}{L(\sigma_{m-1})} = n_{\mu_1}(\sigma_{m-1})\frac{L^{\mu_1\mu_2\cdots\mu_m}(\sigma_m)}{L(\sigma_m)}. \tag{3.15}$$

This expression can be proved with techniques similar to those that led to (3.14).

IV. EXTERIOR DIFFERENTIATION

Consider a complex ρ_3 that has been subdivided into a set of three-simplexes. The integral of any two-form A^* over a two-dimensional subcomplex ρ_2 of ρ_3 is defined, in a coordinate frame, as

$$I(\rho_2,\rho_3)=\sum_{\sigma_2 \text{in } \rho_2}\int_{\sigma_2} A^*_{\mu\nu}(x^\alpha)dx^\mu\wedge dx^\nu. \tag{4.1}$$

Similarly, the integral of a three-form B^* over the complex is defined as

$$I(\rho_3)=\sum_{\sigma_3 \text{in } \rho_3}\int_{\sigma_3} B^*_{\mu\nu\tau}(x^\alpha)dx^\mu\wedge dx^\nu\wedge dx^\tau. \tag{4.2}$$

Define the quantities $A_{\mu\nu}(\sigma_2)$ and $B_{\mu\nu\tau}(\sigma_3)$ via the equations

$$A_{\mu\nu}(\sigma_2)M(\sigma_2)=\int_{\sigma_2} A^*_{\mu\nu}(x^\alpha)d^2S, \tag{4.3a}$$

$$B_{\mu\nu\tau}(\sigma_3)M(\sigma_3)=\int_{\sigma_3} B^*_{\mu\nu\tau}(x^\alpha)d^3S, \tag{4.3b}$$

with d^iS and $M(\sigma_i)$ being the differential and total measures of the σ_i, respectively. The $A_{\mu\nu}(\sigma_2)$ and $B_{\mu\nu\tau}(\sigma_3)$ are the averages of their associated forms over the simplexes σ_2 and σ_3.

The relations (4.1) and (4.2) may now be rewritten as

$$I(\rho_2,\rho_3)=\sum_{\sigma_2 \text{in } \rho_2} A_{\mu\nu}(\sigma_2)L^{\mu\nu}(\sigma_2) \tag{4.4a}$$

and

$$I(\rho_3)=\sum_{\sigma_3 \text{in } \rho_3} B_{\mu\nu\tau}(\sigma_3)L^{\mu\nu\tau}(\sigma_3). \tag{4.4b}$$

Suppose now that the subcomplex ρ_2 is the boundary of ρ_3. Our aim is to show that $I(\partial\rho_3,\rho_3)$ may be evaluated either directly from (4.4a) or via an expression similar to (4.4b). The expression (4.4a) may be rewritten as a sum over all σ_3's of the complex by introducing

$$J(\sigma_3)=\sum_{\sigma_2 \text{in } \partial\sigma_3} A_{\mu\nu}(\sigma_2)L^{\mu\nu}(\sigma_2). \tag{4.5}$$

Then

$$I(\partial\rho_3,\rho_3)=\sum_{\sigma_3 \text{in } \rho_3} J(\sigma_3), \tag{4.6}$$

since all σ_2's on the interior of ρ_3 will be counted twice, each with opposite orientations, and will therefore cancel each other. Substitution of (3.14) in (4.15) and the resultant expression in (4.6) leads to

$$\begin{aligned} I(\partial\rho_3,\rho_3)&=\sum_{\sigma_2 \text{in } \partial\rho_3} A_{\mu\nu}(\sigma_2)L^{\mu\nu}(\sigma_2)\\ &=\sum_{\sigma_3 \text{in } \rho_3}\sum_{\sigma_2 \text{in } \partial\sigma_3} n_\rho(\sigma_2)A_{\mu\nu}(\sigma_2)\frac{L(\sigma_2)}{L(\sigma_3)}L^{\rho\mu\nu}(\sigma_3). \end{aligned} \tag{4.7}$$

This expression is greatly simplified by writing

$$A(\sigma_2)=A_{\mu\nu}(\sigma_2)L^{\mu\nu}(\sigma_2), \tag{4.8a}$$

and

$$dA(\sigma_3)=\sum_{\sigma_2 \text{in } \partial\sigma_3} n_\rho(\sigma_2)A_{\mu\nu}(\sigma_2)\frac{L(\sigma_2)}{L(\sigma_3)}L^{\rho\mu\nu}(\sigma_3), \tag{4.8b}$$

for then

$$I(\partial\rho_3,\rho_3)=\sum_{\sigma_2 \text{in } \partial\rho_3} A(\sigma_2)=\sum_{\sigma_3 \text{in } \rho_3} dA(\sigma_3). \tag{4.9}$$

In this form the similarity of this expression with the usual continuum form of Stokes' theorem is quite apparent. The relation (4.8a) defines the value of the two-form A on σ_2 and (4.8b) defines its exterior derivative evaluated on σ_3.

An analysis similar to that which lead to (4.8a), (4.8b), and (4.9) may be applied to complexes of dimension other than 3. Consider a complex ρ_n of dimension n. Suppose there is defined an m-form $A(\sigma_m)$ on each of the σ_m's of ρ_n. Thus put

$$A(\sigma_m)=A_{\mu_1\mu_2\cdots\mu_m}(\sigma_m)L^{\mu_1\mu_2\cdots\mu_m}(\sigma_m). \tag{4.10}$$

Then the exterior derivative of A evaluated on σ_{m+1} is defined as

$$\begin{aligned} dA(\sigma_{m+1})=&\sum_{\sigma_m \text{in}\partial\sigma_{m+1}} n_{\mu_0}(\sigma_m)A_{\mu_1\mu_2\cdots\mu_m}(\sigma_m)\\ &\times\frac{L(\sigma_m)}{L(\sigma_{m+1})}L^{\mu_0\mu_1\cdots\mu_m}(\sigma_{m+1}), \end{aligned} \tag{4.11}$$

and Stokes' theorem takes the form

$$\begin{aligned} I(\partial\rho_{m+1},\rho_{m+1})&=\sum_{\sigma_m \text{in}\partial\rho_{m+1}} A(\sigma_m)\\ &=\sum_{\sigma_{m+1} \text{in}\rho_{m+1}} dA(\sigma_{m+1}). \end{aligned} \tag{4.12}$$

If the complex consists of only one σ_{m+1} then this expression reduces to

$$dA(\sigma_{m+1})=\sum_{\sigma_m \text{in}\partial\sigma_{m+1}} A(\sigma_m). \tag{4.13}$$

This provides an alternative yet equivalent method for computing the exterior derivative. In some situations this expression may be more useful than (4.11). As an example it will now be shown that the value of a form, twice exterior differentiated, is zero. Consider a set of numbers $B(\sigma_{m-1})$ on the σ_{m-1} of ρ_{m-1}. Suppose that each number arose as the value of an $(m-1)$-form B on each of the σ_{m-1} of ρ_{m+1}. The exterior derivative of B, evaluated on each σ_m, gives rise to another set of numbers $A(\sigma_m)$ distributed on the σ_m of ρ_{m+1}. Thus

$$A(\sigma_m)=dB(\sigma_m)=\sum_{\sigma_{m-1} \text{in}\,\partial\sigma_m} B(\sigma_{m-1}). \tag{4.14}$$

Now the exterior derivative of $A(\sigma_m)$ is

$$\begin{aligned} dA(\sigma_{m+1})&=\sum_{\sigma_m \text{in}\partial\sigma_{m+1}} A(\sigma_m)\\ &=\sum_{\sigma_m \text{in}\partial\sigma_{m+1}}\sum_{\sigma_{m-1} \text{in}\,\partial\sigma_m} B(\sigma_{m-1}). \end{aligned}$$

However each σ_{m-1} is counted twice, each time with opposite orientations, thus

$$dA(\sigma_{m+1})=d\,dB(\sigma_m)=0.$$

Exactly the same result occurs in the continuum theory of differential forms.

As another example consider the flux of a constant vector A, with components A^μ, over the surface of one m-sim-

plex in an m-complex. Clearly this quantity vanishes and is expressed as

$$0=\sum_{\sigma_{m-1}\text{in}\,\partial\sigma_m} A^{\mu} n_{\mu}(\sigma_{m-1}) L(\sigma_{m-1}).$$

As this expression is true for any constant field A it follows that

$$0=\sum_{\sigma_{m-1}\text{in}\,\partial\sigma_m} n_{\mu}(\sigma_{m-1}) L(\sigma_{m-1}).$$

Unfortunately, since n_{μ} need not be continuous across each σ_{m-1}, this expression cannot be applied directly to complexes of more than one m-simplex. However after a contraction with $L^{\mu\mu_1\mu_2\cdots\mu_{m-1}}(\sigma_m)$ and using (3.15) this expression reduces to

$$0=\sum_{\sigma_{m-1}\text{in}\,\partial\sigma_m} L^{\mu_1\mu_2\cdots\mu_{m-1}}(\sigma_{m-1}),$$

which is easily extended to complexes, thus

$$0=\sum_{\sigma_{m-1}\text{in}\,\partial\rho_m} L^{\mu_1\mu_2\cdots\mu_{m-1}}(\sigma_{m-1}).$$

This expression can also be proved directly from the definition (3.9).

V. THE CONTINUUM LIMIT

The definitions (4.10) and (4.11) may be extended to complexes built from blocks other than simplexes. For example, an initial manifold could be constructed by piecing together a sequence of three-dimensional cubes. Each such cube could be subdivided, by the addition of extra vertices, legs, and faces, into a set of three-simplexes thus producing a three-complex. To this complex the identity (4.12) would apply. However the terms of this expression may be regrouped so that those terms involving the faces of the three-simplexes are combined into terms involving the faces of the cubes. Similarly the terms involving the three-simplexes would be grouped into terms involving the cubes. In effect the expression (4.12) is unaltered except that the objects in the summation are now parallelograms and parallel cubes instead of triangles and tetrahedrons.

To show that the similarity of (4.9) and (4.12) with Stokes' theorem is not just a consequence of formal algebraic manipulations, the nature of (4.9), over a sequence of complexes, will now be investigated. The following assumptions are necessary.

(i) The dimension of the complex is 3. A similar analysis may be used for higher dimensions.

(ii) The sequence of complexes converges, as the number of σ_3's is increased without limit while keeping the total measure, fixed, to a smooth differentiable manifold.

(iii) The σ_3's of each complex are sufficiently small that the values of $A^{*}_{\mu\nu}$ on the faces σ_2 of σ_3 may be derived from a Taylor series based at some point within σ_3. Thus

$$A^{*}_{\mu\nu}(x^{\alpha})=A^{*}_{\mu\nu}+A^{*}_{\mu\nu,\rho}\delta x^{\rho}+O(\delta x)^2, \tag{5.1}$$

with $\delta x^{\alpha}=x^{\alpha}-x_0^{\alpha}$, and x_0^{α} is the point, within σ_3, from which the Taylor series is developed.

(iv) All σ_3's are three-cubes (parallelepipeds).

For a cube the inward pointing normals for two opposite faces are equal apart from their directions. Thus the terms in (4.8b) may be regrouped as

$$dA(\sigma_3)=\sum_{\substack{\text{three adjacent}\\ \text{faces}}} n_{\rho}(\sigma_2)\Delta A_{\mu\nu}(\sigma_2)\frac{L(\sigma_2)}{L(\sigma_3)}L^{\rho\mu\nu}(\sigma_3). \tag{5.2}$$

However, from (4.3a)

$$\Delta A_{\mu\nu}(\sigma_2)L(\sigma_2)=\int_{\sigma_2-\sigma_{2^*}} A^{*}_{\mu\nu}(x^{\alpha})d^2S, \tag{5.3}$$

with σ_{2^*} being the face opposite σ_2. Substitution of (5.1) into (5.3) and noting that $A^{*}_{\mu\nu}$ and $A^{*}_{\mu\nu,\rho}$ are constant throughout σ_3 results in

$$\Delta A_{\mu\nu}(\sigma_2)L(\sigma_2)=A^{*}_{\mu\nu,\rho}\int_{\sigma_2-\sigma_{2^*}}\delta x^{\rho}\,d^2S.$$

By projecting δx^{ρ} onto the normal and tangential vectors of σ_2 it is not hard to show that this last integral equals $n^{\rho}L(\sigma_3)$. Thus

$$\Delta A_{\mu\nu}(\sigma_2)L(\sigma_2)=A^{*}_{\mu\nu,\rho}n^{\rho}(\sigma_2)L(\sigma_3)$$

and consequently (4.8b) becomes

$$dA(\sigma_3)=A^{*}_{\mu\nu,\rho}\sum_{\substack{\text{three adjacent}\\ \text{faces}}} n_{\alpha}(\sigma_2)n^{\rho}(\sigma_2)L^{\alpha\mu\nu}(\sigma_3).$$

But from (3.10a) and (3.10b) the summation reduces to $L^{\rho\mu\nu}(\sigma_3)$. Thus

$$dA(\sigma_3)=A^{*}_{\mu\nu,\rho}(\sigma_3)L^{\rho\mu\nu}(\sigma_3)$$

and (4.7) becomes

$$I(\partial\rho_3,\rho_3)=\sum_{\sigma_2\text{in}\,\partial\rho_3} A_{\mu\nu}(\sigma_2)L^{\mu\nu}(\sigma_2)$$

$$=\sum_{\sigma_3\text{in}\,\rho_3} A_{\mu\nu,\rho}(\sigma_3)L^{\rho\mu\nu}(\sigma_3), \tag{5.4}$$

with $A_{\mu\nu,\rho}(\sigma_3)=A^{*}_{\mu\nu,\rho}$.

This last result shows clearly that this definition of exterior differentiation does reduce to the usual form when the Regge manifold and the forms built on it are made smooth and differentiable.

VI. CONCLUSION

It has been shown that the concept of exterior differentiation has a natural extension to the Regge calculus. Results similar to (4.9) may be found in references 8–10. The motivation for the development of a Regge version of exterior differentiation arises in the attempt to show that certain Regge expressions "converge" to their usual classical counterparts under certain conditions. An example of this process, that our version of Stokes' theorem reduces to its usual form when applied to differtiable forms, has been presented in Sec. V. A more ambitious project would be to prove (or disprove) that the Regge field equations reduce to the Einstein field equations when an appropriate limiting process is applied. This may form the basis of a future investigation.

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Series representations for calculations in quantum statistics

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The mathematical methods used to average a function of energy over the Maxwell–Boltzmann (MB), Bose–Einstein (BE), and Fermi–Dirac(FD) statistics are compared. Blankenbecler's method converts the FD integrals into a series of differentiations which converge rapidly if the Fermi energy is large compared to kT. The BE integrals may be obtained from the corresponding MB integral by setting the chemical potential equal to zero and multiplying by a slowly converging numerical series. In each case a single integral of general form is used to calculate familiar quantities like chemical potential, energy, and heat capacity.

I. INTRODUCTION

The purpose of this paper is to illustrate three convenient, but very different, mathematical methods used to average a function of energy over a Maxwell–Boltzmann (MB), Bose–Einstein (BE), or Fermi–Dirac (FD) distribution.

When these distribution functions are seen in compact form they appear to differ only slightly:

$$f(\epsilon,\tau) = 1/\exp[(\epsilon-\mu)/\tau]^{+0}_{\text{or}\,+1}. \tag{1}$$

Each is a function of energy ϵ, Boltzmann's constant k, temperature T, and chemical potential μ. From a physical as well as a mathematical point of view, the three numbers in the denominator are crucial. The zero is associated with MB statistics, the minus one with BE, and the plus one with FD. It is helpful to write (1) in terms of the dimensionless parameters $x = \epsilon/\tau$ and $y = \mu/\tau$.

II. THE MAXWELL–BOLTZMANN INTEGRALS

As a first example, we average $C\epsilon^p$ over the MB distribution.

$$I_{\text{MB}} = C\int_0^\infty \frac{\epsilon^p\,d\epsilon}{\exp[(\epsilon-\mu)/\tau]} = Ce^y\tau^{p+1}\int_0^\infty x^p e^{-x}dx$$
$$= Ce^y\tau^{p+1}\Gamma(p+1). \tag{2}$$

This expression yields familiar results[1] for the chemical potential, energy, and heat capacity for a classical gas.

(a) The chemical potential can be obtained by setting $p = \frac{1}{2}$ and $C = (2I+1)(V/4\pi^2)(2M/\hbar^2)^{3/2}$, where I is the spin, V is the volume, M is the particle mass, and $\hbar$ is Planck's constant divided by 2π. This integral is the density of states averaged over the distribution and is equal to N, the total number of particles. Solving for $y = \mu/kT$ yields

$$\mu = kT\ln[n/(2I+1)n_Q], \tag{3}$$

where $n = N/V$ is the particle concentration and

$$n_Q = (M\tau/2\pi\hbar^2)^{3/2} \tag{4}$$

is the quantum concentration. MB statistics are applicable for $n \ll n_Q$.

(b) The energy and heat capacity follow directly from (2) and (3) for $p = \frac{3}{2}$:

$$U = \tfrac{3}{2}NkT, \tag{5}$$

$$C_V = \left(\frac{dU}{dT}\right)_V = \frac{3}{2}Nk.$$

III. THE BOSE–EINSTEIN INTEGRALS

As a second example, we average $C\epsilon^p$ over the BE distribution.[2]

$$I_{\text{BE}} = C\int_0^\infty \frac{\epsilon^p\,d\epsilon}{\exp[(\epsilon-\mu)/kT]-1}$$
$$= C\tau^{p+1}\int_0^\infty \frac{x^p}{e^{-y}e^x-1}\,dx. \tag{6}$$

We set $\exp(-y)\approx 1$, an approximation we justify later. Divide the numerator and denominator of the integrand by $\exp(x)$ and note that

$$\frac{e^{-x}}{1-e^{-x}} = \sum_{m=1}^{\infty} e^{-mx}.$$

Then

$$I_{\text{BE}} \approx C\tau^{p+1}\int_0^\infty x^p \sum e^{-mx}\,dx, \tag{7}$$

with $y' = mx$,

$$I_{\text{BE}} = \sum_1^\infty \frac{1}{m^{p+1}} C\tau^{p+1}\int_0^\infty y'^p e^{-y'}\,dy'$$
$$= \sum_1^\infty \frac{1}{m^{p+1}} C\tau^{p+1}\Gamma(p+1). \tag{8}$$

Comparing (8) with (2),

$$I_{\text{BE}} = \sum_1^\infty \frac{1}{m^{p+1}}\,[I_{\text{MB}}e^{-y}], \tag{9}$$

where the $\exp(-y)$ in the square brackets is a function of the chemical potential (3).

Equation (8) or (2) and (9) can be used to calculate the Einstein condensation temperature, the chemical potential, the energy, and the heat capacity for a degenerate boson gas.

(a) The number N_e of bosons in excited energy states is the density of states summed over the BE distribution. Take $p = \frac{1}{2}$ and $C = (V/4\pi^2)(2M/\hbar^2)^{3/2}$ for a spinless particle. Then from (8)

$$N_e = 2.612\,n_Q V. \tag{10}$$

The Einstein condensation temperature T_E is defined as that

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temperature for which $N_e = N$, the total number of particles. Using (4) for n_Q

$$T_E = \frac{1}{k}\left(\frac{n}{2.612}\right)^{2/3}\frac{2\pi\hbar^2}{M}. \tag{11}$$

(b) The chemical potential below T_E is small and negative. If N_0 is the occupation number of the ground state energy,

$$N_0 = \frac{1}{e^{-y}-1} \approx -\frac{1}{y} = \frac{1}{-\mu/kT}, \tag{12}$$

or

$$\mu \simeq -kT/N_0.$$

Here

$$N_0 = N\left[1-(T/T_E)^{3/2}\right]. \tag{13}$$

(c) The calculation of the internal energy $U_{\rm BE}$ requires $p = 3/2$. It follows immediately that

$$U_{\rm BE} = \sum_{m=1}^{\infty}\frac{1}{m^{5/2}}\left(\frac{n_Q}{n}\right)\frac{3NkT}{2}$$
$$= 1.341\left(\frac{n_Q}{n}\right)\frac{3NkT}{2}. \tag{14}$$

This expression invovles a quantum factor times a classical factor $3NkT/2$.

(d) The heat capacity

$$C_V = \left(\frac{dU}{dT}\right)_V = 3.35\left(\frac{n_Q}{n}\right)\frac{3}{2}Nk \tag{15}$$

also has a quantum factor times the familiar classical factor $3Nk/2$. Here C_V decreases as $T^{3/2}$, as a result of the temperature dependence of n_Q. It approaches 0 as $T \to 0$, in accordance with the third law of thermodynamics.

IV. FERMI–DIRAC INTEGRALS

As a final example we average $C\epsilon^p$ over the FD distribution. This approach follows that of Blankenbecler[3] except that we use a contour integral and the calculus of residues to put the FD integral in its final form as a series of differentiations:

$$I_{\rm FD} = C\int_0^{\infty}\frac{e^p}{\exp[(\epsilon-\mu)/kT]+1}$$
$$= C\tau^{p+1}\int_0^{\infty}\frac{x^p\,dx}{e^{x-y}+1}. \tag{16}$$

Define

$$F(x) = C\tau^{p+1}\int x^p\,dx = \frac{(C\tau^{p+1}x^{p+1})}{(p+1)}. \tag{17}$$

Integrating (16) by parts,

$$I_{\rm FD} = F(x)\frac{1}{e^{x-y}+1}\Big|_0^{\infty} + \int_0^{\infty}\frac{F(x)e^{x-y}}{(e^{x-y}+1)^2}. \tag{18}$$

Let $x' = x - y$, then

$$I_{\rm FD}(y) = \int_{-y}^{\infty}\frac{F(x'+y)e^{x'}}{(e^{x'}+1)^2}\,dx'. \tag{19}$$

Now let $\delta = \partial/\partial y$ and expand $F(x'+y)$ about $F(y)$,

$$F(x'+y) = F(y) + x'\delta F(y) + \frac{(x'\delta)^2}{2!}F(y) + \cdots$$
$$= e^{x'\delta}F(y), \tag{20}$$

$$I_{\rm FD}(y) = \int_{-y}^{\infty}\frac{dx'\,e^{x'}e^{x'\delta}}{(e^{x'}+1)^2}F(y). \tag{21}$$

With $\eta = \exp(x')$, there is considerable simplification

$$I_{\rm FD}(y) = \int_{e^{-y}}^{\infty}\frac{d\eta\,\eta^{\delta}}{(\eta+1)^2}F(y). \tag{22}$$

In most calculations y is sufficiently large so that $\exp(-y) \approx 0$. A convenient approach for the evaluation of the integral over η is by means of a contour integration and the calculus of residues. Consider

$$\oint dz\,\frac{z^{\delta}}{(z+1)^2} = 2\pi i a_{-1}. \tag{23}$$

At $z = -1 = e^{\pi i}$, there is a pole of order 2. The residue $a_{-1} = -\delta e^{\pi i\delta}$. At $z = 0$ there is a branch point. We use the contour integral shown in Fig. 1,

$$\int_{AB}+\int_{BC}+\int_{CD}+\int_{DE}$$
$$= \int_{\epsilon}^{R}d\eta\,\frac{\eta^{\delta}}{(\eta+1)^2} + \int_0^{2\pi}d\theta\,\frac{iRe^{i\theta}(Re^{i\theta})^{\delta}}{(Re^{i\theta}+1)^2}$$
$$+\int_R^{\epsilon}\frac{d\eta(\eta e^{2\pi i})^{\delta}}{(\eta e^{2\pi i}+1)^2} + \int_{2\pi}^{0}d\theta\,\frac{i\epsilon e^{i\theta}(\epsilon e^{i\theta})^{\delta}}{(\epsilon e^{i\theta}+1)^2}$$
$$= -\delta e^{\pi i\delta}. \tag{24}$$

In the limit as $R \to \infty$ and $\epsilon \to 0$, the second and fourth integrals vanish. Then

$$(1-e^{2\pi i\delta})\int_0^{\infty}d\eta\,\frac{\eta^{\delta}}{(\eta+1)^2} = -2\pi i\delta e^{\pi i\delta} \tag{25}$$

or

$$\int_0^{\infty}d\eta\,\frac{\eta^{\delta}}{(\eta+1)^2} = \pi\delta\csc\pi\delta. \tag{26}$$

When expanded in a power series this operator acts on $F(y) = [Cy^{p+1}/(p+1)][\tau^{p+1}]$, so

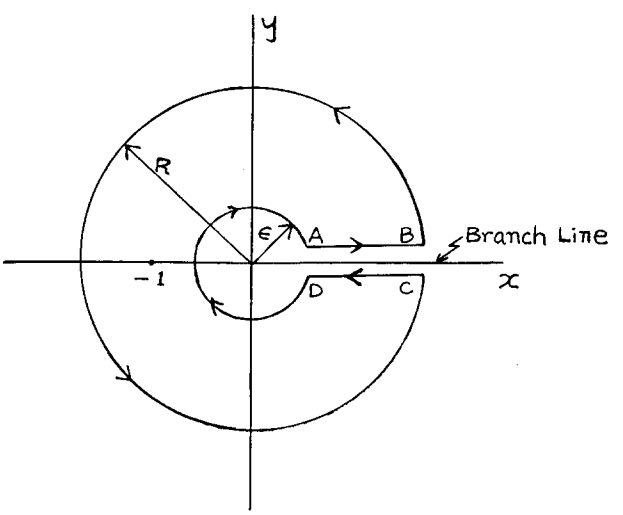

FIG. 1. The contour integral used to evaluate $\int_0^{\infty} d\eta\,\eta^{\delta}/(\eta+1)^2$.

$$I_{\mathrm{FD}}(y)=\left[1+\frac{\pi^2}{6}\frac{\partial^2}{\partial y^2}+\frac{7\pi^4}{3\cdot 5!}\frac{\partial^4}{\partial y^4}+\cdots+\frac{2(2^{2n+1}-1)}{(2n+2)!}\pi^{2n+2}B_{2n+1}\frac{\partial^{2n+2}}{\partial y^{2n+2}}\right]\times\frac{C\tau^{p+1}y^{p+1}}{p+1},\tag{27}$$

where $n=0,1,2,\ldots$, and $B_1=\frac{1}{6}$, $B_3=\frac{1}{30}$, $B_5=\frac{1}{42}$, $B_7=\frac{1}{30},\ldots$.

Equation (27) can be used to calculate the Fermi energy, the internal energy, and the heat capacity for a degenerate Fermi gas.

(a) The number N of fermions is the density of states summed over the FD distribution. Take $p=\frac{1}{2}$ and $C=(V/2\pi^2)(2M/\hbar^2)^{3/2}$ for a spin-$\frac{1}{2}$ particle. Then from (27)

$$\mu_0=(\hbar^2/2M)(3\pi^2 n)^{2/3},\tag{28}$$

and

$$\mu=\mu_0\left[1-\frac{\pi^2}{12}\left(\frac{kT}{\mu_0}\right)^2-\frac{7\pi^4}{8\cdot 15!}\left(\frac{kT}{\mu_0}\right)^4\cdots\right].\tag{29}$$

(b) The internal energy and the heat capacity follow from (27) with $p=3/2$. Then

$$U=\frac{3}{5}N\mu_0\left[1+\frac{5\pi^2}{12}\left(\frac{kT}{\mu_0}\right)^2-\frac{\pi^4}{16}\left(\frac{kT}{\mu_0}\right)^4+\cdots\right],\tag{30}$$

and

$$C_V=\left(\frac{dU}{dT}\right)_V=\frac{\pi^2}{2}\frac{NkT}{T_{\mathrm{F}}}\left(1-\frac{3}{10}\pi^2\frac{\mathrm{T}^2}{\mathrm{T}_{\mathrm{F}}^2}+\cdots\right),\tag{31}$$

where $T_{\mathrm{F}}=\mu_0/k$ is the Fermi temperature at absolute zero.

V. DISCUSSION

The MB integrals may be evaluated exactly. Approximations are used in both the BE and FD integrals. In the BE case $e^{-\mu/kT}\approx 1$. In the FD case $e^{-\mu/kT}\approx 0$. The BE and FD integrals are expressed in series representations. The numerical series in the BE expression converge rather slowly and can best be handled by a simple computer program.[4] The terms in the FD series converge rapidly for $\mu_0 \gg kT$.

It is tempting to use the Blankenbecler procedure for the BE calculation. This can be done formally. However, this leads to a blind alley. The repeated differentiations generate terms with increasingly large negative powers of $y=\mu/kT$ as in the FD series. But y in the BE case is very small indeed, whereas y in the FD case is large. The series diverges.

Each of the averages were made for $C\epsilon^p$. The results can easily be generalized for any function of energy which can be expanded in a McClaurin series. This probably includes most cases of physical interest.

VI. CONCLUSION

The principal results of this paper are embodied in Eqs. (2), (5), and (27). These represent averages of the energy, raised to any power p, taken over the MB, BE, and FD distribution functions. In the FD case, the Blankenbecler method converts the integral into a series of differentiations which rapidly converge, if the Fermi energy is large compared to kT. This method is not appropriate for the BE distribution where the chemical potential is small compared to kT. Rather the solution to this type of integral is an infinite series $\Sigma_1^\infty m^{-p-1}$, times the corresponding MB integral with μ_{BE} and μ_{MB} set equal to zero. To illustrate their utility, Eqs. (2), (5), and (27) are used to calculate the chemical potential, energy, and heat capacity.

[1] C. Kittel and H. Kroemer, *Thermal Physics* (Freeman, San Francisco, 1980), p. 121.

[2] This method is a generalization of a discussion in Kittel and Kroemer,[1] p. 204.

[3] Except where indicated this method follows the method of R. Blankenbecler, Am. J. Phys. **25**, 279 (1957).

[4] Here are a few of these sums: $\Sigma_1^\infty m^{-3/2}=2.612$, $\Sigma_1^\infty m^{-5/2}=1.341$, $\Sigma_1^\infty m^{-7/2}=1.127$, $\Sigma_1^\infty m^{-9/2}=1.055$.

A theorem on Lyapunov stability for dynamical systems and a conjecture on a property of entropy

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For a general dynamical system, it is proved that an equilibrium state belonging to a continuous family of conditionally stable equilibrium states is stable. The result is applied to quantum thermodynamics to clarify in what restricted sense the entropy functional $s(\rho) = -k \operatorname{Tr} \rho \ln \rho$ can provide a Lyapunov criterion for the stability of thermodynamic equilibrium. A conjecture on a special positive-definiteness property of $-k \operatorname{Tr} \rho \ln \rho$ remains to be proved.

I. INTRODUCTION

In this note we address the question of whether entropy is indeed a Lyapunov function of the kind often implied in some thermodynamics literature on the stability of the maximum entropy equilibrium states.[1]

For a general dynamical system,[2] we call L functions those Lyapunov functions[3] that satisfy the hypothesis of Lyapunov's stability theorem.[4] We also define a special class of nondecreasing functions, called S functions, that satisfy the hypothesis of a conditional stability theorem. We prove a theorem giving a sufficient condition for the stability of equilibrium: an equilibrium state is stable if it belongs to a continuous family of conditionally stable equilibrium states (Theorem 3).

We apply the theorem to quantum thermodynamics to clarify the open question whether the entropy functional $s(\rho) = -k \operatorname{Tr} \rho \ln \rho$, together with the principle of nondecrease of entropy, indeed provides a Lyapunov criterion for the stability of thermodynamic equilibrium. We show that $s(\rho)$ is not an L function. We conjecture (Sec. III) that $s(\rho)$ is an S function, but provide only heuristic arguments in support of the conjecture. Thus, the open question remains unresolved, and calls for a technical study of the conjecture.

In view of our result, statements to the effect that the second law of thermodynamics "can be formulated as a dynamical principle in terms of the existence of a Lyapunov variable,[1]" should be taken *cum grano salis*, for they are either unnecessarily strong, if by Lyapunov variable is meant an L function,[1] or too weak, if by Lyapunov function is meant an S function.

Section II presents the general context of the problem. Section III presents its application to quantum thermodynamics.

II. L FUNCTIONS AND S FUNCTIONS

Definition 1: A *dynamical system*[2] on a metric space $(\mathscr{X}, d)$ is a mapping $u: \mathbb{R}^+ \times \mathscr{X} \to \mathscr{X}$ such that

(1.1) $u(\cdot, x)$: $\mathbb{R}^+ \to \mathscr{X}$ is continuous;
(1.2) $u(t, \cdot)$: $\mathscr{X} \to \mathscr{X}$ is continuous;
(1.3) $u(0, x) = x$;
(1.4) $u(t + s, x) = u(t, u(s, x))$;

for all t, s in $\mathbb{R}^+$, and x in $\mathscr{X}$.

The mapping $u(\cdot, x)$ is called the *motion* passing through x at time $t = 0$. The set $\mathscr{X}$ is also called the *state space*, and $u(t,x)$ is the *state* at time t for a motion passing through state x at time 0. A part of a motion $u(\cdot, x)$ over an interval $[t_1, t_2]$ in $\mathbb{R}^+$, $t_2 > t_1$, with $u(t_1, x) = x_1$ and $u(t_2, x) = x_2$, is called a *process from* state x_1 *to* state x_2.[5] The metric d: $\mathscr{X} \times \mathscr{X} \to \mathbb{R}$ is such that $d(x,y) = 0$ if and only if $x = y$, $d(x,y) = d(y,x) \geq 0$, and $d(x,y) + d(y,z) \geq d(x,z)$ for all x, y, z in $\mathscr{X}$.

The dynamical system is determined by a one-parameter *semigroup* $\Lambda(t)$: $\mathscr{X} \to \mathscr{X}$ such that $\Lambda(t)x = u(t, x)$ for all t in $\mathbb{R}^+$ and x in $\mathscr{X}$, and that the inverse $\Lambda(t)^{-1}$ does not necessarily exist, so that the semigroup may not be extendable to a group with $\Lambda(-t) = \Lambda(t)^{-1}$.

Definition 2: A state x_e is an *equilibrium state* if and only if $u(t, x_e) = x_e$ for all t in $\mathbb{R}^+$.

Next, we recall the definitions of stability and instability according to Lyapunov. We will use the term local stability instead of Lyapunov stability to leave room for nonlocal stability concepts, such as that of metastability.[6]

Definition 3: An equilibrium state x_e is *locally stable* if and only if for each $\epsilon > 0$ there is a $\delta(\epsilon) > 0$ such that $d(x, x_e) < \delta(\epsilon)$ implies $d(u(t, x), x_e) < \epsilon$ for all $t > 0$ and every x in $\mathscr{X}$.

Definition 4: An equilibrium state x_e is *unstable* if and only if it is not locally stable, i.e., there is an $\epsilon > 0$ such that for every $\delta > 0$ there is a $t > 0$ and an x in $\mathscr{X}$ with $d(x, x_e) < \delta$ such that $d(u(t, x), x_e) \geq \epsilon$.

For any $r > 0$, $\mathscr{B}_r(x_e)$ will denote any open neighborhood of x_e containing the open ball with radius r and center x_e, i.e., all the states x such that $d(x, x_e) < r$.

Definition 5: A function $L(\cdot)$: $\mathscr{X} \to \mathbb{R}$ is an *L function* on an open neighborhood $\mathscr{B}_r(x_e)$ of an equilibrium state x_e if and only if the following conditions hold.

(5.1) $L(x) - L(x_e) \geq a(d(x, x_e))$ for every x in $\mathscr{B}_r(x_e)$ and some function $a(\cdot)$: $\mathbb{R} \to \mathbb{R}$ such that $a(0) = 0$, $\epsilon > 0$ implies $a(\epsilon) > 0$, and $a(r) < a(s)$ implies $r < s$.

(5.2) $L(u(t, x)) \leq L(x)$ for all $t > 0$ and every x in $\mathscr{B}_r(x_e)$.

(5.3) $L(\cdot)$: $\mathscr{X} \to \mathbb{R}$ is continuous at x_e, i.e., for each $\zeta > 0$ there is a $\delta'(\zeta) > 0$ such that $|L(x) - L(x_e)| < \zeta$ for every x in $\mathscr{X}$ with $d(x, x_e) < \delta'(\zeta)$.

L functions are the special class of Lyapunov functions[3] considered in the hypothesis of the classical Lyapunov stability theorem.[4]

Theorem 1. Lyapunov Stability Theorem: If $L(\cdot)$: $\mathscr{X} \to \mathbb{R}$ is an L function on an open neighborhood $\mathscr{B}_r(x_e)$ of an equilibrium state x_e, then x_e is a locally stable equilibrium state.

Proof: For each $\epsilon > 0$ (we may suppose $\epsilon < r$ with no loss of generality), let $\zeta(\epsilon) = a(\epsilon) > 0$, where $a(\cdot)$ is the function in

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condition (5.1). By conditions (5.3) and (5.1), there is a $\delta(\epsilon)=\delta'(\zeta(\epsilon))>0$ such that $L(x)-L(x_e)<a(\epsilon)$ for every x with $d(x,x_e)<\delta(\epsilon)$. By conditions (5.1) and (5.2),

$$a(d(u(t,x),x_e))\leqslant L(u(x,t))-L(x_e)\leqslant L(x)-L(x_e)<a(\epsilon), \tag{1}$$

for every $t>0$ and, hence, $d(u(t,x),x_e)<\epsilon$, i.e., x_e satisfies Definition 3. Thus, Theorem 1 is proved.

Definition 6: A single-valued function $E(\cdot)$: $\mathscr{X}\to\mathbb{R}^k$ is an *invariant* if and only if $E(u(t,x))=E(x)$ for all t in $\mathbb{R}^+$ and every x in $\mathscr{X}$.

Definition 7: A subset $\mathscr{C}(E)$ of $\mathscr{X}$ is a *constant-E subset* if and only if $E(x)=E$ for all x in $\mathscr{C}(E)$ and $E(\cdot)$ is an invariant.

Clearly, $\mathscr{C}(E)$ coincides with $\mathscr{X}$ if $E(\cdot)$ is a trivial invariant, e.g., the constant functions $E(\cdot)=E$. If $E(\cdot)$ is a nontrivial invariant with a range R_E in $\mathbb{R}^k$, then each x in $\mathscr{X}$ belongs to one and only one constant-E subset $\mathscr{C}(E(x))$ and every motion $u(\cdot,x)$ lies entirely in $\mathscr{C}(E(x))$, i.e., $u(t,x)$ is in $\mathscr{C}(E(x))$ for all t in $\mathbb{R}^+$.

Definition 8: An equilibrium state x_e is *conditionally locally stable* with respect to an invariant $E(\cdot)$ if and only if for each $\eta>0$ there is a $\delta(\eta)>0$ such that $d(x,x_e)<\delta(\eta)$ implies $d(u(t,x),x_e)<\eta$ for all $t>0$ and every x in $\mathscr{C}(E(x_e))$.

A conditionally locally stable equilibrium state x_e [with respect to a nontrivial invariant $E(\cdot)$] is not necessarily also locally stable because stability with respect to "perturbations" that bring the state off the constant-E subset $\mathscr{C}(E(x_e))$ is not guaranteed by Definition 8.

For any $r>0$, $\mathscr{D}_r(x_e)$ will denote any constant-E neighborhood of x_e containing the open disk in $\mathscr{C}(E(x_e))$ with radius r and center x_e, i.e., all the states x such that $d(x,x_e)<r$ and $E(x)=E(x_e)$.

Definition 9: A function $S(\cdot)$: $\mathscr{C}(E(x_e))\to\mathbb{R}$ is an *S function* on a constant-E neighborhood $\mathscr{D}_r(x_e)$ of an equilibrium state x_e if and only if the following conditions hold.

(9.1) $S(x_e)-S(x)\geqslant a(d(x,x_e))$ for every x in $\mathscr{D}_r(x_e)$ and some function $a(\cdot)$: $\mathbb{R}\to\mathbb{R}$ such that $a(0)=0$, $\epsilon>0$ implies $a(\epsilon)>0$, and $a(r)<a(s)$ implies $r<s$.

(9.2) $S(u(t,x))\geqslant S(x)$ for all $t>0$ and every x in $\mathscr{D}_r(x_e)$.

(9.3) $S(\cdot)$: $\mathscr{C}(E(x_e))\to\mathbb{R}$ is continuous at x_e, i.e., for each $\zeta>0$ there is a $\delta'(\zeta)>0$ such that $|S(x_e)-S(x)|<\zeta$ for every x in $\mathscr{C}(E(x_e))$ with $d(x,x_e)<\delta'(\zeta)$.

S functions acquire importance in view of the following conditional stability theorem.

Theorem 2. Lyapunov Conditional Stability Theorem: If $S(\cdot)$: $\mathscr{C}(E(x_e))\to\mathbb{R}$ is an S function on a constant-E neighborhood $\mathscr{D}_r(x_e)$ of an equilibrium state x_e, then x_e is conditionally locally stable with respect to the invariant $E(\cdot)$.

The proof of this theorem is completely analogous to that of Theorem 1 and will not be repeated.

Clearly, if $L(\cdot)$ is an L function then $S(\cdot)=-L(\cdot)$ is an S function. However, the converse is not true necessarily, i.e., if $S(\cdot)$ is an S function, $L(\cdot)=-S(\cdot)$ is not necessarily an L function. For example, condition (9.1) holds only on a constant-E neighborhood of x_e, whereas condition (5.1) is required to hold on an unconstrained neighborhood of x_e.

For applications such as thermodynamics (see Sec. III), it may be easier to construct S functions than L functions. The following theorem gives a sufficient condition under which stability can be proved even if no L function can be found. The condition requires the existence of a continuous family of conditionally stable equilibrium states in the neighborhood of x_e.

Theorem 3: Given an equilibrium state x_e, if there exist an invariant $E(\cdot)$: $\mathscr{X}\to R_E$ and a single-valued family of equilibrium states $x_e(\cdot)$: $R_E\to\mathscr{X}$ such that the following conditions hold, then x_e is a stable equilibrium state.

(3.1) $E(\cdot)$ is continuous at x_e, and $E(x_e)=E_e$.

(3.2) $x_e(\cdot)$ is continuous at E_e, and $x_e(E_e)=x_e$.

(3.3) For some $\xi>0$, every $x_e(E)$ with $d(x_e(E),x_e)<\xi$ is conditionally locally stable with respect to the invariant $E(\cdot)$.

(3.3)′ For some $\xi>0$, there is an S function on a constant-E neighborhood of each equilibrium state $x_e(E)$ with $d(x_e(E),x_e)<\xi$.

By virtue of Theorem 2, conditions (3.3) and (3.3)′ are equivalent.

Proof: We must show that for each $\epsilon>0$ there is a $\delta(\epsilon)>0$ such that $d(x,x_e)<\delta(\epsilon)$ implies $d(u(t,x),x_e)<\epsilon$ for all $t>0$. Let $\epsilon>0$ be given. With no loss of generality, we may suppose $\epsilon<\xi$.

For each E such that $d(x_e(E),x_e)<\epsilon/2$, we define

$$\eta(\epsilon,E)=\inf\{d(x,x_e(E))\,|\,E(x)=E,\ d(x,x_e)\geqslant\epsilon\} \tag{2}$$

so that $E(x)=E$ and $d(x,x_e(E))<\eta(\epsilon,E)$, i.e., $d(x,x_e(E(x)))<\eta(\epsilon,E(x))$, implies $d(x,x_e)<\epsilon$, because $d(x,x_e)\geqslant\epsilon$ would imply $d(x,x_e(E))\geqslant\eta(\epsilon,E)$. Moreover, $\eta(\epsilon,E)>0$ because the triangular inequality $d(x,x_e(E))+d(x_e(E),x_e)\geqslant d(x,x_e)$, for each x with $E(x)=E$ and $d(x,x_e)\geqslant\epsilon$, implies $d(x,x_e(E))\geqslant\epsilon-\epsilon/2=\epsilon/2$, but $\eta(\epsilon,E)$ is the greatest lower bound of $d(x,x_e(E))$ and, therefore, $\eta(\epsilon,E)\geqslant\epsilon/2>0$.

Because $x_e(E)$ is conditionally stable (Condition 3.3), there is a $\delta(\eta(\epsilon,E))>0$ such that $E(x)=E$ and $d(x,x_e(E))<\delta(\eta(\epsilon,E))$ imply $d(u(t,x),x_e(E))<\eta(\epsilon,E)$ for all $t>0$ (Definition 8). We denote by $\delta(\epsilon,E)$ the lowest upper bound of all the δ's that satisfy Definition 8 for a given $\eta(\epsilon,E)$, i.e., $\delta(\epsilon,E)=\inf\{\delta(\eta(\epsilon,E))\}$, and we define

$$\gamma'(\epsilon)=\inf\{\delta(\epsilon,E)\,|\,E \text{ such that } d(x_e(E),x_e)<\epsilon/2\}, \tag{3}$$

so that $\delta(\epsilon,E)\geqslant\gamma'(\epsilon)\geqslant\delta(\eta(\epsilon,E))>0$ because $\gamma'(\epsilon)$ is the greatest lower bound of $\delta(\epsilon,E)$.

We now let $\gamma(\epsilon)=\min\{\epsilon,\gamma'(\epsilon)\}$ and define

$$\delta'(\epsilon)=\inf\{d(x,x_e)\,|\,d(x,x_e(E(x)))\geqslant\gamma(\epsilon),\ d(x_e(E(x)),x_e)<\gamma(\epsilon)/2\}, \tag{4}$$

so that $d(x,x_e)<\delta'(\epsilon)$ and $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2$ imply $d(x,x_e(E(x)))<\gamma(\epsilon)$ because $d(x,x_e(E(x)))\geqslant\gamma(\epsilon)$ would imply $d(x,x_e)\geqslant\delta'(\epsilon)$. Moreover, $\delta'(\epsilon)>0$ because the triangular inequality $d(x,x_e)+d(x_e(E(x)),x_e)\geqslant d(x,x_e(E(x)))$, for each x with $d(x,x_e(E(x)))\geqslant\gamma(\epsilon)$ and $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2$, implies $d(x,x_e)\geqslant\gamma(\epsilon)-\gamma(\epsilon)/2=\gamma(\epsilon)$, but $\delta'(\epsilon)$ is the greatest lower bound of $d(x,x_e)$ and, therefore, $\delta'(\epsilon)\geqslant\gamma(\epsilon)/2>0$.

Because of conditions (3.1) and (3.2), $x_e(E(\cdot))$ is continuous at x_e and, therefore, there is a $\delta''(\epsilon)>0$ such that $d(x,x_e)<\delta''(\epsilon)$ implies $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2$. If we now let $\delta(\epsilon)=\min\{\delta''(\epsilon),\delta'(\epsilon)\}$, then $d(x,x_e)<\delta(\epsilon)$ implies $d(x_e(E(x)),x_e)<\gamma(\epsilon)/2\leqslant\epsilon/2$ and $d(x,x_e(E(x)))<\gamma(\epsilon)\leqslant\gamma'(\epsilon)\leqslant\delta(\epsilon,E(x))$. Therefore, $d(u(t,x),x_e(E(x)))<\eta(\epsilon,E(x))$ and $d(u(t,x),x_e)<\epsilon$. Thus, Theorem 3 is proved.

III. APPLICATION TO QUANTUM THERMODYNAMICS

Within quantum theory, Theorem 3 is immediately applicable to study the stability of equilibria of (possibly nonlinear) generalized evolution equations for irreversible dynamics.

Let us consider an isolated physical system with associated Hilbert space $\mathscr{H}$ ($\dim \mathscr{H} \leqslant \infty$), and Hamiltonian operator H (possibly unbounded). For simplicity, let the number operators N_i for each type i of elementary constituent be c-number operators, i.e., $N_i = \mathrm{N}_i I$. If H is unbounded, we further assume that $\mathrm{Tr}\exp(-\beta H) < \infty$ for all β with $0 < \beta < \infty$,[7] and that the energy functional

$$E(\rho) = \mathrm{Tr}\, H\rho \tag{5}$$

is continuous[7] on the set of self-adjoint, non-negative-definite, unit-trace operators on $\mathscr{H}$ with respect to the metric $d(\rho_1,\rho_2) = \mathrm{Tr}|\rho_1 - \rho_2|$.

We then define the *state space* $\mathscr{S}_c$ to be the set of all self-adjoint, non-negative-definite, unit-trace operators ρ on $\mathscr{H}$ with energy $\mathrm{Tr}\, H\rho \leqslant c$, with c a given finite constant, i.e.,

$$\mathscr{S}_c = \{\, \rho \text{ on } \mathscr{H} | \rho^\dagger = \rho,\ \rho \geqslant 0,\ \mathrm{Tr}\,\rho = 1,\ \mathrm{Tr}\, H\rho \leqslant c < \infty \,\}. \tag{6}$$

Operators ρ are called *state operators* for, within quantum thermodynamics, they represent the states of the physical system.

The entropy functional

$$s(\rho) = -k\,\mathrm{Tr}\,\rho\ln\rho \tag{7}$$

is concave[8] and continuous[9] on $\mathscr{S}_c$. Moreover, for a given value E in the range R_E, i.e., for

$$\inf\{E(\rho) | \rho \text{ in } \mathscr{S}_c\} < E < \sup\{E(\rho) | \rho \text{ in } \mathscr{S}_c\} \tag{8}$$

the entropy functional $s(\rho)$ has a unique maximum on the set

$$\mathscr{C}(E) = \{\rho \text{ in } \mathscr{S}_c | E(\rho) = E\} \tag{9}$$

at the state

$$\rho_0(E) = \exp(-\beta(E)H)/\mathrm{Tr}\exp(-\beta(E)H), \tag{10}$$

where $\beta(E)$ is one-to-one and continuous in the specified range for E (see Refs. 10 and 11). Namely $s(\rho_0(E)) > s(\rho)$ for every $\rho \neq \rho_0(E)$ in $\mathscr{C}(E)$. Thus, the family of states $\rho_0(E)$ is single valued and continuous in E.

Now, let us assume that the causal evolution of state operators forms a *dynamical system* on $(\mathscr{S}_c, d)$ such that the energy functional is a nontrivial invariant and the entropy functional is nondecreasing, i.e., for every ρ in $\mathscr{S}_c$ the motion $u(\cdot,\rho)$ is such that

$$E(u(t,\rho)) = E(\rho), \tag{11}$$

$$s(u(t,\rho)) \geqslant s(\rho), \tag{12}$$

for all $t \geqslant 0$.

Consider a state $\rho_0(E)$ [Eq. (10)]. Because $E(\rho)$ is an invariant, $u(t,\rho_0(E))$ is in $\mathscr{C}(E)$ for every $t \geqslant 0$. Because $s(\rho)$ is nondecreasing, $s(u(t,\rho_0(E))) \geqslant s(\rho_0(E))$ for every $t \geqslant 0$. But $s(\rho) < s(\rho_0(E))$ for every $\rho \neq \rho_0(E)$ in $\mathscr{C}(E)$. Therefore, $u(t,\rho_0(E)) = \rho_0(E)$, i.e., each $\rho_0(E)$ is an equilibrium state (Definition 2). We conclude that conditions (3.1), (3.2), and (3.3) of Theorem 3 are satisfied for each equilibrium state $\rho_0(E)$. If each such equilibrium state were shown to be conditionally locally stable then it would also be locally stable by virtue of Theorem 3.

It is noteworthy that, because in any neighborhood of every equilibrium state $\rho_0(E)$ [excluding the state with $E = c$ and the state with $\beta(E) = 0$, if H is bounded] there is another state $\rho_0(E')$ such that $s(\rho_0(E')) > s(\rho_0(E))$, the functions $L_1(\cdot) = -s(\cdot)$ and $L_2(\cdot) = s(\rho_0(E(\cdot))) - s(\cdot)$ are not L functions on any neighborhood of any stable equilibrium state in $\mathscr{S}_c$ with entropy less than the absolute maximum on $\mathscr{S}_c$. Indeed, we could have $L_1(\rho_0(E')) - L_1(\rho_0(E)) < 0$ and $L_2(\rho_0(E')) - L_2(\rho_0(E)) = 0$ even though $d(\rho_0(E'),\rho_0(E)) > 0$ and, therefore, neither $L_1(\cdot)$ nor $L_2(\cdot)$ could satisfy condition (5.1).

The physical importance of showing that the maximum entropy equilibrium states are locally stable emerges from the second law of thermodynamics which requires them to be the only (locally) stable equilibrium states.[12] For the dynamical system to be consistent with the second law of thermodynamics, it must necessarily imply that the maximum entropy equilibrium states are locally stable, and that any other equilibrium state is unstable.

For example, a unitary (Hamiltonian) dynamical system with $u(t,\rho) = U(t)\rho U(t)^{-1}$, $U(t) = \exp(-iH/\hbar)$, would satisfy conditions (11) and (12) with $s(u(t,\rho)) = s(\rho)$. However, it would imply the existence of other stable equilibrium states in addition to those with maximum entropy for a given energy E. Indeed, every equilibrium state ρ_e of such a dynamical system, i.e., every state operator with $\rho_e H = H\rho_e$, would be locally stable because $d(u(t,\rho),\rho_e) = d(\rho,\rho_e)$ for all t and every ρ, i.e., each motion would remain at a fixed distance from every equilibrium state,[13] and, therefore, Definition 3 would be satisfied for each $\epsilon > 0$ with $\delta(\epsilon) = \epsilon$. Thus, a unitary (Hamiltonian) dynamical system would not be consistent with the second law of thermodynamics.

In general, the existence of *dissipative* motions, i.e., motions with $s(u(t,\rho)) > s(\rho)$ for some $t > 0$, reduces both the number of equilibrium states and the number of equilibrium states that are stable. For example, the dynamical system generated by the nonlinear evolution equation recently proposed by the author in the framework of quantum thermodynamics[14,15] not only satisfies conditions (11) and (12), but seems also to contain enough dissipative motions to imply that only the maximum entropy equilibrium states are locally stable, whereas the many other equilibrium states are all unstable, which is consistent with the second law of thermodynamics.

This paper addresses only the question of whether the principle of nondecrease of entropy [condition (12)], together with the properties of the entropy functional [Eq. (7)] and the specific structure of the maximum entropy states [Eq. (10)], is sufficient to imply the local stability of the maximum entropy thermodynamic equilibrium states. In view of Theorem 3, we concluded that it would suffice to show that the entropy functional is an S function and, specifically, that it satisfies condition (9.1) for each equilibrium state $\rho_0(E)$.

In some thermodynamic literature, it is usually stated that entropy provides a Lyapunov criterion for the stability of the thermodynamic equilibrium states.[1,16] However, a rig-

orous justification of these assertions is found nowhere in the literature.

The question would be resolved if we could prove that the functional $s(\rho_0(E)) - s(\rho)$, when restricted to the constant-E subset containing $\rho_0(E)$, is positive definite in the sense made precise by the conjecture below. If the conjecture could be proved, then condition (9.1) would be satisfied, entropy would be an S function in the neighborhood of each maximum entropy equilibrium state, and Theorem 3 would guarantee the local stability of such states. Only then, and in the strict sense specified here, would it be correct to aver that entropy provides a Lyapunov criterion for the stability of thermodynamic equilibrium.

Conjecture: Given a state operator of the form

$$\rho_0 = \frac{\exp(-\Sigma_j \lambda_j R_j)}{\mathrm{Tr}\exp(-\Sigma_i \lambda_i R_i)}, \tag{13}$$

such that $\mathrm{Tr}\exp(-\Sigma_j \lambda_j R_j) < \infty$, there is a function $a(\cdot)$: $\mathbf{R} \to \mathbf{R}$ such that $a(0) = 0$, $\epsilon > 0$ implies $a(\epsilon) > 0$, $a(r) < a(s)$ implies $r < s$, and

$$\mathrm{Tr}\,\rho \ln \rho - \mathrm{Tr}\,\rho_0 \ln \rho_0 \geqslant a(\mathrm{Tr}|\rho - \rho_0|), \tag{14}$$

for every state operator ρ such that $\mathrm{Tr}\,R_j\rho = \mathrm{Tr}\,R_j\rho_0$ for every j, and $\mathrm{Tr}\,|\rho - \rho_0| < \xi$ for some $\xi > 0$.

We have no proof of this conjecture. But its validity seems to be plausible in view of the following facts: (1) state operator ρ_0 is the unique state maximizing $-\mathrm{Tr}\,\rho \ln \rho$ over the set of states with $\mathrm{Tr}\,R_j\rho = \mathrm{Tr}\,R_j\rho_0$; (2) $-\mathrm{Tr}\,\rho \ln \rho$ is continuous in ρ_0 (see Ref. 9); (3) $-\mathrm{Tr}\,\rho \ln \rho$ is strictly concave (see Ref. 8); and (4) state operator ρ_0 is strictly positive. Heuristically, there should be a way to expand the functional $-\mathrm{Tr}\,\rho \ln \rho$ (restricted over the set with $\mathrm{Tr}\,R_j\rho = \mathrm{Tr}\,R_j\rho_0$) in a Taylor series about ρ_0 to find

$$-\mathrm{Tr}\,\rho \ln \rho = -\mathrm{Tr}\,\rho_0 \ln \rho_0 + D_1\,\mathrm{Tr}(\rho - \rho_0) + D_2\,\mathrm{Tr}(\rho - \rho_0)^2 + \cdots . \tag{15}$$

Then, D_1 should equal zero because ρ_0 maximizes $-\mathrm{Tr}\,\rho \ln \rho$ over the restricted set, and D_2 should be defined and strictly negative because ρ_0 is strictly positive and $-\mathrm{Tr}\,\rho \ln \rho$ is strictly concave. A proof on these lines, however, would involve several technical problems of the kind discussed in Ref. 8, such as the essential singularity of function $-y \ln y$ at $y = 0$, the delicate question of continuity of $-\mathrm{Tr}\,\rho \ln \rho$, the question of differentiability of $-\mathrm{Tr}\,\rho \ln \rho$, and so on.

We hope that the arguments just outlined in support of the conjecture will provide sufficient motivation for a rigorous technical study that would settle an important open question in the field of thermodynamics.

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[2] See, e.g., J. A. Walker, *Dynamical Systems and Evolution Equations* (Plenum, New York, 1980), p. 86, and references therein.

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[5] A given process from state x_1 to state x_2 is *reversible* if and only if in the dynamical system there is a process from x_2 to x_1, i.e., the dynamical system contains a "restoring" motion $u(\cdot, x_r)$ such that $u(t', x_r) = x_2$ and $u(t'', x_r) = x_1$ with $t'' > t'$. Otherwise, the process from x_1 to x_2 is *irreversible*. It is noteworthy that if a motion $u(\cdot, x)$ gives rise to a reversible process then the motion is periodic, i.e., there is a $t > 0$ such that $u(t, x) = x$. Clearly, should there be a function $S(\cdot)$: $\mathscr{X} \to \mathbf{R}$ such that $S(u(t, x)) \geqslant S(x)$ for all x in $\mathscr{X}$ and t in $\mathbf{R}^+$, then any process from x_1 to x_2 with $S(x_2) > S(x_1)$ would be irreversible.

[6] We have not found clear definitions of the concepts of metastability and global stability of the equilibrium states of a dynamical system anywhere in the literature. These definitions would be of much importance in the thermodynamics framework described in Sec. III, however, they are not needed in this paper.

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Dynamics of para-Bose coherent states

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The most general form of the Hamiltonian is obtained under the restriction that initially coherent states of a multimode para-Bose system remain coherent at all times. The equation of motion for the square of the annihilation operator for the multimode system using this Hamiltonian is solved.

I. INTRODUCTION

The coherent state for bosons and the one-mode para-Bose system[1] is defined as an eigenstate of annihilation operator, i.e.,

$$a_i|z_1,z_2,...,z_i,...\rangle = z_i|z_1,z_2,...,z_i,...\rangle \tag{1.1a}$$

(for bosons), and

$$a|z,L\rangle = z|z,L\rangle \tag{1.1b}$$

(for the one-mode para-Bose system).

Here L is an integer and known as the order of parastatistics.[2] For bosons $L=1$, and for parabosons $L>1$. For the multimode para-Bose system the coherent state cannot be defined as the eigenstate of annihilation operator because

$$[a_i,a_j] \neq 0. \tag{1.2}$$

But the squares of annihilation operators and ladder operators $J_{jk}=\frac{1}{2}[a_k,a_j]$ commute among themselves for multimode para-Bose system ($J_{jk}=0$ for bosons). Therefore a multimode para-Bose coherent state[3] $|\psi\rangle \equiv |z_1,z_2,...,z_i,...,z_{12},z_{13},...,z_{jk},...,L\rangle$ is defined as the simultaneous eigenstate of a_i^2 ($i=1,2,...$) and J_{jk} ($j,k=1,2,...$), i.e.,

$$a_i^2|\psi\rangle = z_i^2|\psi\rangle, \tag{1.3a}$$

$$J_{jk}|\psi\rangle = z_{jk}|\psi\rangle. \tag{1.3b}$$

The dynamics of the states $|\psi\rangle$ will be discussed in this paper. It may be recalled that for coherent states, Glauber[4] has shown that if the time derivative of the annihilation operator does not involve functional dependence on the creation operator, i.e.,

$$\frac{da_k(t)}{dt} = f_k(a_j(t),t), \tag{1.4}$$

then the states which are initially coherent remain coherent for all times. Similarly for multimode para-Bose coherent states to remain coherent for all times the following conditions should be satisfied:

$$\frac{da_k^2(t)}{dt} = f_k(a_j(t),t), \tag{1.5}$$

and

$$\frac{dJ_{jk}(t)}{dt} = f_{jk}(J_{lm}(t),t). \tag{1.6}$$

In Sec. II, time evolution of multimode para-Bose coherent states will be discussed and a general form of the Hamiltonian consistent with the conditions (1.5) and (1.6) will be obtained.

II. TIME EVOLUTION OF PARA-BOSE COHERENT STATES

The time evolution can be worked out in either the Heisenberg or Schrödinger representation.

Heisenberg representation: The Heisenberg equation of motion for a_i^2 ($i=1,2,...$) is defined as

$$\eta \frac{da_i^2(t)}{dt} = [a_i^2(t),H(t)] \quad (\eta=\sqrt{-1}). \tag{2.1}$$

Here H is the Hamiltonian of the para-Bose system. For infinitesimal δt we obtain from Eq. (2.1)

$$a_i^2(t+\delta t) - a_i^2(t) = -\eta \delta t\,[a_i^2(t),\ H(t)]. \tag{2.2}$$

For $|\psi\rangle$ to remain an eigenstate of $a_i^2(t+\delta t)$ with eigenvalue $z_i^2(t+\delta t)$ at instant $t+\delta t$, we have

$$a_i^2(t+\delta t)|\psi\rangle = \left(z_i^2(t) + \delta t \frac{\partial z_i^2(t)}{\partial t}\right)|\psi\rangle. \tag{2.3}$$

From Eqs. (2.1)–(2.3) we readily obtain

$$[a_i^2(t),\ H(t)]|\psi\rangle = \eta \frac{\partial z_i^2(t)}{\delta t}|\psi\rangle, \tag{2.4}$$

and it follows that $|\psi\rangle$ is also an eigenstate of the operator $[a_i^2(t),\ H(t)]$ with eigenvalue $\eta\,\partial z_i^2(t)/\partial t$. Therefore $a_i^2(t)$ and $[a_i^2(t),\ H(t)]$ should commute, i.e.,

$$[a_i^2(t),[a_i^2(t),\ H(t)]] = 0. \tag{2.5}$$

From the Green's[2] trilinear commutation relations for parabosons of any order of statistics L, it readily follows that

$$[a_i^2(t),\ H(t)] = f(a_k(t),\ t). \tag{2.6}$$

The Eq. (2.6) is valid for all i's, therefore H can be at the most linear in creation operators. The general form of the Hamiltonian consistent with its Hermitian nature and Eq. (2.6) is

$$H = \sum_i \sum_j \frac{1}{2} w_{ij}\{a_i(t),a_j^+(t)\} + \sum_i (F_i(t)a_i^+(t) + F_i^*(t)a_i(t)) + \alpha(t). \tag{2.7}$$

Here $w_{ij}(t) = w_{ji}^*$, and $\alpha(t)$ has real values only. The Hamiltonian given by Eq. (2.7) is consistent with the condition (1.5), but it should simultaneously satisfy the condition (1.6). Proceeding similarly, from the Heisenberg equation of motion for the ladder operator J_{jk} we obtain a relation

$$[J_{jk},[J_{lm},H]] = 0. \tag{2.8}$$

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For this relation to be satisfied, the Hamiltonian can have only bilinear combinations of annihilation and creation operators. Thus for initially para-Bose coherent states to remain coherent for all times, the Hamiltonian for the system should be of the form

$$H=\sum_i\sum_j\frac{1}{2}w_{ij}\{a_i(t),a_j^+(t)\}. \tag{2.9}$$

For the one mode para-Bose coherent state as defined by Eq. (1.1b), it can be verified that the Hamiltonian should identically be of the form $H=\frac{1}{2}w\{a(t),a^+(t)\}$ for initially coherent states to remain coherent at all times.

We can arrive at the same conclusion by working in the Schrödinger representation.

Schrödinger representation: Here the operators are fixed and the state changes with time. The Schrödinger equation for the state $|\psi(t)\rangle$ is given by

$$\eta\frac{d}{dt}|\psi(t)\rangle=H|\psi(t)\rangle. \tag{2.10}$$

For $|\psi(t+\delta t)\rangle$ to remain an eigenstate of a_i^2 and J_{jk} at the instant $t+\delta t$, where δt is infinitesimal, we obtain, using Eq. (2.10),

$$|\psi(t+\delta t)\rangle=|\psi(t)\rangle-\eta\,\delta t\,H|\psi(t)\rangle. \tag{2.11}$$

We also have

$$a_i^2|\psi(t+\delta t)\rangle=\left(z_i^2(t)+\delta t\frac{\partial z_i^2(t)}{\partial t}\right)|\psi(t+\delta t)\rangle, \tag{2.12a}$$

$$J_{jk}|\psi(t+\delta t)\rangle=\left(z_{jk}(t)+\delta t\frac{\partial z_{jk}(t)}{\partial t}\right)|\psi(t+\delta t)\rangle. \tag{2.12b}$$

From Eqs. (2.11) and (2.12) it readily follows that

$$[a_i^2,H]|\psi(t)\rangle=\eta\frac{\partial z_i^2(t)}{\partial t}|\psi(t)\rangle, \tag{2.13a}$$

and

$$[J_{jk},H]|\psi(t)\rangle=\eta\frac{dz_{jk}(t)}{\partial t}|\psi(t)\rangle. \tag{2.13b}$$

From the similarity of these relations with those obtained in the Heisenberg picture, it readily follows that the general form of the Hamiltonian, consistent with the requirement that initially para-Bose coherent states remain coherent for all times, is given by

$$H=\sum_i\sum_j\frac{1}{2}w_{ij}(t)\{a_i,a_j^+\}. \tag{2.14}$$

The Hamiltonian H can also be expressed in terms of position (q_k) and momentum (p_k) operators using the relations

$$a_k=(2w_k)^{-1/2}(w_kq_k+\eta p_k), \tag{2.15a}$$

and

$$a_k^+=(2w_k)^{-1/2}(w_kq_k-\eta p_k). \tag{2.15b}$$

Here w_k is the frequency of the k th para-Bose oscillator and $\hbar=1$. The Hamiltonian contains terms bilinear in q_k and p_k.

III. EQUATION OF MOTION

The operator a_i^2 satisfies the following equation of motion with Hamiltonian H given by Eq. (2.9):

$$\frac{da_i^2}{dt}=-\eta[a_i^2,H]$$

$$=-\eta\sum_j\frac{1}{2}w_{ij}(a_ia_j+a_ja_i). \tag{3.1}$$

In matrix form Eq. (3.1) is written as

$$\frac{da^2}{dt}=-2\eta wa^2. \tag{3.2}$$

The solution of Eq. (3.2) is given by

$$a^2(t)=U(t)a^2(0). \tag{3.3}$$

Here $U(t)$ is a unitary matrix such that

$$U(t)=\left[\exp\left(-2\eta\int_0^t w(t')\,dt'\right)\right]_+, \tag{3.4}$$

with the subscript $+$ denoting the time ordering operator.[5] If $w(t)$ is such that

$$[w(t),\ w(t')]=0, \tag{3.5}$$

for all t and t', then Eq. (3.4) simplifies to

$$U(t)=\exp\left(-2\eta\int_0^t w(t')\,dt'\right). \tag{3.6}$$

For one-mode para-Bose coherent states we can arrive at the same solution by considering explicitly the time derivative of the annihilation operator with Hamiltonian $H=\frac{1}{2}w\{a,a^+\}$.

We conclude with the observation that the Hamiltonian for a para-Bose system, consistent with the requirement that initially coherent states remain coherent at all times, contains only bilinear combinations of a_i and a_j^+ $(i,j=1,2,...)$. The terms linear either in a_i or a_j^+ do not occur, unlike the case of coherent states for bosons.[6] This is because commutation relations $[a_i,\ a_i^+]$, etc. for para-Bose operators are not C numbers.

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Euclidean invariant integral representations for Schwinger functionals

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It is shown that if the Schwinger functions of a Wightman theory with a mass gap can be represented as moments of a complex measure, there is also such a representation by a measure that is invariant under the Euclidean group. A necessary and sufficient condition is also given for the exponential of a quadratic form on the test function space to be the characteristic functional of a complex measure.

I. INTRODUCTION

In Ref. 1 a necessary and sufficient condition was given for the Schwinger functions of a Wightman quantum field theory to admit an integral representation in terms of a complex measure on the space of tempered distributions. It remained an open problem whether the measure can always be chosen to be invariant under the Euclidean group in the same way as the Schwinger functions. While this is almost obvious in the case of a positive measure, the question is more delicate for signed or complex measures: For instance, the time-ordered functions of the free field can be represented by a signed measure, but no representing measure is invariant under the translation group.[2] In the present paper we come back to this question and give at least a partial answer to it: For a Wightman theory with a unique vacuum and a lower mass gap, no additional conditions besides those of Ref. 1 are needed to ensure the existence of an invariant representing measure for the Schwinger functions. For theories without a mass gap one can reasonably conjecture the answer to be the same; a proof by the method of the present paper, however, would require a sharpening of some results of Ref. 1.

We would now like to make a few comments on the reasons for considering signed or complex measures and not just positive measures. First, even if one were only interested in positive measures, it is useful to know precisely when at least a representation with a signed measure exists. Secondly, although the measures appearing in the two- and three-dimensional models constructed rigorously so far are positive, this seems rather to be a lucky coincidence than a fundamental property of Wightman fields. In fact, these models can be obtained as limits of cutoff models which are perturbations of the free field. It so happens that the free field can be represented by a positive measure, and this holds also for the cutoff interacting theories, because the Euclidean Lagrangians considered are formally real. On the other hand, it is not even clear that the Schwinger functions of the Wick powers of the free field in dimensions $\geqslant 4$ are moments of a positive measure. Also, there might well exist scalar Wightman fields whose Schwinger functions are not real and can thus at best be represented by complex measures. Thirdly, in gauge theories there occur many formal expressions which have the appearance of complex measures (cf. Ref. 3, p. 110). It is unlikely that these expressions can be used to define σ-additive, finite, complex measures, but one might in some cases be able to find such measures having the same moments, which are after all the main objects of interest. Fourthly, there has recently been an attempt to use complex measures in constructive field theory.[4] It was shown in Theorem 2.1 in Ref. 4 that the Schwinger functions of $:\exp \Phi_0:$, where Φ_0 is a free field, are the moments of an invariant, complex measure on the space of Jaffe distributions. The arguments in Ref. 4 are in fact more general and cover a whole class of theories having a certain continuity property (Theorem 5.1 in Ref. 4). Theorem 3.2 of the present paper can easily be extended to other test function spaces than $\mathcal{S}$ and would then imply Theorem 2.1 in Ref. 4.

In this paper "measure" always means a σ-additive, finite, complex Borel measure on the space $\mathcal{S}'_R$ of real, tempered distributions on $\mathbf{R}^d$. The reason for considering only finite measures is that we would like a formula like $\int d\mu(\omega) = 1$ to hold in the sense of standard integration theory. It is, however, quite possible that in some cases when a finite representing measure exists, another kind of representation, similar to the Feynman path integrals with a real time coordinate (cf., e.g., Ref. 5), might turn out to be more convenient. A complex measure may for instance have moments with a Gaussian structure, although no finite measure with these moments has a Gaussian characteristic functional. In fact, as we show in Sec. IV such moments define a Gaussian complex measure iff the real part of the two-point function is positive (semi-) definite and the imaginary part is given by a Hilbert–Schmidt operator in the corresponding Hilbert space.

Since Euclidean invariance of the measure is not an additional restriction on the Schwinger functions, one might ask what the Osterwalder–Schrader (OS) positivity of the Schwinger functions implies for the measure. This point has already been discussed in Ref. 6; the result was that if the measure is invariant under time translations and satisfies an extended form of the OS positivity, then the measure is necessarily positive. The proof is rather simple, but it uses standard integration theory and might therefore be invalid in the case of more general integral representations.

The proof of the main result of this paper, Theorem 3.2, is based on an averaging procedure for a generating functional for the truncated Schwinger functions. For this procedure to work it is essential that the truncated Schwinger functions decrease sufficiently rapidly; hence it must fail for the time-ordered Wightman functions, as mentioned above. The general method is discussed in Sec. II, its application to

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the Schwinger functions in Sec. III. Finally, Sec. IV contains some remarks on characteristic functionals of complex measures.

II. A CONSTRUCTION OF INVARIANT MEASURES

As usual we denote Borchers's test function algebra by $\underline{\mathscr{S}}$; this is the tensor algebra over Schwartz's space $\mathscr{S} = \mathscr{S}(\mathbb{R}^d)$, completed in its natural topology. We write its elements as $\underline{f} = (f_0, \ldots, f_N, 0, \ldots)$ with $f_0 \in \mathbb{C}, f_n \in \mathscr{S}_n = \mathscr{S}(\mathbb{R}^{d \cdot n})$. The dual space $\underline{\mathscr{S}}'$ consists of sequences $T = (T_0, T_1, \ldots)$ with $T_0 \in \mathbb{C}$ and $T_n \in \mathscr{S}_n'$. A functional $T \in \underline{\mathscr{S}}'$ is called totally symmetric, if $T_n(f_1 \otimes \cdots \otimes f_n) = T_n(f_{\pi 1} \otimes \cdots \otimes f_{\pi n})$ for all permutations π of $\{1, \ldots, n\}$, all $f_1, \ldots, f_n \in \mathscr{S}$, and all n. The real part of $\mathscr{S}$ is denoted by $\mathscr{S}_R$ and the space of real, tempered distributions over $\mathbb{R}^d$ by $\mathscr{S}_R'$. If $\omega \in \mathscr{S}_R'$ we denote by χ_ω the corresponding Hermitian character in $\underline{\mathscr{S}}'$: $\chi_\omega = (1, \omega, \omega^{\otimes 2}, \ldots)$. By means of the characters χ_ω we can identify the symmetric tensor algebra over $\mathscr{S}$ with the algebra of all functions on $\mathscr{S}_R'$ of the form $\omega \mapsto \chi_\omega(\underline{f}), \underline{f} \in \underline{\mathscr{S}}$. We refer also to this algebra as the polynomials over $\mathscr{S}_R'$ and denote it by $\mathscr{P}$. Here $\mathscr{P}$ is a subalgebra of a larger algebra $\mathscr{F}$, consisting of all functions on $\mathscr{S}_R'$ of the form $\omega \mapsto g(\chi_\omega(\underline{f}_1), \ldots, \chi_\omega(\underline{f}_n))$, where g is continuous and polynomially bounded on $\mathbb{R}^N$ and $\underline{f}_1, \ldots, \underline{f}_N \in \underline{\mathscr{S}}$. The positive functionals on $\mathscr{F}$ are in 1–1 correspondence with positive Borel measures $d\nu$ on $\mathscr{S}_R'$ such that all functions in $\mathscr{P}$ are integrable and $\underline{f} \mapsto \int \chi_\omega(\underline{f}) d\nu(\omega)$ is continuous (cf. Theorem 2.7 and Lemma 2.5 in Ref. 1). Such measures will be referred to as *positive measures with continuous moments*.

A functional $T \in \underline{\mathscr{S}}'$ will be called *strongly positive* if it is positive (i.e., non-negative) on all $\underline{f} \in \underline{\mathscr{S}}$ such that $\omega \mapsto \chi_\omega(\underline{f})$ is a positive function; equivalently if it is totally symmetric and the corresponding functional on $\mathscr{P}$ is positive on positive polynomials. By using extension theorems of one sort or another one shows[7–9] the following.

Theorem 2.1: The following are equivalent for $T \in \underline{\mathscr{S}}'$.

(i) There is a positive measure $d\nu$ on $\mathscr{S}_R'$ with continuous moments such that

$$T(\underline{f}) = \int \chi_\omega(\underline{f}) d\nu(\omega),$$

for all $\underline{f} \in \underline{\mathscr{S}}'$.

(ii) T is strongly positive.

By Minlos's theorem the characteristic functionals $E(f) = \int \exp i\omega(f) d\nu(\omega)$ of positive meaasures $d\nu$ on $\mathscr{S}_R'$ are precisely those continuous functionals E on $\mathscr{S}_R$ which are *positive definite*, i.e., such that $\sum \bar{\lambda}_i E(f_i - f_j) \lambda_j \geq 0$ for all finite sequences of $f_i \in \mathscr{S}_R$ and $\lambda_i \in \mathbb{C}$. The measure is uniquely determined by E. The existence of the moments of $d\nu$ implies that $(\lambda_1, \ldots, \lambda_N) \mapsto E(\lambda_1 f_1 + \cdots + \lambda_N f_N)$ is a C^∞ function on $\mathbb{R}^N$ for all $f_1, \ldots, f_N \in \mathscr{S}_R$. Conversely, if E is the characteristic functional of a *positive* measure $d\nu$, and if $\lambda \mapsto E(\lambda f)$ is infinitely often differentiable at $\lambda = 0$ for all f, then all the moments of $d\nu$ exist (cf., e.g., Ref. 10, Theorem 2.1.1), and E is a generating functional for them:

$$\int d\nu(\omega) = E(0),$$

$$\int \omega(f_1) \cdots \omega(f_n) d\nu(\omega) = (-i)^n \frac{\partial^n}{\partial \lambda_1 \cdots \partial \lambda_n} E(\lambda_1 f_1 + \cdots + \lambda_n f_n)|_{\lambda_1 = \cdots = \lambda_n = 0}. \tag{2.1}$$

In view of Theorem 2.1 and Minlos's theorem we thus see that a functional $T \in \underline{\mathscr{S}}'$ is strongly positive iff it can be generated by a positive definite continuous functional on $\mathscr{S}_R$.

Let G be a group and $\tau \mapsto \alpha_\tau$ a representation of G by continuous linear transformations α_τ of $\mathscr{S}_R$. The dual transformations α_τ' map $\mathscr{S}_R' \to \mathscr{S}_R'$ and α_τ extends in a natural way to a * automorphism of $\underline{\mathscr{S}}$ and also of $\mathscr{P}$ and $\mathscr{F}$. We may thus speak of G-invariant functionals on $\mathscr{S}_R$, $\underline{\mathscr{S}}$, and $\mathscr{F}$ and also of G-invariant measures on $\mathscr{S}_R'$. A measure is invariant iff its characteristic functional is invariant iff the corresponding functional on $\mathscr{F}$ is invariant.

For integral representations with positive, invariant measures we have the following simple result (cf. Ref. 9, Theorem 3.8, and Ref. 2, Proposition 6.1).

Theorem 2.2: Suppose G is an amenable, topological group and $\tau \mapsto \alpha_\tau f$ is continuous, $G \to \mathscr{S}_R$, for all $f \in \mathscr{S}_R$. The following are equivalent for $T \in \underline{\mathscr{S}}'$.

(i) There is a G-invariant, positive measure $d\nu$ such that

$$T(\underline{f}) = \int \chi_\omega(\underline{f}) d\nu(\omega),$$

for all $\underline{f} \in \underline{\mathscr{S}}$.

(ii) T is G invariant and strongly positive.

Proof: The implication (i)$\Rightarrow$(ii) is clear. As already mentioned, the measures in question correspond uniquely to positive, invariant functionals on the function algebra $\mathscr{F}$. If T is a strongly positive functional on the algebra $\mathscr{P}$ of polynomials, then T has in any case a positive extension $\hat{T}$ to $\mathscr{F}$ by Theorem 2.1. Moreover, if T is G invariant, $\hat{T} \circ \alpha_\tau$ is also a positive extension of T for all τ. Since any function in $\mathscr{F}$ can be dominated by a function in $\mathscr{P}$, it follows that $\tau \to \hat{T} \circ \alpha_\tau(f)$ is a bounded function on G for all $f \in \mathscr{F}$. Applying an invariant mean thus leads to the desired positive and invariant extension of T.

We now turn the attention to signed or complex measures on $\mathscr{S}_R'$. We shall only consider such measures $d\mu$ with *continuous moments*; this means that all functions in $\mathscr{P}$ should be integrable with respect to the positive measure $d|\mu|$. An equivalent definition is that $d\mu = (d\mu_1 - d\mu_2) + i(d\mu_3 - d\mu_4)$, where the $d\mu_i$ are positive measures with continuous moments.

The basic result on the moment problem with complex measures is the following.

Theorem[1] 2.3: The following are equivalent for $T \in \underline{\mathscr{S}}'$.

(i) There is a complex measure $d\mu$ on $\mathscr{S}_R'$ with continuous moments such that

$$T(\underline{f}) = \int \chi_\omega(\underline{f}) d\mu(\omega),$$

for all $\underline{f} \in \underline{\mathscr{S}}$.

(ii) T is totally symmetric, and there are continuous se-

minorms $\|\cdot\|_k$, $k = 1, 2, \ldots$ on $\mathscr{S}$ such that

$$|T_n(f_1 \otimes \cdots \otimes f_n)| \leqslant \|f_1\|_1 \cdots \|f_n\|_n,$$

for all $f_1, \ldots, f_n \in \mathscr{S}$ and all n.

The characteristic functional of a finite complex measure $d\mu$ is defined in the same way as for positive measures, $E(f) = \int \exp i\omega(f) d\mu(\omega)$. If $d\mu$ is a measure with continuous moments, E is a generating functional for them, i.e., a formula like (2.1) holds. There does not seem to exist any simple description of those functionals on $\mathscr{S}_R$ which are characteristic functionals of finite, complex measures, except the obvious one: $E = (E_1 - E_2) + i(E_3 - E_4)$, where the E_i are characteristic functionals of positive measures, i.e., continuous and positive definite. We note in any case that E is necessarily a bounded function on $\mathscr{S}_R$. The characteristic functional determines the measure uniquely, and the same is true for the functional which a measure with continuous moments defines on $\mathscr{F}$. On the other hand, the measure is never uniquely determined by the moments, i.e., by the functional it defines on $\mathscr{P}$ (cf. Sec. IV). A moment problem with a positive measure need not have a unique solution either, but the positive extensions from $\mathscr{P}$ to $\mathscr{F}$ of a given functional on $\mathscr{P}$ form at least a bounded set in the dual space of $\mathscr{F}$, and this was the main point in the proof of Theorem 2.2. For complex measures this boundedness no longer holds, and the question of an invariant solution to the moment problem is therefore more difficult for complex measures than for positive measures.

We now come to the proper subject of this section, namely, to establish a sufficient condition for a functional on $\mathscr{S}$ to have a representation by an invariant, complex measure. We start by recalling the definition and some properties of the s product of functionals in $\mathscr{S}'$ (Ref. 11).

Suppose $T, S \in \mathscr{S}'$. Their s product is defined by

$$(T \mathbin{s} S)_0 = T_0 S_0,$$

$$(T \mathbin{s} S)_n (f_1 \otimes \cdots \otimes f_n)$$

$$= \sum T_k (f_{i_1} \otimes \cdots \otimes f_{i_k})\, T_l (f_{j_1} \otimes \cdots \otimes f_{j_l}),$$

where the sum ranges over all partitions of $\{1, \ldots, n\}$ into ordered subsets $(i_1, \ldots, j_k)$, $(j_1, \ldots, j_l)$ with $i_1 < \cdots < i_k$, $j_1 < \cdots j_l$, $k + l = n$. One has the following.

(i) The s product is commutative and associative and

$$T \mathbin{s} (S + R) = (T \mathbin{s} S) + (T \mathbin{s} R), \tag{2.2}$$

for all $T, R, S \in \mathscr{S}'$.

(ii) If $A(x) = \sum a_n x^n$ is a power series with radius of convergence a, then

$$A(T)_{|_s} := \sum_n a_n\, T \mathbin{s} \cdots \mathbin{s} T$$

converges in $\mathscr{S}'$ for all T with $|T_0| < a$.

In particular, $\exp_{|_s} T = \sum (1/n!) T^n_{|_s}$ is defined for all T, and

$$T^t := \log_{|_s} T$$

$$= \log T_0 + \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n \cdot T_0^n} (T - T_0)^n_{|_s}$$

is defined for all T with $T_0 \neq 0$. T^t is called the *truncated functional* of T; one has $T = \exp_{|_s} T^t$. If T is normalized so that $T_0 = 1$, one has the usual formula

$$T^t_0 = 0,$$

$$T_n(f_1 \otimes \cdots \otimes f_n)$$

$$= \sum_{\text{Part}} T^t_{n_1} (f_{i_{1,1}} \otimes \cdots \otimes f_{i_{1,n_1}}) \cdots T^t_{n_k} (f_{i_{k,1}} \otimes \cdots \otimes f_{i_{k,n_k}}), \tag{2.3}$$

where the sum ranges over all partitions of $\{1, \ldots, n\}$ into disjoint ordered subsets $(i_{1,1}, \ldots, i_{1,n_1}) \cdots (i_{k,1}, \ldots, i_{k,n_k})$ with $i_{l,1} < \cdots < i_{l,n_l}$, $n_1 + \cdots + n_k = n$.

The s product corresponds to the usual product for generating functionals: If E (resp. F) are generating functionals for totally symmetric functionals T (resp. $S) \in \mathscr{S}'$, then $f \to E(f) \cdot F(f)$ is a generating functional for $T \mathbin{s} S$. Also, if $A(x)$ is a power series, then $A(E(f))$ is a generating functional for $A(T)_{|_s}$.[12] In particular, if we can write $E(f) = \exp \Gamma(f)$, then Γ is a generating functional for T^t.

A functional Γ on $\mathscr{S}_R$ is called *conditionally positive definite* (cf. Ref. 13, Chap. III, Sec. 4.3) if $\sum \bar{\lambda}_i \Gamma(f_i - f_j) \times \lambda_j \geqslant 0$ for all finite sequences of $f_i \in \mathscr{S}_R$ and $\lambda_i \in \mathbb{C}$ with $\sum \lambda_i = 0$, and if Γ satisfies moreover the reality condition $\Gamma(-f) = \Gamma(f)^*$. A linear functional $T \in \mathscr{S}'$ will be called *conditionally strongly positive*, if it can be generated by a conditionally positive functional. (Included in this definition is in particular that T should be totally symmetric and Hermitian.) An equivalent definition is as follows: T is Hermitian, and positive on all positive polynomials without a constant term. We shall, however, not need this second form of the definition.

It is well known, that if Γ is conditionally positive definite, then $\exp \Gamma(f)$ is positive definite (Ref. 13, Theorem 4, Chap. III, Sec. 4.3). It follows that if T^t is conditionally strongly positive, then $T = \exp_{|_s} T^t$ is strongly positive (see also Ref. 14 for a variant of this result). We now want to prove the following.

Proposition 2.4: Suppose $T^t \in \mathscr{S}'$ is conditionally strongly positive and G invariant. Then there exists for any $\lambda \in \mathbb{C}$ strongly positive and G-invariant functionals $T^{(\nu)}$, $\nu = 1, \ldots, 4$, such that

$$\exp_{|_s} \lambda T^t = (T^{(1)} - T^{(2)}) + i(T^{(3)} - T^{(4)}).$$

Remark 2.5: A corresponding statement for characteristic functionals is wrong: If $\langle \cdot, \cdot \rangle$ is a positive scalar product on $\mathscr{S}_R$, then $\Gamma(f) = -\langle f, f \rangle$ is conditionally positive definite and $E(f) = \exp \Gamma(f)$ is the characteristic functional of a positive, Gaussian measure. However, $f \to \exp(-\Gamma(f))$ is not the characteristic functional of any bounded measure, for it is not bounded on $\mathscr{S}_R$.

For the proof of Proposition 2.4 we shall need several simple facts which we list as lemmas below. Recall that a sequence $\{\alpha_n\}_{n=0,1,\ldots}$ of complex numbers is said to be of positive type if $\sum \bar{\lambda}_i \alpha_{i+j} \lambda_j \geqslant 0$ for all finite sequences of $\lambda_i \in \mathbb{C}$; this is equivalent to the existence of a positive measure $d\rho$ on $\mathbf{R}$ with $\alpha_n = \int x^n d\rho(x)$.

Lemma 2.6: For any sequence $\{c_n\}$ of positive numbers there is another sequence $\{\gamma_n\}$, such that for any seminorm $\|\cdot\|$ on $\mathscr{S}$ one has

$$\sum_n c_n \, ||f_n|| \leq \sup || \sum_n \alpha_n f_n ||,$$

for all $f \in \underline{\mathscr{S}}$, where the supremum is taken over all sequences $\{\alpha_n\}$ of positive type with $|\alpha_n| \leq \gamma_n$ for all n.

Proof: This is essentially the same statement as Lemma 3.1 in Ref. 1, or statement 3 in Ref. 15. In fact,

$$\sum c_n \, ||f_n|| \leq \sup_n c_n \cdot 2^{n+1} || f_n ||$$

$$< \sup_{\substack{\{\beta_n\} \\ |\beta_n| < c_n \cdot 2^{n+1}}} || \sum \beta_n f_n ||.$$

Now every sequence $\{\beta_n\}$ can be written as a linear combination of four sequences of positive type $\{\alpha_n^{(i)}\}$, $i = 1,\ldots, 4$, and a bound for β_n implies a bound for $\alpha_n^{(i)}$. Since $|\beta_n| < 2^{n+1} c_n$, there exist constants γ_n', independent of $\{\beta_n\}$, such that $|\alpha_n^{(i)}| \leq \gamma_n'$. The statement thus holds with $\gamma_n = 4\gamma_n'$.

Lemma 2.7: Let T and $S \in \underline{\mathscr{S}}'$ be strongly positive, and $\{\alpha_n\}$ a positive definite sequence. Then $T_{\{\alpha_n\}} := (\alpha_0 T_0, \alpha_1 T_1, \ldots)$ and $T \mathbin{s} S$ are also strongly positive.

Proof: By Theorem 2.1, T (resp. S) are generated by characteristic functionals E (resp. F) of positive measures. If $d\rho$ is a positive measure on $\mathbf{R}$ with $\alpha_n = \int x^n \, d\rho(x)$, then the positive definite functional $f \mapsto \int E(xf) \, d\rho(x)$ generates $T_{\{\alpha_n\}}$, and $f \mapsto E(f) \cdot F(f)$ is positive definite and generates $T \mathbin{s} S$.

The last lemma is contained in the proofs of Propositions 1.21 and 1.15 in Ref. 16. It is basically an application of the Hahn–Banach theorem.

Lemma 2.8: Let V be a real vector space and C a convex cone (or wedge) in V. Let $\|\cdot\|$ be a monotone seminorm on V with respect to the ordering defined by C, i.e.,

$$\|x\| \leq \|x + y\|,$$

for all $x, y \in C$. If T is a linear functional on E with

$$|T(x)| \leq \|x\|,$$

for all x, there are positive, linear functionals $T^{(1)}$, $T^{(2)}$, on V, and a $\lambda \in [0,1]$, such that $T = T^{(1)} - T^{(2)}$, and

$$|T^{(1)}(x)| \leq \lambda \, \|x\|, \quad |T^{(2)}(x)| \leq (1 - \lambda)\|x\|.$$

Proof of Proposition 2.4: Suppose first that $\lambda = \alpha \in \mathbf{R}$. We assert that for any n there is a $c_n(\alpha) \geqslant 0$ such that for all $f_n \in \mathscr{S}_n$ we have

$$|\exp_{|_s} \alpha T^t(f_n)| \leq c_n(\alpha) \sup_{0 \leq \epsilon \leq 1} |\exp_{|_s} \epsilon T^t(f_n)|.$$

In fact, one has

$$\exp_{|_s} \epsilon T^t(f_n) = \sum_{k=1}^{n} \epsilon^k \left(\sum_{\mathrm{Part}_k} T^t_{n_1} \otimes \cdots \otimes T^t_{n_k}(f_n) \right),$$

where the sum in the parentheses is an abbreviation of an expression like the right-hand side of (2.3), but with k fixed. For every f_n this is a polynomial in ϵ of degree at most n. The sup over $\epsilon \in [0,1]$ defines a norm on the finite-dimensional vector space of such polynomials. The evaluation of a polynomial at a particular point $\epsilon = \alpha$ is a linear functional on this space, so the assertion follows. Next, we conclude from Lemma 2.6 that there is a sequence $\{\gamma_n(\alpha)\}$, such that

$$|\exp_{|_s} \alpha T^t(\underline{f})| \leq \sup |(\exp_{|_s} \epsilon T^t) \{\alpha_n\}(\underline{f})|,$$

for all $\underline{f} \in \underline{\mathscr{S}}$, where the sup is now taken over $\epsilon \in [0,1]$ and sequences $\{\alpha_n\}$ of positive type with $|\alpha_n| \leq \gamma_n(\alpha)$. The right-hand side defines a continuous seminorm on $\underline{\mathscr{S}}$. Since $\exp_{|_s} \epsilon T^t$ is strongly positive for all $\epsilon > 0$ and this holds also for $(\exp_{|_s} \epsilon T^t)_{\{\alpha_n\}}$ by Lemma 2.7, the seminorm is monotone with respect to the order defined by the wedge $\{\underline{f} | \chi_\omega(\underline{f}) \geqslant 0 \text{ for all } \omega\}$ in the Hermitian part of $\underline{\mathscr{S}}$. The positive functionals with respect to this order are precisely the strongly positive functionals. Moreover, G invariance of T^t implies that the seminorm vanishes on $K_G := \mathrm{cl\,lin\,span}\{\alpha_\tau \underline{f} - \underline{f} | \tau \in G, \underline{f} \in \underline{\mathscr{S}}\}$. By Lemma 2.8 it follows that $\exp_{|_s} \alpha T^t$ is the difference of two strongly positive functionals, which also vanish on K_G and are thus G invariant. In a similar way we treat $\exp_{|_s} \lambda T^t$ if $\lambda = i\beta$, $\beta \in \mathbf{R}$: By the same argument as before we have

$$|\sin_{|_s} \beta T^t(f_n)|$$

$$= \left| \sum_{k \,\mathrm{odd}} \beta^k \left(\sum_{\mathrm{Part}_k} T_{n_1} \otimes \cdots \otimes T_{n_k} \right)(f_n) \right|$$

$$\leq c_n'(\beta) \sup_{0 \leq \epsilon \leq 1} |\exp_{|_s} \epsilon T^t(f_n)|,$$

and analogously for $\cos_{|_s} \beta T^t$. Hence $\exp_{|_s} i\beta T^t$ is a linear combination of strongly positive, G-invariant functionals.

Finally, by (2.2)

$$\exp_{|_s} (\alpha + i\beta) T^t = (\exp_{|_s} \alpha T^t) \mathbin{s} (\exp_{|_s} i\beta T^t),$$

and we obtain the statements for arbitrary $\lambda = \alpha + i\beta$ using (2.1) and Lemma 2.7.

We can now prove the following.

Theorem 2.9: Suppose G is an amenable group and $T \in \underline{\mathscr{S}}'$, $T_0 \neq 0$. The following are equivalent.

(i) T has an integral representation with a G-invariant complex measure on $\mathscr{S}_R'$.

(ii) T^t can be written as a linear combination of G-invariant, conditionally strongly positive functionals.

Proof: The implication (ii) $\Rightarrow$ (i) follows from Proposition 2.4 and Theorem 2.2, using Eq. (2.2): If $T^t = (R_1 - R_2) + i(R_3 - R_4)$ with R_i conditionally positive and G invariant, then

$$T = \exp_{|_s} T^t$$

$$= (\exp_{|_s} R_1) \mathbin{s} (\exp_{|_s}(-R_2)) \mathbin{s} (\exp_{|_s}(iR_3)) \mathbin{s} (\exp_{|_s}(iR_4))$$

is a linear combination of strongly positive, G-invariant functionals. The other implication (i) $\Rightarrow$ (ii) follows from

$$T^t = \log T_0 + \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n \cdot T_0 \, n} (T - T_0)^n_{|_s},$$

using Lemma 2.7 and (2.2). This formula shows in fact that T^t is a linear combination of strongly positive, G-invariant functionals.

Remark 2.10: Because

$$T = (\log \exp T)|_*$$
$$= T_0 + \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} e^{-nT_0}(e^T - e^{T_0})|_*^n,$$

we see that another equivalent condition is the following.

(iii) T is a linear combination of conditionally strongly positive, G-invariant functionals. For the present purpose, however, condition (ii) turns out to be the most useful one.

We now specialize to the case that G is the Euclidean group ISO(d), which acts in a natural way on $\mathscr{S}_R$. It is in fact only the translation group $\mathbf{R}^d$ that causes a problem, for the rotation group SO(d) is compact, and one can obtain an invariant measure by integrating over it. The next theorem gives a sufficient criterion for a functional $T \in \mathscr{S}'$ to admit a representation by an $\mathbf{R}^d$-invariant measure. This criterion combines the estimate (ii) of Theorem 2.3 with the condition that T_n' decreases rapidly at infinity in the difference variables for all n. A remark on the notation: If $\alpha = (\alpha^0, \ldots, \alpha^{d-1})$ is a multiindex we write $|\alpha| = \alpha^0 + \cdots + \alpha^{d-1}$ as usual. Also, D_i^{α} is the corresponding differential operator with respect to $x_i \in \mathbf{R}^d$. A continuous function on $\mathbf{R}^d$ is said to be of rapid decrease, if $\sup|(1 + |x|^N)\, g(x)| < \infty$ for all $N \in \mathbf{N}$.

Theorem 2.11: Suppose $T \in \mathscr{S}'$ is totally symmetric and $\mathbf{R}^d$ invariant with $T_0 \neq 0$. If there exist constants k_n and rapidly decreasing, continuous functions g_n such that

$$|T_n'(f_1 \otimes \cdots \otimes f_n)|$$
$$\leqslant \max_{|\alpha_i| \leqslant k_i} \sup_{x_1, \ldots, x_n} \left| \prod_{j=2}^{n} g_n(x_1 - x_j)\, D_1^{\alpha_1} f(x_1) \cdots D_n^{\alpha_n} f(x_n) \right|$$

for all $f_1, \ldots, f_n \in \mathscr{S}$, $n = 1, 2, \ldots$, then T has a representation by an $\mathbf{R}^d$-invariant, complex measure on $\mathscr{S}_R'$.

Proof: The decrease of T_n' implies that we can divide with a function in $\mathscr{S}_{n-1}$ and still retain a similar estimate. More precisely, by the Lemma in the Appendix there exists a positive function $h \in \mathscr{S}$ such that

$$\sup_{x_1, \ldots, x_n} \left| \prod_{i=2}^{n} g_n(x_i - x_1) \prod_{j=1}^{n} D_j^{\alpha_j}\, \overline{h^{\otimes n}}(x_1, \ldots, x_n)^{-1} \right| < \infty,$$

for all $\alpha_1, \ldots, \alpha_n$, where

$$\overline{h^{\otimes n}}(x_1, \ldots, x_n) := \int h(x_1 + a) \cdots h(x_n + a)\, da.$$

It follows that $T_n' := T_n' \cdot (\overline{h^{\otimes n}})^{-1}$ is a well-defined tempered distribution with

$$|T_n'(f_1 \otimes \cdots \otimes f_n)| \leqslant c_n \cdot \sup_{|\alpha_i| \leqslant k_i} |D_1^{\alpha_1} f_1(x_1) \cdots D_n^{\alpha_n} f_n(x_n)|,$$

for all $f_1, \ldots, f_n \in \mathscr{S}$, with some constants $c_n < \infty$. By Theorem 2.3 the T_n' are moments of a complex measure $d\nu(\omega)$.

Let $F(f) = \int \exp i\omega(f)\, d\nu(\omega)$ be the characteristic functional of this measure and consider the functional

$$\Gamma(f) := \int (F(h \cdot f_a) - F(0))\, da.$$

We assert that Γ is a linear combination of invariant, conditionally positive definite functionals and that it is a generating functional for the T_n'. To show this, we remark first that if $\|\cdot\|$ is a continuous seminorm on $\mathscr{S}$ and $h \in \mathscr{S}$, then

$$f \mapsto \left(\int \|h \cdot f_a\|^n\, da \right)^{1/n},$$

with $f_a(x) := f(x - a)$ also a continuous seminorm on $\mathscr{S}$ for all n. Now we can write $F = (F^{(1)} - F^{(2)}) + i(F^{(3)} - F^{(4)})$, where the $F^{(i)}$ are characteristic functionals of positive measures $d\nu^{(i)}$ with continuous moments $S_n^{(i)}$. We have for all $f \in \mathscr{S}_R$

$$|F^{(i)}(f) - F^{(i)}(0)| \leqslant \int |e^{i\omega(f)} - 1|\, d\nu^{(i)}(\omega) \leqslant S_2^{(i)}(f^{\otimes 2})$$

and hence

$$\int |F^{(i)}(h \cdot f_a) - F^{(i)}(0)|\, da \leqslant \int S_2^{(i)}((h f_a)^{\otimes 2})\, da < \infty.$$

Thus Γ is well defined, and it is a linear combination of the conditionally positive, invariant functionals

$$\Gamma^{(i)}(f) = \int (F^{(i)}(h \cdot f_a) - F^{(i)}(0))\, da.$$

The continuity of $\Gamma^{(i)}$ follows in the same way from the continuity of $S_2^{(i)}$. Finally, $\lambda \mapsto \Gamma^{(i)}(\lambda f)$ is n-times differentiable at zero for all n and all f, because differentiation under the integral sign gives $\int S_n^{(i)}((h \cdot f_a)^{\otimes n})\, da$ which converges by the remark above. It follows that Γ is a generating functional for the n-point distribution

$$\int ((S_n^{(1)} - S_n^{(2)}) + i(S_n^{(3)} - S_n^{(4)}))$$
$$\times ((h \cdot f_{1,a}) \otimes \cdots \otimes (h \cdot f_{n,a}))\, da$$
$$= \int T_n'((h \cdot f_{1,a}) \otimes \cdots \otimes (h \cdot f_{n,a}))\, da$$
$$= \int T_n'((h_{-a} \cdot f_1) \otimes \cdots \otimes (h_{-a} \cdot f_n))\, da$$
$$= T_n'(\overline{h^{\otimes n}} \cdot (f_1 \otimes \cdots \otimes f_n))$$
$$= T_n(f_1 \otimes \cdots \otimes f_n),$$

where the invariance of T_n' was used to shift the integration variable from f to h. We have thus shown that the T_n' fulfill condition (ii) of Theorem 2.9 and the proof is complete.

Remark 2.12: The theorem could equivalently be stated in terms of the T_n themselves instead of T_n', cf. Remark 2.10. Using this, we obtain the following corollary.

Theorem 2.13: The linear span of those functionals in $\mathscr{S}'$ which have a representation by an $\mathbf{R}^d$-invariant, positive measure on $\mathscr{S}_R'$ is strongly dense in the space of all totally symmetric, $\mathbf{R}^d$-invariant functionals in $\mathscr{S}'$.

Proof: Since $\mathscr{S}$ is reflexive, strong density is the same as weak density. Every functional $T \in \mathscr{S}'$ can obviously be approximated weakly by functionals of the form $(T_0, T_1 h_1, \ldots, T_N \cdot h_N, 0, \ldots)$, where the $h_n \in \mathscr{S}(\mathbf{R}^{d(n-1)})$ are functions of the difference variables, taking the value 1 on increasingly large subsets of $\mathbf{R}^{d(n-1)}$. These functionals satisfy the condition of Theorem 2.11.

Remark 2.14: The sufficient criterium of Theorem 2.11 is by no means necessary, not even for functionals with cluster property, i.e., such that the T_n' go to zero at infinity. For instance, one can define a Gaussian measure for any positive

definite two-point function, and such function can decrease at least as slowly as $|x_1 - x_2|^{-(d-1)}$ at infinity. The reason for the rather stringent condition in Theorem 2.11 is that Theorem 2.3 does not give any information about the moments of the measures $d\nu^{(i)}$, except that they are tempered distributions. Thus, in order to ensure the convergence of the integrals $\int (F^{(i)}(h \cdot f_a) - F^{(i)}(0))da$, one must take h to be of rapid decrease at infinity. If Theorem 2.3 could be improved, so that one had a control over the behavior of the moments of $d\nu^{(i)}$, this would result in a corresponding strengthening of Theorem 2.11.

III. APPLICATION TO SCHWINGER FUNCTIONALS

Although Theorem 2.11 does not give a complete answer to the question when invariant functionals in $\mathscr{S}'$ have invariant integral representations, it can be applied to Schwinger functionals because of the following property.

Lemma 3.1: Let S_n^t $(n = 1, 2,...)$ be the truncated Schwinger functions of a Wightman field theory with a unique vacuum and a lowest mass $m > 0$. Then for all n, and all $\epsilon > 0$, there are constants $a_{n,\epsilon}$, $N_n < \infty$, $b_n > 0$ such that

$$|S_n^t(x_1,..., x_n)| \leqslant a_{n,\epsilon} \left(\max_{i,j} |x_i - x_j|\right)^{N_n} e^{-b_n \max_{ij} |x_i - x_j|}$$

if $|x_i - x_j| \geqslant \epsilon$ for all $i \neq j$.

Proof: The arguments are more or less standard. Using the compactness of the unit sphere in $\mathbb{R}^d$ one shows easily (cf., e.g., Ref. 17, Lemma 5.2) that there is a constant $c_n > 0$, such that for any $(x_1,..., x_n) \in \mathbb{R}^{d \cdot n}$ one can choose a rotation $R \in SO(d)$ such that $|(Rx_i)^0 - (Rx_j)^0| \geqslant c_n |x_i - x_j|$ for all i, j. Using the Euclidean invariance of S_n^t we can thus for a given $(x_1,..., x_n)$ assume that the time axis points in a direction such that $|x_j^0 - x_j^0| \geqslant c_n |x_i - x_j|$. Moreover, by total symmetry of S_n^t we have

$$S_n^t(x_1,..., x_n) = S_n^t(x_{\pi 1},..., x_{\pi n}),$$

where the permutation π is such that $x_{\pi 1}^0 < \cdots < x_{\pi n}^0$; we can thus without restriction assume that $x_1^0 < \cdots < x_n^0$, and

$$|x_n^0 - x_1^0| \geqslant c_n \max_{i,j} |x_i - x_j|.$$

At such time-ordered points S_n^t is the Fourier–Laplace transform of the truncated Wightman distribution W_n^t, i.e.,

$$S_n^t(x_1,..., x_n) = \int \exp\left(-\sum_{\nu=2}^{n} q_\nu^0 (x_\nu^0 - x_{\nu-1}^0)\right) \times \exp\left(i \sum_{\nu=2}^{n} \mathbf{q}_\nu \cdot (\mathbf{x}_\nu - \mathbf{x}_{\nu-1})\right) \times \tilde{W}_n^t(q_2,..., q_n) dq_2 \cdots dq_n,$$

where $\tilde{W}_n^t$, the Fourier transform of W_n^t in the difference variables, has support in $\overline{V}_{m_0}^+ \times \cdots \times \overline{V}_{m_0}^+ = \{(q_2,..., q_n) | q_\nu \cdot q_\nu > m_0^2, q_\nu^0 > 0 \text{ for all } \nu\}$. Write $\tilde{W}_n^t = \Sigma_{|\alpha| < k} D^\alpha F_\alpha$, where the F_α are continuous and polynomially bounded with support in $\overline{V}_{m_0}^+ \times \cdots \times \overline{V}_{m_0}^+$. This is possible because one can map this set smoothly onto a product of half-spaces, where such a representation holds, e.g., by the BEG lemma (cf. Ref. 18, Lemma IX, 15). Thus S_n^t is a sum of terms of the form

$$P_\alpha(x_2 - x_1,..., x_n - x_{n-1}) \times \int \exp\left(-\sum_{\nu=2}^{n} q^0(x_\nu^0 - x_{\nu-1}^0)\right) \times \exp\left(i \sum_{\nu=2}^{n} \mathbf{q}_\nu \cdot (\mathbf{x}_\nu - \mathbf{x}_{\nu-1})\right) \times F_\alpha(q_2,..., q_n) dq_2 \cdots dq_n,$$

where P_α is a polynomial. Because of the support properties of F_α, this can for $|x_i - x_j| \geqslant \epsilon$ be estimated by

$$\sum_\alpha \max_{i,j} |x_i - x_j|^{N_\alpha} \exp\left(-\frac{m_0}{2} |x_n^0 - x_1^0|\right) \times \int \exp\left(-\frac{m-1}{2} c_n \epsilon \sum_{\nu=2}^{n} q_\nu^0\right) \times |F(q_2,..., q_n)| dq_2 \cdots dq_n \leqslant a_{n,\epsilon} \cdot \max_{ij} |x_i - x_j|^{N_n} \exp(-b_n \max_{i,j} |x_l - x_j|),$$

with $b_n = -(m_0/2) c_n$.

Lemma 3.1 says that the condition of rapid decrease at infinity is automatically satisfied for the truncated Schwinger functions if there is a mass gap. On the other hand, it is easily verified that estimate (ii) of Theorem 2.3 holds for the truncated Schwinger functions if and only if it holds for the Schwinger functions themselves. Combining Theorem 2.11, Lemma 3.1, and Theorem 5.1 in Ref. 1, we thus obtain the following.

Theorem 3.2: Let S_n, $n = 0, 1,...$ be the Schwinger functions of a Wightman field theory with a unique vacuum and a lowest mass $m_0 > 0$. The following are equivalent.

(i) There is a Euclidean invariant, complex measure $d\mu$ on $\mathscr{S}_R'$ with continuous moments, such that

$$S_n(f_1 \otimes \cdots \otimes f_n) = \int \omega(f_1) \cdots \omega(f_n) d\mu(\omega),$$

for all $f_1,..., f_n \in \mathscr{S}$ with nonoverlapping supports. The right-hand side defines then an extension of S_n as distribution to all of $\mathbb{R}^{d \cdot n}$.

(ii) There are continuous seminorms $\|\cdot\|_i$, $i = 1, 2,...$ on $\mathscr{S}$ such that

$$|S_n(f_1 \otimes \cdots \otimes f_n)| \leqslant \|f_1\|_1 \cdots \|f_n\|_n,$$

for all $f_1,..., f_n \in \mathscr{S}$, all n.

(iii) There are constants c_n and k_n, $n = 1, 2,...$ such that

$$|S_n(x_1,..., x_n)| \leqslant c_n \cdot \sum_{\nu=2}^{n} \sum_{i_1 < \cdots < i_\nu} d(x_{i_1},..., x_{i_\nu})^{-k_\nu},$$

with $d(y_1,..., y_m) := \max_{i,j} |y_i - y_j|$.

Remarks 3.3: (i) The uniqueness of the vacuum is not a very serious restriction: If the theory is a superposition of theories with unique vacuums:

$$S_n = \int S_{n,\zeta} \, d\rho(\zeta),$$

where $d\rho$ is a probability measure, and the Schwinger functions $S_{n,\zeta}$ have the cluster property with exponential decay, uniform in ζ, then one can simply form the measure

$d\mu = \int d\mu_\zeta \, d\rho(\zeta)$, where $d\mu_\zeta$ is the measure representing $S_{n,\zeta}$. It is at present not clear whether Theorem 3.2 holds true in more general cases, in particular if there is no mass gap at all, cf. Remark 2.14.

(ii) If the Schwinger functions are real (i.e., if the theory is invariant under time inversion), then the measure $d\mu$ can of course be chosen real valued. Now it should be remembered that the Schwinger functions are to begin with only defined at points $(x_1,\ldots, x_n)\in\mathbb{R}^{d\cdot n}$, with $x_i \neq x_j$ for all $i\neq j$ (noncoinciding points). Thus the following question arises naturally: Is it always possible to extend real Schwinger functions to coinciding points in such a way that they have a representation by an invariant, *positive* measure? To put it differently, can a positive measure with continuous moments always be dominated by a positive measure whose moments have support at coinciding points? Theorem 2.2 in Ref. 19 is an indication that this might be true, but this is an unsolved problem at the moment.

IV. GENERAL REMARKS ON THE MOMENT PROBLEM WITH COMPLEX MEASURES

In this final section we want to point out some differences between complex measures and positive measures, as far as the moment problem is concerned.

Remark 4.1: The moment problem with a complex measure has never a unique solution. To see this, note that there are nonzero, signed measures $d\zeta$ or $\mathbb{R}$ such that all $|x|^n$ are integrable with respect to $d|\zeta|$ and $\int x^n \, d\zeta(x) = 0$ for all n.[20] If E is the characteristic functional of a positive measure $d\nu(\omega)$ or $\mathscr{S}'_R$ with continuous moments, then $f \Rightarrow \int E(xf) d\zeta(x)$ is the characteristic functional of a signed, nonzero measure or $\mathscr{S}'_R$, with all moments vanishing. Such a measure can be added to any solution of the moment problem to obtain a different solution.[22]

Remark 4.2: The formula

$$E(f) = \sum_{n=0}^{\infty} \frac{i^n}{n!} T_n(f^{\otimes n}),$$

with

$$E(f) = \int \exp i\omega(f) d\mu(\omega), \quad T_n = \int \omega^{\otimes n} \, d\mu(\omega),$$

is in general not true for complex measures, even if

$$\sum_{n=0}^{\infty} (n!)^{-1} |T_n(f^{\otimes n})| < \infty,$$

for all f.

In fact, in order to interchange integration and sum we would have to know that

$$\sum_{n=0}^{\infty} (n!)^{-1} \int |\omega(f)|^n \, d|\mu|(\omega) < \infty.$$

We illustrate this with two examples.

Suppose $\omega_0 \neq 0$ is some fixed distribution in $\mathscr{S}'_R$ and define T and $S \in \mathscr{S}'$ by

$$T_{2n} = 0, \quad T_{2n+1} = \omega_0^{\otimes (n+1)},$$

respectively,

$$S_{2n} = 0, \quad S_{2n+1} = (-1)^{n+1} \omega_0^{\otimes (n+1)},$$

for all n. Both functionals satisfy the condition of Theorem 2.3 and have an integral representation by a signed measure on $\mathscr{S}'_R$. In the case of T one such measure can easily be written down:

$$d\mu(\omega) = \tfrac{1}{2}\delta(\omega - \omega_0) - \tfrac{1}{2}\delta(\omega + \omega_0)$$

and one has in fact

$$\int \exp i\omega(f) d\mu(\omega) = i \sin \omega_0(f)$$

$$= \sum_{n=0}^{\infty} \frac{i^n}{n!} T_n(f^{\otimes n}).$$

On the other hand,

$$\sum_{n=0}^{\infty} \frac{i^n}{n!} S_n(f^{\otimes n}) = i \sinh \omega_0(f)$$

is not the characteristic functional of a finite, complex measure, because it is not bounded as a function or $\mathscr{S}_R$. These examples show clearly, that an estimate on $|T_n^{\otimes n}|$ is of no use for deciding whether the characteristic functional can be obtained by summing up the moments or not. This is further substantiated by the next remark.

Remark 4.3: Gaussian moments need not be the moments of a Gaussian measure. By Gaussian moments we here mean that the T_n are determined by T_2 in the usual way:

$$T_{2n+1} = 0,$$

$$T_{2n}(f_1 \otimes \cdots \otimes f_{2n}) = \sum_{\text{Pairings}} T_2(f_{i_1} \otimes f_{j_1}) \cdots T_2(f_{i_n} \otimes f_{j_n}), \tag{4.1}$$

and by a (normalized) complex Gaussian measure we mean a measure $d\mu(\omega)$ such that

$$\int e^{i\omega(f)} \, d\mu(\omega) = e^{-(1/2)Q(f)},$$

where Q is a continuous, quadratic form on $\mathscr{S}_R$. A Gaussian measure has continuous moments, which are given by the formula (4.1) with $T_2(f^{\otimes 2}) = Q(f)$. Conversely, if the T_n have the form (4.1), one has

$$\sum_n \frac{i^n}{n!} T_n(f^{\otimes n}) = e^{-(1/2) T_2(f^{\otimes 2})},$$

but this is in general not the characteristic functional of a measure; the time-ordered function of a free field provides a counterexample, for if $e^{-(1/2) T_2(f^{\otimes 2})}$ were the characteristic functional of a measure on $\mathscr{S}'_R$, this measure would be $\mathbb{R}^d$ invariant, which is not possible (cf. Ref. 2, Sec. 6). The fact that the time-ordered functions are not the moments of a finite, Gaussian measure was noted long ago by Cameron.[23] His argument was not based on the $\mathbb{R}^d$ invariance, but on a direct calculation of the total mass of the complex Gaussian cylinder measures defined by T_2. The following proposition is an elaboration of Cameron's observation. It should probably be classified as a folk theorem although the present author has not found it explicitly stated in the literature.

Proposition 4.4: Let Q be a complex quadratic form on $\mathscr{S}_R$. In order that there is a (finite, σ-additive) complex measure $d\mu$ on $\mathscr{S}'_R$ with

$$e^{-(1/2)Q(f)} = \int_{\mathscr{S}'_R} e^{i\omega(f)}\, d\mu(\omega),$$

it is necessary and sufficient that

$$Q(f) = \langle f,f\rangle + i\langle f,Bf\rangle,$$

where $\langle\cdot,\cdot\rangle$ is a positive semidefinite, continuous scalar product on $\mathscr{S}_R$ and B is a self-adjoint Hilbert–Schmidt operator with respect to this scalar product. The measure $d\mu$ is in this case absolutely continuous with respect to the positive Gaussian measure with covariance $\langle\cdot,\cdot\rangle$.

Proof: We show first the necessity of the condition. To begin with Q must be continuous if $d\mu$ is σ additive: If $f_n \to f$ in the topology of $\mathscr{S}_R$, then $e^{i\omega(f_n)} \to e^{i\omega(f)}$ for all ω and hence $e^{-(1/2)Q(f_n)} \to e^{-(1/2)Q(f)}$ by the dominated convergence theorem for the positive measure $d|\mu|$. Since Q is a quadratic form it suffices to show its continuity in a neighborhood of 0. But $f_n \to 0$ implies $\exp(-\frac{1}{2}Q(f_n)) \to 1$, which implies $Q(f_n) = -2\log\exp(-\frac{1}{2}Q(f_n)) \to 0$. Now for every $f_1,\ldots,f_N \in \mathscr{S}_R$ we have a complex measure $d\mu_{f_1\cdots f_N}$ on $\mathbf{R}^N$, defined by

$$\int_{\mathbf{R}^N} F(t_1,\ldots,t_N)\, d\mu_{f_1\cdots f_N}(t_1,\ldots,t_N) = \int_{\mathscr{S}'_R} F(\omega(f_1),\ldots,\omega(f_N))\, d\mu(\omega),$$

for bounded, continuous functions F. The total mass of the $d\mu_{f_1,\ldots,f_N}$ is uniformly bounded:

$$\int d|\mu_{f_1,\ldots,f_N}| \leq \int d|\mu| < \infty.$$

Since Q is a quadratic form, we can write

$$Q(f) = \langle f,f\rangle + i(f,f),$$

with symmetric, real-valued, bilinear forms $\langle\cdot,\cdot\rangle$ and $(\cdot,\cdot)$ on $\mathscr{S}_R$. It is evident that $\langle f,f\rangle \geq 0$ for all f, for otherwise $\exp(-\frac{1}{2}\lambda^2 Q(f)) = \int \exp i\lambda t\, d\mu_f(t)$ would be an unbounded function of λ for some f, in contradiction to $\int d|\mu_f| < \infty$.

Similarly, $(\cdot,\cdot)$ must be bounded with respect to $\langle\cdot,\cdot\rangle$, because

$$\int d|\mu_f| = (1 + (f,f)^2/\langle f,f\rangle^2)^{1/4}.$$

Thus $|(f,f)| \leq c\langle f,f\rangle$, for some c, independent of f. It follows that we can write $(f,g) = \langle f,Bg\rangle$, where B is a s.a. bounded operator on the Hilbert space defined by $\langle\cdot,\cdot\rangle$. Let $\{f_i\}$ be any orthonormal basis in $\mathscr{S}_R$ corresponding to the scalar product $\langle\cdot,\cdot\rangle$. Let $B^{(n)}$ denote the symmetric matrix $\langle f_i, Bf_j\rangle$, with $i,j = 1,\ldots,n$. If $\beta_1^{(n)},\ldots,\beta_n^{(n)}$ are its eigenvalues we have

$$\sum_{n=1}^{n} \beta_k^{(n)2} = \sum_{k,l=1}^{n} |\langle f_k, Bf_e\rangle|^2.$$

Since

$$\int d|\mu|(\omega) > \int d|\mu_{f_1,\ldots,f_n}|(t_1,\ldots,t_n) = \prod_{k=1}^{n} (1+\beta_k^{(n)2})^{1/4} > \left(\sum_{k=1}^{n} \beta_k^{(n)2}\right)^{1/4} = \left(\sum_{k,l=1}^{n} |\langle f_k, Bf_l\rangle|^2\right)^{1/4},$$

we conclude that

$$\sum_{k,l=1}^{\infty} |\langle f_l, Bf_l\rangle|^2 < \infty,$$

so B is a Hilbert–Schmidt operator.

To prove that the condition is sufficient one can use similar arguments as in the proof of the theorem on mutual absolute continuity of positive Gaussian measures (the Feldman–Hajek theorem, cf., e.g., Ref. 24). Completing $\mathscr{S}_R$ modulo null space in the scalar product $\langle\cdot,\cdot\rangle$ we obtain a Hilbert space $\mathscr{H}$. Let $\{e_k\}_{k=1,2,\ldots}$ be an orthonormal basis of eigenvectors of B: $Be_k = \beta_k e_k$, with $\Sigma\beta_k^2 < \infty$. Once a basis has been introduced the positive Gaussian measure $d\nu$ with covariance $\langle\cdot,\cdot\rangle$ can be realized as a product measure on $\mathbf{R}^\infty$:

$$d\nu(x) = \prod_{k=1}^{\infty} d\nu_k(x_k),$$

with

$$d\nu_k(x_k) = \frac{1}{(2\pi)^{1)2}} e^{-(1/2)x_k^2}\, dx_k.$$

Since $\int x_k x_l\, d\nu(x) = \delta_{kl}$, Fubini's theorem implies that for every $v = (v_1, v_2,\ldots)$ with $\Sigma v_k^2 < \infty$ the sum $\Sigma x_k v_k$ converges in L_2 sense, and hence in measure, to an L_2 function on $\mathbf{R}^\infty$. We denote this function of x by $x\cdot v$. If we identify v with $\Sigma v_k e_k \in \mathscr{H}$ we can write

$$\exp(-\tfrac{1}{2}\langle v,v\rangle) = \int \exp ix\cdot v\, d\nu(x)$$

by the dominated convergence theorem. Now define

$$\psi_k(x_k) = (1+i\beta_k)^{-1/2} \exp(\tfrac{1}{2}(1+i\beta_k)^{-1} i\beta_k x_k^2),$$

where the square root is determined by $\mathrm{Re}(1+i\beta)^{1/2} > 0$, $\beta \in \mathbf{R}$. We have

$$\int \exp(ix_k v_k)\psi_k(x_k)\, d\nu_k(x_k) = \exp\left(-\frac{1}{2}(1+i\beta_k)v_k^2\right), \tag{4.2}$$

$$\int |\psi_k(x_k)|\, d\nu_k(x_k) = (1+\beta_k^2)^{1/4}, \tag{4.3}$$

and

$$\int |\psi_k(x_k)|^2\, d\nu_k(x_k) = (1-\beta_k^2)^{-1/2}, \quad \text{for } \beta_k < 1. \tag{4.4}$$

From (4.2)–(4.4) we compute for $m > n$, $\beta_k < 1$ for $k > n$

$$\int \left|\prod_{k=1}^{n}\psi_k(x_k) - \prod_{k=1}^{m}\psi_k(x_k)\right| d\nu(x) < \prod_{k=1}^{n}(1+\beta_k^2)^{1/4}\left(\int \left|1 - \prod_{k=n+1}^{m}\psi_k(x_k)\right|^2 d\nu(x)\right)^{1/2} = \prod_{k=1}^{n}(1+\beta_k^2)^{1/4}\left(\prod_{k=n+1}^{m}(1-\beta_k^2)^{-1/2} - 1\right)^{1/2},$$

where in the last equation we used $\int \Pi_{k=n+1}^{m}\psi_k(x_k)\, d\nu(x) = 1$. Since $\Sigma\beta_k^2 < \infty$ it follows that $\Pi_{k=1}^{n}\psi_k(x_k)$ converges in L_1 norm to an L_1 function on $\mathbf{R}$, denoted by ψ, and the dominated convergence theorem gives

$$\int \exp(ix\cdot v)\psi(x)\, d\nu(x) = \exp\left(-\frac{1}{2}(\langle v,v\rangle + i\langle v,Bv\rangle)\right)$$

and

$$\int |\psi(x)|d\nu(x) = \prod_{k=1}^{\infty} (1+\beta_k^2)^{1/4} < \infty.$$

The measure on $\mathbb{R}^\infty$ is now transported into a measure on $\mathscr{S}'_R$ by using the nuclearity of $\mathscr{S}_R$. Since $\langle v,v\rangle = \int |x\cdot v|^2 \, d\nu(x)$, we can identify $\mathscr{H}$ with a subspace of $L_2(\mathbb{R}^\infty, d\nu)$, consisting of the functions $x \to x\cdot v$ with $v \in \mathscr{H}$. Since the canonical mapping $\mathscr{S}_R \to \mathscr{H}$ is continuous, it follows from the nuclear spectral theorem (Ref. 25, cf. also Ref. 6, Lemma 2.3) that $\mathscr{S}_R \ni f \mapsto x\cdot f$ is continuous, i.e., a distribution in $\mathscr{S}'_R$, for almost all x. Hence we can write

$$\exp\left(-\frac{1}{2}Q(f)\right) = \int_{\mathscr{S}'_R} \exp i\omega(f) d\mu(\omega),$$

where $d\mu(\omega)$ is the complex measure on $\mathscr{S}'_R$ corresponding to the complex measure $\psi(x)d\nu(x)$ on $\mathbb{R}^\infty$.

Remark 4.5: If T_n, $n = 0, 1,...$ have the Gaussian structure (4.1), they can always be written as moments of a complex measure, because the condition of Theorem 2.3 is obviously fulfilled. On the other hand, if T_2 does not satisfy the condition of Proposition 4.4, there is no such measure with characteristic functional $\exp(-\frac{1}{2}T_2(f^{\otimes 2}))$. Nevertheless, one can define more general objects than σ-additive measures, such that a formula like $\int e^{i\omega(f)} d\mu(\omega) = \exp(-T_2(f^{\otimes 2}))$ makes sense.[5] One disadvantage of this approach is that the usual convergence theorems of integration theory need not hold for these objects. It thus depends on the problems treated whether such generalized Gaussian integrals are a useful analytical tool or not.

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APPENDIX: A TECHNICAL LEMMA

We prove here a technical lemma that is needed in the proof of Theorem 2.11.

Lemma: Let g_n, $n = 1, 2,...$ be rapidly decreasing, continuous functions on $\mathbb{R}^d$. There exists a function $h \in \mathscr{S}$ with $h(x) > 0$ for all $x \in \mathbb{R}^d$, such that for all n and all multiindices $\alpha_1,..., \alpha_n$,

$$\sup_{x_1,...,x_n} \left| \prod_{i=2}^{n} g(x_i - x_1) D_1^{\alpha_1}\cdots D_n^{\alpha_n} \times \overline{(h^{\otimes n}}(x_1,..., x_n))^{-1} \right| < \infty,$$

where $\overline{h^{\otimes n}}$ denotes the function $\int h(x_1 + a)\cdots h(x_n + a)da$.

Proof: Define $\| g_n \|_k = \sup_x |(1 + |x|^k) g_n(x)|$,

$$\epsilon_n^{(k)} = (1 + \|g_n\|_k)^{-1} \cdot 2^{-n} \quad \text{and} \quad \epsilon_n = \min_{k \le n} \epsilon_n^{(k)}.$$

Then $\epsilon_n > 0$ for all n and $\Sigma_n \epsilon_n \| g_n \|_k < \infty$ for all k.

In particular, the series $\Sigma_n \epsilon_n |g_n(x)|$ converges uniformly on $\mathbb{R}$ and defines a positive, rapidly decreasing, continuous function g such that $|g_n(x)| \le \epsilon_n^{-1} g(x)$ for all n.

Define $f(x) = \sup_{y+z=x} g(y)g(z)$.

Then f is also continuous and rapidly decreasing, for if $y + z = x$, then either $|y| \ge \frac{1}{2}|x|$ or $|z| \ge \frac{1}{2}|x|$. Consider now the function M or $\mathbb{R}$ defined by

$$M(r) = \begin{cases} \sup_{|x| > r} f(x), & \text{if } r \ge 0, \\ f(0) & \text{if } r < 0. \end{cases}$$

Here, M is rapidly decreasing for $r > 0$, continuous and monotone with $M(|x|) \ge f(x)$ for all x.

Consider next the function $\gamma(s) = \exp -(1 + s^2)^{1/2}$. This is a positive function in $\mathscr{S}(\mathbb{R})$, and for every $n \in \mathbb{N}$ there is a $c_n < \infty$, such that $|\gamma^{(n)}(s)| \le c_n |\gamma(s)|$ for all s.

The function h is now defined by

$$h(x) = \int_{-\infty}^{\infty} \gamma((1 + |x|^2)^{1/2} - r) M(r) dr.$$

It is easy to see that h is C^∞ and rapidly decreasing, and since γ and M are monotone and positive with $M(|x|) (\ge f(x)$ we have

$$h(x) \ge \int_{-\infty}^{|x|} \gamma((1 + |x|^2)^{1/2} - r) M(r) dr \ge \left(\int_1^\infty \gamma(s) ds \right) f(x).$$

Also, differentiating under the integral sign gives

$$|D^\alpha h(x)| \le \int |\gamma^{|\alpha|}((1 + |x|^2)^{1/2} - r)| \, M(r) dr \le C_{|\alpha|} \, h(x).$$

We claim that there exist a $\delta > 0$ and constants $c_{\alpha_1,...,\alpha_n} < \infty$, such that

$$|\overline{h^{\otimes n}}(x_1,..., x_n)| \ge \delta \prod_{i=2}^{n} g(x_i - x_1) \tag{A1}$$

and

$$|D_1^{\alpha_1}\cdots D_n^{\alpha_n} \overline{h^{\otimes n}}(x_1,..., x_n)| \le C_{\alpha_1\cdots\alpha_n} \overline{h^{\otimes n}}(x_1,..., x_n). \tag{A2}$$

For the first inequality remember that $h(x) \ge \text{const} f(x) \ge \text{const} \sup_{x=z+y} g(z)g(y)$, so

$$\int h(x_1 + a)\cdots h(x_n + a) da = \int h(a)h(x_2 - x_1 + a)\cdots h(x_n - x_1 + a) da \ge \left(\int h(a) g(a)^{n-1} da \right) \prod_{i=2}^{n} g(x_i - x_1),$$

and the second inequality follows from $|D^\alpha h| \le c_{|\alpha|}$.

Finally, the statement of the Lemma follows from (A1) and (A2) by induction over the degree of the differential operators, using the formula

$$0 = \sum_{\beta_1,...,\beta_n} \binom{\alpha_1}{\beta_1}\cdots\binom{\alpha_n}{\beta_n} D^{\beta_1}\cdots D^{\beta_n} (\overline{h^{\otimes n}})^{-1} D^{\alpha_1 - \beta_1} \cdots D^{\alpha_n - \beta_n} \overline{h^{\otimes n}}.$$

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The action of a general gauge field theory: Minimum or stationary

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Unless both the Cartan–Killing metric $(C_{\alpha\beta})$ and the space metric (g_{ij}) are positive definite, a solution of the field equations always represents a stationary value of the action and never a minimum or maximum. In the Euclidean case, with $(C_{\alpha\beta})$ positive definite, the action is a strict local minimum at a solution of the field equations. The validity of imposing certain gauge conditions is also discussed.

I. INTRODUCTION

Ever since the fundamental paper by Yang and Mills[1] on isotopic invariance, there has been considerable interest in gauge field theories from physicists and mathematicians. The literature is quite extensive, and Refs. 2–4 are a small selection of review articles. It is standard practice to use a calculus of variations approach, and the action functional $S[A]$ [defined in Eq. (3.3) below] is well known. The purpose of this paper is to find general conditions determining whether $S[A]$ is minimum, or whether a solution of the field equations is only a stationary point of $S[A]$. The problem has been investigated for the special case of self-dual or anti-self-dual solutions[4–6]; also the nonminimality of some Yang–Mills–Higgs solutions has been shown.[7] The technique to be used in this paper is a development of that used to study the action functional of general relativity.[8]

Section II is concerned with the calculus of variations. Notation and certain known results which will be used later are summarized. In Sec. III, these results are applied to a general gauge field theory. It will be shown that unless both the space metric and the Cartan–Killing metric are positive definite, the action functional $S[A]$ is never minimum.[9] The positive definite case requires a special method which necessitates the imposition of a Lorentz gauge condition. This matter is discussed in Sec. IV, and since gauge conditions are used elsewhere in gauge field theory, the conclusions of this section may be of wider interest. In Sec. V it is shown that $S[A]$ is strictly locally minimum in the positive definite case. The Conclusion (Sec. VI) summarizes the results obtained and suggests a possible area for further study.

The properties of the action are important to the Feynman path integral approach to quantum field theory,[10,11] and so the results obtained in this paper may be of relevance to the quantization of gauge field theories.[3,4]

II. THE CALCULUS OF VARIATIONS

Consider the action functional

$$S_\Omega[u] = \int_\Omega L\,(x^j; u^A; u^A{}_{,k})\, d^n x, \tag{2.1}$$

where the independent variables are $x^j = (x^1,\ldots,x^n)$, the dependent variables are $u^A = (u^1,\ldots,u^R)$, $u^A{}_{,k} = \partial u^A/\partial x^k$, and the domain $\Omega \subset \mathbb{R}^n$. It will be assumed throughout that both L and u are sufficiently smooth (say C^∞) functions of their arguments. The basic problem of the calculus of variations is to find those functions $u(x)$ such that $S_\Omega[u]$ is minimum or stationary. More precisely, consider $S_\Omega[\bar{u}] = S_\Omega[u+\epsilon\psi]$, where $\epsilon\psi^A(x)$ is a small variation in the sense that $1 \geqslant \epsilon > 0$ and $\sup_{A,i,\Omega}(|\psi^A(x)|, |\psi^A{}_{,i}(x)|) < 1$. The variation ψ must satisfy the boundary condition

$$\psi = 0 \quad \text{on the boundary} \quad \partial\Omega. \tag{2.2}$$

Now, $S_\Omega[\bar{u}]$ may be expanded as a Taylor series

$$S_\Omega[u+\epsilon\psi] = S^{(0)}_\Omega + \epsilon S^{(1)}_\Omega + \epsilon^2 S^{(2)}_\Omega + \cdots, \tag{2.3}$$

where

$$S^{(0)}_\Omega = S_\Omega[u], \tag{2.4}$$

$$S^{(1)}_\Omega[u,\psi] = \int_\Omega \left(\frac{\partial L}{\partial u^A}\psi^A + \frac{\partial L}{\partial u^A{}_{,k}}\psi^A{}_{,k} \right) d^n x, \tag{2.5}$$

$$S^{(2)}_\Omega[u,\psi] = \int_\Omega \left(\frac{1}{2}\frac{\partial^2 L}{\partial u^A\,\partial u^B}\psi^A\psi^B + \frac{\partial^2 L}{\partial u^A{}_{,k}\,\partial u^B}\psi^A{}_{,k}\psi^B + \frac{1}{2}\frac{\partial^2 L}{\partial u^A{}_{,k}\,\partial u^B{}_{,l}}\psi^A{}_{,k}\psi^B{}_{,l} \right) d^n x. \tag{2.6}$$

The following results are standard. The action $S_\Omega[u]$ is *stationary* (and the function u is called a critical point) if and only if $S^{(1)}_\Omega[u,\psi] = 0$, $\forall\psi$, and this condition is satisfied if and only if u satisfies the well-known Euler–Lagrange equations. The action $S_\Omega[u]$ is *strictly minimum* at u if and only if $S_\Omega[u+\epsilon\psi] > S_\Omega[u]$, $\forall\psi \neq 0$. Note that $S_\Omega[u]$ strictly minimum implies that both $S^{(1)}_\Omega[u,\psi] = 0$, $\forall\psi$ and $S^{(2)}_\Omega[u,\psi] \geqslant 0$, $\forall\psi \neq 0$, and also note that both $S^{(1)}_\Omega[u,\psi] = 0$, $\forall\psi$ and $S^{(2)}_\Omega[u,\psi] > 0$, $\forall\psi \neq 0$, imply that $S_\Omega[u]$ is strictly minimum at u.

At this stage it is useful to note a particular example, the simple harmonic oscillator in the time interval $(0,t_0)$. In this case $R = n = 1$ and

$$S = \int_0^{t_0} \frac{1}{2}(\dot{u}^2 - u^2)\, dt, \quad S^{(2)} = \int_0^{t_0} \frac{1}{2}(\dot{\psi}^2 - \psi^2)\, dt. \tag{2.7}$$

The minimum value of $S^{(2)}$ occurs when $\psi \propto \sin \pi t/t_0$, from which it is clear that $S^{(2)} > 0$, $\forall\psi$ if $t_0 < \pi$, and $S^{(2)}$ may be positive or negative if $t_0 > \pi$. In this example, $t = 0$ and $t = \pi$ are (Jacobi) conjugate points. It is therefore clear that whether $S_\Omega[u]$ is strictly minimum may depend upon the domain Ω. The following definition is made. The action $S_\Omega[u]$ is *locally strictly minimum* at u if and only if $\forall x_0 \in \Omega$, $\exists\, \Omega_0 \ni x_0$ such that S_{Ω_0} is strictly minimum.

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Conditions for $S_\Omega[u]$ to be minimum have been known for some time. Define

$$\tau = \xi_i \xi_j v^A v^B \frac{\partial^2 L(u)}{\partial u^A{}_{,i} \partial u^B{}_{,j}}, \quad \xi_i \in \mathbb{R}^n, \quad v^A \in \mathbb{R}^R. \tag{2.8}$$

Theorem 2.1 (Legendre–Hadamard condition): $S_\Omega[u]$ has a minimum at u implies that $\tau \geqslant 0$, $\forall \xi_i$, v^A, $x \in \Omega$.

The theorem is most useful in the converse sense, that is if it can be shown that $\exists \xi_i$, v^A such that τ can be both positive and negative, then $S_\Omega[u]$ cannot be minimum or maximum but is only stationary at the critical point u.

Theorem 2.2: Suppose that $\exists k > 0$ such that $\tau \geqslant k |\xi|^2 |v|^2$, $\forall \xi_i$, v^A, $x \in \Omega$, and suppose that u is a critical point, then $S_\Omega[u]$ is locally strictly minimum at u.

The above theorems are generalizations of Legendre's well-known result for the case $R = n = 1$, and are amply discussed in the literature.[12–15] Theorem 2.2 is a less general statement of Theorem 2 in Ref. 12.

III. GAUGE FIELD THEORY

In this section, Theorems 2.1 and 2.2 will be applied to the action integral of a general classical gauge field theory. The notation to be used will follow closely that in the recent review by Rund.[2] The gauge potentials are $A_i^\alpha(x)$, where $\alpha = 1,...,M$ and $i = 1,...,n$ with $n > 1$; thus there are M vector potentials. The gauge field is defined by

$$F_{hj}^\alpha = A_{[h,j]}^\alpha + C_{\epsilon\beta}^\alpha A_j^\epsilon A_h^\beta, \tag{3.1}$$

where $C_{\epsilon\beta}^\alpha$ is the structure constant of the Lie group. The Cartan–Killing metric is defined by

$$C_{\alpha\beta} = C_\alpha{}^\lambda{}_\mu \, C_\beta{}^\mu{}_\lambda, \tag{3.2}$$

and the action functional is

$$S_\Omega[A_h^\alpha, A_{h,j}^\alpha] = \frac{1}{4} C_{\alpha\beta} \int_\Omega F_{hj}^\alpha F_{kl}^\beta g^{hk} g^{jl} d^n x, \tag{3.3}$$

where g_{ij} is the metric on the space, which will be taken as flat so that $g_{ij} = \text{diag}(\pm 1,..., \pm 1)$. The quantities defined obey some symmetry properties:

$$C_{\epsilon\beta}^\alpha = -C_{\beta\epsilon}^\alpha, \quad F_{hj}^\alpha = -F_{jh}^\alpha, \quad C_{\alpha\beta} = C_{\beta\alpha}. \tag{3.4}$$

It is a straightforward exercise to calculate the quantity τ defined by Eq. (2.8). The result is

$$\tau = C_{\alpha\beta}\{(\mathbf{v}^\alpha \cdot \mathbf{v}^\beta)(\boldsymbol{\xi} \cdot \boldsymbol{\xi}) - (\mathbf{v}^\alpha \cdot \boldsymbol{\xi})(\mathbf{v}^\beta \cdot \boldsymbol{\xi})\}, \tag{3.5}$$

where $\cdot$ is the inner product defined by the metric g_{ij}, and $\boldsymbol{\xi}$ and $\mathbf{v}^\alpha$ are vectors $\in \mathbb{R}^n$. Since $C_{\alpha\beta}$ is symmetric, it may be diagonalized to $C'_{\gamma\gamma}$. Of course, the diagonalization process will also change $\mathbf{v}^\alpha \to \mathbf{v}'^\gamma$. But since $\mathbf{v}^\alpha$ is arbitrary, and since the transformation to diagonal form is an isomorphism, $\mathbf{v}'^\gamma$ is also arbitrary. Thus the $'$ may be dropped, and

$$\tau = \sum_\gamma C_{\gamma\gamma}\{(\mathbf{v}^\gamma \cdot \mathbf{v}^\gamma)(\boldsymbol{\xi} \cdot \boldsymbol{\xi}) - (\mathbf{v}^\gamma \cdot \boldsymbol{\xi})^2\}. \tag{3.6}$$

Applying Theorems 2.1 and 2.2 to Eq. (3.6) the following can be deduced.

(a) If the eigenvalues $C_{\gamma\gamma}$ of $C_{\alpha\beta}$ are both positive and negative, then τ can be both positive and negative and the action (3.3) is neither minimum nor maximum, but only stationary.

(b) If the signature $(g_{ij}) \neq n$, and $n \geqslant 3$, then consider, without loss of generality, the case $g_{11} = -g_{22} = -g_{33}$, and let (i) $v_1^\alpha = 1$, $\xi_2 = 1$, all other components 0: $\tau = -1$, (ii) $v_2^\alpha = 1$, $\xi_3 = 1$, all other components 0: $\tau = +1$. Thus, the action (3.3) is neither minimum nor maximum but is stationary. If $n = 2$ and signature $(g_{ij}) = 0$ then $\tau \leqslant 0$, with equality possible. The theorems do not determine whether a critical point is or is not a maximum.

(c) If all the eigenvalues $C_{\gamma\gamma}$ are positive, and if the metric g_{ij} is Euclidean [$= \text{diag}(1,...,1)$] then $\tau \geqslant 0$ with equality if and only if all the $\mathbf{v}^\gamma$ and $\boldsymbol{\xi}$ are parallel (that is there exist constants k^γ such that $\mathbf{v}^\gamma = k^\gamma \boldsymbol{\xi}$). Theorem 2.2 cannot be applied, and the action (3.3) may or may not be minimum. A direct method for considering this case will be given below.

IV. GAUGE CONDITIONS

Before proceeding further, it will be helpful to understand why Theorem 2.2 could not be applied in case (c) above. To this end, consider the simplest gauge field theory — electromagnetism. Writing a variation as $\bar{A}_i = A_i + \epsilon \mathscr{A}_i$,

$$S[\bar{A}] = \frac{1}{4} \int_\Omega \bar{A}^2_{[i,h]} d^4 x,$$

$$S^{(2)}[A, \mathscr{A}] = \frac{1}{4} \int_\Omega \mathscr{A}^2_{[i,h]} d^4 x. \tag{4.1}$$

(Because the metric is Euclidean, the indices i, j, k, etc. may be regarded as representing the components of a Cartesian tensor; all indices are written as covariant and the metric tensor is omitted.) Suppose the variation $\mathscr{A}$ is a gauge transformation, that is, for some scalar field ϕ

$$\mathscr{A}_i = \phi_{,i}. \tag{4.2}$$

Then clearly $S^{(2)}[A, \phi] = 0$ for nonzero variation ϕ. A general theorem on minimality must have $S^{(2)} > 0$ so that the higher-order variations, $S^{(3)}$, etc. may be ignored. It is because of the existence of gauge transformations that Theorem 2.2 could not be applied. [However, in the particular case of electromagnetism the semi-positive-definiteness of $S^{(2)}$ is sufficient to ensure (nonstrict) minimality of a critical point because the Lagrangian is quadratic in A, and so $S^{(p)} = 0$ for $p \geqslant 3$.]

It is therefore desirable to permit only those variations which are not gauge transformations; a gauge condition must be imposed. Since the problem in case (c) arises when the $\mathbf{v}^\gamma$ are parallel to $\boldsymbol{\xi}(\sim \partial/\partial x^i)$, it is natural to consider the gauge condition

$$A_{i,i}^\alpha = 0, \tag{4.3}$$

which is analogous to the Lorentz condition of electromagnetism. It is also known as the Landau gauge or the Hodge gauge.

Let $A_i^\alpha(x)$ be a given vector field, and suppose a gauge transformation described by M scalar fields $\mu^\alpha(x)$ is made, with $\mu^\alpha = 0$ being the identity transformation. Then we have (Ref. 2, Eq. 8.12)

$$A(\mu)_i^\alpha = G_\beta^\alpha(\mu) A_i^\beta - \lambda_\beta^\alpha(\mu) \mu^\beta{}_{,i}, \tag{4.4}$$

where $G_\beta^\alpha(0) = \lambda_\beta^\alpha(0) = \delta_\beta^\alpha$, and matrices G_β^α and λ_β^α are

always invertible. The gauge condition (4.3) may be imposed provided there exist $\mu(x)$ such that $A(\mu)^{\alpha}_{i,i} = 0$, i.e., such that

$$0 = \frac{\partial G^{\alpha}_{\beta}}{\partial \mu^{\epsilon}} \mu^{\epsilon}{}_{,i} A^{\beta}_{i} + G^{\alpha}_{\beta} A^{\beta}_{i,i} - \frac{\partial \lambda^{\alpha}_{\beta}}{\partial \mu^{\epsilon}} \mu^{\epsilon}{}_{,i} \mu^{\beta}{}_{,i} - \lambda^{\alpha}_{\beta} \mu^{\beta}{}_{,ii}, \tag{4.5}$$

equivalently

$$\mu^{\alpha}{}_{,ii} = \lambda^{-1\alpha}{}_{\gamma} \frac{\partial G^{\gamma}_{\beta}}{\partial \mu^{\epsilon}} \mu^{\epsilon}{}_{,i} A^{\beta}_{i} + \lambda^{-1\alpha}{}_{\gamma} G^{\lambda}_{\beta} A^{\beta}_{i,i} - \lambda^{-1\alpha}{}_{\gamma} \frac{\partial \lambda^{\gamma}_{\beta}}{\partial \mu^{\epsilon}} \mu^{\epsilon}{}_{,i} \mu^{\beta}{}_{,i}. \tag{4.6}$$

Equation (4.6) has a linear approximation about $\mu = 0$

$$\mu^{\alpha}{}_{,ii} = C^{\alpha}_{\beta\epsilon} \mu^{\epsilon}{}_{,i} A^{\alpha}_{i} + A^{\alpha}_{i,i} + A^{\beta}_{i,i} \mu^{\epsilon} (C^{\alpha}_{\beta\epsilon} + a^{\alpha}_{\beta\epsilon}). \tag{4.7}$$

The existence of a local solution to a nonlinear elliptic system of partial differential equations has been considered by Morrey[13] (pp. 266–277), and it may be asserted that given $\mu^{\alpha} = 0$ at a point $x_0 \in \Omega$, $\exists$ a solution $\mu^{\alpha}(x)$ to equation (4.6) in a neighborhood $\Omega_0 \ni x_0$. The problem of existence and uniqueness of a global solution to (4.6) is much more difficult, and henceforth attention will be confined to the linear approximation (4.7). It may be asserted that, under suitable smoothness conditions, the Dirichlet problem for Eq. (4.7) in a bounded domain Ω has a solution, and further, provided Ω is small enough, the solution is unique.[16] [The solution to (4.7) is not unique if Ω is sufficiently large; this is the Gribov effect.[17]]

V. THE EUCLIDEAN CASE: THE ACTION IS LOCALLY MINIMIZED

In this section it will be shown that the unsolved case (c) of Sec. III is in fact a strict local minimum. The domain of integration will be Ω_0, which will be considered as small so that the gauge condition (4.3) may be imposed. The norm $\| \ \|_{L_2(\Omega_0)}$ will be written for brevity as $\| \ \|$. Let $A^{\alpha}_{i}(x)$ be a critical point and let $\bar{A}^{\alpha}_{i}(x)$ be a variation, both satisfying the gauge condition (4.3). (Because the action is gauge invariant, $S_{\Omega_0}[A]$ and $S_{\Omega_0}[\bar{A}]$ may be evaluated in any convenient gauge.) Let the variation $\mathscr{A}^{\alpha}_{i}$ be defined by $\bar{A}^{\alpha}_{i} = A^{\alpha}_{i} + \epsilon \mathscr{A}^{\alpha}_{i}$, so that $\mathscr{A}$ also obeys the gauge condition

$$\mathscr{A}^{\alpha}_{i,i} = 0. \tag{5.1}$$

By Eq. (2.1),

$$\mathscr{A}^{\alpha}_{i} = 0 \quad \text{on} \quad \partial \Omega_0, \tag{5.2}$$

and the following lemma may be proved.

Lemma 5.1: Given conditions (5.1) and (5.2), then

$$\| \mathscr{A}^{\alpha}_{[k,j]} \|^2 = \tfrac{1}{2} \| \mathscr{A}^{\alpha}_{k,j} \|^2. \tag{5.3}$$

Proof: Consider

$$\| \mathscr{A}^{\alpha}_{[k,j]} \|^2 - \| \mathscr{A}_{(k,j)} \|^2 = \sum_{\alpha} \int_{\Omega_0} \mathscr{A}^{\alpha}_{[k,j]}{}^2 - \mathscr{A}^{\alpha}_{(k,j)}{}^2 \, d^n x, \tag{5.4}$$

which after a short calculation reduces to

$$\begin{aligned} &- \sum_{\alpha} \int_{\Omega_0} \mathscr{A}^{\alpha}_{k,j} \mathscr{A}^{\alpha}_{j,k} \, d^n x \\ &= \sum_{\alpha} \int_{\Omega_0} - (\mathscr{A}^{\alpha}_{j} \mathscr{A}^{\alpha}_{k,j})_{,k} + \mathscr{A}^{\alpha}_{j} \mathscr{A}^{\alpha}_{k,jk} \, d^n x \\ &= \sum_{\alpha} \int_{\partial \Omega_0} - \mathscr{A}^{\alpha}_{j} \mathscr{A}^{\alpha}_{k,j} n_k \, d^{n-1} x \\ &\quad + \sum_{\alpha} \int_{\Omega_0} \mathscr{A}^{\alpha}_{j} (\mathscr{A}^{\alpha}_{k,k})_{,j} \, d^n x. \end{aligned} \tag{5.5}$$

The first term is zero by condition (5.2) and the second term is zero by condition (5.1). Hence $\| \mathscr{A}^{\alpha}_{[k,j]} \|^2 = \| \mathscr{A}^{\alpha}_{(k,j)} \|^2$. Now,

$$\| \mathscr{A}^{\alpha}_{k,j} \|^2 = \| \mathscr{A}^{\alpha}_{[k,j]} + \mathscr{A}^{\alpha}_{(k,j)} \|^2 = \| \mathscr{A}^{\alpha}_{[k,j]} \|^2 + \| \mathscr{A}^{\alpha}_{(k,j)} \|^2,$$

and the stated result follows.

The main result may now be proved:

$$S^{(2)}_{\Omega}[A, \mathscr{A}] = \frac{1}{4} C_{\alpha\beta} \int_{\Omega_0} \mathscr{A}^{\alpha}_{[j,k]} \mathscr{A}^{\beta}_{[j,k]} + O(\mathscr{A}^2, \mathscr{A} \nabla \mathscr{A}) \, d^n x. \tag{5.6}$$

Diagonalizing $C_{\alpha\beta}$, the variation $\mathscr{A}$ is transformed linearly to $\mathscr{A}'$, and therefore conditions (5.1) and (5.2) remain satisfied by $\mathscr{A}'$:

$$S^{(2)}_{\Omega_0}[A, \mathscr{A}'] = \frac{1}{4} \sum_{\gamma} C_{\gamma\gamma} \int_{\Omega_0} \mathscr{A}'^{\gamma}_{[j,k]}{}^2 + O(\mathscr{A}'^2, \mathscr{A}' \nabla \mathscr{A}') d^n x. \tag{5.7}$$

Let $8k > 0$ be the smallest value of $C_{\gamma\gamma}$. Then

$$\begin{aligned} S^{(2)}_{\Omega_0}[A, \mathscr{A}'] &\geqslant 2k \| A'^{\gamma}_{[j,k]} \|^2 + \int_{\Omega_0} O(\mathscr{A}'^2, \mathscr{A}' \nabla \mathscr{A}') \, d^n x \\ &= k \| A'^{\gamma}_{j,k} \|^2 + \int_{\Omega_0} O(\mathscr{A}'^2, \mathscr{A}' \nabla \mathscr{A}') \, d^n x, \end{aligned} \tag{5.8}$$

by the lemma proved above. By Holder's inequality[18] the order term above may be written

$$\int_{\Omega_0} O(\mathscr{A}'^2, \mathscr{A}' \nabla \mathscr{A}') \, d^n x = O(\| \mathscr{A}' \|^2, \| \mathscr{A}' \| \, \| \nabla \mathscr{A}' \|). \tag{5.9}$$

By Poincaré's inequality (Ref. 13, p. 69), $\| \mathscr{A}' \| \leqslant a \| \mathscr{A}' \|$, where a is the radius of the smallest ball that can contain Ω_0. Hence

$$S^{(2)}_{\Omega_0}[A, \mathscr{A}'] \geqslant \| \nabla \mathscr{A}' \|^2 (k + O(a^2, a)). \tag{5.10}$$

Thus for a small enough, $S^{(2)}_{\Omega_0}[A, \mathscr{A}'] > 0$ for $\mathscr{A}' \neq 0$ (and $\mathscr{A}' \neq 0 \Rightarrow \mathscr{A} \neq 0$), so that the critical point A is a strict local minimum of the action.

VI. CONCLUSION

It has been shown that [apart from the special but uninteresting case $n = 2$ and signature $(g_{ij}) = 0$], unless both the Cartan–Killing metric $C_{\alpha\beta}$ and the space metric g_{ij} are positive definite, the action $S_{\Omega}[A]$ is never minimum or maximum but is only stationary at a critical point A. In the latter case it has been shown that a critical point is a strict local minimum of the action.

It may or may not be possible to remove the "local" requirement, that is, to show that the action is strictly mini-

mum for any domain of integration Ω. This would be a much more difficult problem because, in the local case, the solution of the field equations $A_i^{\alpha}(x)$ can be ignored; S_2 is essentially a functional only of the variation $\mathscr{A}$. In the global case this would not be true and, at the very least, some properties of $A_i^{\alpha}(x)$ would have to be taken into account.

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Surface integrals in lower dimensions from higher-order Chern classes and a class of solutions in three dimensions

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It is shown that surface integrals, involving gauge and Higgs fields, in both odd and even dimensions can be obtained by dimensional reduction from Chern classes in higher dimensions. For odd dimensions, the physically useful dimensional reduction is characterized by $\mathcal{M}_N = E_{N-p} \times S^p$, and for even dimensions by $\mathcal{M}_N = E_{N-p} \times S^2 \times \cdots \times S^2$ ($\frac{1}{2}p$ times). The existence of a family of field configurations for which these surface integrals in three dimensions exist, and are nonzero, is presented. This family includes a Yang–Mills–Higgs (YMH) system with an algebra-valued Higgs field and one with the Higgs field in the reducible representation adjoint ⊕ scalar.

I. INTRODUCTION

The relationship between finite action (energy) solutions of classical gauge field theories and the topological properties of the same theories has been recognized since the discovery of monopole[1] and instanton[2] solutions. These topological properties derive from certain topological invariants, which, subject to normalization, have an integer spectrum—for example, the monopole charge and the Pontryagin index. In turn these topological invariants are expressed as surface integrals, whose values are determined by the asymptotic properties of the relevant classical field configurations. For instantons, the second Chern class

$$q^2 \simeq \epsilon_{\mu\nu\rho\sigma} \int \operatorname{tr} F_{\mu\nu} F_{\rho\sigma}\, d_4x \tag{1.1}$$

leads to the Pontryagin index by normalization. The corresponding surface integral is given by the Chern–Simons formula

$$q^{(2)} \simeq \epsilon_{\mu\nu\rho\sigma} \int \partial_\mu \operatorname{tr} A_\nu \left(F_{\rho\sigma} - \frac{2}{3} A_\rho A_\sigma \right) d_4x. \tag{1.1'}$$

In this case, the relevant asymptotic behavior of A_μ is

$$A_\mu(x) \underset{|x| \to \infty}{\to} \partial_\mu g g^{-1}, \tag{1.2}$$

where $g \in G$, and G is the gauge group. Clearly then, only the last term of the integrand in (1.1′) contributes on an infinitely large surface. Using an explicit parametrization of $g \in G$, it can be shown that the integrand in (1.1′) is the Jacobian for the transformation of x_μ to the coordinates of S^3 and that carrying out the angular integrations gives rise to the normalization factor times an integer.

Indeed, field configurations satisfying the condition (1.2) have been found as the (self-dual) solutions[2] of the Yang–Mills (YM) system. It is natural, then, to expect other gauge field configurations to be associated with the higher-order Chern classes $q^{(N/2)}$, for even N-dimensional manifolds.

In the cases of six- and eight-dimensional manifold (which we shall be discussing in detail) the corresponding Chern classes are

$$q^{(3)} \simeq i\epsilon_{M_1M_2\cdots M_6} \int d_6x \operatorname{tr} F_{M_1M_2} F_{M_3M_4} F_{M_5M_6}, \tag{1.3a}$$

$$q^{(4)} \simeq \epsilon_{M_1\cdots M_8} \int d_8x \operatorname{tr} F_{M_1M_2} \cdots F_{M_7M_8}, \tag{1.3b}$$

and in Chern–Simons form they can be written

$$\begin{aligned} q^{(3)} \simeq i\epsilon_{M_1\cdots M_6} \int d^6x\, \partial_{M_1} \operatorname{tr} A_{M_2} [& F_{M_3M_4} F_{M_5M_6} \\ & - A_{M_3} A_{M_4} F_{M_5M_6} + \tfrac{2}{5} A_{M_3} A_{M_4} A_{M_5} A_{M_6}], \end{aligned} \tag{1.3a'}$$

$$\begin{aligned} q^{(4)} \simeq \epsilon_{M_1\cdots M_8} \int d^8x\, \partial_{M_1} \operatorname{tr} A_{M_2} [& F_{M_3M_4} F_{M_5M_6} F_{M_7M_8} \\ & - \tfrac{4}{5} F_{M_3M_4} F_{M_5M_6} A_{M_7} A_{M_8} - \tfrac{2}{5} F_{M_3M_4} A_{M_5} F_{M_6M_7} A_{M_8} \\ & + \tfrac{4}{5} F_{M_3M_4} A_{M_5} A_{M_6} A_{M_7} A_{M_8} \\ & - \tfrac{4}{35} A_{M_3} A_{M_4} A_{M_5} A_{M_6} A_{M_7} A_{M_8}]. \end{aligned} \tag{1.3b'}$$

The factors of i occur in (1.3a) and (1.3a′) because we are using anti-Hermitian representations of $\mathcal{G}$, the algebra of G.

The question as to whether there exist field configurations over the N-dimensional manifold with the property (1.2), and for *what* dynamical systems these occur, does not interest us directly in this paper. A preliminary investigation into that question is presented in Ref. 3. In this paper we are interested in the physically relevant dimensions $N = 2,3$, and 4, as far as the dynamical gauge field systems are concerned. It is for this reason that the calculus of dimensional reduction is an indispensable tool for what follows.

Indeed, the monopole[1] solutions of the Yang–Mills–Higgs (YMH) system are characterized by their magnetic

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charge, which is a surface integral derived from the second Chern class[1] by dimensional reduction. Here the four-dimensional manifold may be regarded as $\mathcal{M}_4 = E_3 \times S^1$, with x_i $(i = 1,2,3)$ the coordinates of E_3. Then, requiring that $A_M = (A_i, A_4)$ be symmetric under the SO(2) subgroup of G is actually equivalent to requiring that A_M be independent of x_4, the coordinate on S^1. The field $A_4 = \Phi$ is identified as the Higgs field, which takes its values in $\mathcal{G}$. Reduction of the second Chern class (1.1) in this manner leads to the expression

$$q^{(2)} \simeq \epsilon_{ijk} \int d_3x \ \mathrm{tr}\ \Phi F_{jk}, \tag{1.1''}$$

where the integration over x_4 has been performed. This is the well-known monopole charge of the YMH system. When this dimensional reduction is performed on the four-dimensional YM Lagrangian, one obtains the three-dimensional YMH Lagrangian *without* a Higgs potential term. The existence of finite energy solutions is guaranteed by imposing the *finite energy condition*

$$D_i \Phi \underset{r \to \infty}{\to} 0, \tag{1.2'}$$

which is the analog of (1.2). The absence of a Higgs potential is not harmful, as long as the Higgs fields "remember" that they have to satisfy (1.2'), and hence that

$$\mathrm{tr}\ \Phi^2 \underset{r \to \infty}{\to} \eta^2 = \mathrm{const.} \tag{1.2''}$$

Many solutions of this type, for $G = \mathrm{SU}(2)$, are known.[4] These are the self-dual solutions obeying the Bogomolnyi[5] equations. Indeed the Bogomolnyi equations themselves can be obtained from the YM self-duality equations using the above dimensional reduction. These, however, are not the only field configurations for which the surface integral (1.1'') is nonzero. There are non-self-dual[1,6] field configurations of the YMH system with a nonvanishing Higgs potential that are known to have magnetic charge (1.1'') and finite energy. This is in contrast with the situation for the YM system in four dimensions, where only self-dual solutions are known to exist.[2,7]

Thus, in a gauge field system endowed with a Higgs field, the surface integral (1.1'') has a central role to play. On the other hand the condition (1.2') implies that the asymptotic value of the Higgs field may be one of the several diagonal elements of $\mathcal{G}$. Throughout the following we shall suppose that $G = \mathrm{SU}(n)$, for the sake of illustration. As such, there are $(n-1)$ different possible Higgs vaccua satisfying (1.2'). Again YMH configurations of this type are known to exist,[6,8] and the self-dual[8] ones are known explicitly.

It is to describe the "magnetic" charges of such solutions, that Taubes[9] generalized the formula (1.1'') to

$$q_{(k)} \simeq \epsilon_{ijk} \int d_3x \ \mathrm{tr}\ \Phi^k F_{jl}, \tag{1.1'''}$$

$k = 1,\ldots,(n-1)$ for $\mathrm{SU}(n)$.

In a recent article,[10] we have shown that the surface integrals (1.1''') are obtained from a dimensional reduction of the higher Chern classes (1.3a) and (1.3b). The dimensional reduction in question from six(eight) to three dimensions reduces a SU(nm) gauge field theory over six(eight) dimensions, with gauge field A_M, down to a SU(n) gauge field Higgs system, with fields (A_i, Φ), over three dimensions. More precisely we have shown that the higher Chern classes (1.3a) and (1.3b), which are surface integrals in N dimensions by virtue of their Chern–Simons formulas (1.3a') and (1.3b'), reduce, subject to some symmetries, to surface integrals on the three-dimensional manifold and that these surface integrals involve the various Taubes invariants (1.1''').

In the present paper we wish to extend the analysis begun in our earlier article in a number of directions. (i) In the earlier work we concentrated on a reduction to three-dimensional manifolds. Now we will include the reduction to any odd-dimensional submanifold. (ii) The surface integrals of Taubes (1.1''') are written in terms of an adjoint representation Higgs field. By extending our analysis to include dimensional reduction schemes in which the Higgs field belongs to other irreducible representations, or even reducible representations, we extend the definition of the Taubes invariants (1.1''') to these cases also. (iii) We also extend the analysis to include the reduction of the higher Chern classes to lower *even*-dimensional manifolds, an example of which is the relationship between the second Chern class in four dimensions, $\mathcal{M}_4 = E_2 \times S^2$, and the vortex number[11,12] expressed as a surface integral in two dimensions. (iv) The final aim of the paper is to present a class of non-self-dual solutions of the SU(n) YMH system in three dimensions, endowed with topological integrals of the type (1.1''').

Throughout the paper the calculus of dimensional reduction used is that of Schwarz and Tyupkin (ST),[13] who developed the method of Forgács and Manton.[14] These dimensional reduction schemes are designed to yield a genuine symmetry breaking type of Higgs potential in the residual gauge Higgs field theory. These potentials ensure that the modulus of the Higgs field has nonzero vacuum values, which in turn can guarantee that there exist classical field configurations with finite action/energy. It is not a coincidence, therefore, that we employ the ST reduction scheme, since on very general grounds we would expect that the existence of the (topological) surface integrals is linked to the existence of regular finite action/energy solutions of the corresponding Euler–Lagrange equations.

In Sec. II we review the ST dimensional reduction scheme, and adapt it to suit our particular needs. For pedagogical reasons, we restrict the presentation to that of the reduction by an odd number of dimensions. In Sec. III we apply this method to the reduction of Chern classes to *odd*-dimensional manifolds, with particular emphasis on E_3 and E_5. Section IV is given over to the study of the reduction of the higher Chern classes to *even*-dimensional manifolds. In this section we further adapt the formalism of dimensional reduction by an *odd* number of steps given in Sec. II, to apply also to reduction by an *even* number of steps. In Sec. V we present a class on non-self-dual solutions to the YMH system in three dimensions, for the cases where the Higgs field belongs to the adjoint representation and where the Higgs field belongs to the adjoint $\oplus$ scalar representation. Section VI contains a discussion of our results.

We hope that our results, apart from their intrinsic interest, will be useful in the study of anomalies[15] as well.

II. DIMENSIONAL REDUCTION

By means of the procedure of dimensional reduction it is possible to contain within the formalism of a simple field theory over N dimensions the formalism of a field theory with more complicated structure over $N-p$ dimensions, where $p>0$. This procedure has proved very useful in gravity (the Kaluza–Klein theories), supergravity and, indeed, gauge theories in general. Interest in recent years in the application of dimensional reduction to gauge theories has been sparked by the work of Lohe, Forgács–Manton,[14] and Schwarz–Tyupkin.[13]

The basic idea of the MF and ST methods is that we start with a pure gauge theory on an N-dimensional manifold $\mathscr{M}_N$, whose topology we specify as that of the Cartesian product of an $(N-p)$-dimensional (flat) Euclidean manifold and a p sphere,

$$\mathscr{M}_N = E_{N-p}\times S^p. \tag{2.1}$$

The gauge fields are denoted by $A_M=(A_\mu,\ A_a)$ for $\mu=1,\ldots,N-p$ and $a=1,\ldots,p$. The dependence of the gauge fields on the coordinates x_a of S^p is determined by the requirement of spherical symmetry on S^p, i.e., A_M, after a SO$(p+1)$ rotation on S^p, is gauge equivalent to the gauge field before the rotation.

In this work we prefer to use the ST scheme. This method is distinguished from that of MF in that it makes use of a fixed point calculus previously developed by Schwarz[16] and others for three-dimensional spherical symmetry. In addition to its intrinsic elegance and efficiency the ST method can be adapted straightforwardly to reduction by an arbitrary number of dimensions. This we now present.

One of the features of these dimensional reduction methods applied to gauge theories is that, though we begin with a gauge group K over $\mathscr{M}_N$, after reduction to E_{N-p} the residual gauge group is a subgroup of K—the dimensional reduction procedure itself breaks the gauge group.

To illustrate the ST method let us start with a gauge group SU(nm), where n and m are integers whose relevance will become apparent shortly. To write down the conditions for spherical symmetry we must specify a homomorphism from the SO$(p+1)$ defined over S^p to a SO$(p+1)$ subgroup of SU(nm). If we denote the fixed point of S^p by ξ, with stability group SO(p), then the conditions for spherical symmetry can be written in terms of SO(p), rather than SO$(p+1)$, as shown in Ref. 13:

$$A_\mu(x_\mu,\xi_a)=\mu(h)A_\mu(x_\mu,\xi_a)\mu^{-1}(h), \tag{2.2}$$

$$A_a(x_\mu,\xi_a)=h^{\ b}_a\mu(h)A_b(x_\mu,\xi_a)\mu^{-1}(h), \tag{2.3}$$

where μ maps the stability group SO(p) into the gauge group SU(nm), i.e., $\mu(h)\in$ SU(nm) for $h\in$ SO(p).

The structure of the dimensionally reduced theory (its gauge group and field content) are determined by the following three steps: (i) make a particular choice of the mapping μ; (ii) solve Eq. (2.2)—this will define the residual gauge group; and (iii) solve Eq. (2.3)—this will define the field content.

(i) Choice of μ: For $h\in$ SO(p), $\mu(h)$ is an $nm\times nm$ matrix. The canonical choice for μ is

$$\mu(h)=\mathbf{1}_n\otimes\hat{\mu}(h), \tag{2.4}$$

where $\hat{\mu}(h)$ is an $m\times m$ matrix representation of SO(p). In fact this is the simplest possibility. More complicated embeddings are considered in Ref. 13 but, as we shall see shortly, it is possible to achieve the same results starting with a mapping such as (2.4).

(ii) Choice of gauge group: If we use the form of $\mu(h)$ given by (2.4) in Eq. (2.2) then it is clear that the solution will be of the form

$$A_\mu(x,\xi)=\mathscr{A}_\mu(x)\otimes\mathbf{1}_m, \tag{2.5}$$

where $\mathscr{A}_\mu(x)$ is an $n\times n$ anti-Hermitian traceless matrix and $\mathbf{1}_m$ is the $m\times m$ unit matrix. One solution corresponds to $\mathscr{A}_\mu(x)\in$ su(n) giving rise to SU(n) as the residual gauge group. This solution, however, it not unique.

(iii) Choice of field content: In view of the structure of $\mu(h)$ in (2.5) the solution of (2.3) can be written in the form

$$A_a(x,\xi)=\chi(x)\otimes\hat{\Gamma}_a, \tag{2.6}$$

where $\hat{\Gamma}_a$ are $m\times m$ numerical tensors (essentially Clebsch–Gordan coefficients), which satisfy the equation

$$\hat{\mu}(h)\hat{\Gamma}_a\hat{\mu}^{-1}(h)=h^{\ b}_a\hat{\Gamma}_b, \tag{2.7}$$

and $\chi(x)$ is an $n\times n$ spin-0 field. Equation (2.7) was solved in detail for the case $p=3$, i.e., $h\in$ SO(3), in Ref. 13. For the purposes of generalizing to $p>3$, however, it is more useful to make use of a particular solution of (2.7) that generalizes to arbitrary p, namely

$$\hat{\Gamma}_a=iL_{a,p+1}, \tag{2.8}$$

where $\{L_{ab},L_{a,p+1}\}$ is the $m\times m$ Γ matrix generated representation of SO$(p+1)$ (Appendix A). It is clear that this choice of $\hat{\Gamma}_a$ establishes the role of the integer m,

$$m=\begin{cases}2^{(1/2)(p-1)}, & p \text{ odd},\\ 2^{(1/2)p}, & p \text{ even}.\end{cases} \tag{2.9}$$

The $n\times n$ spin-0 field $\chi(x)$ can be decomposed into irreducible representations of the residual gauge group. *For example,* let us consider the case of SU(n). Denoting the spin-0 field by $\phi(x)$ in this case, we note that since the $\hat{\Gamma}_a$ are traceless it follows that $\phi(x)$ is not necessarily traceless. In fact, we can write

$$\phi=\Phi+\Theta\mathbf{1}_n,\quad \Theta=(1/n)\operatorname{tr}\phi, \tag{2.10}$$

where Φ belongs to the adjoint representation of su(n) and Θ to the scalar representation. Other possibilities will be considered shortly.

Having solved the spherical symmetry conditions (2.1) and (2.4) at the fixed point, there remains to evaluate the components of $F_{MN}(x,\xi)$. For this we need the derivatives $\partial_\mu A_\nu,\partial_\mu A_a,\partial_a A_\mu$, and $\partial_a A_b$ evaluated at the fixed point. Following the infinitesimal analysis of Refs. 13 and 16 we see that

$$\begin{aligned}&\partial_\mu A_\nu(x,\xi)=\partial_\mu A_\nu\otimes\mathbf{1}_m,\\ &\partial_\mu A_a(x,\xi)=\partial_\mu\chi\otimes\hat{\Gamma}_a,\\ &\partial_a A_\mu(x,\xi)=0,\\ &\partial_a A_b(x,\xi)=-\tfrac{1}{2}\eta^2 f_{ab\alpha}T_\alpha,\end{aligned} \tag{2.11}$$

where η^2 is a dimensional parameter ($1/\eta$ is the radius of S^p) and T_α are the generators of so(p) in the representation μ.

Clearly, then,

$$T_\alpha = \mathbf{1}_n \otimes \hat{T}_\alpha, \tag{2.12}$$

where $\hat{T}_\alpha$ are the SO(p) generators in the representation $\hat{\mu}$. The numerical tensors f_{abc} are structure constants which occur in the following way: If $\{\hat{h}_\alpha, \alpha = 1,\ldots,\frac{1}{2}p(p-1)\}$ denote the SO(p) generators and $\{\hat{v}_a, a = 1,\ldots,p\}$ denote the generators of the orthogonal complement of so(p) in so($p+1$), then

$$[\hat{v}_a, \hat{v}_b] = f_{abc}\hat{h}_\alpha + f_{abc}\hat{v}_c. \tag{2.13}$$

With our choice of SO($p+1$) generators (cf. Appendix A) we see that $\partial_a A_b$ can be written as

$$\partial_a A_b(x,\xi) = -\tfrac{1}{2}\eta^2 \mathbf{1}_n \otimes L_{ab}. \tag{2.14}$$

A. Residual gauge group SU(n): Field strengths

The components of the field strength $F_{MN}(x,\xi)$ can now be written down for the case when the residual gauge group is SU(n):

$$\begin{aligned} F_{\mu\nu}(x,\xi) &= \mathcal{F}_{\mu\nu} \otimes \mathbf{1}_m, \\ F_{\mu a}(x,\xi) &= \mathcal{D}_\mu \phi \otimes \hat{\Gamma}_a, \\ F_{ab}(x,\xi) &= -(\eta^2 \mathbf{1}_n + \phi^2) \otimes L_{ab}, \end{aligned} \tag{2.15}$$

where

$$\begin{aligned} \mathcal{F}_{\mu\nu}(x) &= \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu + [\mathcal{A}_\mu, \mathcal{A}_\nu], \\ \mathcal{D}_\mu \phi(x) &= \partial_\mu \phi + [\mathcal{A}_\mu, \phi]. \end{aligned} \tag{2.16}$$

Thus we see that the reduced model over E_{N-p} will consist of a SU(n) gauge field $\mathcal{A}_\mu(x)$ interacting with spin-0 fields Φ and Θ in the adjoint and scalar representations of SU(n), respectively.

B. Residual gauge group SU($n-1$)×U(1): Field strengths

As an illustration of the wide range of models over E_{N-p} that this method can give rise to, let us return to step (ii) above and make use of a different solution of Eq. (2.2), namely,

$$A_\mu(x,\xi) = \left[\begin{array}{c|c} \mathcal{A}_\mu(x) & 0 \\ \hline 0 & ia_\mu(x) \end{array}\right] \otimes \mathbf{1}_m. \tag{2.17}$$

Here $\mathcal{A}_\mu(x)$ is an anti-Hermitian SU($n-1$) gauge field while $a_\mu(x)$ is a Hermitian U(1) gauge field. This solution corresponds to the residual gauge group SU($n-1$)×U(1).

It is now appropriate to examine the solution to Eq. (2.3)

$$A_a(x,\xi) = \chi(x) \otimes \hat{\Gamma}_a,$$

with a view to decomposing $\chi(x)$ into irreducible SU($n-1$) multiplets. We find

$$\chi(x) = \left[\begin{array}{c|c} \phi(x) & -i\psi(x) \\ \hline -i\psi^\dagger(x) & \beta(x) \end{array}\right], \tag{2.18}$$

where $\psi(x)$ belongs to the fundamental representation of SU($n-1$), $\phi(x)$ can be decomposed as $\phi(x) = \Phi(x) + \Theta(x)\mathbf{1}_{n-1}$ with Φ and Θ belonging to the adjoint and scalar representations of SU($n-1$), respectively, $\beta(x)$ belongs to the scalar representation of SU($n-1$) and the factors of i are for Hermiticity reasons. The field strengths then are given by

$$\begin{aligned} F_{\mu\nu}(x,\xi) &= \left[\begin{array}{c|c} F_{\mu\nu} & 0 \\ \hline 0 & if_{\mu\nu} \end{array}\right] \otimes \mathbf{1}_m, \\ F_{\mu a}(x,\xi) &= \left[\begin{array}{c|c} \mathcal{D}_\mu \phi & -i\mathcal{D}_\mu \psi \\ \hline -i(\mathcal{D}_\mu \psi)^\dagger & \partial_\mu \beta \end{array}\right] \otimes \hat{\Gamma}_a, \\ F_{ab}(x,\xi) &= -(\eta^2 \mathbf{1}_n + \chi^2) \otimes L_{ab}, \end{aligned} \tag{2.19}$$

where $\mathcal{F}_{\mu\nu}$ and $\mathcal{D}_\mu \phi$ are defined as in (2.16), but now are $(n-1)\times(n-1)$ matrices,

$$\begin{aligned} \mathcal{D}_\mu \psi &= \partial_\mu \psi + (\mathcal{A}_\mu - ia_\mu \mathbf{1}_{n-1})\psi, \\ f_{\mu\nu} &= \partial_\mu a_\nu - \partial_\nu a_\mu, \end{aligned} \tag{2.20}$$

and

$$\begin{aligned} \chi^2 &= \left[\begin{array}{c|c} \phi & -i\psi \\ \hline -i\psi^\dagger & \beta \end{array}\right]^2 \\ &= \left[\begin{array}{cc} \phi^2 - \psi\psi^\dagger & -i(\phi\psi + \beta\psi) \\ -i(\psi^\dagger\phi + \beta\psi^\dagger) & \beta^2 - \psi^\dagger\psi \end{array}\right]. \end{aligned} \tag{2.21}$$

In this case the reduced model is a SU($n-1$)×U(1) gauge model with spin-0 fields in the scalar, fundamental and adjoint representations of SU($n-1$). We notice that if we wish to end up with a SU(n)×U(1) gauge model over E_{N-p}, we should start the procedure with an SU($(n+1)m$) gauge theory over $\mathcal{M}_N$, with $m = 2^{(1/2)(p-1)}$.

C. General dimensional reduction procedure

On the basis of these two illustrative examples it is clear that we can summarize the dimensional reduction procedure as follows.

(1) We begin with a pure gauge field theory defined over $\mathcal{M}_N = E_{N-p} \times S^p$, with gauge group K. The choice of gauge group K depends on what we want as residual gauge group over E_{N-p}, and it also depends on the reduction procedure.

(2) We specify that the gauge fields over $\mathcal{M}_N$ are *spherically symmetric* over S^p, i.e., a rotation on S^p leads to a gauge equivalent gauge field, which gives us conditions on the gauge fields.

(3) We make a particular choice of mapping μ: SO(p) $\to K$. Taken in conjunction with the conditions on the gauge fields [such as (2.2) and (2.3)] the effect of this choice is to cause some matrix elements of A_μ and A_a to vanish. This choice defines (i) the *maximal* residual gauge group R_M (defined by matrix elements of A_μ not required to vanish) and (ii) the *maximal* spin-0 field content in the reduced theory (corresponding to those matrix elements of A_a not required to vanish).

(4) We make a particular choice of residual gauge group. We can choose, in effect, *any subgroup R of R_M*. This corresponds to choosing nonzero matrix elements of A_μ appropriate to R.

(5) We make a choice of spin-0 field content. Given the gauge group R we can decompose into irreducible representations of R the matrix elements of A_a, which remain after (3) above. According to our needs, we may choose to set certain of the spin-0 representation fields to vanish. Indeed, we can set scalar representations to be constant without violating the residual gauge symmetry.

To illustrate this point, we consider the second example discussed above where $K = \mathrm{SU}(nm)$ and

$R = \mathrm{SU}(n-1)\times\mathrm{U}(1)$. In this case we could choose the adjoint representation Φ to vanish and the scalar representations Θ and β to be constant over E_{N-p}. Indeed Θ and β are both scalar representations of $\mathrm{SU}(n-1)$, while under the U(1) transformations with parameter α we see that

$$\begin{bmatrix} \Phi+\Theta\mathbf{1} & -i\psi \\ -i\psi^\dagger & \beta \end{bmatrix} \underset{\alpha}{\to} \begin{bmatrix} \Phi+\Theta\mathbf{1} & -ie^{in\alpha}\psi \\ -ie^{-in\alpha}\psi^\dagger & \beta \end{bmatrix},$$

i.e., Θ and β do not transform under the $\mathrm{SU}(n-1)\times\mathrm{U}(1)$ gauge group. In that case the components of the field strength tensor would be

$$\begin{aligned} F_{\mu\nu}(x,\xi) &= \begin{bmatrix} \mathscr{F}_{\mu\nu} & 0 \\ 0 & if_{\mu\nu} \end{bmatrix} \otimes \mathbf{1}_m, \\ F_{\mu a}(x,\xi) &= \begin{bmatrix} 0 & -i\mathscr{D}_\mu\psi \\ -i(\mathscr{D}_\mu\psi)^\dagger & 0 \end{bmatrix} \otimes \hat{\Gamma}_a, \qquad (2.22) \\ F_{ab}(x,\xi) &= -(\eta^2\mathbf{1}_n + \chi^2)\otimes L_{ab}, \end{aligned}$$

where

$$\chi^2 = \begin{bmatrix} -\psi\psi^\dagger + \Theta^2\mathbf{1}_{n-1} & -i(\Theta+\beta)\psi \\ -i(\Theta+\beta)\psi^\dagger & \beta^2 - \psi^\dagger\psi \end{bmatrix}.$$

We see that the reduced model is a $\mathrm{SU}(n-1)\times\mathrm{U}(1)$ gauge field theory with fundamental spin-0 field representation. The role of the two constants Θ and β is to define the self-interaction term for the spin-0 field, namely a symmetry breaking Higgs potential.

The dimensional reduction procedure presented above is quite general. For our applications of this procedure in the succeeding sections we will usually restrict our attention to the unitary groups, as they are the most widely used.

III. REDUCTION OF CHERN CLASSES TO SURFACE INTEGRALS IN ODD DIMENSIONS

We have seen in Sec. II that a pure gauge field theory over an N-dimensional manifold can be related, by dimensional reduction, to a gauge-field–Higgs theory over an $(N-p)$-dimensional manifold. In this section we wish to investigate this relationship in the particular context of the topological Chern classes $q^{(N/2)}$ associated with an (even) N-dimensional manifold. The Chern class, defined by

$$q^{(N/2)} = (-i)^{N/2}\epsilon_{M_1M_2\cdots M_{N-1}M_N}\int d_N x\ \mathrm{tr}\, F_{M_1M_2}\cdots F_{M_{N-1}M_N}, \qquad (3.1)$$

where each of the N indices $M_i, i = 1,\ldots,N$, runs over the values $1,\ldots,N$ (even), is the quantity we focus on in this section. Other invariant quantities, such as

$$\epsilon_{M_1M_2\cdots M_{r-1}M_rM_{r+1}M_{r+2}\cdots M_N} \times \int d_N x\ \mathrm{tr}\, F_{M_1M_2}\cdots F_{M_{r-1}M_r}\ \mathrm{tr}\, F_{M_{r+1}M_{r+2}}\cdots F_{M_{N-1}M_N}, \qquad (3.2)$$

which exist for N sufficiently large, also may be considered, but they do not feature in our analysis.

The result of our investigation can be stated as folows: In all of the cases that we have examined the reduction of a Chern class, of the type (3.1), by an odd number of dimensions yields a surface integral over the odd-dimensional Euclidean manifold, i.e., for p odd,

$$q^{(N/2)}(\mathscr{M}_N = E_{N-p}\times S^p) = \int_{\Sigma_{N-p}} d^{(N-p-1)}S\,\mathbf{n}\cdot\mathbf{J}, \qquad (3.3)$$

where the current $\mathbf{J}$ is given in terms of the gauge and Higgs fields over E_{N-p}.

To illustrate this result we consider two types of models, which are distinguished by the structure of the reduced theory as follows: (I) ST reduction leading to a $\mathrm{SU}(n)$ gauge group, where the reducible Higgs field belongs to the adjoint $\oplus$ scalar representation of $\mathrm{SU}(n)$; and (II) ST reduction leading to a $\mathrm{SU}(n-1)\times\mathrm{U}(1)$ gauge group with Higgs field in the fundamental representation of $\mathrm{SU}(n-1)$. For the purposes of the explicit calculations of this section we restrict our attention to the two cases $N=6$ and $N=8$, i.e., to the third and fourth Chern classes $q^{(3)}$ and $q^{(4)}$. Corresponding to each of I and II above there will then be five different cases:

(1) $K = \mathrm{SU}(2n)$, $\mathscr{M}_6 = E_3\times S^3$,
(2) $K = \mathrm{SU}(2n)$, $\mathscr{M}_8 = E_5\times S^3$,
(3) $K = \mathrm{SU}(4n)$, $\mathscr{M}_8 = E_3\times S^5$,
(4) $K = \mathrm{SU}(n)$, $\mathscr{M}_6 = E_5\times S^1$,
(5) $K = \mathrm{SU}(n)$, $\mathscr{M}_8 = E_7\times S^1$.

We do not consider the cases (4) and (5), as the proof of the result (3.3) involves the elementary dimensional reduction that yields (1.1″) from (1.1), and is trivial. Indeed, the results follow directly from the Chern–Simons formulas (1.3′).

In the six examples considered the calculations are straightforward. The basic idea is to substitute into the Chern class the field strength components that result from the appropriate ST reduction *Ansatz*, as discussed in Sec. II, to carry out the integral over the compact dimensions and finally to regroup the terms in the integral over the remaining euclidean dimensions.

Let us consider the various cases of type I. In each of these cases the field strength components are given by Eq. (2.15) and the trace identities involving the L_{ab} and $\hat{\Gamma}_a$ matrices used in the calculations are given in Appendix A.

(I.1) Third Chern Class, $\mathscr{M}_6 = E_3\times S^3$: $p=3$; $i,j,\ldots = 1,2,3$; $a,b,\ldots = 1,2,3$. In terms of the field strength components the third Chern class is

$$q^{(3)} = \epsilon_{ijk}\epsilon_{abc}\int d_3x\int d_3\Omega \times \mathrm{tr}\left[F_{ij}F_{ka}F_{bc} + F_{ij}F_{ab}F_{kc} - \tfrac{4}{3}F_{ia}F_{jb}F_{kc}\right], \qquad (3.4)$$

and upon reduction we find the surface integral

$$q^{(3)} \simeq \int d^2S\,\mathbf{n}\cdot\left[\eta^2\,\mathrm{tr}\,\phi\mathscr{B} + \frac{1}{3}\mathrm{tr}\,\phi^3\mathscr{B} - \frac{1}{3!}\mathrm{tr}\,\phi(\mathscr{D}\phi\times\mathscr{D}\phi)\right], \qquad (3.5)$$

where $\mathscr{B}_i = \frac{1}{2}\epsilon_{ijk}\mathscr{F}_{jk}$ and $\int d_3\Omega$ is the integral over S^3.

(I.2) Fourth Chern Class, $\mathscr{M}_8 = E_5\times S^3$: $p=3$; $i,j = 1\ldots,5$; $a,b = 1,2,3$. In terms of the field strength components the fourth Chern class is

$$q^{(4)} = \epsilon_{ijklm}\epsilon_{abc}\int d_3x \int d_3\Omega$$
$$\times \mathrm{tr}[F_{ij}F_{kl}F_{ab}F_{mc} + F_{ij}F_{kl}F_{ma}F_{bc}$$
$$+ F_{ij}F_{ka}F_{lm}F_{bc} - 4F_{ij}F_{ka}F_{lb}F_{mc}], \quad (3.6)$$

and upon reduction we find the surface integral

$$q^{(4)} = \int d^4S\, n_i \epsilon_{ijklm}[3\eta^2 \,\mathrm{tr}\,\phi\mathscr{F}_{jk}\mathscr{F}_{lm}$$
$$+ \mathrm{tr}\,\phi^3\mathscr{F}_{jk}\mathscr{F}_{lm} - 2\,\mathrm{tr}\,\phi\mathscr{D}_j\phi\mathscr{D}_k\phi\mathscr{F}_{lm}]. \quad (3.7)$$

(I.3) Fourth Chern Class, $\mathscr{M}_8 = E_3 \times S^5$: $p = 5$, $i,j,\ldots = 1,2,3$; $a,b,\ldots = 1,\ldots,5$. In terms of the field strength components the fourth Chern class is

$$q^{(4)} = \epsilon_{ijk}\epsilon_{abcde}\int d_3x \int d_5\Omega$$
$$\times \mathrm{tr}[F_{ij}F_{ka}F_{bc}F_{de} + F_{ij}F_{ab}F_{kc}F_{de}$$
$$+ F_{ij}F_{ab}F_{cd}F_{ke} - 4F_{ia}F_{jb}F_{kc}F_{de}], \quad (3.8)$$

which upon reduction yields the surface integral

$$q^{(4)} \simeq \int d^2S\,\mathbf{n}\cdot[3\eta^4\,\mathrm{tr}\,\phi\mathscr{B} + 2\eta^2\,\mathrm{tr}\,\phi^3\mathscr{B}$$
$$- \eta^2\,\mathrm{tr}\,\phi(\mathscr{D}\phi\times\mathscr{D}\phi) + \tfrac{3}{5}\,\mathrm{tr}\,\phi^5\mathscr{B}$$
$$- \tfrac{2}{3}\,\mathrm{tr}\,\phi^3(\mathscr{D}\phi\times\mathscr{D}\phi) + \tfrac{1}{3}\,\mathrm{tr}\,\phi^2(\mathscr{D}\phi\times\phi\mathscr{D}\phi)]. \quad (3.9)$$

In the cases (I.1) and (I.3) the surface integral is over the two-dimensional surface at infinity in a three-dimensional Euclidean manifold. The $\mathscr{B}$-dependent terms in (3.5) and (3.9) are very similar to the Taubes invariants (1.1″′). However, in the case of the Taubes formulas, Φ is understood to belong to the adjoint representation of the gauge group. In the cases above, ϕ is not an irreducible representation of the residual gauge group SU(n). If we decompose ϕ into irreducible components, $\phi = \Phi + \Theta 1_n$, where Φ belongs to the adjoint representation of SU(n), we can rewrite the $\mathscr{B}$-dependent terms in (3.5) and (3.9):

$$q^{(3)} \simeq \int d^2S\,\mathbf{n}\cdot[(\eta^2 + \Theta^2)\mathrm{tr}\,\Phi\mathscr{B} + \Theta\,\mathrm{tr}\,\Phi^2\mathscr{B}$$
$$+ \tfrac{1}{3}\,\mathrm{tr}\Phi^3\mathscr{B} - (1/3!)\mathrm{tr}\Phi(\mathscr{D}\Phi\times\mathscr{D}\Phi)], \quad (3.5')$$

$$q^{(4)} \simeq \int d^2S\,\mathbf{n}\cdot[3(\eta^2 + \Theta^2)^2\,\mathrm{tr}\,\Phi\mathscr{B} + 6(\eta^2 + \Theta^2)\mathrm{tr}\,\Phi^2\mathscr{B}$$
$$+ 2(\eta^2 + 3\Theta^2)\mathrm{tr}\,\Phi^3\mathscr{B} + 3\Theta\mathrm{tr}\,\Phi^4\mathscr{B} + \tfrac{3}{5}\,\mathrm{tr}\,\Phi^5\mathscr{B}$$
$$- \eta^2\,\mathrm{tr}\,\phi(\mathscr{D}\phi\times\mathscr{D}\phi) - \tfrac{2}{3}\,\mathrm{tr}\,\phi^3(\mathscr{D}\phi\times\mathscr{D}\phi)$$
$$+ \tfrac{1}{3}\,\mathrm{tr}\,\phi^2(\mathscr{D}\phi\times\phi\mathscr{D}\phi)]. \quad (3.9')$$

If we now set the scalar representation Θ to be a constant then we see that of the Taubes invariants

$$\int d^2S\,\mathbf{n}\cdot\mathrm{tr}\,\Phi^k\mathscr{B}, \quad k = 1,\ldots,(n-1), \quad (3.10)$$

the first three occur in (3.5′), while the first five occur in (3.9′).

It is clear that, in this way, the dimensionally reduced Chern class $q^{(N/2)}$ ($\mathscr{M}_N = E_3\times S^{N-3}$), for N even, will involve the Taubes invariants (3.10) for $k = 1,\ldots,N-3$, provided $n > N-3$. If $n < N-3$, then, in the surface integrals at infinity, $\Phi^k(\infty)$ for $n \leqslant k \leqslant N-3$ can be reexpressed in terms of $\Phi(\infty),\Phi^2(\infty),\ldots,\Phi^{n-1}(\infty)$, thus modifying the coefficients of the Taubes invariants that occur. To ensure that all of the relevant Taubes invariants occur it is necessary to choose the order of the Chern class $> (n+1)/2$.

It must be pointed out that the surface integrals (3.5′) and (3.9′) do not depend on the above *Ansatz* for Θ for their significance. Indeed, as we shall see in the sequel, it is not necessary to assume Θ to be a constant to establish the existence of field configurations for which these surface integrals are nontrivial.

Other surface integrals: The occurrence of surface integrals in the dimensional reduction of the third and fourth Chern classes does not depend on the representation employed for the Higgs field in the reduction. As we shall now see, surface integrals occur also when we employ fundamental Higgs representations. Such models are of intrinsic interest—classical field configurations with the Higgs field in the fundamental representation have featured in the recent studies[17] of saddle point solutions to the YMH systems.

For these cases the field strength components are formally given by (2.19) and the results of the calculations are as follows.

(II.1) Third Chern Class, $\mathscr{M}_6 = E_3\times S^3$:

$$q^{(3)} \simeq (\Theta + \beta)\int d^2S\,\mathbf{n}\cdot\langle\psi,(\mathscr{B} + i\mathbf{b})\psi\rangle. \quad (3.11)$$

(II.2) Fourth Chern class, $\mathscr{M}_8 = E_5\times S^3$:

$$q^{(4)} \simeq (\Theta + \beta)\int d^4S\, n_i\epsilon_{ijklm}$$
$$\times\langle\psi,(\mathscr{F}_{jk}\mathscr{F}_{lm} + i\mathscr{F}_{jk}f_{lm} - f_{jk}f_{lm})\psi\rangle. \quad (3.12)$$

(II.3) Fourth Chern class, $\mathscr{M}_8 = E_3\times S^5$:

$$q^{(4)} \simeq (\Theta + \beta)\int d^2S\,\mathbf{n}\cdot\{-(2\Theta^2 + \beta^2 + 3\eta^2)$$
$$\times\langle\psi,(\mathscr{B} + i\mathbf{b})\psi\rangle - (\beta^2 - \Theta^2)\langle\psi,i\mathbf{b}\psi\rangle$$
$$+ \langle\psi,\psi\rangle[\langle\psi,\mathscr{B}\psi\rangle + 2i\mathbf{b}\langle\psi,\psi\rangle$$
$$- \langle\mathscr{D}\psi,\times\mathscr{D}\psi\rangle]\}, \quad (3.13)$$

where we employ the notation $\langle\psi,A\psi\rangle = \psi^+A\psi$ and $b_i = \frac{1}{2}\epsilon_{ijk}f_{jk}$, cf. (2.20).

It is interesting to point out that in these three cases we must be careful not to choose $(\Theta + \beta)$ to be zero, or the Chern class will vanish trivially. We recall that the imaginary constants Θ and β originate from the scalar spin-0 field representations.

We notice that the surface integrals (3.11) and (3.13) involve the following analog of the Taubes invariants (3.10):

$$\int d^2S\,\mathbf{n}\cdot\langle\psi,(\mathscr{B} + i\mathbf{b})\psi\rangle\langle\psi,\psi\rangle^k, \quad (3.14)$$

for $k = 0,1$. Quite naturally the ψ fields occur in pairs as they are column vectors. It is clear that by going to high Chern classes we can generate the integrals (3.14) for other values of k.

IV. SURFACE INTEGRALS IN EVEN DIMENSIONS

Since the Chern classes are defined on even-dimensional manifolds, the subject matter of this section involves the reduction of Chern classes by an even number of dimensions. This is not as straightforward as the reduction of Chern classes by an odd number of dimensions described in the previous section.

As explained in the Introduction, our aim in reducing Chern classes and action densities is twofold. On the one hand we wish to obtain from the Chern class a surface integral, while at the same time from the action density we wish to produce a Higgs potential for spin-0 fields. The latter will allow for field configurations that yield nontrivial surface integrals. The adaptation of the ST *Ansatz* for the reduction characterized by $\mathcal{M}_N = E_{N-P}\times S^P$ to the case of *even* p(2) was given in Ref. 10(b). We briefly review the relevant formulas here. To start with, the solutions (2.5) and (2.6) of (2.2) and (2.3), respectively, change. This is because for even p the symmetry group of S^p, namely SO($p+1$), has two possible $m\times m$ spinor representations, cf. (2.9), each inside those of SO($p+2$). The elements of the corresponding algebras are given by (A1). In addition the elements h of SO(p), the stability group of S^p, commute with the last element $L_{p+1,p+2}\simeq\Gamma^{(p+1)}$ of so($p+2$). This results immediately in the more general solutions of (2.2),

$$A_\mu(x,\xi) = \mathcal{A}_\mu(x)\otimes \mathbf{1}_m + \mathcal{B}_\mu(x)\otimes iL_{p+1,p+2}, \tag{4.1}$$

$$A_a(x,\xi) = \phi(x)\otimes iL_{a,p+1} + \chi(x)\otimes iL_{a,p+2}. \tag{4.2}$$

The resulting field strengths can then be computed[13] to give

$$\begin{aligned} F_{\mu\nu}(x,\xi) &= \mathcal{F}_{\mu\nu}\otimes \mathbf{1} + \mathcal{D}_{[\mu}\mathcal{B}_{\nu]},\\ F_{\mu a}(x,\xi) &= \mathfrak{B}_\mu\otimes iL_{a,p+1} + \mathfrak{A}_\mu\otimes iL_{a,p+2}, \qquad (4.3)\\ F_{ab}(x,\xi) &= -(\eta^2 L_n + \phi^2 + \chi^2)\otimes L_{ab} - [\phi,\chi]\otimes\Gamma^{p+1}L_{ab}, \end{aligned}$$

where

$$\mathfrak{B}_\mu = \mathcal{D}_\mu\phi - i\{\mathcal{B}_\mu,\chi\},\quad \mathfrak{A}_\mu = \mathcal{D}_\mu\chi + i\{\mathcal{B}_\mu,\phi\},$$
$$\mathcal{D}_\mu = \partial_\mu + [\mathcal{A}_\mu,\cdot\,].$$

It was found in Ref. 10(b) that substituting (4.3) into the third Chern–Pontryagin integral over $\mathcal{M}_6 = E_2\times S^4$ resulted, after integration over the S^4 variables, in a surface integral $\int J_\mu dS_\mu$ on E_2 given by the current

$$\begin{aligned} J_\mu(x) = \epsilon_{\mu\nu}\,\mathrm{tr}[\,& i\eta^2(\chi\mathcal{D}_\nu\phi - \phi\mathcal{D}_\nu\chi)\\ &+ i(\chi\phi\chi - \phi^3)\mathcal{D}_\nu\chi - i(\phi\chi\phi - \chi^3)\mathcal{D}_\nu\phi\\ &+ ((\eta^2\mathbf{1} + \phi^2 + \chi^2)^2 - [\phi,\chi]^2)\mathcal{B}_\nu\,]. \end{aligned} \tag{4.4}$$

Similar formulas are obtained for higher dimensions, as presented in Ref. 10(b). However, concerning the physical applicability of formulas like (4.4), the situation is not so clear.[10(b)] Based on arguments of *finite energy* (*action*), it can be concluded that the covariant derivative of a Higgs field has the same asymptotic behavior as a curvature, or the curl of a vector field. Accordingly it was argued that the surface integral of (4.4) gave a vanishing contribution. Similar conclusions[10(b)] were arrived at for higher-dimensional examples. Accordingly, we must search for other paths of descent $\mathcal{M}_n = E_{N-P}\times M_p$, where M_p is different from S^p, e.g., $M_p = S^{p_1}\times\cdots\times S^{p_n}$, $\Sigma_1^n p_i = p$, with the purpose of achieving a current with nonvanishing surface integral.

To this end, we consider the example $\mathcal{M}_8 = E_2\times S^3\times S^3$, which is the simplest nontrivial case with each $p_i > 2$. (The cases with $p_i = 2$ are privileged and will be considered below separately.)

To this end, we consider the case when p is even but $p/2$ is odd. In this case we might examine $\mathcal{M}_N = E_{N-p}\times S^{p/2}\times S^{p/2}$ with spherical symmetry over each $S^{p/2}$ factor. Application of this reduction to a Chern class will lead to a surface integral. Furthermore, it will also lead to a symmetry breaking type of Higg's potential. The simplest nontrivial example that we can consider is $\mathcal{M}_8 = E_2\times S^3\times S^3$.

To describe the reduction *Ansatz* in this case we proceed in two stages.

(i) $\mathcal{M}_8 = \mathcal{M}_5\times S^3$, initial gauge group SU($4n$), field strengths F_{LN}. If $L,N = 1,\ldots,8$; $i,j = 1,\ldots,5$ and $\alpha,\beta = 6,7,8$, the reduction *Ansatz* can be written

$$\begin{aligned} &F_{ij}|_{\xi_1} = G_{ij}\otimes\mathbf{1}_2,\quad F_{i\alpha}|_{\xi_1} = D_i\phi\otimes\hat{\Gamma}_\alpha,\\ &F_{\alpha\beta}|_{\xi_1} = -(\eta^2\mathbf{1}_{2n} + \phi^2)\otimes L_{\alpha\beta}, \end{aligned} \tag{4.5}$$

where G_{ij} is a SU($2n$) field strength.

(ii) $\mathcal{M}_5 = E_2\times S^3$. If $\mu,\nu = 1,2$; $a,b = 3,4,5$, the second reduction *Ansatz* is, for the SU($2n$) field strengths,

$$\begin{aligned} &G_{\mu\nu}|_{\xi_2} = \mathcal{F}_{\mu\nu}\otimes\mathbf{1}_2,\quad G_{\mu a}|_{\xi_2} = \mathcal{D}_\mu\chi\otimes\hat{\Gamma}_a,\\ &G_{ab}|_{\xi_2} = -(\rho^2\mathbf{1}_n + \chi^2)\otimes L_{ab}, \end{aligned} \tag{4.5'}$$

from (2.15), where $\mathcal{F}_{\mu\nu}$ is a SU(n) field strength, and for the Higgs field $\phi = \varphi\otimes\mathbf{1}_2$,

$$\begin{aligned} &D_\mu\phi|_{\xi_2} = \mathcal{D}_\mu\varphi\otimes\mathbf{1}_2,\quad D_a\phi|_{\xi_2} = [\chi,\phi]\otimes\hat{\Gamma}_4,\\ &\phi^2|_{\xi_2} = \varphi^2\otimes\mathbf{1}_2. \end{aligned} \tag{4.5''}$$

The resulting SU(n) YHM system with two Higgs fields φ and χ (neither of which is necessarily traceless) has the potential term in the Lagrangian, of the form

$$\mathrm{tr}[(\eta^2\mathbf{1}_n + \varphi^2)^2 + (\rho^2\mathbf{1}_n + \chi^2)^2 + \tfrac{1}{4}[\varphi,\chi]^2].$$

Substitution of Eqs. (4.5), (4.5'), and (4.5'') into the third Chern integral and integrating over $S^3\times S^3$ yields the current

$$\begin{aligned} J_\mu = \epsilon_{\mu\nu}\,\mathrm{tr}[\,& -6\eta^2\rho^2\chi\overleftrightarrow{\mathcal{D}}_\nu\varphi - \chi^3\mathcal{D}_\nu\varphi^3 + \tfrac{1}{2}(\chi\varphi\chi\varphi\chi\mathcal{D}_\nu\varphi - \varphi\chi\varphi\chi\varphi\mathcal{D}_\nu\chi)\\ &+ 3(\rho^2\varphi\chi\varphi\mathcal{D}_\nu\varphi - \eta^2\chi\varphi\chi\mathcal{D}_\nu\chi) - 3(\rho^2\chi\mathcal{D}_\nu\varphi^3 - \varphi\mathcal{D}_\nu\chi^3)\\ &- (\varphi\chi^2\varphi\chi\mathcal{D}_\nu\varphi - \chi\varphi^2\chi\varphi\mathcal{D}_\nu\chi) + (\varphi\chi\varphi\chi^2\mathcal{D}_\nu\varphi - \chi\varphi\chi\varphi^2\mathcal{D}_\nu\chi)\\ &- (\chi\varphi^2\chi^2\mathcal{D}_\nu\varphi - \varphi\chi^2\varphi^2\mathcal{D}_\nu\chi) + (\varphi\chi^3\varphi\mathcal{D}_\nu\varphi - \chi\varphi^3\chi\mathcal{D}_\nu\chi)\,]. \end{aligned} \tag{4.6}$$

As $\int_{E_2\times S^3\times S^3}$ is manifestly a surface integral, in which the current (4.6) is integrated over a large surface in E_2, and as the Higg's potential (4.4) in the action density is of a suitable form, we appear to have achieved our objective.

The structure of the current (4.6), however, is such that it may be useless for any practical (i.e., physical) application. We notice that the lowest-order term in (4.6), $\eta^2\rho^2\epsilon_{\mu\nu}\,\mathrm{tr}\,\chi\overleftrightarrow{\mathscr{D}}_\nu\varphi$, does not involve the curvature field $\mathscr{F}_{\mu\nu}$. Indeed this is a persistent feature in all such reductions. For example, for the reduction $\mathscr{M}_{10}=E_4\times S^3\times S^3$, the substitution of (4.5), (4.5'), and (4.5'') into the fifth Chern class yields a current very similar to (4.6) in which the lowest-order term is

$$\eta^2\rho^2\epsilon_{\mu\nu\rho\sigma}\,\mathrm{tr}\,\chi\mathscr{D}_\nu\varphi\mathscr{F}_{\rho\sigma}, \tag{4.7a}$$

and *not*

$$\epsilon_{\mu\nu\rho\sigma}\,\mathrm{tr}\,\mathscr{A}_\nu\left[\mathscr{F}_{\rho\sigma}-\tfrac{2}{3}\mathscr{A}_\rho\mathscr{A}_\sigma\right], \tag{4.7b}$$

the Chern–Simons form of the Pontryagin density. On a large surface the asymptotic properties of the Pontryagin density (4.7b) are those of the product $\mathscr{A}_\nu\mathscr{A}_\rho\mathscr{A}_\sigma$, while the asymptotic properties of (4.7a) are those of $\mathscr{D}_\nu\varphi\mathscr{A}_\rho\mathscr{A}_\sigma$. Now, the finite energy conditions (1.2') imply that $\mathscr{D}_\nu\varphi$ must tend to zero at infinity at a faster rate than the field $\mathscr{A}_\nu$. Therefore, the density (4.7a) tends to zero faster than (4.7b), and consequently the lower-order term (4.7a) makes no contribution to the surface integral. Furthermore, the asymptotic properties of the higher-order terms are also such that they make no contribution to the surface integral. We conclude that in such reduction schemes the surface integral vanishes.

This is a general feature of all reduction schemes

$$\mathscr{M}_N=\mathscr{M}_{N-p}\times S^{m_1}\times\cdots\times S^{m_q},\quad m_i\ \text{odd},\quad i=1,\ldots,q,$$

with the exception of the case $M_N=M_{N-p}\times S^1\times\cdots\times S^1$ (p times).

For example, if $\mathscr{M}_6=E_3\times S^1\times S^1\times S^1$ the third Chern class reduces to the surface integral

$$\begin{aligned}q^{(3)}=&\frac{i}{2}\epsilon_{ijk}\int d^2S\,n_i\\&\times\mathrm{tr}\big[F_{jk}(\{\Phi_1,[\Phi_2,\Phi_3]\}+\text{cyclic perm.})\\&-(\Phi_1\{D_j\Phi_2,D_k\Phi_3\}+\text{cyclic perm.})\big],\end{aligned} \tag{4.8}$$

which does not vanish when the finite energy condition (1.2') is imposed. In this case, however, the YMH Lagrangian density is endowed with the potential term

$$\mathrm{tr}([\Phi_1,\Phi_2]^2+[\Phi_2,\Phi_3]^2+[\Phi_3,\Phi_1]^2),$$

which on its own is not a symmetry-breaking potential. Thus it cannot be guaranteed that field configurations exist for which the surface integral (4.8) is nonvanishing.

The results (4.4) and (4.6) suggest that if the residual gauge theory has more than one Higgs field, the resulting Higgs potential is of the symmetry breaking type, and the surface integrals obtained from the corresponding Chern classes vanish. Fortunately, this does not always follow. In the above analysis we have used S^{m_i} factors where m_i is odd. In such cases the result does hold. However, we shall see shortly that if we allow the m_i to be even ($=2$) then the result does not automatically follow.

Qualitatively we note that in multiple stage ST *Ansätze* there normally occurs more than one Higgs field, e.g., φ and χ in the case treated above, as was the case with the single stage ST reduction for even $p>2$. Furthermore if we were to choose our *Ansätze* (4.5), (4.5'), and (4.5''), such that either φ or χ were to vanish then the current (4.6) and the associated surface integrals would identically vanish. We shall see shortly that the attainment of a nonvanishing surface integral after a multiple stage ST reduction $\mathscr{M}_N=E_{N-p}\times S^{m_1}\times\cdots\times S^{m_q}$ will depend on our ability to perform the reduction in such a way that in the residual model there is *only one Higgs field*.

So far we have not considered one important even p case—$p=2$, i.e., reduction by two dimensions induced by $\mathscr{M}_N=E_{N-2}\times S^2$. The results of the application of this reduction to Chern classes are *nontrivial*, and are well known from some investigations[11,12,18] on vortices. The qualitative difference between the $p=2$ and even $p>2$ ST reductions is due to the imposition of SO$(p+1)$ spherical symmetry on S^p. Since this is implemented by solving (2.3), where h belongs to the stability group of the fixed point of S^p, we find in the case of S^2 the stability group SO(2), which is Abelian, in contrast with all other $p(>2)$ cases where h belongs to a non-Abelian group.

Let us review briefly the details of the reduction by two dimensions. To start with we must specify the mapping μ from SO(2) into the initial gauge group, and then we must solve (2.2) and (2.3). In the case of initial gauge group SU(n) we have $\mu=\exp iM\varphi$, $M=\mathrm{diag}(m_1,\ldots,m_n)$, $\Sigma_{i=1}^n m_i=0$. The m_i, $i=1,\ldots,n$, characterize the SO(3) spherical symmetry on S^2. The solutions of (2.2) and (2.3) are then readily obtained[13,16]:

$$\begin{aligned}&A_\mu(x)_{ij}|_\xi=0,\quad m_i\neq m_j,\\&A_1(x)_{ij}|_\xi=A_2(x)_{ij}|_\xi=0,\quad\text{if } |m_i-m_j|\neq 1\\&A_2(x)_{ij}|_\xi=i\,\mathrm{sgn}(m_i-m_j)A_1(x)_{ij}|_\xi,\\&\text{if } |m_i-m_j|=1,\end{aligned} \tag{4.9}$$

where $\mu=1,2,\ldots,N-2$. Again, one can show that the $(N/2)$th Chern class in N dimensions reduces to a surface integral in $N-2$ dimensions. To illustrate, we give the explicit formulas for the surface integral $\int\partial_\mu J_\mu^{(N-2)}d^{(N-2)}x$ for $N=4,6,8$:

$$J_\mu^{(2)}=-2\epsilon_{\mu\nu}\,\mathrm{tr}\left[i\eta^2MA_\nu+\tfrac{1}{2}\epsilon_{ab}A_aD_\nu A_b\right], \tag{4.10a}$$

$$\begin{aligned}J_\mu^{(4)}=&-4\epsilon_{\mu\nu\rho\sigma}\,\mathrm{tr}\big[i\eta^2MA_\nu(F_{\rho\sigma}-\tfrac{2}{3}A_\rho A_\sigma)\\&+\epsilon_{ab}A_aD_\nu A_bF_{\rho\sigma}\big],\end{aligned} \tag{4.10b}$$

$$\begin{aligned}J_\mu^{(6)}=&-4\epsilon_{\mu\nu\rho\sigma\tau\lambda}\,\mathrm{tr}\big[i\eta^2MA_\nu(F_{\rho\sigma}F_{\tau\lambda}\\&-A_\rho A_\sigma F_{\tau\lambda}+\tfrac{2}{5}A_\rho A_\sigma A_\tau A_\lambda)\\&+\epsilon_{ab}A_aD_\nu A_bF_{\rho\sigma}F_{\tau\lambda}-\tfrac{1}{2}\epsilon_{ab}A_aF_{\rho\sigma}D_\nu A_bF_{\tau\lambda}\big].\end{aligned} \tag{4.10c}$$

To derive these results we need the following consequences of (4.9):

$$\begin{aligned}&F_{ab}|_\xi=-i\eta^2\epsilon_{ab}M+[A_a,A_b],\\&F_{\mu a}|_\xi=D_\mu A_a=\partial_\mu A_a+[A_\mu,A_a],\quad a=1,2,\\&[A_\mu,M]=0,\quad[D_\mu,M]=0.\end{aligned} \tag{4.11}$$

We infer from (4.10) thgat the ST reduction induced by $M_N = E_{N-2} \times S^2$ always reduces the $(N/2)$th Chern class to a surface integral in $(N-2)$ dimensions. Furthermore, the corresponding Lagrangian density is endowed with a Higgs potential of the desired form. Of course, it is only in the cases $N=4$ and $N=6$ that the surface integrals which result from this *Ansatz* [i.e., (4.10a) and (4.10b)] would be of any physical interest—in all other cases the surface integral would be in a nonphysical space of dimension $\geqslant 6$.

Despite our earlier discussion when we considered the extra dimensions to be an even product of spheres of odd dimension it is possible to construct an ST type reduction so that the $(N/2)$th Chern class will reduce to *nonvanishing* surface integrals in two- and four-dimensional spaces. We end this section by giving such a reduction scheme, namely $p/2$ successive reductions by two dimensions. As seen earlier, such a scheme would be expected to give rise to more than one Higgs field, like φ and χ in (4.2) and (4.3), with the undesirable feature that the resulting surface integrals vanish. One solution to this problem is to find a multiple stage ST reduction scheme in which each (except the last) of the Higgs fields vanishes by the requirement of spherical symmetry on the extra dimensions at the given stage of reduction. This objective can be achieved easily if the reduction is induced by $\mathcal{M}_N = E_{N-P} \times S^2 \times \cdots \times S^2$.

To see this let us consider a SU(n) gauge field theory interacting with a Higgs field ψ in the *fundamental representation* of SU(n), which is subjected to a reduction by two dimensions. The equation, expressing the spherical symmetry of the Higgs field ψ, analogous to (2.2), reads

$$\psi(x_\rho, \xi_a) = \mu(h)\psi(x_\mu, \xi_a), \tag{4.12}$$

where $\mu(h) = \exp iM\theta$. In infinitesimal form this reads

$$M\psi = 0. \tag{4.12'}$$

Therefore, if we arrange this stage of the reduction scheme to be characterized by $M = \mathrm{diag}(m_1, \ldots, m_n)$ with $m_i \neq 0$ for all $i = 1, \ldots, n$, (4.12') implies that every component of ψ must vanish by virtue of the spherical symmetry.

Thus, if every stage of $\mathcal{M}_N = E_{N-p} \times S^2 \times \cdots \times S^2$ ($p/2$ times) is arranged to be of this type, then the only nonvanishing Higgs field in the $(N-p)$-dimensional theory is the one arising from the last stage of the reduction scheme. In that case the potential term in the corresponding Lagrangian density will be of the type $\mathrm{tr}\, F_{12}^2$ [cf. (4.11)], i.e., of the symmetry breaking type.

To illustrate this scheme we present the simplest possible example, induced by $\mathcal{M}_6 = E_2 \times S^2 \times S^2$. Let the initial gauge group be SU(4), and let the first stage of the reduction be characterized by

$$M_1 = \mathrm{diag}(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}, -\tfrac{3}{4}) \propto \lambda_{15} \in \mathrm{su}(4). \tag{4.13}$$

This yields a SU(3)×U(1) theory with curvature $\mathcal{G}_{ij} + (i/2)\lambda_{15} g_{ij}$ [where $\mathcal{G}_{ij} \in \mathrm{su}(3)$ and $g_{ij} = \partial_i b_j - \partial_j b_i$ is the U(1) field] and with a SU(3) fundamental Higgs field ψ. We let the second stage of the reduction be characterized by

$$M_2 = \mathrm{diag}(\tfrac{1}{3}, \tfrac{1}{3}, -\tfrac{2}{3}) \propto \lambda_8 \in \mathrm{su}(3) \tag{4.14}$$

for the SU(3) factor. With this choice, $\mathcal{G}_{ij}$ yields a SU(2)×U(1) system with curvature $\mathcal{F}_{\mu\nu} + (i/2)\lambda_8 f_{\mu\nu}$, where $\mathcal{F}_{\mu\nu} \in \mathrm{su}(2)$ and $f_{\mu\nu} = \partial_\mu a_\nu - \partial_\nu a_\mu$ is the second U(1) field, and a SU(2) fundamental Higgs field φ. The effect of (4.14) on the Higgs field ψ and $D_\mu \psi$ is, because of (4.12'),

$$\psi = 0, \quad D_\tau \psi = 0. \tag{4.15}$$

Finally there remains the imposition of spherical symmetry on the U(1) gauge field $b_i = (b_\mu, b_a)$. As U(1) does not possess the structure of SU(n), it is clear that, at the fixed point, the solution of Eqs. (4.9) applied to b_i yields

$$b_\mu(x) \neq 0, \quad b_a(x) = 0. \tag{4.16}$$

Thus, with the exception of $g_{\mu\nu}$, all the components of g_{ij} vanish on the fixed point of S^2.

Thus, from an initial SU(4) gauge theory we end up with a SU(2)×U(1)×U(1) gauge model on E_2 with one Higgs field, the SU(2) fundamental representation φ. Substitution into the third Chern class of the first stage reduction together with (4.15) yields

$$q^3 \simeq -i\eta^2 \int d^2x\, d_2\Omega\, \epsilon_{ijkl}\, \mathrm{tr}\, \mathcal{G}_{ij} \mathcal{G}_{kl}. \tag{4.17}$$

Application of the second stage of the reduction to (4.17) leads to the simple surface integral given by (4.10a).

V. A CLASS OF SOLUTIONS

In establishing the existence of the vortex solution in two dimensions, the procedure adopted was to establish the form of the relevant surface integral in two dimensions, then the form of the action and finally to look for finite action field configurations, which give rise to nontrivial surface integrals.

In essence, we wish to pursue an analogous procedure for the non-self-dual 't Hooft–Polyakov monopole and its generalizations. Indeed, having presented surface integrals involving all powers of the Higgs field in Sec. III, the natural question arises: are there topological solutions with Higgs vacua contributing to (1.1'") for $k > 1$?

The answer is that many classes of such solutions are known in three dimensions—for example, the spherically symmetric SU(n) ($n \geqslant 3$) YMH monopole of Bais *et al.*,[8] and the axisymmetric SU(3) monopole of Ward,[19] both of which are self-dual field configurations. However, there is only one non-self-dual (spherically symmetric) SU(3) monopole with a λ_8-like vacuum, namely that found by Burzlaff.[6]

In this section we will establish the existence of finite action field configurations, which give rise to nontrivial surface integrals of the type discussed in Sec. III, in three dimensions. In fact we will present a class of solutions for the spherically symmetric non-self-dual YMH systems that have Higgs vacua that contribute in (1.1'") for $k > 1$. The YMH systems in question are those obtained from a higher-dimensional YM system by using the ST reduction *Ansatz* of type (I), as outlined in Secs. II and III. In this case, since we are dealing solely with the action density in three dimensions, the dimension of the manifold from which we are reducing is immaterial. The SU(n) YMH system in three dimensions with action density

$$\mathcal{L} \simeq \mathrm{tr}\left[\mathcal{F}_{ij}^2 + \tfrac{1}{4}(\mathcal{D}_i \phi)^2 - \tfrac{1}{4}(\eta^2 \mathbf{1}_n + \phi^2)^2\right] \tag{5.1}$$

is obtained from the six-dimensional YM system. The YMH

action in three dimensions similarly derived from an N-dimensional YM system would differ from (5.1) only in the (unimportant) magnitude of the constant coefficients of the terms in (5.1). What is important is the sign of each term—each term in (5.1) is negative definite, since ϕ, $\mathscr{D}_i\phi$, and $\mathscr{F}_{ij}$ are anti-Hermitian, for all such reductions.

We shall seek spherically symmetric field configurations for the system (5.1) in three dimensions. Spherical symmetry in three dimensions has been studied very fully.[8,16] We adopt the notation of Ref. 8 to make the spherically symmetric *Ansatz* for the YMH system. This approach also makes use of a fixed point framework—the fixed point is the point where the z axis intersects S^2 in E_3. Then the *Ansatz* for the spherically symmetric configuration of the system (25) is

$$\begin{aligned}
&\mathscr{B} = (1/r)M_1'\mathbf{i} + (1/r)M_2'\mathbf{j} + (1/r^2)([M_1,M_2] - T_3)\mathbf{k}\,,\\
&\mathscr{D}\phi = (1/r)[M_2,\phi]\mathbf{i} - (1/r)[M_1,\phi]j + \phi'\mathbf{k}\,,\\
&(M_1)_{\alpha\beta} = -(i/2)(\delta_{\alpha,\beta-1}a_\alpha + \delta_{\alpha-1,\beta}a_\beta) \quad \text{(no sum)}\,,\\
&(M_2)_{\alpha\beta} = -(i/2)(\delta_{\alpha,\beta-1}a_\alpha - \delta_{\alpha-1,\beta}a_\beta) \quad \text{(no sum)}\,,\\
&\Phi = -(i/2)\mathrm{diag}(\phi_1,\phi_2-\phi_1,\ldots,-\phi_{n-1})\,,\\
&\Theta = -i\theta,\\
&T_3 = -i\,\mathrm{diag}\left(\frac{n-1}{2},\frac{n-1}{2}-1,\ldots,-\frac{n-1}{2}\right),
\end{aligned} \tag{5.2}$$

where the functions θ, ϕ_α, a_α, $\alpha = 1,\ldots,n-1$ and their derivatives θ', ϕ_α', a_α' depend on the radial variable only and ϕ and Φ are related as in (2.10).

To prove the existence of spherically symmetric field configurations that have finite energy and give rise to nontrivial surface integrals such as (3.5) and (3.9), we need the energy integral in terms of the functions $\theta,\phi_1,\ldots,\phi_{n-1}$, $a_1,\ldots,a_{n-1}$; it is

$$\begin{aligned}
\mathscr{E} = \int_0^\infty dr\Big\{&4[(a_1')^2 + (a_2')^2 + \cdots + (a_{n-1}')^2]\\
&+ \tfrac{1}{2}r^2[(\phi_1')^2 + (\phi_2' - \phi_1')^2\\
&+ \cdots + (\phi_{n-1}' - \phi_{n-2}')^2 + (\phi_{n-1}')^2] + 2r^2(\theta')^2\\
&+ \tfrac{1}{2}[a_1^2(\phi_2 - 2\phi_1)^2 + a_2^2(\phi_3 - 2\phi_2 + \phi_1)^2\\
&+ \cdots + a_{n-1}^2(-2\phi_{n-1} + \phi_{n-2})^2]\\
&+ (1/r^2)[(a_1^2 - n + 1)^2 + (a_2^2 - a_1^2 - n + 3)^2\\
&+ \cdots + (n - 1 - a_{n-1}^2)^2]\\
&+ \tfrac{2}{3}r^3\Big[\Big(\Big(\frac{\phi_1}{2} + \theta\Big)^2 - \eta^2\Big)^2 + \Big(\Big(\frac{\phi_2 - \phi_1}{2} + \theta\Big)^2 - \eta^2\Big)^2\\
&+ \cdots + \Big(\Big(-\frac{\phi_{n-1}}{2} + \theta\Big)^2 - \eta^2\Big)^2\Big]\Big\}\,.
\end{aligned} \tag{5.3}$$

The method we use to establish the existence of solutions is that due to Fate'ev, Tyupkin, and Schwarz[20] (FTS). To start with, we know that the Euler–Lagrange equations of the system (5.1) arising with respect to the variations $\delta\Theta$, $\delta\Phi$, $\delta\mathscr{A}_i$, are solved[8,16] by those w.r.t. $\delta\theta$, $\delta\phi_\alpha$, δa_α ($\alpha = 1,\ldots,n-1$), of the energy integral (5.3). Thus it is sufficient to prove existence for the problem determined by the functional (5.3). Indeed the FTS method consists of verifying that the functional $\mathscr{E}(\theta,a_\alpha,\phi_\alpha)$ attains its minimal value for some set of functions θ, a_α, ϕ_α.

At this point we must decide whether we will use (5.1) as our YMH system, to which correspond surface integrals of the type (3.5), (3.9), etc., or if we will specialize the ST *Ansatz* by assuming $\Theta = \text{const}$ (and $\theta' = 0$), to which correspond the surface integrals of the type (3.5'), (3.9'), etc., or simply (1.1''). As the latter system is the more conventional in that the Higgs field Φ resides in su(n), we will first deal with that case. From now on, θ is a constant parameter.

To begin with let us examine the consequences of the finite energy condition, $\mathscr{E}(a_\alpha,\phi_\alpha) < \infty$. The convergence of the integral as a whole and the positivity of each term in the integrand ensures that each term must converge separately. In particular the final term, the Higgs potential term, must converge. This result allows us to infer the asymptotic limits of $\phi_\alpha(r)$, $\alpha = 1,\ldots,n-1$, namely $\phi_\alpha(\infty)$, $\alpha = 1,\ldots,n-1$. Indeed, for any given n, there are many different sets of asymptotic values. However, to establish our result below it is necessary to restrict our attention to those asymptotic values that give rise to nonzero values for

$$(\phi_2 - 2\phi_1),(\phi_3 - 2\phi_2 + \phi_1),\ldots,(-2\phi_{n-1} + \phi_{n-2})\,, \tag{5.4}$$

whose squares are the coefficients of $a_1^2,a_2^2,\ldots,a_{n-1}^2$ in the gauge-field–Higgs-field interaction term. A simple analysis shows that for each n, there are just two sets of solutions (related by a minus sign). However, these solutions exist only if the hitherto arbitrary constant parameter θ takes on specified values. The solutions fall into two classes according as n is odd or even.

n odd: In this case $\theta = \pm(1/n)\eta$. We list below the asymptotic values $\phi_\alpha(\infty)$ in units of $(4/n)\eta$, i.e., $\hat{\phi}_\alpha = \phi_\alpha(\infty)/(4/n)\eta$:

$$\begin{aligned}
&n=3,\quad \hat{\phi}_1 = \pm 1,\quad \hat{\phi}_2 = \mp 1,\\
&n=5,\quad \hat{\phi}_1 = \pm 2,\quad \hat{\phi}_2 = \mp 1,\quad \hat{\phi}_3 = \pm 1,\quad \hat{\phi}_4 = \mp 2,\\
&n=7,\quad \hat{\phi}_1 = \pm 3,\quad \hat{\phi}_2 = \mp 1,\quad \hat{\phi}_3 = \pm 2,\quad \hat{\phi}_4 = \mp 2,\quad \hat{\phi}_5 = \pm 1,\quad \hat{\phi}_6 = \mp 3\,;\\
&\text{arbitrary odd } n\,,\quad \hat{\phi}_i = \begin{cases} \pm(n-i)/2\,, & i \text{ odd}\,,\\ \mp i/2\,, & i \text{ even}\,.\end{cases}
\end{aligned} \tag{5.5}$$

n even: in this case $\theta = 0$. We list below the asymptotic values $\phi_\alpha(\infty)$ in units of 2η, i.e., $\hat{\phi}_\alpha = \phi_\alpha(\infty)/2\eta$:

$$\begin{aligned}
&n=2,\quad \hat{\phi}_1 = \pm 1,\\
&n=4,\quad \hat{\phi}_1 = \pm 1,\quad \hat{\phi}_2 = 0,\quad \hat{\phi}_3 = \pm 1,\\
&n=6,\quad \hat{\phi}_1 = \pm 1,\quad \hat{\phi}_2 = 0,\quad \hat{\phi}_3 = \pm 1,\quad \hat{\phi}_4 = 0,\quad \hat{\phi}_5 = \pm 1\,;
\end{aligned} \tag{5.5'}$$

arbitrary even n, $\hat{\phi}_i = \begin{cases} \pm 1, & i \text{ even}, \\ 0, & i \text{ odd}. \end{cases}$

The asymptotic values of the functions $\phi_\alpha(r)$ lead to the following vacuum orbits for the adjoint Higgs fields:

$$n \text{ odd}, \quad \Phi(\infty) = \pm \operatorname{diag} 2\eta\left(1-\frac{1}{n}, -\left(1+\frac{1}{n}\right), 1-\frac{1}{n}, -\left(1+\frac{1}{n}\right), \ldots, -\left(1+\frac{1}{n}\right), 1-\frac{1}{n}\right)$$

$$\left.\begin{array}{ll} \text{invariance} \\ \text{group of } \Phi(\infty) \end{array}\right\}: \quad \begin{array}{ll} n=3, & \mathrm{SU}(2)\times\mathrm{U}(1), \\ n>3, & \mathrm{SU}((n+1)/2)\times\mathrm{SU}((n-1)/2); \end{array} \tag{5.6}$$

$$n \text{ even}, \quad \Phi(\infty) = \pm \operatorname{diag} 2\eta(1,-1,1,-1,\ldots,1,-1),$$

$$\left.\begin{array}{ll} \text{invariance} \\ \text{group of } \Phi \end{array}\right\} \quad \begin{array}{ll} n=2, & \mathrm{U}(1), \\ n>2, & \mathrm{SU}(n/2)\times\mathrm{SU}(n/2). \end{array} \tag{5.6'}$$

To recast the energy functional (5.3) into a form to which the FTS proof is applicable, it is convenient to reparametrize the Higgs field in terms of the diagonal matrix $\tau = \operatorname{diag}(\tau_1,\ldots,\tau_n)$ defined by

$$\tau = \Phi - \Phi(\infty), \quad \text{i.e., } \tau(\infty) = 0. \tag{5.7}$$

The functions $\tau_i(r)$ are then defined by

$$\tau_i(r) = \phi_i(r) - \phi_{i-1}(r) + 2\eta\epsilon_i,$$

$$\epsilon_i = \begin{cases} (-1)^i(1+(-1)^i/n), & n \text{ odd}, \\ (-1)^i, & n \text{ even}, \end{cases} \tag{5.7'}$$

where $\phi_0(r) = \phi_n(r) = 0$ and we have chosen the positive asymptotic limits. If we introduce the functions

$$\mu_\alpha = a_\alpha(\tau_{\alpha+1} - \tau_\alpha + (-1)^\alpha 4\eta), \quad \alpha = 1,\ldots,n-1,$$

$$\nu_i = (1/r)[a_i^2 - a_{i-1}^2 - n + 2i - 1], \tag{5.8}$$

$$i = 1,\ldots,n, \quad a_0 = a_n = 0,$$

$$\rho_i = (1/\sqrt{6})\, r\tau_i(\tau_i - (-1)^i 4\eta), \quad i = 1,..,n,$$

then the energy functional can be written in the form

$$\mathscr{E} = \int_0^\infty dr\left\{4\sum_{\alpha=1}^{n-1}(a'_\alpha)^2 + \frac{1}{2}r^2\sum_{i=1}^{n}(\tau'_i)^2 + \frac{1}{2}\sum_{\alpha=1}^{n-1}(\mu_\alpha)^2 + \sum_{i=1}^{n}(\nu_i)^2 + \sum_{i=1}^{n}(\rho_i)^2\right\}. \tag{5.9}$$

With the energy functional in this form, we can proceed with the FTS proof. Given that functions a_α and τ_i exist, which gives rise to finite energy, we choose from such solutions a minimizing set of sequences of functions $\{a_\alpha^m, \tau_i^m\}$ with the property that

$$\lim_{m\to\infty} \mathscr{E}(a_\alpha^m, \tau_i^m) = \inf \mathscr{E}(\alpha_\alpha, \tau_i). \tag{5.10}$$

To establish the existence of solutions that minimize $\mathscr{E}$ it is sufficient to show the $\inf \mathscr{E}(a_\alpha, \tau_i)$ is attained for the set of functions $\{a_\alpha^0, \tau_i^0\}$—the limit of the above minimizing set of sequences.

The proof of this result is very technical and for this reason we leave the details to Appendix B. Most of the work goes into establishing convergence properties of the induced sequences of functions $\{\mu_\alpha^m, \nu_i^m, \rho_i^m\}$, in terms of the convergence properties of $\{a_\alpha^m, \tau_i^m\}$. Having established the strong convergence $a_\alpha^m \to a_\alpha^0$, $\tau_i^m \to \tau_i^0$ in $C(a,b)$, it follows that the sequences $\{\mu_\alpha^m, \nu_i^m, \rho_i^m\}$ converge weakly in $L^2(0,\infty)$ to $\{\mu_\alpha^0, \nu_i^0, \rho_i^0\}$. The other induced sequences $\{a_\alpha'^m, r\tau_i'^m\}$ also converge weakly in $L^2(0,\infty)$ as a result of the finiteness of $\mathscr{E}$.

Once these convergence properties are established, we make use of a property of the scalar product in $L^2(0,\infty)$, namely that

$$\langle \text{weak limit, weak limit} \rangle \leqslant \lim \langle 0,0 \rangle$$

to give us

$$\mathscr{E}(a_\alpha^0, \tau_i^0) \leqslant \lim_{m\to\infty} \mathscr{E}(a_\alpha^m, \tau_i^m). \tag{5.11}$$

Together with (5.10) above we see that the infinium is attained for the functions (a_α^0, τ_i^0).

This establishes the result that the YMH system in three dimensions, with a fixed value for the coupling constant of the Higgs potential, obtained from the ST dimensional reduction of the YM system in some higher even-dimensional manifold, possesses finite energy *monopole* solutions. These solutions have asymptotic Higgs fields (on the z axis) given by (5.6) and (5.6') for the gauge group SU(n), n odd and n even, respectively. Of these, (5.6') for $n = 2$ is the Higgs vacuum for the 't Hooft–Polyakov monopole,[1] with a fixed value for the coupling constant, while (5.6) for $n = 3$ is the non-self-dual monopole orbit found by Burzlaff.[6] Of course, the whole family of solutions presented here are non-self-dual.

In the spherical symmetry *Ansatz* (5.2), the SU(n) system is characterized by $(2n-1)$ radial functions, namely $\theta, \phi_1, \ldots, \phi_{n-1}, a_1, \ldots, a_{n-1}$. However, for the moment we are dealing with the case $\Theta = \text{const}$. On the surface this reduces the number of radial functions to $2(n-1)$. However, imposing this constraint on the Euler–Lagrange equations of the system gives rise to a constraint on the ϕ_α, a_α functions, further reducing their number.

Consider the Euler–Lagrange equation of the field multiplet ϕ of (5.1),

$$\mathscr{D}_i\mathscr{D}_i\phi + 2(\eta^2 + \phi^2)\phi = 0. \tag{5.12}$$

If we take the trace of this equation we find the equation of motion for Θ, namely,

$$n\Delta\Theta = -2\operatorname{tr}[\Phi^3 + 3\Theta\Phi^2] - 2n\Theta(\eta^2 + \Theta^2). \tag{5.13}$$

Clearly $\Theta = \text{const}$ is a consistent solution of this equation only if the right-hand side vanishes, i.e.,

$$\operatorname{tr}[\Phi^3 + 3\Theta\Phi^2] + n\Theta(\eta^2 + \Theta^2) = 0. \tag{5.14}$$

This one scalar condition reduces the number of independent radial $\phi_\alpha(r)$ functions by at least 1. We will return to this

point in the next section where we discuss the solutions obtained above.

From the viewpoint of Sec. III these solutions are very interesting because they provide field configurations for which each term in the surface integrals (3.5') and (3.9') contributes distinctly, provided that we take the gauge group $G = \mathrm{SU}(n)$ to be sufficiently large. For example, in the case of (3.5') each term will contribute distinctly if $G = \mathrm{SU}(5)$.

To evaluate these surface integrals it is sufficient to specify the Higgs orbit (5.6) or (5.6') and the corresponding values of the constant parameter $\Theta = -i\eta/n$ for odd n, and $\Theta = 0$ for even n. The asymptotic properties of $\mathscr{B}_i$ and $\mathscr{D}_i\phi$ can be deduced simply from the Euler–Lagrange equations of the action (5.3), namely that both $\mathscr{B}_i$ and $\mathscr{D}_i\phi$ asymptotically behave as $O(1/r^2)$. This result ensures that the terms involving $\mathscr{D}_i\phi$ in the surface integrals (3.5), (3.9), (3.5'), and (3.9') do not contribute.

The existence proof outlined above, and given in Appendix B, does not depend critically on the assumption of constant θ. Indeed, with minor modifications, the proof can be extended to cover this case. For instance, the asymptotic limits on the singlet function $\theta(r)$ turn out to be

$$\theta(\infty) = \pm(1/n)\eta, \quad \text{for } n \text{ odd},$$
$$= 0, \quad \text{for } n \text{ even}.$$

The other modification is to the spin-0 field parametrization, where it is more convenient, for the purposes of the proof, to parametrize the Higgs field by

$$\phi = (i/2)\mathrm{diag}(\chi_1,\chi_2,\cdots,\chi_n),$$

rather than in terms of Φ and Θ separately. These, however, are very minor modifications that in no way affect the details of the proof. The solutions obtained will of course be a distinct family of monopole solutions with reducible Higgs fields in the adjoint $\oplus$ scalar representations. It is clear that the constraint (5.14), which reduced the number of radial functions in the $\Theta = \text{const}$ case, does not now arise.

VI. DISCUSSION

A. Surface integrals

The main results of this paper are those obtained in Secs. III and IV. Our task in those sections was to derive surface integrals in odd- and even-dimensional spaces from Chern classes defined on manifolds of arbitrary (even) dimension. This was achieved by imposing symmetries on the original manifold using the ST calculus for dimensional reduction. It is very important to stress that the surface integrals in the lower-dimensional manifolds converge for certain field configurations, in the sense that the corresponding Lagrangian systems (in the lower dimensions) have finite energy (action) solutions. The existence of such solutions is guaranteed by the fact that the particular dimensional reduction schemes employed give rise to the symmetry breaking type of Higgs potential. In fact, it is this qualitative requirement that makes our prescription nontrivial.

In Sec. III we treated the case where the reduced space is of odd dimensions, with particular emphasis on the physically relevant three-dimensional case. Our objective in this section was twofold. We wished to demonstrate that Taubes' topologically invariant surface integrals[9] occur in some particular reduction of Chern classes of arbitrarily high order. The reduction in question is one where, in three dimensions, the gauge convariant scalar (Higgs) field belongs to the adjoint representation of the residual gauge group. The second objective was to generate (via dimensional reduction) gauge-field–Higgs systems endowed with topological integrals where the Higgs field belongs to either some other irreducible representation or to some reducible representation of the residual gauge group. For simplicity we only performed the reductions leading to the adjoint $\oplus$ scalar Higgs representation,[10] and to a fundamental Higgs representation,[17] as illustrative examples. Although the latter systems[17] are in principle equally as interesting as the conventional one with just the adjoint representation Higgs field, no minimum energy (action) solutions with finite topological integral are known for them. One reason for the absence of such solutions may be the fact that for the YMH systems in question there are no self-duality equations, whereas all known *exact* solutions are self-dual. However, unstable solutions (which maximize the energy) for a fundamental SU(2) Higgs field have recently been found.[17]

Our objective in Sec. IV—obtaining surface integrals in even-dimensional submanifolds—was not so easily attained. First, we found that the reduction by an even number of dimensions, induced by $\mathscr{M}_N = E_{N-p} \times S^p$, p even, resulted in the vanishing of all Chern integrals except in the case of reduction by two dimensions. That the $p = 2$ case is not trivial was known to us from previous work,[12,18] but the trivial nature of the even $p > 2$ cases meant that to obtain nonzero surface integrals we would have to use more complicated reduction schemes. As a first attempt we found that generating such a reduction by means of two separate reductions by odd numbers of dimensions led to a gauge-field–Higgs system with two Higgs fields where, however, the surface integral vanished identically due to the finite energy condition and the special dependence of the integral on the two Higgs fields. Fortunately we could find a prescription yielding a nonvanishing surface integral in the (even) lower dimensions—namely a succession of ST reductions by two dimensions. This was achieved by arranging for the Higgs field arising from each stage of the reduction to vanish except for the Higgs field arising from the last stage of the reduction. The vanishing of these Higgs fields was not arranged arbitrarily but by the imposition of symmetries.

B. Solutions and constraints

A subsidiary result of this paper is the proof of existence of the two families of solutions for both the YMH system with an adjoint representation Higgs field and the YMH system with adjoint $\oplus$ scalar representation Higgs field, which we presented in Sec. V. The relevance of these solutions to the above is that, using the YMH system as a vehicle, we have presented field configurations that lead to finite values for the topological integrals of type I derived in Sec. III. Unfortunately we are not in a position to present a proof of the existence of field configurations that lead to nonvanishing values for the surface integrals of type (II) of Sec. III. Indeed the only known finite energy solutions of such mod-

els[17] give rise to vanishing surface integrals. Thus we complete the analogy with the reduction from four dimensions to two dimensions, considered in Sec. IV, where the vortex surface integral given by (4.10a) has finite value for the field configurations of Ginzburg and Landau.[11]

In particular, the solutions of the YMH system with adjoint representation SU(n) Higgs field separate naturally into two families, one for even n and the other for odd n. The first member of the even n family is the archetypal SU(2) 't Hooft–Polyakov[1] solution, while the first member of the odd n family is equivalent to the SU(3) solution found by Burzlaff.[6]

As mentioned in Sec. V, these families of solutions to the adjoint representation model are subject to certain constraints. Indeed, this constraint reduces our SU(3) solution[10] to a two function field configuration. This result can be seen to follow directly from the constraint (5.14). Let us consider first the *odd n* cases. The constraint in this case reads

$$\operatorname{tr}\Phi^2(i\Phi+(3/n)\eta)=-\eta^3(1-1/n^2)\,. \tag{6.1}$$

The $n=3$, i.e., SU(3), constraint is particulary simple, namely

$$(\phi_1-4\eta/3)(\phi_2+4\eta/3)(\phi_2-\phi_1-4\eta/3)=0\,. \tag{6.2}$$

Of the three solutions of this constraint equation, $\phi_2-\phi_1=4\eta/3$ is not consistent with the asymptotic conditions (5.5), but the remaining two solutions

$$\phi_1=4\eta/3\,,\quad \phi_2=-4\eta/3 \tag{6.3}$$

are both acceptable. When these constraints are substituted into the equations of motion for the functions $\phi_1(r)$ and $\phi_2(r)$, they lead, respectively, to further constraints

$$a_1=0\,,\quad a_2=0\,. \tag{6.4}$$

Thus, for SU(3) our field configuration is parametrized in terms of only two radial functions, either (ϕ_1,a_1) or (ϕ_2,a_2), and not four.

Now let us consider the *even n* case. The constraint then reads

$$\operatorname{tr}\Phi^3=0\,, \tag{6.5}$$

as for even n, $\Theta=0$. The $n=4$, i.e., SU(4), constraint is again particularly simple, namely

$$\phi_2(\phi_3-\phi_1)(\phi_1+\phi_3-\phi_2)=0\,. \tag{6.6}$$

The solution $\phi_1+\phi_3=\phi_2$ is not consistent with the asymptotic conditions (5.5'), but the remaining two solutions

$$\phi_2=0\,,\quad \phi_1=\phi_3 \tag{6.7}$$

are both acceptable. These solutions lead in turn to the further constraints

$$a_2=0\,,\quad a_1=\pm a_3\,, \tag{6.8}$$

respectively. Consequently we see that there are two classes of solutions. Class (I) is characterized by $\phi_2=a_2=0$, so that there are four radial functions (ϕ_1,ϕ_3,a_1,a_3). However, in this case the equations decouple into two identical sets of SU(2) equations for (ϕ_1,a_1) and (ϕ_3,a_3). Class (II), on the other hand, is characterized by the four functions (ϕ_1,ϕ_2,a_1,a_2) and in this case the equations of motion do not decouple. The class (II) solutions then are true four function solutions.

For $n>4$ the constraint equations can be solved by inspection in the manner we now outline. Again the cases n odd and n even are treated separately. Let us first consider the case of *n odd*. It is straightforward to see that the constraint (6.1) is solved by each of the following sets of constraints:

$$\phi_1=\left(\frac{n-1}{2}\right)\frac{4\eta}{n}\,,\quad \phi_3=\left(\frac{n-3}{2}\right)\frac{4\eta}{n}\,,\ldots,\phi_{n-2}=\frac{4\eta}{n}\,, \tag{6.9a}$$

$$\phi_2=-\frac{4\eta}{n}\,,$$

$$\phi_4=-2\left(\frac{4\eta}{n}\right),\ldots,\phi_{n-1}=-\left(\frac{n-1}{2}\right)\frac{4\eta}{n}\,. \tag{6.9b}$$

Substitution of (6.9a) and (6.9b) in turn into the Euler–Lagrange equations leads to the further constraints

$$a_1=a_3=\cdots=a_{n-2}=0\,, \tag{6.10a}$$

$$a_2=a_4=\cdots=a_{n-1}=0\,. \tag{6.10b}$$

The resulting equations of motion for the remaining $(n-1)$ functions (ϕ_α,a_α), $\alpha=2,4,\ldots,n-1$, or $\alpha=1,3,\ldots,n-2$ decouple for each α separately. The pairs of uncoupled differential equations are all different, however, so that the corresponding field configuration is parametrized by $(n-1)$ different radial functions.

On the other hand, for even n, it can easily be shown that the constraint (6.5) can be solved by each of the following sets of constraints:

$$\phi_2=\phi_4=\cdots=\phi_{n-2}=0\,, \tag{6.11a}$$

$$\phi_1=\phi_3=\cdots=\phi_{n-3}\,,\quad \phi_{n-2}=0\,. \tag{6.11b}$$

When substituted into the equations of motion these constraints lead, respectively to

$$a_2=a_4=\cdots=a_{n-2}=0\,, \tag{6.12a}$$

$$a_1^2=a_3^2=\cdots=a_{n-1}^2\,. \tag{6.12b}$$

When the constraints (6.11a) and (6.12a) are used the equations of motion decouple; the remaining n functions (ϕ_α,a_α), $\alpha=1,3,\ldots,n-1$, satisfy identical differential equations for each value of α. Thus the solutions of the differential equations are identical, and we have a two function field configuration, as seen above for $n=4$. However, the constraints (6.11b) and (6.12b) lead to n differential equations for the n radial functions (ϕ_α,a_α), $\alpha=1,2,4,6=n-4$, and (a_{n-2},ϕ_{n-1}), which *do not decouple*. The resulting field configuration is parameterized by n different radial functions.

We have not found any field configurations parametrized by more than $n-1$ (n) different radial functions for n odd (n even). Field configurations do exist, however with fewer than $n-1$ (n) different radial functions. An exhaustive survey of all the solutions was not our aim in this analysis—such a survey wil be reported upon elsewhere. Rather, our aim was to establish the existence of nontrivial multifunction finite energy (action) field configurations.

Of course, in the adjoint $\oplus$ scalar representation model there are also two families of solutions, again separating into the even n and odd n cases. The constraints, discussed above, which reduce the number of radial functions in the adjoint representation model, simply do not occur in this model.

Thus for SU(n) there are $2n-1$ different radial functions in the spherically symmetric *Ansatz*, namely $\theta(r),\phi_1(r),\ldots,\phi_{n-1}(r),a_1(r),\ldots,a_{n-1}(r)$. Solutions of this type have not been presented before.

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APPENDIX A: Γ-MATRIX TRACES

In our adaptation of the ST scheme to the reduction of p dimensions ($p \geq 2$), we have used the matrices $\hat{\Gamma}_a = iL_{a,p+1}$ for *odd* p, and $\hat{\Gamma}_a = iL_{a,p+1}$ and $iL_{a,p+2}$ for *even* p, where L_{ab} are the $m \times m$ (spinor) representations of so(p) (the stability subalgebra), with m given by (2.9), namely

$$\begin{aligned} m &= 2^{(p-1)/2}, \quad p \text{ odd}, \\ &= 2^{p/2}, \quad p \text{ even}. \end{aligned}$$

the so($p+2$) algebra, which these $\hat{\Gamma}_a$ belong to, can be defined in terms of the $m \times m$ Γ matrices (of p dimensions):

$$\begin{aligned} &L_{ab} = -\tfrac{1}{4}[\Gamma_a,\Gamma_b], \quad L_{\alpha,p+1} = \pm(i/2)\Gamma_a, \\ &L_{a,p+1} = \tfrac{1}{2}\Gamma^{p+1}\Gamma_a, \quad L_{p+1,p+2} = \mp(i/2)\Gamma^{p+1}, \end{aligned} \tag{A1}$$

where $\Gamma^{p+1} = i^{(1/2)(p-2)}\Gamma_1\cdots\Gamma_p$ is the chirality operator, and it plays a role in our considerations *only* for even p.

The traces involved in our computation in Secs. III and IV are of the following forms for p odd/even:

$$T^{(\text{odd})} = \epsilon_{a_1\cdots a_p} \operatorname{tr} \Gamma^{p+1} L_{a_1a_2}\cdots L_{a_{p-1},p}, \tag{A2}$$

$$T^{(\text{even})} = \epsilon_{a_1\cdots a_p} \operatorname{tr} L_{a_1a_2}\cdots L_{a_{p-2},a_{p-1}}\hat{\Gamma}_{a_p}. \tag{A3}$$

To evaluate (A2) and (A3) we make use of the following Γ-matrix identity, for Γ_μ matrices in p dimensions:

$$[\Gamma_{\mu_1},\Gamma_{\mu_2}] = [2/(p-2)!]\epsilon_{\mu_1\cdots\mu_p}\Gamma^{p+1}\Gamma_{\mu_3}\cdots\Gamma_{\mu_p}. \tag{A4}$$

This follows directly from the definition of the Γ in p dimensions and the spinor identity

$$[\gamma_\mu,\gamma_\nu] = -\epsilon_{\mu\nu\rho\sigma}\gamma_5\gamma_\rho\gamma_\sigma, \tag{A4'}$$

for the 4×4 γ matrices.

APPENDIX B: THE EXISTENCE PROOF

In this Appendix we are concerned with the existence proof of Sec. V, and in particular with the technical details omitted there.

The energy functional is given by

$$\mathscr{E} = \int_0^\infty dr\left[4\sum_{\alpha=1}^{n-1}(a'_\alpha)^2 + \frac{1}{2}r^2\sum_{i=1}^{n}(\tau'_i)^2 + \frac{1}{2}\sum_{\alpha=1}^{n-1}\mu_\alpha^2 + \sum_{i=1}^{n}\nu_i^2 + \sum_{i=1}^{n}\rho_i^2\right], \tag{B1}$$

where

$$\begin{aligned} &\mu_\alpha = a_\alpha(\tau_{\alpha+1} - \tau_\alpha + (-1)^\alpha 4\eta), \quad \alpha = 1,\ldots,n-1, \\ &\nu_i = (1/r)(a_i^2 - a_{i-1}^2 - n + 2i - 1), \\ &i = 1,\ldots,n, \quad a_0 = a_n = 0, \\ &\rho_i = (1/\sqrt{6})\, r\,\tau_i(\tau_i - (-1)^i 4\eta), \quad i = 1,\ldots,n. \end{aligned} \tag{B2}$$

We denote the minimizing set of sequences of functions by $\{a_\alpha^m,\tau_i^m\}$.

The first technical step is to establish that the sequences $\{\tau_i^m\}$ are bounded in the Sobelev space $\mathscr{H}_1$ with norm

$$\|\tau\|_1 = \left(\int_0^\infty r^2|\tau'|^2\,dr + |\tau(1)|^2\right)^{1/2}. \tag{B3}$$

Using the Cauchy–Schwarz inequality we see that

$$\int_B^\infty |\tau_i^{m\prime}|dr \leq \left(\int_B^\infty \frac{dr}{r^2}\right)^{1/2}\left(\int_B^\infty r^2(\tau_i^{m\prime})^2\,dr\right)^{1/2} \leq \frac{c_i}{\sqrt{B}} \tag{B4}$$

as the convergence of $\mathscr{E}$ implies the convergence of $\int_B^\infty r^2(\tau_i^{m\prime})^2\,dr$. However,

$$\int_B^\infty |\tau_i^{m\prime}|dr \geq |\,|\tau_i^m(\infty)| - |\tau_i^m(B)|\,| \tag{B5}$$

and we know that $\tau_i^m(\infty) = 0$, so that

$$\int_B^\infty |\tau_i^{m\prime}|dr \geq |\tau_i^m(B)|, \tag{B6}$$

which gives us the result

$$|\tau_i^m(B)| \leq c_i/\sqrt{B}, \tag{B7}$$

i.e., the sequences $\{\tau_i^m(B)\}$ are bounded.

In particular we choose $B = 1$, and use (B7) to see that

$$\left(\int_0^\infty r^2(\tau_i^{m\prime})^2\,dr + |\tau_i^m(1)|^2\right)^{1/2}$$

is bounded for all m, and for all i. Thus the sequences of functions $\{\tau_i^m: i = 1,\ldots,n\}$ are indeed bounded in $\mathscr{H}_1$.

The second technical step is to show that the sequences of functions $\{\theta_\alpha^m:\ \alpha = 1,\ldots,n=1\}$ are bounded in the Sobelev space $\mathscr{H}_2$ with norm

$$\|a_2\| = \left(\int_0^\infty (a')^2\,dr + |a(1)|^2\right)^{1/2}. \tag{B8}$$

The convergence of $\mathscr{E}(a_\alpha^m,\phi_\alpha^m)$ for each m ensures that $\int_0^\infty (a_\alpha^{m\prime})^2\,dr$ and $\int_0^\infty (\mu_\alpha^m)^2\,dr$ are bounded sequences. The latter can be rewritten as

$$\int_0^\infty (a_\alpha^m)^2(\tau_{\alpha\mp1}^m - \tau_\alpha^m + (-1)^\alpha 4\eta)^2\,dr \leq \text{const}. \tag{B9}$$

It is at this stage that the assertion made in (5.4) is relevant. The asymptotic limits have been chosen to ensure that the next argument holds:

$$\begin{aligned} &|\tau_{\alpha+1}^m(r) - \tau_\alpha^m(r) + (-1)^\alpha 4\eta| \\ &\quad \geq 4\eta - |\tau_{\alpha+1}^m(r) - \tau_\alpha^m(r)| \\ &\quad \geq 4\eta - (|\tau_{\alpha+1}^m(r)| + |\tau_\alpha^m(r)|) \\ &\quad \geq 4\eta - (c_{\alpha+1} + c_\alpha)/\sqrt{r} \\ &\quad \geq 4\eta - (c_{\alpha+1} + c_\alpha)/\sqrt{B}, \quad \text{if } r > B. \end{aligned} \tag{B10}$$

In the second last step we have used (B6) above. Using (B9) we see that

$$\begin{aligned} \text{const} &\geq \int_B^\infty (a_\alpha^m)^2(\tau_{\alpha+1}^m - \tau_\alpha^m + (-1)^\alpha 4\eta)^2\,dr \\ &\geq \int_B^\infty (a_\alpha^m)^2(4\eta - (c_{\alpha+1} + c_\alpha)/\sqrt{B})\,dr, \end{aligned}$$

whence we see that

$$\int_B^\infty (a_\alpha^m)^2\,dr \leqslant \frac{\text{const}}{(4\eta - (c_{\alpha+1}+c_\alpha)/\sqrt{B})^2}. \tag{B11}$$

It now follows that

$$(a_\alpha^m(B))^2 \leqslant 2\int_B^\infty |a_\alpha^m(r)|\,|a_\alpha^m(r)'|\,dr \quad \text{by (B6)}$$

$$\leqslant 2\left(\int_B^\infty (a_\alpha^m(r))^2\,dr\right)^{1/2}\left(\int_B^\infty (a_\alpha^{m\prime}(r))^2\,dr\right)^{1/2}$$

by Cauchy–Schwarz inequality

$$\leqslant \text{const}/\left[4\eta - (c_{\alpha+1}+c_\alpha)/\sqrt{B}\,\right], \tag{B12}$$

i.e., $\{a_\alpha^m(B)\colon \alpha = 1,\ldots,n-1\}$ is a set of bounded sequences. In particular we choose $B = 1$, and see that

$$\|a_\alpha^m\|_2 = \left(\int_0^\infty (a_\alpha^m(r)')^2\,dr + |a_\alpha^m(1)|^2\right)^{1/2}$$

is bounded for all m, and for all α. Hence the sequences of functions $\{a_\alpha^m\colon \alpha = 1,\ldots,n-1\}$ are bounded in $\mathscr{H}_2$.

With the above two results established, the remaining steps in the proof follow systematically.

(i) The bounded sequences $\{\tau_i^m\colon i = 1,\ldots,n\}$ and $\{a_\alpha^m\colon \alpha = 1,\ldots,n-1\}$ contain weakly convergent subsequences; without loss of generality,

$$\begin{aligned} &\tau_i^m \to \tau_i^0 \text{ weakly in } \mathscr{H}_1, \\ &a_\alpha^m \to a_\alpha^0 \text{ weakly in } \mathscr{H}_2. \end{aligned} \tag{B13}$$

(ii) It follows that $\tau_i^m \to \tau_i^0$, $a_\alpha^m \to a_\alpha^0$ weakly in $W_1^2(a,b)$, the space of functions with norm $\left[\int_a^b |\varphi'|^2 dr + |\varphi(a)|^2\right]^{1/2}$.

(iii) It now follows that $\tau_i^m \to \tau_i^0$, $a_\alpha^m \to a_\alpha^0$ strongly in $C(a,b)$ the space of continuous functions defined on the interval $[a,b]$, as $W_1^2(a,b)$ is densely embedded in $C(a,b)$.

(iv) This result implies, for the induced sequences, the strong convergence in $C(a,b)$, $\mu_\alpha^m \to \mu_\alpha^0$, $\nu_i^m \to \nu_i^0$, $\rho_i^m \to \rho_i^0$, where

$$\begin{aligned} \mu_\alpha^0 &= a_\alpha^0(\tau_{\alpha+1}^0 - \tau_\alpha^0 + (-1)^\alpha 4\eta), \\ \nu_i^0 &= (1/r)\left[(a_i^0)^2 - (a_{i-1}^0)^2 - n + 2i - 1\right], \\ \rho_i^0 &= (1/\sqrt{6})\, r\,\tau_i^0(\tau_i^0 - (-1)^i 4\eta). \end{aligned} \tag{B14}$$

(v) The convergence of $\mathscr{E}(a_\alpha^m,\tau_i^m)$ for each m ensures that $\{\mu_\alpha^m,\nu_i^m,\rho_i^m\}$ are bounded sequences of functions in $L^2(0,\infty)$. Without loss of generality, we deduce that $\mu_\alpha^m \to \mu_\alpha^0$, $\nu_i^m \to \nu_i^0$, $\rho_i^m \to \rho_i^0$ weakly in $L^2(0,\infty)$. Up to step (iv) above we are establishing the limits of the induced sequences. Step (v) establishes the weak convergence result quoted in the text.

(vi) The convergence of $\mathscr{E}(a_\alpha^m,\tau_i^m)$ for each m ensures that $\{a_\alpha^{m\prime}, r\,\tau_i^{m\prime}\}$ are bounded sequences of functions in $L^2(0,\infty)$, and without loss of generality we can deduce that $a_\alpha^{m\prime} \to a_\alpha^{0\prime}$, $r\,\tau_i^{m\prime} \to r\,\tau_i^{0\prime}$ weakly in $L^2(0,\infty)$.

We have now established all the convergence properties needed. The proof is completed by using the property of the scalar product in $L^2(0,\infty)$, namely that the scalar product of weak limits is less than or equal to the limit of the scalar product, as shown in Sec. V.

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Construction of hyperbolic monopoles

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Methods are presented for explicit construction of hyperbolic monopoles as defined by Atiyah [M. F. Atiyah, Commun. Math. Phys. **93**, 437 (1984); and "Magnetic monopoles in hyperbolic space," unpublished lecture notes, 1984]. The techniques permit the extraction of flat-space self-dual monopoles trivially through a simple rescaling. Relationships to previous works of the present author are indicated.

I. INTRODUCTION

Atiyah has proposed the following definition of hyperbolic monopoles.[1]

Let

$$ds^2 = dx_0^2 + dx_1^2 + dx_2^2 + dx_3^2 \tag{1.1}$$

$$= u^2[d\sigma^2 + u^{-2}(du^2 + dx_1^2 + dx_2^2)] \tag{1.2}$$

$$= u^2[d\sigma^2 + u^{-2}(du^2 + dv^2 + v^2 d\varphi^2)], \tag{1.3}$$

where

$$x_0 \pm ix_3 = ue^{\pm i\sigma}, \tag{1.4}$$

$$x_1 \pm ix_2 = ve^{\pm i\varphi}. \tag{1.5}$$

The conformal equivalence

$$R^4 - R^2 \sim S^1 \times H^3 \tag{1.6}$$

permits one to interpret the S^1-invariant (S^1: $\sigma\in[0,2\pi]$) instantons on R^4 (or S^4) as static monopoles on H^3. Atiyah has analyzed the notion of S^1 invariance that leads to suitable classes of solutions and has studied the parameter space of such solutions.[1] The explicit construction of the solutions and the explicit extraction of flat-space finite-energy BPS monopoles as limits remain difficult through his approach. Exactly these two problems are tackled here using methods showing complementary virtues.

I have studied in a series of papers[2] explicit construction of S^1-invariant instantons. The S^1 in question was selected in the following way.

Let

$$ds^2 = dx_0^2 + dx_1^2 + dx_2^2 + dx_3^2$$

$$= dt^2 + dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta\, d\varphi^2 \tag{1.7}$$

$$= (\cosh\rho + \cos\tau)^{-2}[d\tau^2 + d\rho^2 + \sinh^2\rho(d\theta^2 + \sin^2\theta\, d\varphi^2)]. \tag{1.8}$$

Here t, r, θ, and φ are spherical coordinates and

$$(t + ir) = \tan\tfrac{1}{2}(\tau + i\rho) \tag{1.9}$$

maps

$$t\in[-\infty,\infty], \quad r\in[0,\infty]$$

on

$$\tau\in[-\pi,\pi], \quad \rho\in[0,\infty]. \tag{1.10}$$

In this context, S_1-invariance refers to τ. Again, setting

$$\tau = t'/\alpha, \quad \rho = r'/\alpha, \quad \alpha\to\infty, \tag{1.11}$$

$$(4\alpha^2)ds^2 \equiv ds'^2 = dt'^2 + dr'^2 + r'^2(d\theta^2 + \sin^2\theta\, d\varphi^2). \tag{1.12}$$

This leads very simply, in the limit, to flat-space BPS monopoles of arbitrary charge from τ-independent instantons.[2] I have described repeatedly and in detail my motivations for constructing such "τ-static chains" of instantons with their remarkable properties.[2] Here I will adapt my techniques (Bäcklund-type transformations and Lax-type pairs) to (1.3). This will permit (i) explicit construction of σ-static instantons, and (ii) trivial extraction of flat-space BPS monopoles through a rescaling like (1.11).

By σ-static I mean that in some suitable gauge the components $A_\sigma, A_u, A_v, A_\varphi$, or $A_\sigma, A_u, A_{x_1}, A_{x_2}$ must be independent of σ explicitly. I will often use the following coordinates.

Let

$$u = e^{-\zeta}, \quad u\in[0,\infty], \quad \zeta\in[-\infty,\infty], \tag{1.13}$$

when

$$ds^2 = e^{-2\zeta}[d\sigma^2 + d\zeta^2 + e^{2\zeta}(dv^2 + v^2 d\varphi^2)]. \tag{1.14}$$

(The change $u\to\zeta$ is evidently slight but helpful in certain respects.) Setting

$$\sigma = t'/\alpha, \quad \zeta = z'/\alpha, \quad v = v'/\alpha, \quad \alpha\to\infty, \tag{1.15}$$

$$\alpha^2 ds^2 \equiv ds'^2 = dt'^2 + dz'^2 + dv'^2 + v'^2 d\varphi^2 \tag{1.16}$$

is the line element in cylindrical coordinates.

Correspondingly rescaled solutions will turn out to the flat-space BPS monopoles in the formalism of Forgacs, Horvath, and Palla.[3]

Setting

$$u = (\cosh\chi + \sinh\chi\cos\psi)^{-1}, \tag{1.17}$$

$$v = \sinh\chi\sin\psi(\cosh\chi + \sinh\chi\cos\psi)^{-1}, \tag{1.18}$$

$$\chi\in[0,\infty], \quad \psi\in[0,\pi],$$

$$ds^2 = (\cosh\chi + \sinh\chi\cos\psi)^{-2}[d\sigma^2 + d\chi^2 + \sinh^2\chi\, d\Omega] \tag{1.19}$$

$$(d\Omega \equiv d\psi^2 + \sin^2\psi\, d\varphi^2),$$

since

$$u^{-2}(du^2 + dv^2) = d\chi^2 + \sinh^2\chi\, d\psi^2.$$

(The symbols χ and ψ are used in Ref. 2 with different meanings.)

Comparing (1.8) with (1.19), it is evident (remembering conformal properties of gauge fields) that I could have taken over previous solutions[2] through the substitution

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$$(\tau,\rho,\theta) \to (\sigma,\chi,\psi), \tag{1.20}$$

respectively.

The relations of the two sets to the original x_μ's are quite different. Thus

$$\begin{aligned}
&\tanh\rho = 2r(1 + r^2 + t^2)^{-1},\\
&\quad t = x_0, \quad r = (x_1^2 + x_2^2 + x_3^2)^{1/2}, \qquad (1.21)\\
&\tanh\chi = [\{(u+1)^2 + v^2\}\{(u-1)^2\\
&\qquad + v^2\}]^{1/2}(1 + u^2 + v^2)^{-1},\\
&\quad u = (x_0^2 + x_3^2)^{1/2}, \quad v = (x_1^2 + x_2^2)^{1/2}. \qquad (1.22)
\end{aligned}$$

It is, however, interesting to develop an equivalent formalism from the beginning in terms of (1.14). This will maintain throughout, step by step, a closer contact with other approaches based on the standard quaternionic combinations $\{(x_0 \pm ix_3), (x_1 \pm ix_2)\}$. This can be, for example, helpful in trying to understand the relation to the Atiyah–Drinfeld–Hitchin–Manin (ADHM) formalism.[4] Anyhow, though the equations in the following sections will be in terms of (ζ,v) or (u,v), the combinations of (u,v) corresponding to (1.22) (and its generalizations to be discussed) will enter into the solutions in crucial fashion.

In Secs. II and III, I will present the essential steps of the formalism. The structure of the equations will be almost identical to those of Ref. 2. The meaning or content of the symbols will change. This will permit a concise presentation, to be compared throughout with Ref. 2. As sets of prescriptions, however, the presentation will be self-contained.

II. SU(2): AXIAL SYMMETRY

For

$$ds^2 \approx d\sigma^2 + d\zeta^2 + e^{2\zeta}(dv^2 + v^2\,d\varphi^2), \tag{2.1}$$

$$F_{\mu\nu} + \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu], \quad \epsilon_{\sigma\zeta\nu\varphi} = 1, \tag{2.2}$$

the self-duality equations are

$$F_{\sigma\varphi} = vF_{\zeta v}, \quad F_{\varphi\zeta} = vF_{\sigma v}, \quad F_{v\varphi} = e^{2\zeta}vF_{\sigma\zeta}. \tag{2.3}$$

To solve them, I construct Harrison–Neugebauer-type transformations. [Compare with Refs. 2(a) and 2(d) and the sources quoted there.]

Let

$$M_j(\zeta,v), \quad N_j(\zeta,v), \quad j = 1,2 \tag{2.4}$$

be functions independent of σ and φ. The ansatz is

$$\begin{aligned}
A_\sigma &= (M_1 + M_2 + N_1 + N_2)(\tau_3/2)\\
&\quad - i(M_1 - M_2 - N_1 + N_2)(\tau_1/2),\\
A_\zeta &= -i(M_1 - M_2 - N_1 + N_2)(\tau_2/2), \qquad (2.5)\\
e^{-\zeta}A_v &= -(M_1 - M_2 + N_1 - N_2)(\tau_2/2),\\
e^{-\zeta}v^{-1}A_\varphi &= -i(M_1 + M_2 - N_1 - N_2)(\tau_3/2)\\
&\quad - (M_1 - M_2 + N_1 - N_2)(\tau_1/2).
\end{aligned}$$

For Hermiticity

$$M_1 = \overline{N}_1, \quad M_2 = \overline{N}_2, \tag{2.6}$$

where "$-$" denotes complex conjugation.

Define

$$\partial_\pm = \tfrac{1}{2}(\partial_\zeta \pm ie^{-\zeta}\partial_v), \tag{2.7}$$

and

$$X_\pm = \tfrac{1}{2}\partial_\pm \ln(e^{-\zeta}v) = \tfrac{1}{4}(-1 \pm i/e^\zeta v). \tag{2.8}$$

The self-duality equations reduce to

$$\begin{aligned}
\partial_- M_i &= -M_i(N_i - N_j) + (M_i - N_j)X_+,\\
\partial_+ N_i &= -N_i(M_i - M_j) + (N_i - M_j)X_-, \qquad (2.9)\\
&\quad (i,j) = (1,2), (2,1).
\end{aligned}$$

The relations (upper or lower signs)

$$\partial_\mp X_\pm = (X_\pm - X_\mp)X_\pm \tag{2.10}$$

ensure the validity of the Neugebauer–Kramer, I transformations

$$\begin{aligned}
&IM_1 = -M_2 + X_+, \quad IM_2 = -M_1 + X_+,\\
&IN_1 = -N_1 + X_-, \quad IN_2 = -N_2 + X_-.
\end{aligned} \tag{2.11}$$

Thus (IM_i, IN_i), $i = 1,2$, satisfy (2.9) if (M_i,N_i) do so.

One now has to find a p such that (upper or lower signs)

$$(p^2 - 1)^{-1}\partial_\pm p = p^{\pm 1}X_\pm. \tag{2.12}$$

Let

$$p = e^{i\delta}, \quad Y = \cot\delta. \tag{2.13}$$

Then

$$\partial_\zeta Y = Y + (e^\zeta v)^{-1}, \quad e^{-\zeta}\partial_v Y = 1 - (e^\zeta v)^{-1}Y. \tag{2.14}$$

The solution is, λ being a constant,

$$\cot\delta(\lambda) = Y(\lambda) = (2uv)^{-1}(\lambda^2 + v^2 - u^2), \tag{2.15}$$

or

$$p(\lambda) = \left(\frac{Y+i}{Y-i}\right)^{1/2} = \left[\frac{\lambda^2 + (v+iu)^2}{\lambda^2 + (v-iu)^2}\right]^{1/2} \quad (u = e^{-\zeta}). \tag{2.16}$$

For real λ, δ is real, but complex λ will be needed. The following relation will turn out to be important.

Let

$$\partial_\pm \chi(\lambda) = \tfrac{1}{2}e^{\pm i\delta(\lambda)} \tag{2.17}$$

giving

$$\begin{aligned}
&\cosh\chi(\lambda) = (2\lambda u)^{-1}(\lambda^2 + u^2 + v^2),\\
&\sinh\chi(\lambda) = (2\lambda u)^{-1}[\{(u+\lambda)^2 + v^2\}\{(u-\lambda)^2 + v^2\}]^{1/2}.
\end{aligned} \tag{2.18}$$

For $\lambda = 1$, one has from (1.17), (1.18), and (1.22)

$$\chi(1) = \chi.$$

Define q through the relations

$$\begin{aligned}
\partial_+ q &= (M_2 - M_1)q + p(M_2 - M_1q^2),\\
\partial_- q &= (N_1 - N_2)q + p^{-1}(N_1 - N_2q^2),
\end{aligned} \tag{2.19}$$

and set

$$\tilde{q} = -(p+q)/(1+pq). \tag{2.20}$$

The Harrison transformations are defined as

$$\begin{aligned}
HM_1 &= q\tilde{q}^{-1}M_1 + (1 + p\tilde{q}^{-1})X_+,\\
HM_2 &= \tilde{q}q^{-1}M_2 + (1 + p\tilde{q})X_+,\\
HN_1 &= q^{-1}\tilde{q}^{-1}N_1 + (1 + p^{-1}\tilde{q}^{-1})X_-,\\
HN_2 &= q\tilde{q}N_2 + (1 + p^{-1}\tilde{q})X_-.
\end{aligned} \tag{2.21}$$

Using (2.10), (2,12), and (2.19) one can show that the set

$H(M_1,M_2,N_1,N_2)$ satisfies (2.9) if the set (M_1,M_2,N_1,N_2) does so.

A useful combination is

$$B = IH. \tag{2.22}$$

Since evidently $I^2 = 1$,

$$H = IB. \tag{2.23}$$

Start with the "seed solution"

$$M_1^{(0)} = M_2^{(0)} = N_1^{(0)} = N_2^{(0)} = \alpha/4, \tag{2.24}$$

α being, to start with, an arbitrary real parameter. Injecting (2.24) in (2.19), and using (2.17)

$$(1-q^2)^{-1}\partial_\pm q = \tfrac{1}{4}\alpha e^{\pm i\delta(\lambda)} = \partial_\pm(\tfrac{1}{2}\alpha\chi(\lambda)), \tag{2.25}$$

or

$$q = \tanh \tfrac{1}{2}(\alpha\chi(\lambda) - \beta), \tag{2.26}$$

where β is an integration constant.

Using (2.12) it can be shown[2,3] that in the composition $H(q',p_2)H(q_1,p_1)$,

$$q' = \frac{\tilde q_1 p_2 - \tilde q_2 p_1}{q_1(\tilde q_1 p_1 - \tilde q_2 p_2)}. \tag{2.27}$$

Here $p_i = p(\lambda_i)$ and q_i is the corresponding solution (2.26). In this way one can iterate any number of H transformations using the q's of (2.26) with suitable (λ_i,β_i), $i = 1,2,\ldots$.

For the general n-step solution a remarkable structure thus emerges, which will be indicated later.

The first step is as follows. Let

$$\begin{aligned}(M_1,M_2,N_1,N_2) &= IH(M_1^{(0)},M_2^{(0)},N_1^{(0)},N_2^{(0)})\\ &= IH(\alpha/4,\alpha/4,\alpha/4,\alpha/4).\end{aligned} \tag{2.28}$$

In (2.26), set $\lambda = 1, \beta = 0$. From (2.18), $\chi(1) = \chi$. Hence now

$$q = \tanh \tfrac{1}{2}\alpha\chi, \tag{2.29}$$

and

$$\begin{aligned}\tilde q &= -(p+q)(1+pq)^{-1}\\ &= -(e^{i\delta}+q)(1+e^{i\delta}q)^{-1}\\ &= e^{i\beta},\end{aligned} \tag{2.30}$$

say. From (1.17), (1.18), and (2.15) [see also (A29) and (A30)],

$$\cos\delta = \frac{\sinh\chi + \cosh\chi\cos\psi}{\cosh\chi + \sinh\chi\cos\psi},$$
$$\sin\delta = \frac{\sin\psi}{\cosh\chi + \sinh\chi\cos\psi} \qquad (\lambda = 1). \tag{2.31}$$

One substitutes

$$\cos\beta = -\frac{\sinh(\alpha+1)\chi + \cosh(\alpha+1)\chi\cos\psi}{\cosh(\alpha+1)\chi + \sinh(\alpha+1)\chi\cos\psi},$$
$$\sin\beta = -\frac{\sin\psi}{\cosh(\alpha+1)\chi + \sinh(\alpha+1)\chi\cos\psi}. \tag{2.32}$$

From (2.5), (2.11), (2.21), and (2.29) one obtains

$$\begin{aligned}A_\sigma &= (\coth\chi - \alpha\coth\alpha\chi)[\cos\beta(\tau_3/2) + \sin\beta(\tau_1/2)],\\ A_\zeta &= \sin\beta(\coth\chi - \alpha\coth\alpha\chi)(\tau_2/2),\end{aligned}$$

$$e^{-\zeta}A_v = \left(\frac{\alpha\cos\beta}{\sinh\alpha\chi} - \frac{\sin\beta\cot\psi}{\sin\chi}\right)\frac{\tau_2}{2}, \tag{2.33}$$

$$\begin{aligned}e^{-\zeta}v^{-1}A_\varphi &= \frac{\alpha}{\sinh\alpha\chi}\left(\cos\beta\,\frac{\tau_1}{2} - \sin\beta\,\frac{\tau_3}{2}\right)\\ &\quad - \frac{\cot\psi}{\sinh\chi}\left(\cos\beta\,\frac{\tau_3}{2} + \sin\beta\,\frac{\tau_1}{2}\right).\end{aligned}$$

One sees immediately that a gauge transformation

$$A_\mu^1 = UA_\mu U^{-1} + (i\partial_\mu U)U^{-1},$$

with

$$U = e^{i\beta(\tau_2/2)} \tag{2.34}$$

simplifies (2.33). But one can go further. Note that

$$\partial_\zeta = \cos\delta\,\partial_\chi - \sin\delta\left(\frac{1}{\sinh\chi}\partial_\psi\right),$$
$$e^{-\zeta}\partial_v = \sin\delta\,\partial_\chi + \cos\delta\left(\frac{1}{\sinh\chi}\partial_\psi\right). \tag{2.35}$$

Correspondingly

$$A_\zeta = \cos\delta A_\chi - \sin\delta(\sinh\chi)^{-1}A_\psi,$$
$$e^{-\zeta}A_v = \sin\delta A_\chi + \cos\delta(\sinh\chi)^{-1}A_\psi. \tag{2.36}$$

Also

$$\partial_\chi\beta = (\alpha+1)\sin\beta,$$
$$\partial_\psi\beta = -(\sin\psi)^{-1}\sin\beta. \tag{2.37}$$

Using all these results, after (2.34)

$$\begin{aligned}A'_\sigma &= (\coth\chi - \alpha\coth\alpha\chi)(\tau_3/2),\\ A'_\zeta &= \alpha\sin\delta(\sinh\alpha\chi)^{-1}(\tau_2/2),\\ e^{-\zeta}A'_v &= -\alpha\cos\delta(\sinh\alpha\chi)^{-1}(\tau_2/2),\\ e^{-\zeta}v^{-1}A'_\varphi &= \alpha(\sinh\alpha\chi)^{-1}(\tau_1/2)\\ &\quad - \cot\psi(\sinh\chi)^{-1}(\tau_3/2).\end{aligned} \tag{2.38}$$

Alternatively,

$$\begin{aligned}A'_\sigma &= (\coth\chi - \alpha\coth\alpha\chi)(\tau_3/2),\\ A'_\chi &= 0,\\ A'_\psi &= -\alpha\sinh\chi(\sinh\alpha\chi)^{-1}(\tau_2/2),\\ (\sin\psi)^{-1}A_\varphi &= \alpha\sinh\chi(\sinh\alpha\chi)^{-1}(\tau_1/2)\\ &\quad - \cot\psi\tau_3/2.\end{aligned} \tag{2.39}$$

Apart from a global gauge transformation by $e^{-i\pi\tau_2/2}$, this is formally identical with the one-chain of Ref. 2. But the (χ,ψ) here are functions of (u,v), and the (τ,ρ) in Ref. 2 are functions of (t,r).

The structure of the n-step solution 2(d), 3(a), 3(b) is as follows. Let $D_a^{(n)}$, $a = 1,2,3,4$ be $n\times n$ determinants whose ith rows $[\equiv(D_a^{(n)})_i]$ are, with

$$\begin{aligned}&p_i = p(\lambda_i), \quad q_i = q(\lambda_i,\beta_i),\\ &(D_1^{(n)})_i = (q_i, p_i, p_i^2q_i, p_i^3, p_i^4q_i,\ldots, p_i^{n-1}q_i^\epsilon),\\ &\qquad i = 1,2,\ldots,n; \quad \epsilon = \tfrac{1}{2}(1-(-1)^n),\\ &(D_2^{(n)})_i = (1, p_iq_i, p_i^2, p_i^3q_i, p_i^4,\ldots,\ldots, p_i^{n-1}q_i^{1-\epsilon}),\end{aligned} \tag{2.40}$$

$$(D_3^{(n)})_i = (1, p_i q_i, p_i^2, p_i^3 q_i, p_i^4, \ldots, p_i^{n-2} q_i^\epsilon, p_i^n q_i^\epsilon),$$
$$(D_4^{(n)})_i = (p_i^{-1}, p_i, p_i^2 q_i, p_i^3, p_i^4, q_i, \ldots, p_i^{n-1} q_i^\epsilon).$$

The determinants $\tilde{D}_a^{(n)}$ are defined through the substitutions $q_i \to \tilde{q}_i$.

For $n = 2K$, as many successive H transformations are composed, and for $n = 2K+1$ an additional I transformation is added. One thus obtains for Hermitian solutions

$$M_1^{(n)} = \bar{N}_1^{(n)} = (-1)^n \frac{\tilde{D}_1^{(n)}}{\tilde{D}_2^{(n)}} \left[\frac{D_2^{(n)}}{D_1^{(n)}} M_{(1+\epsilon)}^{(0)} + \frac{D_3^{(n)}}{D_1^{(n)}} X_+ \right], \tag{2.41}$$
$$N_2^{(n)} = \bar{M}_2^{(n)} = (-1)^n \frac{\tilde{D}_1^{(n)}}{\tilde{D}_2^{(n)}} \left[\frac{D_1^{(n)}}{D_2^{(n)}} N_2^{(0)} + \frac{D_4^{(n)}}{D_2^{(n)}} X_- \right].$$

These results are valid for arbitrary seed solutions. Here only (2.24) will be used.

More general seed solutions have been used in Ref. 5. Similar generalizations can be introduced here also.

The total action

$$S = \int_{-\pi}^{\pi} d\sigma \int_{-\infty}^{\infty} d\xi \int_0^{\infty} dv \int_0^{2\pi} d\varphi \left(\frac{1}{2} \sqrt{g} \mathrm{Tr} F_{\mu\nu} F^{\mu\nu} \right) \tag{2.42}$$
$$(\mu,\nu = \sigma,\xi,v,\varphi)$$
$$= 2\pi^2 \int_{-\infty}^{\infty} d\xi \int_0^{\infty} dv\, e^{2\xi} v\, \Delta h^2, \tag{2.43}$$

where

$$\Delta = \partial_\xi^2 + 2\partial_\xi + e^{-2\xi}\left(\partial_v^2 + \frac{1}{v}\partial_v \right) + e^{-2\xi} v^{-1} \partial_\varphi^2$$
$$(\partial_\varphi \approx 0)$$

and

$$h^2 = 2\,\mathrm{Tr}\, A_\sigma^2 = 4(M_1 + N_2)(M_2 + N_1)$$
$$= \{2|M_1 + N_2|\}^2, \tag{2.44}$$

For regular solutions (2.43) can be converted to a more convenient surface integral.

One can also go over to the variables (χ,ψ) when

$$S = 2\pi^2 \int_0^{\pi} \sin\psi\, d\psi [\sinh^2 \chi\, \partial_\chi h^2]_{\chi \to \infty}. \tag{2.45}$$

For (2.39) one gets immediately

$$h^2 = (\alpha \coth \alpha\chi - \coth \chi)^2 \tag{2.46}$$

and

$$S = 8\pi^2(\alpha - 1), \quad \text{for } \alpha > 1. \tag{2.47}$$

For $|\alpha| < 1$, S diverges, for $\alpha = 1$, one has a pure gauge solution, and for $|\alpha| > 1$, $S(-\alpha) = S(\alpha)$.

For multistep solutions, comparison with previously known results[2,3] indicates the following choice of parameters.

For $n = 2k$,

$$\lambda_{2j-1} = \bar{\lambda}_{2j} = e^{-i(2j-1)\pi/\alpha},$$
$$j = 1,\ldots,k, \tag{2.48}$$

and

$$\beta_{2j-1} = i(j-1)\pi, \quad \beta_{2j} = \beta_{2j-1} + i\pi. \tag{2.49}$$

For $n = 2k+1$,

$$\lambda_1 = 1, \quad \beta_1 = 0,$$
$$\bar{\lambda}_{2j} = \lambda_{2j+1} = e^{-ij\pi/\alpha}, \tag{2.50}$$
$$j = 1,\ldots,k,$$
$$\beta_{2j} = i(j\pi) = \beta_{2j+1}. \tag{2.51}$$

The total action after n steps turns out to be[2]

$$S = 8\pi^2 n(\alpha - n), \quad \text{for } \alpha > n. \tag{2.52}$$

I will not enter into a detailed study of this hierarchy in this paper. One final point is the following. The parameter α can be continuous for finite S. But for noninteger α, the A_μ's cannot be both finite and single valued everywhere. When they are finite there are branch points. This aspect has been repeatedly discussed.[2] Hence for finite action solutions with A_μ's everywhere finite and single valued,

$$\alpha = n+1, n+2, \ldots, \quad n = 1,2,\ldots. \tag{2.53}$$

Our technique gives a canonical generalization of the integer spectrum to a continuous one through the inclusion of branch points in A_μ. This should be compared with results of Ref. 6.

III. LINEAR PAIRS FOR THE GENERAL CASE

The formalism of this section is not restricted to axial symmetry nor to SU(2). For comparison see Refs. 2(b)–2(d). I present briefly the essential steps adapted to

$$ds^2 \approx d\sigma^2 + d\xi^2 + e^{2\xi}(dx_1^2 + dx_2^2) \tag{3.1}$$
$$= d\sigma^2 + d\xi^2 + e^{2\xi}(dv^2 + v^2\, d\varphi^2). \tag{3.2}$$

Let

$$a = \tfrac{1}{2}(\xi + i\sigma), \quad \bar{a} = \tfrac{1}{2}(\xi - i\sigma),$$
$$b = \tfrac{1}{2}(x_1 + ix_2), \quad \bar{b} = \tfrac{1}{2}(x_1 - ix_2), \tag{3.3}$$

when

$$ds^2 \approx da\, d\bar{a} + e^{2\xi}\, db\, d\bar{b}. \tag{3.4}$$

The self-duality constraints are

$$F_{ab} = 0 = F_{\bar{a}\bar{b}}, \quad e^{2\xi} F_{a\bar{a}} + F_{b\bar{b}} = 0 \quad (\xi = a + \bar{a}). \tag{3.5}$$

It is known that setting

$$A_\mu = (i\partial_\mu D) D^{-1}, \quad \mu = a,b.$$
$$A_{\bar{\mu}} = (i\,\partial_{\bar{\mu}} D^{+-1}) D^+, \quad \bar{\mu} = \bar{a},\bar{b}, \tag{3.6}$$

where D is a unimodular matrix [$N \times N$ for SU(N)] and D^+ is the Hermitian adjoint, and defining

$$G = D^+ D, \tag{3.7}$$

the self-duality equations reduce to

$$e^{2\xi}(G_a G^{-1})_{\bar{a}} + (G_b G^{-1})_{\bar{b}} = 0 \quad (G_a \equiv \partial_a G, \ldots). \tag{3.8}$$

For the σ-static case,

$$\partial_a \approx \partial_{\bar{a}} \approx \partial_\xi, \quad e^{2\xi}(G_\xi G^{-1})_\xi + (G_b G^{-1})_{\bar{b}} = 0. \tag{3.9}$$

Introducing a spectral parameter Λ, let

$$D_1\Psi = (\partial_\xi - \Lambda e^{-\xi}\partial_{\bar{b}} - \Lambda\,\partial_\Lambda)\Psi = (G_\xi G^{-1})\Psi, \tag{3.10}$$
$$D_2\Psi = (\Lambda e^{\xi}\partial_\xi + \partial_b + e^{\xi}\Lambda^2\,\partial_\Lambda)\Psi = (G_b G^{-1})\Psi, \tag{3.11}$$
$$[D_1, D_2] = 0, \tag{3.12}$$

and

$$[D_1,D_2]\Psi = D_1\{(G_b G^{-1})\Psi\} - D_2\{(G_\zeta G^{-1})\Psi\} = 0 \tag{3.13}$$

gives back (3.9)

One imposes

$$\Psi(\Lambda = 0) = G. \tag{3.14}$$

For SU(N) let the zeroth step (seed solution) be

$$G_0 = \mathrm{diag}(\epsilon_1 e^{k_1\alpha\zeta},...,\epsilon_N e^{k_N\alpha\zeta}) \tag{3.15}$$

$$\epsilon_j = \pm 1, \quad j = 1,...,N,$$

$$k_1 > k_2 > \cdots > k_N,$$

$$k_1 + k_2 + \cdots + k_N = 0. \tag{3.16}$$

Then

$$\Psi_0 = \mathrm{diag}(\epsilon_1 e^{k_1 h},...,\epsilon_N e^{k_N h}), \tag{3.17}$$

where

$$D_1 h = \alpha, \quad D_2 h = 0. \tag{3.18}$$

A solution is

$$h(\Lambda) = \tfrac{1}{2}\alpha(\zeta - \ln\Lambda) = -\tfrac{1}{2}\alpha\ln(u\Lambda), \tag{3.19}$$

but setting

$$B_+(\Lambda) = 2b + \Lambda^{-1}e^{-\zeta},$$

$$B_-(\Lambda) = 2\bar{b} - \Lambda e^{-\zeta} = \overline{B_+(-\bar{\Lambda}^{-1})}, \tag{3.20}$$

$$D_1 B_\pm(\Lambda) = 0 = D_2 B_\pm(\Lambda). \tag{3.21}$$

Hence, a general solution is

$$h = -\tfrac{1}{2}\alpha\ln(e^{-\zeta}\Lambda) + \mathcal{F}(B_+(\Lambda),B_-(\Lambda)). \tag{3.22}$$

The function $\mathcal{F}$, arbitrary to start with, can eventually be restricted to assure suitable properties.

Solitonic solutions can be looked for in the form

$$\Psi_n = \left(I + \sum_{k=1}^{n} R_k(\Lambda - \mu_k)^{-1}\right)\Psi_0 \equiv X(\Lambda)\Psi_0, \tag{3.23}$$

I and R_k being $N\times N$ matrices (I is the unit one) and R_k and μ_k being independent of Λ.

Substituting in (3.10), (3.11), the residues of the double poles on the left must vanish.

Hence the pole equations

$$\partial_\zeta\mu - \mu e^{-\zeta}\partial_{\bar{b}}\mu + \mu = 0,$$

$$\mu e^{\zeta}\partial_\zeta\mu + \partial_b\mu - e^{\zeta}\mu^2 = 0, \tag{3.24}$$

$$B_+(\mu) = 2b + \mu^{-1}e^{-\zeta} = c_+,$$

$$B_-(\mu) = 2\bar{b} - \mu e^{-\zeta} = c_- \tag{3.25}$$

($c_\pm$: constants)

give solutions.

The general solution is

$$H(B_+(\mu),B_-(\mu)) = 0. \tag{3.26}$$

Here H, an arbitrary function of $B_\pm$, has to be suitably chosen to assure regularity and correct asymptotic properties.

One can also construct Ψ_n stepwise as

$$\Psi_n = (I + R_n(\Lambda - \mu_n)^{-1})\Psi_{n-1}$$

$$(n = 1,2,...). \tag{3.27}$$

Exploiting the explicit pole structure in Ψ of the ansatz, the pole equations, and the Hermiticity condition

$$G = X(\Lambda)G_0 X^{+}(-\bar{\Lambda}^{-1}), \tag{3.28}$$

one can solve for Ψ_n algebraically. The details and the original sources can be found in Refs. 2(b)–2(d). General prescriptions exist for writing R_k explicitly. I will not repeat them here.

The above formalism can be restricted to axial symmetry as follows. To make the formalism independent of φ the phase factors $e^{\pm i\varphi}$ in ∂_b and $\partial_{\bar{b}}$, respectively, can be absorbed by a redefinition

$$\Lambda \to e^{-i\varphi}\Lambda. \tag{3.29}$$

This leads to the prescription

$$\partial_b \to \partial_v - v^{-1}\Lambda\,\partial_\Lambda, \tag{3.30}$$

$$\partial_{\bar{b}} \to \partial_v + v^{-1}\Lambda\,\partial_\Lambda.$$

Thus

$$D_1\Psi \equiv [\partial_\zeta - \Lambda e^{-\zeta}(\partial_v - v^{-1}\Lambda\,\partial_\Lambda) - \Lambda\partial_\Lambda]\Psi$$

$$= (G_\zeta G^{-1})\Psi, \tag{3.31}$$

$$D_2\Psi \equiv [\Lambda e^{\zeta}\partial_\zeta + (\partial_v + v^{-1}\Lambda\,\partial_\Lambda) + e^{\zeta}\Lambda^2\partial_\Lambda]\Psi$$

$$= (G_v G^{-1})\Psi. \tag{3.32}$$

Everything is now independent of φ as well as σ. The result

$$[D_1, vD_2] = 0 \tag{3.33}$$

leads, as in (3.13), through

$$[D_1, vD_2]\Psi = 0 \tag{3.34}$$

to

$$e^{2\zeta}(G_\zeta G^{-1})_\zeta + v^{-1}(vG_v G^{-1})_v = 0. \tag{3.35}$$

For G_0 and Ψ_0 of (3.15) and (3.17), respectively, now

$$h = \tfrac{1}{2}\alpha\ln\{e^{2\zeta}(1 + \Lambda e^{\zeta}v)^{-1}\} + \mathcal{F}(B(\Lambda)), \tag{3.36}$$

where

$$B(\Lambda) = (v - \Lambda e^{-\zeta})(v + \Lambda^{-1}e^{-\zeta}). \tag{3.37}$$

Here $B(\Lambda)$ is $B_+(\Lambda)B_-(\Lambda)$ with the factors $e^{\pm i\varphi}$ absorbed and

$$D_{1,2}B(\Lambda) = 0. \tag{3.38}$$

The pole equations are now

$$e^{\zeta}\partial_\zeta\mu - \mu\,\partial_v\mu + (e^{\zeta} - v^{-1}\mu)\mu = 0,$$

$$e^{\zeta}\mu\,\partial_\zeta\mu + \partial_v\mu - (e^{\zeta}\mu + v^{-1})\mu = 0, \tag{3.39}$$

admitting only a one-parameter family of solutions (c being a constant)

$$B(\mu) = (v - e^{-\zeta}\mu)(v + e^{-\zeta}\mu^{-1}) = c. \tag{3.40}$$

An agreeable possibility arises now. Using (2.7) and (2.8) define the "superpotential" V satisfying

$$\partial_\pm V = -(8X_\pm)^{-1}\mathrm{Tr}(\partial_\pm G\cdot G^{-1})^2. \tag{3.41}$$

Self-duality is equivalent to

$$(\partial_\zeta\partial_v - \partial_v\partial_\zeta)V = 0. \tag{3.42}$$

It can be shown that ($\sqrt{g} = e^{2\zeta}v$)

$$\Delta V = (2/\sqrt{g})[\partial_+(\sqrt{g}\,\partial_- V) + \partial_-(\sqrt{g}\,\partial_+ V)],$$
$$= \tfrac{1}{2}\,\mathrm{Tr}(G_\zeta G^{-1})^2. \tag{3.43}$$

Thus ΔV is proportional to the "Higgs length" or the action density. In deriving (3.43) it is convenient to use

$$\partial_\pm(\sqrt{g}/X_\mp) = -4\sqrt{g}. \tag{3.44}$$

For SU(2) a suitable parametrization of G leads to, using (2.5),

$$\partial_+ V = -X_+^{-1} M_1 M_2,$$
$$\partial_- V = -X_-^{-1} N_1 N_2. \tag{3.45}$$

But the main interest of V is for SU(N), $N>2$, where it greatly facilitates the study of regularity constraints [see the discussion in Ref. 2(c), and 2(d) and the sources quoted there].

For the axially symmetric case in (3.26), one must set

$$\mathrm{H} = \prod_i (B(\mu) - c_i) = 0. \tag{3.46}$$

What should be the correct choice for the general case? This is a crucially important aspect not explored in this paper (see the relevant remarks in Sec. V).

IV. FLAT SPACE MONOPOLE LIMIT

The extremely simple limiting process has been indicated in (1.15) and (1.16) and indeed it gives directly the results of Ref. 3. Not only the final results but all the steps of the formalism of Ref. 3 can be extracted easily. I indicate briefly some typical results. Set

$$(\sigma,\zeta,v) \to \alpha^{-1}(t',z',v'), \quad \alpha \to \infty, \tag{4.1}$$
$$(A_\sigma, A_\zeta, A_v) \to \alpha(A_{t'}, A_{z'}, A_{v'}). \tag{4.2}$$

[Henceforth I drop the primes in this section. Even for v this should cause no confusion; ρ is retained as the symbol introduced in (1.9).]

Corresponding to Sec. II one now has

$$\begin{aligned} A_t &= (M_1 + M_2 + N_1 + N_2)(\tau_3/2) \\ &\quad - i(M_1 - M_2 - N_1 + N_2)(\tau_1/2), \\ A_z &= -i(M_1 - M_2 - N_1 + N_2)(\tau_2/2), \\ A_v &= -(M_1 - M_2 + N_1 - N_2)(\tau_2/2), \\ v^{-1}A_\varphi &= -i(M_1 + M_2 - N_1 - N_2)(\tau_3/2) \\ &\quad - (M_1 - M_2 + N_1 - N_2)(\tau_1/2). \end{aligned} \tag{4.3}$$

(Here M_i and N_i are rescaled implicitly; A_t can be replaced by Φ, the Higgs scalar.)

Corresponding to

$$ds^2 = dt^2 + dz^2 + dv^2 + v^2\,d\varphi^2,$$

now

$$\partial_\pm = \tfrac{1}{2}(\partial_z \pm i\,\partial_v), \tag{4.4}$$
$$X_\pm = \pm i(4v)^{-1}. \tag{4.5}$$

(My convention concerning the imaginary factor i is not the same as in Ref. 3. This is a trivial difference.)

The equations defining I, H, q, and so on remain formally the same. But now, setting

$$\lambda = e^{-c/\alpha}, \quad \alpha \to \infty, \tag{4.6}$$

in (2.15) and (2.16),

$$\cot\delta = Y = \frac{z-c}{v}, \quad p = e^{i\delta} = \left(\frac{z-c+iv}{z-c-iv}\right)^{1/2}. \tag{4.7}$$

Now (2.26) reduces to

$$q(c,\beta) = \tanh\tfrac{1}{2}\{[(z-c)^2 + v^2]^{1/2} - \beta\}. \tag{4.8}$$

This follows from

$$\begin{aligned} &\{(u+\lambda)^2 + v^2\}^{1/2} \to 2[1 - (z+c)/2\alpha], \\ &\{(u-\lambda)^2 + v^2\}^{1/2} \to \alpha^{-1}[(z-c)^2 + v^2]^{1/2}. \end{aligned} \tag{4.9}$$

Similarly

$$\chi(\lambda) \to \alpha^{-1}[(z-c)^2 + v^2]^{1/2} \tag{4.10}$$

implies

$$\chi = \chi(1) \to \alpha^{-1}(z^2 + v^2)^{1/2} = \alpha^{-1} r \tag{4.11}$$

and

$$\psi \to \theta = \tan^{-1}(v/z). \tag{4.12}$$

The total action now naturally diverges as $\alpha \to \infty$, $S = 8\pi^2 n(\alpha - n) \to \infty$.

But now one obtains finite energy monopoles with

$$\text{Magnetic charge} = \lim_{\alpha\to\infty}(S/8\pi^2\alpha) = n, \tag{4.13}$$

for the n-step solution.

The formalism of Sec. III can also be subjected to the same process. Now

$$(G_z G^{-1})_z + (G_{\bar y} G^{-1})_{\bar y} = 0 \quad (y = b/\alpha), \tag{4.14}$$

and

$$(\partial_z - \Lambda\,\partial_{\bar y})\Psi = (G_z G^{-1})\Psi, \tag{4.15}$$
$$(\Lambda\,\partial_z + \partial_y)\Psi = (G_y G^{-1})\Psi. \tag{4.16}$$

From (3.19), (3.20), and (3.22),

$$\lim[h - \tfrac{1}{2}\alpha \ln B_+] = (z - \Lambda y), \tag{4.17}$$
$$\lim \tfrac{1}{2}\alpha(1 + B_+ B_-) = (y\Lambda - \bar y\Lambda^{-1} - z). \tag{4.18}$$

These are the combinations used in Ref. 3 to construct Ψ_0. I have deliberately exhibited the forms (3.19)–(3.22) to point out that different, simple, and interesting possibilities can arise for the finite action case. Thus in (3.19) axial symmetry is not already broken at the zeroth level through Ψ_0.

The pole equations are now

$$\begin{aligned} &\partial_z \mu - \mu\,\partial_{\bar y}\mu = 0, \\ &\mu\,\partial_z \mu + \partial_y \mu = 0. \end{aligned} \tag{4.19}$$

Apart from the combination (4.18),

$$y\mu - \bar y\mu^{-1} - z = \text{const}, \quad \mu = \text{const},$$

is now also a solution. Indeed

$$\begin{aligned} &\lim B_+(\mu) = \mu^{-1}, \\ &\lim B_-(\mu) = -\mu. \end{aligned} \tag{4.20}$$

The general solution is thus given by

$$H(\{y\mu - \bar y\mu^{-1} - z\}, \mu) = 0. \tag{4.21}$$

The linearized pair for axial symmetry, (3.31), (3.32), and the

superpotential V of (3.41) can be similarly used to extract the necessary results for flat-space monopoles.

V. REMARKS

From (1.4), (1.5), (1.13), and (2.5),

$$\begin{aligned} A_0 \pm iA_3 &= \pm ie^{\pm i\sigma}u^{-1}\Big\{(M_1+M_2+N_1+N_2)(\tau_3/2) \\ &\quad - i(M_1-M_2-N_1+N_2)\frac{\tau_1 \pm i\tau_2}{2}\Big\} \\ &= \pm ie^{\pm i\sigma}(uf_1)^{-1}\Big\{\partial_\zeta f_1 \frac{\tau_3}{2} + \partial_\zeta f_2 \frac{\tau_1 \pm i\tau_2}{2}\Big\} \\ &= \mp i f_1^{-1}(\partial_0 \pm i\partial_3)\Big\{f_1\frac{\tau_3}{2} + f_2\frac{\tau_1 \pm i\tau_2}{2}\Big\} \end{aligned} \tag{5.1}$$

using (B5). Similarly

$$\begin{aligned} -A_1 \pm iA_2 &= \pm ie^{\mp i\varphi}u^{-1}\Big\{-i(M_1+M_2-N_1-N_2) \\ &\quad \times(\tau_3/2) - (M_1-M_2+N_1-N_2)\frac{\tau_1+i\tau_2}{2}\Big\} \\ &= \pm e^{\mp i\varphi}f_1^{-1}\Big\{\partial_v f_1\frac{\tau_3}{2} + \partial_v f_2\frac{\tau_1 \pm i\tau_2}{2}\Big\} \\ &= \mp i f_1^{-1}(-\partial_1 \pm i\partial_2)\Big\{f_1\frac{\tau_3}{2} + f_2\frac{\tau_1 \pm i\tau_2}{2}\Big\}. \end{aligned} \tag{5.2}$$

Thus the triangularizations of the standard R-gauge are automatically implemented. As stated in the Introduction, this should be helpful in relating the results to other standard formalisms. I have treated the one-step case in detail [(2.28)–(2.39)] to show how in that relatively simple case (5.1) and (5.2) are related to (2.39), the form typical of the "spherical R-gauge" of Ref. 2. Starting directly from (2.39), it would have been difficult to find out (even for this "one-chain" of Ref. 2) the necessary transformations [through (2.32) and (2.34)] to the forms having the structure of (5.1) and (5.2). For an n-step, one can easily imagine the situation. But apart from the problem of comparison with other formalisms the one of Ref. 2 has certain attractive features. Though the intermediate expressions here are often simpler the final solutions are not necessarily so! For spherical symmetry (1.8) is definitely preferable.[2(c)]

Moreover, the coordinate χ, of the line element formally the same as that used in Ref. 2 [compare (1.8) and (1.19)] enters crucially in the solutions. The reason lies in the relation between the dilatations and the pseudotranslations discussed in Appendix A. Different choices of the parameter λ [from (2.15) onwards] correspond in the results to rescalings of (u,v). On the other hand for axially symmetric flat-space monopoles the crucial parameters are imaginary translations along the z axis

$$c = 0,\ \pm i\pi,\ \pm i2\pi, \ldots .$$

So in the finite action solutions, if they are to have monopole limits, a combination $\chi(\lambda)$ such that

$$\lim_{\alpha\to\infty}\chi(c,\alpha) = (1/\alpha)[(z-c)^2+v^2]^{1/2}$$

must play a crucial role.

The results of Sec. II, restricted to SU(2) and axial symmetry, are essentially complete. Flat-space monopoles have been studied for higher-dimensional gauge groups by similar method.[7] But it is really effective for SU(2). Though, thus limited, it has an important quality. It gives (M_i,N_i) and hence A_μ directly in a convenient real gauge. To emphasize this point I have given the ansatz (2.5) directly in terms of (M_i,N_i) shunting the Ernst-type equations to Appendix B. In applications involving gauge and matter fields, invariants involving directly the A_μ's (through covariant derivatives, for example) are important. Explicit forms of A_μ are exactly what are needed in treating fluctuations around classical background fields. A method that delivers them directly is best suited from this point of view.

The method of Sec. III is much more general. There all the necessary steps have been taken except the choice of the explicit form of H in (3.26). Choosing a suitably parametrized form of H is not difficult. Thus the choice

$$H = \tfrac{1}{4}\alpha^2(1+B_+B_-)^2 + c^1(B^2_+ + B^2_-) + c_2 \tag{5.3}$$

in (3.26) gives, in the monopole limit

$$H = (y\mu - \bar{y}\mu^{-1} - z)^2 + c_1(\mu^2+\mu^{-2}) + c_2, \tag{5.4}$$

the choice of Ref. 3(c). But even in the flat-space monopole limit[3] one is led to numerical calculations. This is beyond the scope of this paper. A study of SU(N) solutions ($N>2$) through the superpotential, of course, can be undertaken, starting from (3.41), in a fashion analogous to Ref. 2(c).

Finally note that the class of σ-static instantons is much broader than the previous constructions indicate. Consider, for example, the 't Hooft solutions with all centers in the (x_1, x_2) plane. In our conventions [see (2.2)]

$$\begin{aligned} A_\mu = \sigma_{\mu\nu}\partial_\nu \ln\Big[\sum_{i=0}^{n}\lambda_i^2\{x_0^2 + x_3^2 \\ + (x_1-\alpha_i)^2 + (x_2-\beta_i)^2\}^{-1}\Big]. \end{aligned} \tag{5.5}$$

The gauge transformation by

$$U = e^{i\theta\tau_3/2} \tag{5.6}$$

gives A_σ, A_ζ, A_1, and A_2 in explicitly σ-independent form. But this does not have a monopole limit. The methods of Secs. II and III pick out those with such limits. They are supple and the interpretation of the solutions depends on the S_1 selected. So "φ-static" solutions (not necessarily σ-static) thus constructed can give explicit axially symmetric instantons in higher Atiyah–Ward classes.

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APPENDIX A: FROM DILATATIONS TO PSEUDOTRANSLATIONS

Some useful results concerning the coordinate systems used [(1.2), (1.3), (1.8), and (1.29)], are collected here. It has been noted that setting

$$u = (x_0^2 + x_3^2)^{1/2} = (\cosh\chi + \sinh\chi\cos\psi)^{-1}, \tag{A1}$$

$$v = (x_1^2 + x_2^2)^{1/2}$$
$$= \sinh\chi\sin\psi(\cosh\chi + \sinh\chi\cos\psi)^{-1}, \tag{A2}$$

$$ds^2 = dx_0^2 + dx_1^2 + dx_2^2 + dx_3^2 \tag{A3}$$
$$= u^2\{d\sigma^2 + u^{-2}(du^2 + dv^2 + v^2\,d\varphi^2)\} \tag{A4}$$
$$= u^2\{d\sigma^2 + d\chi^2 + \sinh^2\chi(d\psi^2 + \sin^2\psi\,d\varphi^2)\}. \tag{A5}$$

Defining

$$D_\pm = \{(u \pm 1)^2 + v^2\}^{1/2}, \tag{A6}$$

$$e^{\pm\chi} = (4u)^{-1}(D_+ \pm D_-)^2, \tag{A7}$$

or

$$\cosh\chi = (4u)^{-1}(D_+^2 + D_-^2), \quad \sinh\chi = (2u)^{-1}D_+D_-. \tag{A8}$$

Also

$$\sin\psi = 2v(D_+D_-)^{-1},$$
$$\cos\psi = (1 - u^2 - v^2)(D_+D_-)^{-1}. \tag{A9}$$

Corresponding to the rescaling

$$(u, v) \to (u/\lambda, v/\lambda), \tag{A10}$$

define $\chi(\lambda)$ and $\psi(\lambda)$ such that

$$u(\lambda) \equiv u/\lambda = (\cosh\chi(\lambda) + \sinh\chi(\lambda)\cos\psi(\lambda))^{-1}, \tag{A11}$$

$$v(\lambda) \equiv v/\lambda = \sinh\chi(\lambda)\sin\psi(\lambda)$$
$$\times(\cosh\chi(\lambda) + \sinh\chi(\lambda)\cos\psi(\lambda))^{-1}, \tag{A12}$$

with

$$\chi(1) = \chi, \quad \psi(1) = \psi. \tag{A13}$$

It can be shown that

$$\chi, \psi \to \chi(\lambda), \psi(\lambda)$$

is a "pseudotranslation" in the following sense.

Set

$$\lambda = e^{-c}, \tag{A14}$$

$$\cosh\chi(c) = \cosh c\cosh\chi - \sinh c\sinh\chi\cos\psi, \tag{A15}$$

$$\tan\psi(c) = \sinh\chi\sin\psi$$
$$\times(\cosh c\sinh\chi\cos\psi - \sinh c\cosh\chi)^{-1}. \tag{A16}$$

Consistent with (A11) and (A12),

$$\cosh\chi(c) + \sinh\chi(c)\cos\psi(c) = e^{-c}(\cosh\chi + \sinh\chi\cos\psi), \tag{A17}$$

$$\sinh\chi(c)\sin\psi(c) = \sinh\chi\sin\psi. \tag{A18}$$

For two successive pseudotranslations

$$(\chi, \psi) \xrightarrow{c_1} (\chi_1, \psi_1) \xrightarrow{c_2} (\chi_2, \psi_2), \tag{A19}$$

$$\cosh\chi_2 = \cosh c_2\cosh\chi_1 - \sinh c_2\sinh\chi_1\cos\psi_1$$
$$= \cosh(c_1 + c_2)\cosh\chi - \sinh(c_1 + c_2)\sinh\chi\cos\psi, \tag{A20}$$

$$\sinh\chi_2\sin\psi_2 = \sinh\chi_1\sin\psi_1 = \sinh\chi\sin\psi. \tag{A21}$$

This is the group property.

The relation between pseudotranslations and dilatations was pointed out to me by Comtet[8,9] in the context of stereographic projection of the de Sitter line element:

$$ds^2 = \sum_{i=1}^{5} dz_i^2, \quad \sum_{i=1}^{5} z_i^2 = 1. \tag{A22}$$

Setting

$$(z_1 \pm iz_2)(1 + z_5)^{-1}$$
$$= e^{\pm i\gamma}(\cosh\rho + \sinh\rho\cos\theta)^{-1}, \tag{A23}$$

$$(z_3 \pm iz_4)(1 + z_5)^{-1}$$
$$= e^{\pm i\varphi}\sinh\rho\sin\theta(\cosh\rho + \sinh\rho\cos\theta)^{-1}, \tag{A24}$$

$$ds^2 = (\cosh\rho)^{-2}[d\tau^2 + d\rho^2$$
$$+ \sinh^2\rho(d\theta^2 + \sin^2\theta\,d\varphi^2)]. \tag{A25}$$

In (A23) and (A24) one recognizes the combinations corresponding to (A1) and (A2) in terms of (ρ, θ).

Corresponding to (A11) and (A12) one can define

$$D\pm(\lambda) \equiv [(u \pm \lambda)^2 + v^2]^{1/2}, \tag{A26}$$

with

$$D_\pm(1) = D_\pm.$$

Then

$$e^{\pm\chi(\lambda)} = (4\lambda u)^{-1}(D_+(\lambda) \pm D_-(\lambda))^2, \tag{A27}$$

$$\sin\psi(\lambda) = (2\lambda v)(D_+(\lambda)D_-(\lambda))^{-1},$$
$$\cos\psi(\lambda) = (\lambda^2 - u^2 - v^2)(D_+(\lambda)D_-(\lambda))^{-1}. \tag{A28}$$

Thus for $\delta(\lambda)$ of (2.15) and (2.16),

$$\cos\delta(\lambda) = \frac{\lambda^2 + v^2 - u^2}{D_+(\lambda)D_-(\lambda)}$$
$$= \frac{\sinh\chi(\lambda) + \cosh\chi(\lambda)\cos\psi(\lambda)}{\cosh\chi(\lambda) + \sinh\chi(\lambda)\cos\psi(\lambda)}, \tag{A29}$$

$$\sin\delta(\lambda) = \frac{2uv}{D_+(\lambda)D_-(\lambda)}$$
$$= \frac{\sin\psi(\lambda)}{\cosh\chi(\lambda) + \sinh\chi(\lambda)\cos\psi(\lambda)}. \tag{A30}$$

For $\lambda = 1$ one gets back (2.31) with $\delta(1) = \delta$.

APPENDIX B: ERNST-LIKE EQUATIONS

In (2.5), set

$$M_1 = (2f_1)^{-1}\partial_t(f_1 + if_2), \quad M_2 = (2f_1)^{-1}\partial_t(f_1 - if_2),$$
$$N_1 = (2f_1)^{-1}\partial_-(f_1 - if_2), \quad N_2 = (2f_1)^{-1}\partial_-(f_1 + if_2). \tag{B1}$$

Here $\partial_\pm$ are given by (2.7) and f_1 and f_2 are functions of (ζ, v). The self-duality equations (2.9) become the "Ernst-like" equations

$$f_1\tilde{\Delta}f_1 = (\nabla f_1)^2 - (\nabla f_2)^2,$$
$$f_1\tilde{\Delta}f_2 = 2(\nabla f_1 \cdot \nabla f_2), \tag{B2}$$

where

$$\nabla \equiv (\partial_\zeta, e^{-\zeta}\partial_\nu)\,, \tag{B3}$$

$$\tilde{\Delta} \equiv \partial_\zeta^2 + e^{-2\zeta}(\partial_\nu^2 + \nu^{-1}\partial_\nu)\,. \tag{B4}$$

For Hermitian A_μ's ($M_i = \bar{N}_i$), f_1 and f_2 are real functions.

From (2.5) and (B1),

$$\begin{aligned} A_\sigma &= f_1^{-1}\,\partial_\zeta f_1(\tau_3/2) + f_1^{-1}\,\partial_\zeta f_2\,(\tau_1/2)\,,\\ A_\zeta &= f_1^{-1}\,\partial_\zeta f_2\,(\tau_2/2)\,,\\ A_\nu &= f_1^{-1}\,\partial_\nu f_2\,(\tau_2/2)\,,\\ \nu^{-1}A_\varphi &= f_1^{-1}\,\partial_\nu f_1(\tau_3/2) + f_1^{-1}\,\partial_\nu f_2\,(\tau_1/2)\,. \end{aligned} \tag{B5}$$

From (2.44) and (B5),

$$h^2 = 2\,\mathrm{Tr}\,A_\sigma^2 = f_1^{-2}\,[(\partial_\zeta f_1)^2 + (\partial_\zeta f_2)^2]\,. \tag{B6}$$

APPENDIX C: MORE ABOUT THE ONE-STEP SOLUTION (SEC. II)

This solution [(2.33), (2.38), and (2.39)] is of course, equivalent to the one-chain of Refs. 2 and 10. The following points are useful in understanding the relation. They are presented suppressing details.

Starting with (1.19) and setting

$$t' + ir' = \tan\tfrac{1}{2}(\pi/2 + \sigma + i\chi)\,, \tag{C1}$$

$$ds^2 \simeq dt'^2 + dr'^2 + r'^2\,d\psi^2 + r'^2\sin^2\psi\,d\varphi^2\,. \tag{C2}$$

Consider the solution

$$A'\mu = \sigma_{\mu\nu}\,\partial'_\nu \ln \Sigma'(x') \quad (x'_0 = t',\, x'_3 = r'\cos\psi\,,\ldots)\,,$$

$$\Sigma'(x') = \sum_{k=0}^{\alpha-1} \sec^2\frac{k\pi}{\alpha}\left\{\left(t' - \tan\frac{k\pi}{\alpha}\right)^2 + r'^2\right\}^{-1}. \tag{C3}$$

This is the above mentioned one-chain. The relation between x_μ of (1.1) and x'_μ introduced here can be shown to be

$$(x + c)_\mu = 2(x'_\mu + c_\mu x'^2)(1 + 2c\cdot x' + x'^2)^{-1}\,, \tag{C4}$$

with

$$c = (0, 0, 0, 1)\,, \tag{C5}$$

so that $(x + c) = (x_0, x_1, x_2, x_3 + 1)$ undergoes a special conformal transformation followed by a dilatation. By applying the rules[11] for the transformation of the generating function (C3) under (C4) one obtains

$$\Sigma'(x') \to \Sigma(x) = 4\sum_{K=0}^{\alpha-1}\left\{(x_0 - \sin\frac{k}{\alpha}\,2\pi)^2 + (x_3 + \cos\frac{k}{\alpha}\,2\pi)^2 + x_1^2 + x_2^2\right\}^{-1}. \tag{C6}$$

(The overall factor is irrelevant.) The gauge transformation connecting (2.39) and (C3) can be found in Ref. 10 (with a minor change of convention). Thus (2.39) must be equivalent to

$$A_\mu = \sigma_{\mu\nu}\,\partial_\nu \ln \Sigma(x)\,, \tag{C7}$$

where $\Sigma(x)$ is given by (C6) and can be shown to be

$$\Sigma(x) = i\alpha(4\mu\sinh\chi)^{-1}\left\{\cot\frac{1}{2}\alpha\left(\frac{\pi}{2} + \sigma + i\chi\right) - \cot\frac{1}{2}\alpha\left(\frac{\pi}{2} + \sigma - i\chi\right)\right\}. \tag{C8}$$

Let

$$(x_0, x_1, x_2, 1 + x_3) = \alpha^{-1}(x''_0, x''_1, x''_2, x''_3)\,. \tag{C9}$$

Then

$$\Sigma''(x'') = \lim_{\alpha\to\infty}(\alpha^{-2}\Sigma(x)) = \sum_{k''=-\infty}^{\infty}\{(x''_0 - k''2\pi)^2 + \mathbf{x}''^2\}^{-1}. \tag{C10}$$

This gives the Prasad–Sommerfield monopole in its periodic form [see Ref. 10(a) and sources quoted there]. This can be gauge transformed to the standard static form, which follows directly on rescaling (2.39) as in Refs. 2 and 10.

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Physical state conditions and supersymmetry breaking in quantum mechanics

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It is shown, by giving an explicit example, how the conditions imposed on physically admissible states can affect the pattern of supersymmetry breaking and, as a consequence, the values of physically interesting quantities such as the Witten index. As a by-product an unusual kind of explicit supersymmetry breaking is observed, where the supersymmetry algebra still holds formally, as well as a spontaneous breakdown of supersymmetry, which is not induced by instantons.

I. THE MODEL

Supersymmetric quantum mechanics[1–4] has recently become a matter of both physical[2,3,5] and mathematical[6] interest. A major reason for the physical interest is the hope to get a better insight into the mechanism of supersymmetry breaking.[2,3]

In the present paper we consider a particular model of supersymmetric quantum mechanics where an unexpected kind of explicit supersymmetry breaking occurs, and discuss how this breaking is influenced by the conditions imposed on physical states.

The model is given by the supersymmetry charges

$$Q_\pm = \tfrac{1}{4}(W \pm ip)(\sigma_1 \pm i\sigma_2), \tag{1}$$

with

$$W(q) = bq - c/q, \tag{2}$$

and the Hamiltonian

$$H = \begin{pmatrix} H_1 & 0 \\ 0 & H_0 \end{pmatrix}, \tag{3}$$

with

$$H_\nu = \tfrac{1}{2}\left(p^2 + W^2 - (-1)^\nu \frac{dW}{dq}\right)$$
$$= \tfrac{1}{2}(p^2 + b^2q^2 + c(c+2\nu-1)q^{-2} - b(2c-2\nu+1)). \tag{4}$$

Here the coordinate q takes values in $\mathbb{R}$, $p = -i\,d/dq$, σ_i denote the Pauli matrices, and the indices $\nu = 0,1$ in (3) and (4) refer to the eigenvalue of the "fermion number operator" $f = \tfrac{1}{2}(\sigma_3 + 1)$[3,4]; b and c are real constants, and without loss of generality[4] we can choose $b \geqslant 0$. From (1)–(4) we have the supersymmetry algebra

$$\{Q_\pm, Q_\pm\} = 0,$$
$$\{Q_+, Q_-\} = H, \tag{5}$$
$$[Q_\pm, H] = 0.$$

For the moment we ignore all questions about self-adjointness and domains of the operators $Q_\pm$ and H and regard (5) just as an algebra of "formal differential operators."[7]

It may be noted that (3) is a supersymmetric extension of the ordinary Hamiltonian $\tfrac{1}{2}(p^2 + b^2q^2 + gq^{-2})$, which has been studied by several authors.[8–10]

The solutions of the differential equation $H\phi = E\phi$ are easily found[8,10]; they are

$$\phi_{n\nu A} = \left(\frac{n!\sqrt{b}}{\Gamma(n+\gamma+1)}\right)^{1/2} (bq^2)^{(\gamma/2)+(1/4)} \exp(-\tfrac{1}{2}bq^2)$$
$$\times L_n^\gamma(bq^2)(\operatorname{sgn} q)^A \chi_\nu, \tag{6}$$

where χ_ν are the spinors

$$\chi_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{7}$$

γ is the constant defined by

$$\gamma = (-1)^{[(A-1)/2]}|c + \nu - \tfrac{1}{2}|, \tag{8}$$

where $[x]$ is the biggest integer $< x$, and L_n^α are the generalized Laguerre polynomials.[11] Also, the quantum numbers n, ν, and A in (6) take the following values: $n = 0,1,2,\ldots$, $\nu = 0,1$, and $A = 1,2,3,4$ if $c \neq 0$ and $c \neq 1 - 2\nu$; while in the exceptional cases $c = 0$ or $c = 1 - 2\nu$ only the values $A = 1,4$ are allowed. (This restriction of the values of A occurs because in the exceptional cases H_ν is not singular at $q = 0$; also, using the connection between the Laguerre and the Hermite polynomials,[11] the solutions with $A = 1, 4$ then just reproduce the eigenfunctions of the harmonic oscillator.) The eigenvalues corresponding to the solutions (6) are

$$E_{n\nu1} = E_{n\nu2} = \begin{cases} E'_n, & \text{for } c \leqslant \tfrac{1}{2} - \nu, \\ E_{n\nu}, & \text{for } c \geqslant \tfrac{1}{2} - \nu, \end{cases}$$
$$E_{n\nu3} = E_{n\nu4} = \begin{cases} E_{n\nu}, & \text{for } c \leqslant \tfrac{1}{2} - \nu, \\ E'_n, & \text{for } c \geqslant \tfrac{1}{2} - \nu, \end{cases} \tag{9}$$

where

$$E_{n\nu} = 2b(n + \nu),$$
$$E'_n = 2b(n - c + \tfrac{1}{2}). \tag{10}$$

We now list some properties of the solutions (6). From their behavior at $q = 0$ and at infinity we can immediately decide whether they are square integrable, continuous, or continuously differentiable; we list these properties in Table I. If their energy eigenvalue is zero, they form singlet representations of the superalgebra (5), while for nonzero energy they form doublets whose components transform into each other by supersymmetry transformations; e.g., for $n \neq 0$ the states ϕ_{n01} and

$$Q_+\phi_{n01} = \begin{cases} \sqrt{E'_n}\,\phi_{n12}, & \text{for } c \leqslant -\tfrac{1}{2}, \\ \sqrt{E'_n}\,\phi_{n14}, & \text{for } -\tfrac{1}{2} < c < \tfrac{1}{2}, \\ \sqrt{E_{n0}}\,\phi_{n-1,1,2}, & \text{for } c \geqslant \tfrac{1}{2}, \end{cases} \tag{11}$$

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TABLE I. The range of the parameter $\gamma(8)$ for which the solutions (6) have the following properties: (a) ϕ_{nvA} is square integrable; (b) ϕ_{nvA} is continuous at $q=0$; and (c) $(d/dq)\,\phi_{nvA}$ is continuous at $q=0$.

	(a) square integrable	(b) continuous	(c) continuously differentiable
A even	$\gamma > -1$	$\gamma \geqslant -\frac{1}{2}$	$\gamma = -\frac{1}{2}$ or $\gamma > \frac{1}{2}$
A odd	$\gamma > -1$	$\gamma > -\frac{1}{2}$	$\gamma \geqslant \frac{1}{2}$

form a supersymmetry doublet. Note that the application of $Q_\pm$ changes the parity of the wave functions.

Finally, with the usual definition of the scalar product, the solutions (6) obey, for $\gamma > -1$,

$$(\phi_{nvA}, \phi_{m\mu B}) = \delta_{nm}\delta_{\nu\mu}\delta_{AB}, \tag{12}$$

for $A-B \neq \pm 2$ (for $A=B$ this follows from the orthogonality relation of the Laguerre polynomials,[11] for $A \neq B$ it holds for parity reasons), while for $A-B=2$ we find[12]

$$\begin{aligned}(\phi_{nvA}, \phi_{m\mu B}) = \delta_{\nu\mu}(-1)^{m+n}(n!m!)^{-1/2} \\ \times(\Gamma(n-|\gamma|+1)\Gamma(m+|\gamma|+1))^{1/2} \\ \times(\Gamma(m-n+|\gamma|+1)\Gamma(n-m-|\gamma|+1))^{-1}\end{aligned} \tag{13}$$

(and analogously for $A-B=-2$). In particular the solutions with different energy eigenvalues are in general not orthogonal; as we will see below, this is due to the non-Hermiticity of the Hamiltonians (4).

II. PHYSICAL STATE CONDITIONS

If we want to discuss the eigenvalue problem $H\phi = E\phi$ with H given by (3) and (4) along the lines of the probabilistic interpretation of quantum mechanics, we cannot accept all the solutions (6) as "physically admissible states." First we have to decide whether for the Hamiltonian at hand a probabilistic interpretation is possible at all. Now it is well known[13,14] that for the nonsupersymmetric case such an interpretation is possible if the coupling constant g of the inverse square term gq^{-2} fulfills $g > -\frac{1}{4}$, while for $g \leqslant -\frac{1}{4}$ any solution of the Schrödinger equation has an infinite number of zeroes,[14] which means that the energy spectrum is not bounded from below ("the particle falls to the center") and the physical interpretation is lost. In our case, due to supersymmetry, we automatically have $g \geqslant -\frac{1}{4}$, since

$$g = c(c+2\nu-1) = \gamma^2 - \tfrac{1}{4}, \tag{14}$$

so that we have only to exclude the case $\gamma = 0$, i.e., $c = \frac{1}{2} - \nu$; since the Hamiltonian (3) contains both H_0 and H_1, both $c=\frac{1}{2}$ and $c=-\frac{1}{2}$ have to be excluded. Thus in the following we always assume $c \neq \pm\frac{1}{2}$.

Another restriction of the allowed range of c is obtained from the requirement that the physically acceptable states are square integrable, i.e., belong to the Hilbert space $\mathscr{H} = \mathscr{L}^2(\mathbb{R}) \otimes \mathbb{C}^2$. In addition we may be forced to impose further constraints. In the following we will first consider different choices of conditions; afterwards we will argue which of the choices has to be considered as the physical one. The choices are as follows.

(i) The only requirement is that the solutions (6) belong to $\mathscr{H}$. Ths means that we must have $\gamma > -1$; for $A=1,2$ this imposes no constraint on the parameter c, while for $A=3,4$, c must fulfill

$$-\tfrac{1}{2} - \nu < c < \tfrac{3}{2} - \nu. \tag{15}$$

Thus the following solutions are allowed (we list their respective energy in brackets):

$$\begin{aligned}
&c \in (-\infty, \tfrac{3}{2}]: && \phi_{nv1}, \phi_{nv2}(E'_n), \\
&c \in (-\tfrac{3}{2}, -\tfrac{1}{2}) \setminus \{-1\}: && \phi_{nv1}, \phi_{nv2}(E'_n); \phi_{n13}, \phi_{n14}(E_{n1}), \\
&c \in (-\tfrac{1}{2}, \tfrac{1}{2}) \setminus \{0\}: && \phi_{n01}, \phi_{n02}, \phi_{n13}, \phi_{n14}(E'_n); \\
& && \phi_{n03}, \phi_{n04}(E_{n0}); \phi_{n11}, \phi_{n12}(E_{n1}), \\
&c \in (\tfrac{1}{2}, \tfrac{3}{2}) \setminus \{1\}: && \phi_{nv1}, \phi_{nv2}(E_{nv}); \phi_{n03}, \phi_{n04}(E'_n), \\
&c \in [\tfrac{3}{2}, \infty): && \phi_{nv1}, \phi_{nv2}(E_{nv}),
\end{aligned} \tag{16a}$$

$$\begin{aligned}
&c = -1: && \phi_{nv1}, \phi_{n02}(E'_n); \phi_{n14}(E_{n1}), \\
&c = 0: && \phi_{n01}, \phi_{n14}(E'_n); \phi_{n11}, \phi_{n04}(E_{nv}), \\
&c = 1: && \phi_{nv1}, \phi_{n12}(E_{nv}); \phi_{n04}(E'_n),
\end{aligned} \tag{16b}$$

with $n = 0,1,2,\ldots$ and $\nu = 0,1$. Note that in the range of $\frac{1}{2} < c < \frac{3}{2}$ there are allowed solutions (ϕ_{003}, ϕ_{004}) with negative energy eigenvalues. Also the limits $c \to 0, \pm 1$ do not reproduce the results obtained for these exceptional values; this is an example of the Klauder[15] phenomenon.

(ii) In addition to (i) we require that the solutions are continuous at $q=0$. This means $\gamma \geqslant -\frac{1}{2}$ ($\gamma > -\frac{1}{2}$) for A even (odd) which for $A=1,2$ again imposes no condition on c, while for $A=3,4$ it gives

$$\begin{aligned}
&-\nu < c < 1-\nu, && \text{for } A=3, \\
&-\nu \leqslant c \leqslant 1-\nu, && \text{for } A=4.
\end{aligned} \tag{17}$$

Thus the allowed solutions are as follows:

$$\begin{aligned}
&c \in (-\infty, -1): && \phi_{nv1}, \phi_{nv2}(E'_n), \\
&c \in (-1, -\tfrac{1}{2}): && \phi_{nv1}, \phi_{nv2}(E'_n); \phi_{n13}, \phi_{n14}(E_{n1}), \\
&c \in (-\tfrac{1}{2}, 0): && \phi_{n01}, \phi_{n02}, \phi_{n13}, \phi_{n14}(E'_n); \\
& && \phi_{n11}, \phi_{n12}(E_{n1}), \\
&c \in (0, \tfrac{1}{2}): && \phi_{n01}, \phi_{n02}(E'_n); \phi_{n03}, \phi_{n04}(E_{n0}); \\
& && \phi_{n11}, \phi_{n12}(E_{n1}), \\
&c \in (\tfrac{1}{2}, 1): && \phi_{nv1}, \phi_{nv2}(E_{nv}); \phi_{n03}, \phi_{n04}(E'_n), \\
&c \in (1, \infty): && \phi_{nv1}, \phi_{nv2}(E_{nv}),
\end{aligned} \tag{18a}$$

$$c \in \{-1,0,1\}: \quad \text{same as in (16b).} \tag{18b}$$

Again there is a range of the parameter c, namely $\frac{1}{2} < c \leqslant 1$, where negative energy values occur, and again in the limits $c \to 0, \pm 1$ we find the Klauder phenomenon.

(i') and (ii") In addition to (i) and (ii), we require that the solutions are linearly independent. According to (12) and (13), this amounts to excluding the solutions with two of the four possible values of A such that the case $|A-B| = 2$ cannot occur. This was done in Refs. 10 and 16, where the values $A=2,3$ were excluded; in this case in (16) and (18) all solutions with $A=2,3$ are removed while those with $A=1,4$ are still allowed. In particular there are no longer energywise degenerate solutions with the same value of ν.[16] Also in the case (i') the limits $c \to 0, \pm 1$ are smooth and the Klauder

phenomenon is avoided.

Before going on to (iii), we remark that the requirement of linear independence is ambiguous; instead of following Refs. 10 and 16 we could as well exclude the solutions with $A = 1,2$ or those with $A = 3,4$ to fulfill this requirement; these choices would lead to entirely different energy spectra.

(iii) In addition to (ii) we require that the first derivative of the solutions is continuous at $q = 0$. This means $\gamma = -\frac{1}{2}$ or $\gamma > \frac{1}{2}$ ($\gamma \geqslant \frac{1}{2}$) for A even (odd) which for $A = 1,2$ gives

$$\begin{aligned} &c \geqslant 1-\nu \text{ or } c \leqslant -\nu, \quad \text{for } A = 1, \\ &c > 1-\nu \text{ or } c < -\nu, \quad \text{for } A = 2, \end{aligned} \tag{19}$$

while the solutions with $A = 3$ are no longer accepted at all and of those with $A = 4$ only the exceptional cases $c = 0$, $c = 1 - 2\nu$ remain. The allowed solutions are then as follows.

$$\begin{aligned} &c \in (-\infty, -1): && \phi_{n\nu 1}, \phi_{n\nu 2}(E'_n), \\ &c \in (-1,0): && \phi_{n01}, \phi_{n02}(E'_n), \\ &c \in (0,1): && \phi_{n11}, \phi_{n12}(E_{n1}), \\ &c \in (1,\infty): && \phi_{n\nu 1}, \phi_{n\nu 2}(E_{n\nu}), \end{aligned} \tag{20a}$$

$$c \in \{-1,0,1\}: \quad \text{same as in (16b).} \tag{20b}$$

Again in the limits $c \to 0, \pm 1$ the Klauder phenomenon shows up; in particular in the limit $c \to 1^-$ ($c \to 1^+$) all energies remain positive definite (positive semidefinite) while for $c = 1$ there is still an allowed solution (ϕ_{004}) with negative energy.

To decide which of the above choices has to be considered as physically meaningful, we have to look at the principles of quantum mechanics. These include the requirement[17] that the physical states belong to a Hilbert space, which, in the model under consideration, is $\mathscr{H} = \mathscr{L}^2(\mathbb{R}) \otimes \mathbb{C}^2$ whereas, as stressed in Ref. 10, there is no *a priori* reason to require that the Schrödinger picture wave functions are continuous or continuously differentiable.[17]

Nevertheless it is easy to see that in the present case the latter conditions indeed have to be imposed. Namely, they follow from another axiom of quantum mechanics which states that only self-adjoint operators can be interpreted as observables.[18] This axiom is indispensable for a physical interpretation of quantum mechanics, since it guarantees the reality of the eigenvalues and the orthogonality and completeness of the eigenstates, and thus, in particular, the conservation of probability.

Now if the domain $\mathscr{D}$ of the formal differential operators (4) is understood to be $\mathscr{D} = \mathscr{H}$, then they are not self-adjoint. (For the supersymmetry charges this means that Q_- is not the adjoint of Q_+.) However, as shown in Ref. 13, for $c \neq \frac{1}{2} - \nu$, it is possible to construct from H_ν self-adjoint operators H'_ν by restricting their domain; the mapping prescription for the operators H'_ν is still given by (4), but their domain is[13] $\mathscr{D} = \mathscr{L}^2(\mathbb{R}) \cap C^1(\mathbb{R})$, where $C^1(\mathbb{R})$ denotes the set of continuously differentiable functions on $\mathbb{R}$ (see Ref. 19). Thus we can conclude that of the above choices, only (iii) leads to a physically meaningful interpretation. We remark that the necessity of restricting the domain of H can be understood intuitively. In computing the scalar product $(\phi, H\psi)$ the integration from $-\infty$ to ∞ has to be split into integrations from $-\infty$ to 0 and from 0 to ∞ because of the singular nature of H; thus the physically acceptable solutions have to be well behaved not only at infinity, but also at zero.

As observed above [see Eq. (13)], the solutions (6) corresponding to different eigenvalues are not orthogonal in general; this is simply a consequence of the fact that the operators given by (4) with domain $\mathscr{D} = \mathscr{H}$ are not self-adjoint and even not Hermitian. Note that all eigenvalues are automatically real in our model; one could therefore be led to suppose that a restriction of the domain of H, through the requirement of orthogonality of the eigenfunctions,[20] could be sufficient to obtain a self-adjoint Hamiltonian. However, from the above considerations it is clear that this supposition is not true. Also, we have seen that this requirement is ambiguous and thus a specific choice of orthogonal solutions, e.g., the prescription chosen in Ref. 10, cannot be motivated on physical grounds.

III. SUPERSYMMETRY BREAKING

Supersymmetric systems are commonly classified into the cases where supersymmetry is unbroken, spontaneously broken, or explicitly broken. If supersymmetry is unbroken, then the ground state energy is zero; if it is spontaneously broken, the ground state energy is positive.[2-4] The converse of this is true if and only if supersymmetry is not explicitly broken, which, in the case of supersymmetric quantum mechanics, means that the supersymmetry algebra (5) holds as an operator algebra in $\mathscr{H}$. If (5) does not hold as an operator algebra in $\mathscr{H}$, then supersymmetry is explicitly broken. In particular this is the case if the image $Q_\pm(\mathscr{D})$ of the domain $\mathscr{D}$ of H under the map $Q_\pm$ is not contained in $\mathscr{D}$; in contrast (5) may still be true as an algebra of formal differential operators so that consequences of the explicit breaking of supersymmetry (such as the possible appearance of negative energy values[16]) may occur rather unexpectedly.

As follows directly from the supersymmetry transformation rules (11), the latter situation indeed occurs in the present model for some range of the parameter c. We list the pattern of supersymmetry breaking for the cases discussed above in Table II. We see that the breakdown of supersymmetry is heavily influenced by the conditions that we impose on the physical states. Imposing conditions that are too weak, we can be led to conclude that supersymmetry is un-

TABLE II. The range of the parameter c for which supersymmetry is (a) unbroken, (b) spontaneously broken, and (c) explicitly broken.

	(a) unbroken	(b) spontaneously broken	(c) explicitly broken
Case (i)	$-\frac{1}{2} < c < \frac{1}{2}$ or $c > \frac{3}{2}$	$c \leqslant -\frac{3}{2}$	$-\frac{3}{2} < c < -\frac{1}{2}$ or $\frac{1}{2} < c < \frac{3}{2}$
Case (i')	$-\frac{1}{2} < c < \frac{1}{2}$	...	$c < -\frac{1}{2}$ or $c > \frac{1}{2}$
Case (ii)	$c = 0$ or $c > 1$	$c < -1$	$-1 \leqslant c < 0$ or $0 < c \leqslant 1$
Case (ii')	$c = 0$	...	$c \neq 0$
Case (iii)	$c = 0$ or $c > 1$	$c < -1$	$-1 \leqslant c < 0$ or $0 < c \leqslant 1$

broken in a range of parameters where the full physical conditions show that it is explicitly broken, and also the other way around. We also note that for all $c\neq 0$ $W(q)$ has an even number of zeroes; despite this fact there are ranges of $c\neq 0$ where supersymmetry is unbroken.

Let us exploit the differences between the various cases somewhat further. First we evaluate the value of the Witten index[4,6,21]

$$\Delta = N_0(E=0) - N_1(E=0), \tag{21}$$

where $N_\nu(E=0)$ is the dimension of the zero energy eigenspace of H_ν. Denoting the different cases by a subscript, we find

$$\Delta_{(i)} = \begin{cases} 0, & \text{for } c < -\frac{1}{2}, \\ 1, & \text{for } c = 0,1, \\ 2, & \text{for } c > -\frac{1}{2}, \quad c\neq 0,1, \end{cases} \tag{22a}$$

$$\Delta_{(i')} = \begin{cases} 0, & \text{for } c < -\frac{1}{2}, \\ 1, & \text{for } c > -\frac{1}{2}, \end{cases} \tag{22b}$$

$$\Delta_{(ii)} = \begin{cases} 0, & \text{for } c < 0, \\ 1, & \text{for } c = 0,1, \\ 2, & \text{for } c > 0, \quad c\neq 1, \end{cases} \tag{22c}$$

$$\Delta_{(ii')} = \begin{cases} 0, & \text{for } c < 0, \\ 1, & \text{for } c \geqslant 0, \end{cases} \tag{22d}$$

$$\Delta_{(iii)} = \begin{cases} 0, & \text{for } c < 1, \quad c\neq 0, \\ 1, & \text{for } c = 0,1, \\ 2, & \text{for } c > 1. \end{cases} \tag{22e}$$

Thus Δ changes discontinuously as a function of the parameter c (see Ref. 22). It is commonly stated[4,21] that supersymmetry is unbroken if $\Delta\neq 0$; this is of course only true if the symmetry is not broken explicitly. Indeed according to Table II and (22), there is some range of $c[\frac{1}{2} < c < \frac{3}{2}$ for the cases (i) and (i'), $0 < c \leqslant 1$ for (ii), $c > 0$ for (ii'), and $c = 1$ for (iii)], where $\Delta\neq 0$, but supersymmetry is explicitly broken.

Next consider the "superpartition function"[21,23,24]

$$Y(\beta) = \operatorname{tr}(-1)^f e^{-\beta H}, \tag{23}$$

which is supposed to provide a regularization of the Witten index [which can be formally written as $\Delta = \operatorname{tr}(-1)^f$] and, in addition, is connected to supersymmetry breaking at finite temperature.[24,4] Defining

$$Z_\nu = 2\sum_{n=0}^{\infty} \exp(-\beta E_{n\nu}) = \frac{e^{\beta b(1-2\nu)}}{\sinh(\beta b)}, \quad \nu = 0,1 \tag{24}$$

and

$$Z' = 2\sum_{n=0}^{\infty} \exp(-\beta E'_n) = \frac{e^{2\beta bc}}{\sinh(\beta b)} \tag{25}$$

and making use of $Z_0 - Z_1 = 2$ we find

$$Y_{(i)} = \begin{cases} 0, & \text{for } c \leqslant -\frac{3}{2}, \\ 1, & \text{for } c = 0, \\ 2, & \text{for } -\frac{1}{2} < c < \frac{1}{2}, \ c\neq 0, \text{ or } c \geqslant \frac{3}{2}, \\ -Z_1, & \text{for } -\frac{3}{2} < c < -\frac{1}{2}, \quad c\neq -1, \\ 2+Z', & \text{for } \frac{1}{2} < c < \frac{3}{2}, \quad c\neq 1, \\ \frac{1}{2}(Z'-Z_1), & \text{for } c = -1 \\ 1+\frac{1}{2}(Z'-Z_1), & \text{for } c = 1, \end{cases} \tag{26a}$$

$$Y_{(i')} = \begin{cases} \frac{1}{2}Y_{(i)}, & \text{for } c\neq 0, \pm 1, \\ 1, & \text{for } c = 0, \\ -\frac{1}{2}Z_1, & \text{for } c = -1, \\ 1+\frac{1}{2}Z', & \text{for } c = 1, \end{cases} \tag{26b}$$

$$Y_{(ii)} = \begin{cases} 0, & \text{for } c < -1, \\ -Z_1, & \text{for } -1 < c < 0, \\ 2+Z', & \text{for } 0 < c < 1, \\ 2, & \text{for } c > 1, \\ Y_{(i)}, & \text{for } c = 0, \pm 1, \end{cases} \tag{26c}$$

$$Y_{(ii')} = \begin{cases} \frac{1}{2}Y_{(ii)}, & \text{for } c\neq 0, \pm 1, \\ Y_{(i')}, & \text{for } c = 0, \pm 1, \end{cases} \tag{26d}$$

$$Y_{(iii)} = \begin{cases} 0, & \text{for } c < -1, \\ Z', & \text{for } -1 < c < 0, \\ -Z_1, & \text{for } 0 < c < 1, \\ 2, & \text{for } c > 1, \\ Y_{(i)}, & \text{for } c = 0, \pm 1. \end{cases} \tag{26e}$$

Comparing (22) and (26), we see that $Y(\beta)$ provides a sensible regularization of Δ, i.e.,

$$\Delta = \lim_{\beta\to\infty} Y(\beta), \tag{27}$$

if supersymmetry is unbroken or spontaneously broken [in fact this is true for any choice of $W(q)$ in (1) as long as the energy spectrum does not contain a continuous part beginning at zero[4]] and also for some cases where supersymmetry is explicitly broken. However, in the case of explicit supersymmetry breaking there are also regions in parameter space where (27) ceases to be true [$\frac{1}{2} < c < \frac{3}{2}$ for the cases (i) and (i'), $\frac{1}{2} < c < 1$ for (ii) and (ii'), and $c = 1$ for (iii)] despite the fact that the energy spectrum is purely discrete; this anomalous behavior is due to the fact that in the relevant parameter range there is an allowed solution with negative energy. Also we see again that a change in the conditions defining physical states has drastic consequences on the properties of the model.

Finally we note another peculiarity of the model (1)–(4). According to (26) the relation[4,6,25]

$$Y(\beta) = \tfrac{1}{2}(\operatorname{sgn}(W_+)\operatorname{erf}[\sqrt{\beta W_+^2}\,] - \operatorname{sgn}(W_-)\operatorname{erf}[\sqrt{\beta W_-^2}\,]) \tag{28}$$

(where erf denotes the error function[11]) between the superpartition function Y and the asymptotic values $W_\pm = W(q = \pm\infty)$ of the superpotential $W(q)$ is violated in this model for $c\neq 0$. It is clear that this violation can occur if supersymmetry is explicitly broken, since its derivation[4,6] makes use of the pairing of states which transform into each other under supersymmetry transformations. However, even in the parameter range where supersymmetry is unbroken, in the cases (i), (ii), and (iii), (28) holds only up to a factor of 2; the extra factor of 2 stems from the fact that, due to the singular nature of the supersymmetry charges $Q_\pm$ (1) at $q = 0$, there is a degeneracy in energy between states which only differ by their parity. [In the cases (i') and (ii') one of any two of those energywise degenerate states is excluded by hand so that the extra factor is no longer needed.]

IV. CONCLUSIONS

We discussed a supersymmetric quantum mechanical model where an unusual kind of explicit supersymmetry breaking occurs, namely where the supersymmetry algebra holds as an algebra of formal differential operators but not as an operator algebra in Hilbert space. We find it important to note that such a kind of breaking is possible since many properties of supersymmetric quantum mechanical models are commonly supposed to be due to the supersymmetry algebra as an algebra of formal differential operators (ignoring any domain questions) but are actually valid only if the supersymmetry algebra holds as an operator algebra in Hilbert space. Such properties are in particular the positivity of the energy and the pairing of states[2–4] and thus any properties which make use of these, e.g., the connections among the Witten index, the superpartition function, and the asymptotic values of the superpotential.

The pattern of supersymmetry breaking in the model under consideration was strongly influenced by the conditions imposed on physically admissible states. Consequently, the value of the Witten index and the superpartition function depended on these conditions. We can expect that such a dependence will occur whenever the supersymmetry charges are singular. The first step in a discussion of such models, therefore, always should be a careful definition of the physically admissible states.

We finally note that under the substitution $c \to -c$, $\nu \to 1-\nu$ the Hamiltonian (3) is invariant up to the constant $b(2\nu - 2c - 1) = E'_n - E_{n,1-\nu}$. This is just the difference in the ground state energy between the two cases $c = \pm|c|$. In particular in the range where supersymmetry is broken spontaneously, the ground state energy is analytic in the coupling constant c. This indicates that the spontaneous supersymmetry breakdown in this model is *not* due to instantons. The latter situation does not only occur in our specific model.[26] Indeed, whenever for a given $W(q)$ corresponding to unbroken supersymmetry one can find a solution $\tilde{W}(q)$ of the Ricatti equation $\tilde{W}^2 \pm \tilde{W}' = W^2 \pm W' + E_0$ with some positive constant E_0, then $\tilde{W}$ will describe a model with spontaneously broken supersymmetry and ground state energy E_0. What is specific to our model is that a solution to this Ricatti equation with appropriate choice of E_0 is obtained by just changing the sign of c.

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On the theory of one-parameter subgroups of supergroups

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The one-parameter subgroups of supergroups are defined and their primary properties are delineated. Parametrization schemes analogous to those used in Lie group theory are investigated. In particular, exponentiation is introduced and related to the one-parameter subgroups. Canonical coordinates of three kinds are investigated, the third of which has no analog in conventional Lie theory. We illustrate our results with the examples of the supersymmetric quantum-mechanical superalgebra sqm(2) and the simple superalgebra osp(1/2).

I. INTRODUCTION

Lie algebras and Lie groups play an important role in the description of physical symmetries. In the last decade or so, certain generalizations of Lie algebras have become increasingly significant in theoretical physics,[1] especially within the context of unified theories. These generalized algebras are called "superalgebras"; their generators close under *anticommutation* as well as commutation.

The theory of superalgebras has been developed along lines similar to those of Lie algebras. The simple superalgebras have been classified[2,3] and many features are now well-established.[4] Until recently, however, the situation for the generalization of Lie *groups* was not as clear. We call these generalizations "supergroups."

The first attempts to construct supergroups[5,6] were not entirely satisfactory from a physical viewpoint because the structures involved were not abstract groups. Subsequent attempts included constructions by exponentiation of the algebra via Baker–Campbell–Hausdorff relations[7] or matrix representations.[8] However, these results did not explicitly treat the important problem of the manifold structure of the supergroups.

In 1980, Rogers introduced[9] a global theory of supermanifolds that is mathematically rigorous and is based on an extension of real analysis to Grassmann algebras. It is sufficiently general to include as a subset various earlier supermanifold theories.[6,10,11] This work provided the foundation for a subsequent discussion[12] of supergroups. In Rogers' formalism, supergroups are abstract groups and also superanalytic supermanifolds with composition mappings. This approach provides a direct generalization of the usual theory of Lie algebras and Lie groups to superalgebras and supergroups. It has been further refined mathematically by several authors,[13] and has been used as the basis for supergravity theories[14] and for superlattice theory using discrete supergroups.[15]

In spite of the large amount of literature on the subject of supergroups, only their general structure has been established.[11,12] Many areas remain to be clarified, if supergroups are ever to attain a physical relevance comparable to that of Lie groups. This is especially true for practical calculations, for which few results exist.

In this paper, we tackle one area for which detailed analysis is not available in the literature: the theory of one-parameter subgroups of connected supergroups, based on Rogers' work.[9,12] Our aim is to provide a mathematical description of the theory and also to give examples of practical calculations, including new calculational techniques, that will be useful to the practicing theorist.

We remark that one-parameter subgroups of supergroups have been considered previously by De Witt.[11] His analysis, however, is based upon a definition[11] of supermanifolds that is less general than that of Rogers[9] and therefore may not be applicable to all supergroups of the Rogers type. Throughout our work, we strive to maintain the close relationship between a supergroup and its associated Lie group. This leads to extensions of the work of De Witt. In this way, we obtain the relationships between one-parameter subgroups of supergroups and of the associated Lie groups. We are able to classify supergroup canonical coordinates. Also, we present applications of our methods to the construction of their matrix representations.

In Sec. II, we present a summary of those results of Rogers that we shall use in this paper. We do not repeat the proofs of her results, but instead refer the reader to her published work.[9,12]

Section III provides a comprehensive account of one-parameter subgroups of supergroups, within the framework of Rogers' supermanifolds. Differentiable curves through a point in the supergroup manifold are defined and used to construct the composition rules of one-parameter subgroups in a natural way. We prove that the construction is unique.

The concept of exponentiation is introduced in Sec. IV and related to the one-parameter subgroups. We develop canonical coordinates of *three* kinds, two of which are analogous to the canonical coordinates used in the standard theory of Lie groups. The third type is new.

These results are illustrated in Sec. V with two exam-

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ples. We consider both the supersymmetrical quantum-mechanical superalgebra sqm(2) with two anticommuting generators and the superalgebra osp(1/2). The supergroups and their one-parameter subgroup are explicitly constructed, as are the expressions involving the three types of canonical coordinates.

Appendix A contains a glossary of symbols. To avoid confusion, we have adhered as closely as possible to the notation of Rogers. In Appendix B, we provide a description of a few special superfunctions, i.e., functions of Grassmann-valued variables. The judicious use of such superfunctions can significantly simplify calculations as will be apparent to the reader who works our examples. Finally, we have included in Appendix C some technical details of the calculations that for clarity were omitted from the main text.

II. SUMMARY OF ROGERS' RESULTS

In this section, we state results on supermanifolds and supergroups that will be needed for the subsequent discussion. These facts are taken from the two papers of Rogers, Refs. 9 and 12, which we shall denote by R1 and R2, respectively. For ease of reference in the subsequent discussion, we number the paragraphs in this section. Notation conventions are given in Appendix A.

(1) Denote the real Grassmann algebra over $\mathbb{R}$ by B_L. The "flat superspace" $B_L^{m,n}$ is defined as the Cartesian product of m copies of the even part of B_L with n copies of the odd part. It has $d = 2^{L-1}(m+n)$ dimensions when viewed as a vector space over $\mathbb{R}$. There exists a homeomorphism ι: $B_L^{m,n} \to \mathbb{R}^d$ (R2, Appendix F). We remark here that the extension to complex-valued vectors in Grassmann algebras is possible[15]; however, in this paper we restrict ourselves to the real case.

(2) An (m,n)-dimensional superanalytic supermanifold $S_L^{m,n}$ over B_L is then (R1, Definition 3.1) a Hausdorff space with an atlas such that $S_L^{m,n}$ is locally homeomorphic to $B_L^{m,n}$ and the transition functions are superanalytic in the sense of R1, Definition 2.5.

(3) An (m,n)-dimensional supergroup H is defined to be a set that is an abstract group and an (m,n)-dimensional superanalytic supermanifold with a superanalytic map $H \times H \to H$: $(h_1,h_2) \to h_1 h_2^{-1}$ (R2, Definition 2.1). Paralleling the result for Lie groups, the set W of infinitesimal left translations on the supergroup form a "supermodule," called a "graded Lie module" by Rogers (R2, Definitions 3.1–3.3 and Theorem 3.4).

(4) Due to the homeomorphism ι, H can also be regarded as a $2^{L-1}(m+n)$-dimensional Lie group with Lie algebra $\mathbf{h}$. Then, the even part W_0 of W, regarded as a $2^{L-1}(m+n)$-dimensional Lie algebra, is isomorphic to $\mathbf{h}$ (R2, Proposition 3.5).

(5) Conversely, let W be a left B_L supermodule. If $\mathbf{h}$ is a real Lie algebra such that $\mathbf{h} \cong W_0$ and if H is a real Lie group whose Lie algebra is $\mathbf{h}$, then H can be given the structure of a supergroup over B_L with supermodule W (R2, Theorem 5.5).

(6) Suppose $\{X_1,\ldots,X_{m+n}\}$ is a basis for W. Let β_μ be a basis element in B_L (see Appendix A). Then, $\{X_{i\mu} | X_{i\mu} = \beta_\mu X_i, i = 1,\ldots,m+n, \mu \in M_{L,|i|}\}$ is a basis for W_0 that has the structure of a Lie algebra with commutation relations

$$[X_{j\mu}, X_{k\nu}] = \sum_{l=1}^{m+n} \sum_{\rho \in M_{L,|l|}} B^{l\rho}_{j\mu\, k\nu} X_{l\rho}\,,$$
$$1 \leqslant j,k \leqslant m+n, \quad \mu \in M_{L,|j|}, \quad \nu \in M_{L,|k|}\,. \tag{2.1}$$

(7) Suppose e denotes the identity in H, and let V' and V be open neighborhoods of e. Let ψ_e: $V' \to B_L^{m,n}$ be a chart. Then, the composition function for supergroups is a mapping K: $\psi_e(V') \times \psi_e(V') \to \psi_e(V)$, defined by

$$K(\psi_e(v_1),\psi_e(v_2)) = \psi_e(v_1 v_2), \quad \forall v_1,v_2 \in V'. \tag{2.2}$$

In terms of coordinates,

$$K^j(\underset{\sim}{x},\underset{\sim}{y}) = z^j, \quad 1 \leqslant j \leqslant m+n, \tag{2.3}$$

where $\underset{\sim}{x}, \underset{\sim}{y}, \underset{\sim}{z} \in B_L^{m,n}$.

(8) Since H can also be viewed as a d-dimensional Lie group, we can define the composition rule for H as a Lie group. Let ϕ_e: $V' \to \mathbb{R}^d$ be the chart at e given by

$$\phi_e = \iota \circ \psi_e. \tag{2.4}$$

The composition function is the mapping κ: $\phi_e(V') \times \phi_e(V') \to \phi_e(V)$, where

$$\kappa(\phi_e(v_1),\phi_e(v_2)) = \phi_e(v_1 v_2), \quad \forall v_1,v_2 \in V'. \tag{2.5}$$

In terms of coordinates,

$$\kappa^{j\mu}(\vec{x},\vec{y}) = z^{j\mu}, \quad 1 \leqslant j \leqslant m+n, \quad \mu \in M_{L,|j|}, \tag{2.6}$$

where $\vec{x}, \vec{y}, \vec{z} \in \mathbb{R}^d$.

(9) The supergroup composition rule K^j is related to the Lie group composition function $\kappa^{j\mu}$ by

$$K^j(\underset{\sim}{x},\underset{\sim}{y}) = \sum_{\mu \in M_{L,|j|}} \kappa^{j\mu}(\iota(\underset{\sim}{x}),\iota(\underset{\sim}{y}))\,\beta_\mu, \quad 1 \leqslant j \leqslant m+n \tag{2.7}$$

(R2, Lemma 5.3).

III. ONE-PARAMETER SUBGROUPS OF SUPERGROUPS

In this section, we shall establish the existence and uniqueness of one-parameter subgroups of H, when H is viewed both as a connected Lie group and as a connected supergroup. After developing the concept of a differentiable curve in H, we obtain the differential equations describing those curves associated with the composition functions of H. The main result is then stated and proved.

We begin by characterizing a differentiable curve through the identity e of the supergroup H. Let τ: $\mathbb{R} \to H$ be a mapping such that $\tau(0) = e \in H$. Given a chart (V,ψ_α), where V is a neighborhood of the identity, we can express the differentiable curve in coordinate form as

$$x^j(t) = \Pi^j \circ \psi_e \circ \tau(t), \quad 1 \leqslant j \leqslant m+n, \tag{3.1}$$

such that $x^j(0) = e^j = 0$ for $j = 1,\ldots,m+n$. Here, Π^j is the projection

$$\Pi^j: B_L^{m,n} \to {}^0B_L, \quad 1 \leqslant j \leqslant m, \tag{3.2}$$

$$\Pi^j: B_L^{m,n} \to {}^1B_L, \quad m+1 \leqslant j \leqslant m+n. \tag{3.3}$$

The homeomorphism ι [Sec. II, paragraph (1)] enables us to establish a differentiable curve in H viewed as a Lie group, because

$$\vec{x}(t) = \iota(\underset{\sim}{x}(t)). \tag{3.4}$$

We now obtain expressions for bases of infinitesimal generators of H and differential equations for differentiable curves in terms of the composition functions. Let us start by viewing H as a Lie group. Following the standard method,[16] we rewrite the composition function (2.6) as

$$x^{j\mu}(t+s)=\kappa^{j\mu}(\vec{x}(t),\vec{x}(s)),\quad 1\leqslant j\leqslant m+n,\quad \mu\in M_{L,|j|}. \tag{3.5}$$

A curve satisfying Eq. (3.5) forms a connected one-dimensional analytic subgroup of H called a one-parameter subgroup of the Lie group H.

Differentiating (3.5) with respect to s and setting $s=0$, we obtain a system of first-order ordinary differential equations in the coordinates $x^{j\mu}(t)$. They are expressed as

$$\begin{aligned}\frac{dx^{j\mu}(t)}{dt}&=\sum_{k=1}^{m+n}\sum_{\sigma\in M_{L,|k|}}\left.\frac{\partial\kappa^{j\mu}(\vec{x}(t),\vec{y})}{\partial y^{k\sigma}}\right|_{\vec{y}=0}\left.\frac{dx^{k\sigma}(s)}{ds}\right|_{s=0}\\&=\sum_{k=1}^{m+n}\sum_{\sigma\in M_{L,|k|}}\chi^{j\mu}_{k\sigma}(\vec{x}(t))a^{k\sigma},\\&1\leqslant j\leqslant m+n,\quad \mu\in M_{L,|j|}.\end{aligned} \tag{3.6}$$

Here,

$$\chi^{j\mu}_{k\sigma}(\vec{x})=\left.\frac{\partial\kappa^{j\mu}(\vec{x},\vec{y})}{\partial y^{k\sigma}}\right|_{\vec{y}=0} \tag{3.7}$$

are the group transformation functions, with $1\leqslant j,k\leqslant m+n$ and $\mu\in M_{L,|j|}$. The real variables $a^{k\sigma}$ in (3.6) are

$$a^{k\sigma}=\left.\frac{dx^{k\sigma}(s)}{ds}\right|_{s=0},\quad 1\leqslant k\leqslant m+n,\quad \sigma\in M_{L,|k|}. \tag{3.8}$$

Continuing with the usual approach,[16] the $\chi^{j\mu}_{k\sigma}(\vec{x})$ can be used to construct a basis of infinitesimal generators for H, by defining the vector fields

$$\begin{aligned}X_{k\sigma}&=\sum_{j=1}^{m+n}\sum_{\mu\in M_{L,|j|}}\chi^{j\mu}_{k\sigma}(\vec{x})\partial_{x^{j\mu}},\\&1\leqslant k\leqslant m+n,\quad \sigma\in M_{L,|k|}.\end{aligned} \tag{3.9}$$

These vector fields satisfy commutation relations

$$\begin{aligned}[X_{k\sigma},X_{l\nu}]&=\sum_{p=1}^{m+n}\sum_{\rho\in M_{L,|p|}}B^{p\rho}_{k\sigma\, l\nu}X_{p\rho},\\&1\leqslant k,l\leqslant m+n,\quad \sigma\in M_{L,|k|},\quad \nu\in M_{L,|l|},\end{aligned} \tag{3.10}$$

where the Lie group structure constants are defined as

$$\begin{aligned}B^{p\rho}_{k\sigma\, l\nu}&=\partial_{x^{k\sigma}}\chi^{p\rho}_{l\nu}(\vec{x})|_{\vec{x}=0}-\partial_{x^{l\nu}}\chi^{p\rho}_{k\sigma}(\vec{x})|_{\vec{x}=0},\\&1\leqslant k,l,p\leqslant m+n,\quad \sigma\in M_{L,|k|},\quad \nu\in M_{L,|l|},\quad \rho\in M_{L,|p|}.\end{aligned} \tag{3.11}$$

Let us now repeat the above analysis, viewing H as a supergroup. From (2.3), we have

$$x^j(t+s)=K^j(\underset{\sim}{x}(t),\underset{\sim}{x}(s)),\quad 1\leqslant j\leqslant m+n. \tag{3.12}$$

A curve satisfying Eq. (3.12) forms a connected one-dimensional superanalytic subgroup of H, called a one-parameter subgroup of the supergroup H (cf. Ref. 11, Chap. 3). Now, differentiate (3.12) with respect to s and set $s=0$, as before. Using the chain rule (R1, Proposition 2.12h), we find

$$\begin{aligned}\frac{dx^j(t)}{dt}&=\sum_{k=1}^{m+n}\left.\frac{dx^k(s)}{ds}\right|_{s=0}G_{k(y)}K^j(\underset{\sim}{x}(t),\underset{\sim}{y})|_{\underset{\sim}{y}=0},\\&=\sum_{k=1}^{m+n}a^k\chi^j_k(\underset{\sim}{x}(t)),\quad 1\leqslant j\leqslant m+n.\end{aligned} \tag{3.13}$$

The transformation function,

$$\chi^j_k(\underset{\sim}{x})=G_{k(y)}K^j(\underset{\sim}{x},\underset{\sim}{y})|_{\underset{\sim}{y}=0},\quad 1\leqslant j,k\leqslant m+n, \tag{3.14}$$

is defined as in Ref. 12, and the variables

$$a^k=\left.\frac{dx^k(s)}{ds}\right|_{s=0},\quad 1\leqslant k\leqslant m+n, \tag{3.15}$$

take values in B_L.

A basis for the left B_L supermodule W of H is

$$X_k=\sum_{j=1}^{m+n}\chi^j_k(\underset{\sim}{x})\partial_{x^j},\quad 1\leqslant k\leqslant m+n. \tag{3.16}$$

These satisfy the graded commutation relations

$$[X_k,X_l\}=\sum_{p=1}^{m+n}C^p_{kl}X_p,\quad 1\leqslant k,l\leqslant m+n, \tag{3.17}$$

where the graded structure constants take values in B_L and are defined by

$$C^p_{kl}=G_k\chi^p_l(\underset{\sim}{x})|_{\underset{\sim}{x}=0}-(-)^{|k|\,|l|}G_l\chi^p_k(\underset{\sim}{x})|_{\underset{\sim}{x}=0}. \tag{3.18}$$

At this stage, we have established the formalism necessary for the proof of the principal result of this section. In Lie theory, there is a theorem (e.g., Theorem 3.5.1. of Ref. 16) that asserts the uniqueness of a one-parameter subgroup associated with a vector field in the Lie algebra of the Lie group. We will now extend this idea to a supergroup. Once the existence and uniqueness of the one-parameter subgroup of H associated with a vector field in W_0 has been established, we can then define such important concepts as the exponentiation of an element in W_0.

Thus, in the remainder of this section, we shall be concerned with the proof of the following theorem.

Theorem 1: Let H be an (m,n)-dimensional supergroup and let W be its left B_L supermodule. Furthermore, let $\mathbf{h}$ be the Lie algebra isomorphic to W_0, the even part of W. Given any $X\neq 0$ in W_0, there exists a unique one-parameter subgroup of H whose infinitesimal generator is X.

Proof: For a suitable chart (V,ψ_e) containing the identity e, using (3.16) we have

$$X=\sum_{k=1}^{m+n}a^kX_k=\sum_{k=1}^{m+n}a^k\sum_{j=1}^{m+n}\chi^j_k(\underset{\sim}{x})\partial_{x^j}, \tag{3.19}$$

where the a^k are Grassmann variables, of which at least some are nonzero. We shall be investigating the system of equations (3.13), subject to the conditions $x^j(0)=e^j=0$, $1\leqslant j\leqslant m+n$.

By the conditions of the theorem, $X\in h\cong W_0$, which implies that

$$\begin{aligned}&a^k\in{}^0B_L,\quad 1\leqslant k\leqslant m,\\&a^k\in{}^1B_L,\quad m+1\leqslant k\leqslant m+n.\end{aligned} \tag{3.20}$$

Therefore,

$$a^k=\sum_{\alpha\in M_{L,|k|}}a^{k\alpha}\beta_\alpha,\quad 1\leqslant k\leqslant m+n, \tag{3.21}$$

instead of the unrestricted summation

$$a^k=\sum_{\alpha\in M_L}a^{k\alpha}\beta_\alpha,\quad 1\leqslant k\leqslant m+n, \tag{3.22}$$

and so

$$\begin{aligned}X&=\sum_{k=1}^{m+n}a^kX_k=\sum_{k=1}^{m+n}\sum_{\alpha\in M_{L,|k|}}a^{k\alpha}\beta_\alpha X_k\\&=\sum_{k=1}^{m+n}\sum_{\alpha\in M_{L,|k|}}a^{k\alpha}X_{k\alpha},\end{aligned} \tag{3.23}$$

$\{X_{k\alpha} | X_{k\alpha} = \beta_\alpha X_k,\ 1 \leqslant k \leqslant m+n,\ \alpha \in M_{L,|k|}\}$ forms a basis of $\mathbf{h} \cong W_0$.

To establish the existence and uniqueness of the one-parameter subgroups of H viewed as a supergroup, we shall show that the system (3.13) with the specified initial conditions has a unique solution $x^j = g^j(t)$ and that $g^j(t+s) = K^j(g(t), g(s))$ for sufficiently small s and t. This will be accomplished by virtue of the homeomorphism ι between $B_L^{m,n}$ and $\mathbb{R}^d$ and the uniqueness of the corresponding one-parameter subgroup of H viewed as a Lie group. The composition rule follows from its Lie group analog.

Thus, we wish to obtain the relationship between (3.13) and (3.6). We differentiate (2.7) with respect to $y^{k\sigma}$, $\sigma \in M_{L,|k|}$, and set $\vec{y} = 0$. We get

$$\left.\frac{\partial K^j(\underline{x}, \underline{y})}{\partial y^{k\sigma}}\right|_{\vec{y}=0} = \sum_{\mu \in M_{L,|j|}} \left.\frac{\partial \kappa^{j\mu}(\vec{x}, \vec{y})}{\partial y^{k\sigma}}\right|_{\vec{y}=0} \beta_\mu, = \sum_{\mu \in M_{L,|j|}} \chi_{k\sigma}^{j\mu}(\vec{x})\beta_\mu, \quad 1 \leqslant j,k \leqslant m+n, \quad \sigma \in M_{L,|k|}, \tag{3.24}$$

using (3.14). By Lemma 5.1 and Corollary 5.2 of Ref. 12,

$$\left.\frac{\partial K^j(\underline{x}, \underline{y})}{\partial y^{k\sigma}}\right|_{\vec{y}=0} = \beta_\sigma G_{k(y)} K^j(\underline{x}, \underline{y})\Big|_{\underline{y}=0}, = \beta_\sigma \chi_k^j(\underline{x}), \quad 1 \leqslant j,k \leqslant m+n, \quad \sigma \in M_{L,|k|}. \tag{3.25}$$

Therefore, we find

$$\beta_\sigma \chi_k^j(\underline{x}) = \sum_{\mu \in M_{L,|j|}} \chi_{k\sigma}^{j\mu}(\iota(\underline{x}))\beta_\mu, \quad 1 \leqslant j,k \leqslant m+n, \quad \sigma \in M_{L,|k|}. \tag{3.26}$$

Combining

$$x^j = \sum_{\mu \in M_{L,|j|}} x^{j\mu}\beta_\mu, \quad 1 \leqslant j \leqslant m+n, \tag{3.27}$$

with Eqs. (3.21) and (3.26), we can rewrite Eq. (3.13) as

$$\frac{dx^j(t)}{dt} = \sum_{\mu \in M_{L,|j|}} \frac{dx^{j\mu}(t)}{dt}\beta_\mu, = \sum_{k=1}^{m+n} \sum_{\alpha \in M_{L,|k|}} a^{k\alpha}\beta_\alpha \chi_k^j(\underline{x}(t)), = \sum_{k=1}^{m+n} \sum_{\alpha \in M_{L,|k|}} a^{k\alpha} \sum_{\mu \in M_{L,|j|}} \chi_{k\alpha}^{j\mu}(\iota(\underline{x}(t)))\beta_\mu, \quad 1 \leqslant j \leqslant m+n. \tag{3.28}$$

Since $\{\beta_\mu | \mu \in M_L\}$ is a basis of B_L, we can identify coefficients. Thus,

$$\frac{dx^{j\mu}(t)}{dt} = \sum_{k=1}^{m+n} \sum_{\alpha \in M_{L,|k|}} a^{k\alpha} \chi_{k\alpha}^{j\mu}(\vec{x}(t)), \quad 1 \leqslant j \leqslant m+n, \quad \mu \in M_{L,|j|}, \tag{3.29}$$

which is equivalent to (3.6). We have therefore shown that (3.13) follows from (3.6).

The next step is to assert the existence and uniqueness of one-parameter subgroups from (3.6). Observe that (3.29) is a system of first-order ordinary differential equations, with initial conditions $x^{j\mu}(0) = e^{j\mu} = 0$, $1 \leqslant j \leqslant m+n$, $\mu \in M_{L,|j|}$. The equations are associated with the Lie group H whose Lie algebra of vector fields (3.9) is $\mathbf{h}$. For $X \in \mathbf{h}$, we have

$$X = \sum_{k=1}^{m+n} \sum_{\alpha \in M_{L,|k|}} a^{k\alpha} \sum_{j=1}^{m+n} \sum_{\mu \in M_{L,|j|}} \chi_{k\alpha}^{j\mu}(\vec{x})\partial_{x^{j\mu}}. \tag{3.30}$$

By a standard theorem of Lie theory (e.g., Theorem 3.5.1 of Ref. 16), we know that the system of equations (3.29) has a unique solution

$$x^{j\mu} = g^{j\mu}(t), \quad 1 \leqslant j \leqslant m+n, \quad \mu \in M_{L,|j|}, \tag{3.31}$$

which is analytic at $t = 0$. Furthermore, we know that

$$g^{j\mu}(t+s) = \kappa^{j\mu}(\vec{g}(t), \vec{g}(s)), \quad 1 \leqslant j \leqslant m+n, \quad \mu \in M_{L,|j|}, \tag{3.32}$$

also satisfies (3.29), for s and t sufficiently small. Therefore, the existence and uniqueness of the one-parameter subgroups of H viewed as a Lie group are established.

We can extend these results to H viewed as a supergroup by recalling that the mapping $\iota: B_L^{m,n} \to \mathbb{R}^d$ is a homeomorphism. Thus, $g(t) = \iota^{-1}(\vec{g}(t))$ is a unique solution of (3.13). In terms of components, we write

$$g^j(t) = \sum_{\mu \in M_{L,|j|}} g^{j\mu}(t)\beta_\mu, \quad 1 \leqslant j \leqslant m+n, \tag{3.33}$$

and the one-parameter subgroup of the supergroup H satisfies the composition rule

$$g^j(t+s) = K^j(\underline{g}(t), \underline{g}(s)), = \sum_{\mu \in M_{L,|j|}} \kappa^{j\mu}(\iota(\underline{g}(t)), \iota(\underline{g}(s)))\beta_\mu, \quad 1 \leqslant j \leqslant m+n, \tag{3.34}$$

for sufficiently small s and t.

Thus, Theorem 1 is established.

IV. EXPONENTIATION AND CANONICAL COORDINATES

At this stage, we are able to introduce the concept of exponentiation and to relate it to the one-parameter subgroups of a supergroup H. As for Theorem 1, we will tie the concept to its analog in Lie groups. Once the link has been developed, we will introduce canonical coordinates for H.

Theorem 2: Let H be a supergroup and let $\underline{g}(t)$ be a one-parameter subgroup of H. Let W denote the left B_L supermodule of H. Then, there exists an $X \in W_0$, given by

$$X = \sum_{k=1}^{m+n} a^k X_k, \tag{4.1}$$

where a^k is defined in (3.20), such that

$$\underline{g}(t) = \exp(tX). \tag{4.2}$$

In terms of components,

$$g^j(t) = (\exp(tX))^j, \quad 1 \leqslant j \leqslant m+n, \tag{4.3}$$

and

$$(\exp(t+s)X)^j = K^j(\exp(tX), \exp(sX)), \quad 1 \leqslant j \leqslant m+n. \tag{4.4}$$

Conversely, for any $X \in W_0$, $\underline{g}(t) = \exp(tX)$ is a one-parameter subgroup of H such that (4.4) holds. Formally, we take

$\exp(tX)$ as the solution of Eq. (3.13). An expansion for $\exp(tX)$ is given below in this section.

Proof: H is a d-dimensional Lie group with Lie algebra $\mathbf{h} \cong W_0$. Let $\vec{g}(t)$ be a one-parameter subgroup of the Lie group H. Then, by standard Lie theory,[17] there exists an $X \in \mathbf{h}$, given by

$$X = \sum_{k=1}^{m+n} \sum_{\alpha \in M_{L,|k|}} a^{k\alpha} X_{k\alpha}, \tag{4.5}$$

where $X_{k\alpha}$ is defined in (3.23), such that

$$\vec{g}(t) = \exp(tX). \tag{4.6}$$

The map exp in Eq. (4.6) is the formal solution of Eq. (3.6). Due to the homeomorphism ι, we do not distinguish symbolically between this exp map and the one in Eq. (4.2). In terms of components,

$$g^{j\mu}(t) = (\exp(tX))^{j\mu}, \quad 1 \leqslant j \leqslant m+n, \quad \mu \in M_{L,|j|}, \tag{4.7}$$

and

$$(\exp(t+s)X)^{j\mu} = \kappa^{j\mu}(\exp(tX), \exp(sX)),$$
$$1 \leqslant j \leqslant m+n, \quad \mu \in M_{L,|j|}. \tag{4.8}$$

Conversely, for any $X \in \mathbf{h}$, $\vec{g}(t) = \exp(tX)$ is a unique one-parameter subgroup of H such that (4.8) is valid.

Since $\iota: B_L^{m,n} \to \mathbb{R}^d$ is a homeomorphism, our result can be extended to supergroups. By (3.33), we have

$$g^j(t) = \sum_{\mu \in M_{L,|j|}} g^{j\mu}(t)\beta_\mu = \sum_{\mu \in M_{L,|j|}} (\exp(tX))^{j\mu}\beta_\mu,$$
$$= (\exp(tX))^j, \quad 1 \leqslant j \leqslant m+n. \tag{4.9}$$

Furthermore, by (2.7), we have

$$(\exp(t+s)X)^j = K^j(\exp(tX), \exp(sX))$$
$$= \sum_{\mu \in M_{L,|j|}} \kappa^{j\mu}[\iota(\exp(tX)), \iota(\exp(sX))]\,\beta_\mu, \tag{4.10}$$

for $1 \leqslant j \leqslant m+n$.

Conversely, for any $X \in \mathbf{h} \cong W_0$, we have from (3.23)

$$X = \sum_{k=1}^{m+n} \sum_{\alpha \in M_{L,|k|}} a^{k\alpha} X_{k\alpha}, \tag{4.11}$$

$$= \sum_{k=1}^{m+n} a^k X_k. \tag{4.12}$$

Also,

$$g^j(t) = \sum_{\mu \in M_{L,|j|}} (\exp(tX))^{j\mu}\beta_\mu,$$
$$= (\exp(tX))^j, \quad 1 \leqslant j \leqslant m+n, \tag{4.13}$$

defines a unique one-parameter subgroup, satisfying (4.10).

Thus, Theorem 2 is proved.

In the theory of Lie groups,[16,17] one-dimensional subgroups of a Lie group are obtained by iteration of infinitesimal transformations. As a further illustration of the relationship between Lie group and supergroup structures, we shall develop the analogous notion of finite displacements for supergroups. Simultaneously, we will obtain the expansion of a one-parameter subgroup of a supergroup H by application of Taylor's theorem.

Let (V,ϕ_e) and (V,ψ_e) be charts, as described in paragraphs (7) and (8) of Sec. II. By Eq. (3.4), we have $\vec{x} = \iota(\underset{\sim}{x})$ for $\vec{x} \in V$. Let $f^\mu(\vec{x})$, $\mu \in M_L$, be a set of analytic functions and define

$$f(\underset{\sim}{x}) = \sum_{\mu \in M_L} f^\mu(\iota(\underset{\sim}{x}))\,\beta_\mu, \tag{4.14}$$

such that $f(\underset{\sim}{x})$ is a B_L-valued superanalytic function.

First, consider the action on each $f^\mu(\vec{x})$ of the one-parameter subgroup (4.6) of H viewed as a Lie group. By Taylor's theorem,[16] we have

$$f^\mu(\kappa(\vec{x}, \vec{g}(t))) = [\exp(tX) f^\mu]\,(\vec{x})$$
$$= [(1 + tX + (1/2!)t^2X^2 + \cdots) f^\mu](\vec{x}),$$
$$\mu \in M_L, \tag{4.15}$$

where X is a vector field in h, given by Eq. (4.11). However,

$$f(K(\underset{\sim}{x}, \underset{\sim}{g}(t))) = \sum_{\mu \in M_L} f^\mu(\iota \circ K(\underset{\sim}{x}, \underset{\sim}{g}(t)))\,\beta_\mu$$
$$= \sum_{\mu \in M_L} [\exp(tX) f^\mu]\,(\iota(\underset{\sim}{x}))\,\beta_\mu$$
$$= [\exp(tX) f](\underset{\sim}{x})$$
$$= [(1 + tX + (1/2!)t^2X^2 + \cdots) f](\underset{\sim}{x}), \tag{4.16}$$

where X is now the vector field (4.12) in $W_0 \cong \mathbf{h}$.

Conversely, we can start with $f(x)$ as defined in Eq. (4.14) and apply Taylor's theorem directly to obtain Eq. (4.16). By virtue of Eqs. (4.11)–(4.13) the analysis can be reversed, yielding Eq. (4.15).

Furthermore, if $\underset{\sim}{x}$ is the identity and $f = x^k$, $1 \leqslant k \leqslant m+n$, then

$$g^k(t) = [\exp(tX)x^k]_e, \tag{4.17}$$

Now, from Eqs. (3.16) and (4.12) it follows that

$$X = \sum_{l=1}^{m+n} a^l \sum_{j=1}^{m+n} \chi_l^j(\underset{\sim}{x})\,\partial_{x^j}. \tag{4.18}$$

Therefore, we have

$$g^k(t) = ta^k + \frac{1}{2!}t^2 \sum_{l=1}^{m+n} a^l (X\chi_l^k(\underset{\sim}{x}))_e + \cdots, \tag{4.19}$$

where $g^k(0) = 0$, $1 \leqslant k \leqslant m+n$.

Let us now turn to a consideration of canonical coordinates for H. Ado's theorem for Lie algebras states[18] that every Lie algebra has a faithful finite-dimensional representation. As a consequence, every abstract Lie algebra is isomorphic to a matrix Lie algebra (e.g., theorem 5.9 of Ref. 17).

For superalgebras, Kac[3] has shown the validity of Ado's theorem. Now, for a supergroup H with superalgebra W, the even part W_0 is isomorphic to the Lie algebra $\mathbf{h}$ of H viewed as a Lie group. This means that W_0 has a faithful finite-dimensional matrix representation.

The exponentiation of a finite-dimensional matrix representation makes transparent the applications of Theorem 2. In fact, parametrization schemes for supergroups are considerably facilitated by the use of matrix methods, as in the case of Lie groups. Examples in the next section will illustrate these points.

For Lie groups, there are two canonical parametrization

schemes: canonical coordinates of the first and second kinds.[16,19] In the former case, a one-parameter subgroup of a Lie group is constructed from a one-dimensional subalgebra of the associated Lie algebra h. The parameter is then set to unity. Thus,

$$\vec{g}_{\rm I} = \exp\left(\sum_{j=1}^{m+n} \sum_{\mu \in M_{L,|j|}} a^{j\mu} X_{j\mu}\right). \tag{4.20}$$

Analogously, we define canonical coordinates of the first kind for supergroups by

$$g_{\rm I} = \exp\left(\sum_{j=1}^{m+n} a^j X_j\right), \tag{4.21}$$

where X_j is related to $X_{j\mu}$ by Eqs. (4.11) and (4.12).

For canonical coordinates of the second kind, individual elements of the Lie algebra basis are exponentiated. Products of these exponentials are then constructed. For example,

$$\vec{g}_{\rm II} = \prod_{j=1}^{m+n} \prod_{\mu \in M_{L,|j|}} \exp(a^{j\mu} X_{j\mu}). \tag{4.22}$$

Other product sequences are also possible. Making use of the relation $\beta_\mu X_j = X_{j\mu}$, we can write canonical coordinates of the second kind for supergroups as

$$g_{\rm II} = \prod_{j=1}^{m+n} \prod_{\mu \in M_{L,|j|}} \exp(a^{j\mu} \beta_\mu X_j). \tag{4.23}$$

An interesting point emerges here. A more natural parametrization, analogous to (4.23), would have been

$$g_{\rm III} = \prod_{j=1}^{m+n} \exp(a^j X_j), \tag{4.24}$$

where a^j is given by (3.21). We shall refer to this parametrization as canonical coordinates of the third kind. It has *no* analog in conventional Lie theory.

In a subsequent paper,[20] we develop Baker–Campbell–Hausdorff relations that relate these different schemes.

V. EXAMPLES: SQM(2) AND OSP(1/2)

In this section, we illustrate the formal results of the earlier sections. The two simple examples we have chosen are the semisimple superalgebra of supersymmetric quantum mechanics, sqm (2), and the simple superalgebra osp(1/2).

The superalgebra sqm(N) has[21] one even generator X_1 and N odd generators $X_2,\ldots,X_{N+1}$. It satisfies the graded commutation relations

$$\begin{aligned} &[X_1, X_i] = 0, \\ &\{X_i, X_j\} = X_1 \delta_{ij}, \end{aligned} \tag{5.1}$$

where $i,j = 2,\ldots,N+1$. This general superalgebra, first introduced[21] into physics in 1981, has received most attention in the form sqm(2), although representations for arbitrary N have been considered.[22]

For our example, we shall be concerned with sqm(2). This superalgebra, already known[23] mathematically before its introduction into supersymmetric quantum mechanics by Witten,[21] has in a remarkably short time attracted much attention,[24–26] including two proposed physical applications.[25]

There are three generators of sqm(2). One, X_1, is even and two, X_2 and X_3, are odd. These generators close under the graded commutation relations

$$\begin{aligned} &[X_1,X_2] = [X_1,X_3] = 0, \\ &\{X_2,X_3\} = X_1, \quad \{X_2,X_2\} = \{X_3,X_3\} = 0. \end{aligned} \tag{5.2}$$

This superalgebra has[23] a faithful 2×2 matrix representation[27]

$$X_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad X_3 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{5.3}$$

From it, we shall construct a matrix representation of the (1,2)-dimensional supergroup locally homeomorphic to $B_L^{1,2}$. First, though, let us determine a one-parameter subgroup of the supergroup.

Let

$$X = \sum_{j=1}^{3} a^j X_j = a^1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a^2 \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + a^3 \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{5.4}$$

where $a^1 \in {}^0B_L$ and $a^2, a^3 \in {}^1B_L$. Exponentiating, we get

$$\begin{aligned} \exp(tX) &= \exp t\left(\sum_{j=1}^{3} a^j X_j\right), \\ &= \exp t\left[a^1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + a^2 \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + a^3 \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right] \\ &= e^{a^1 t} \begin{pmatrix} e^{-t^2 a^2 a^3/2} & ta^2 \\ ta^3 & e^{+t^2 a^2 a^3/2} \end{pmatrix}. \end{aligned} \tag{5.5}$$

For details of this calculation, see Appendix C. Equation (5.5) indeed represents a one-parameter subgroup, since

$$\exp(tX)\exp(sX) = \exp(t+s)X. \tag{5.6}$$

Let us now construct a matrix representation of the supergroup, using canonical coordinates of the first kind, Eq. (4.21). Let T_1 be the supergroup representation that we get when we set $t = 1$ in (5.5).

That is, for $\underline{a} = (a^1,a^2,a^3)$,

$$T_1(\underline{a}) = e^{a^1} \begin{pmatrix} e^{-a^2 a^3/2} & a^2 \\ a^3 & e^{+a^2 a^3/2} \end{pmatrix}, \tag{5.7}$$

where the Grassmann variables $\underline{a}$ are canonical coordinates of the first kind. Then, by the homomorphism property,[28]

$$T_1(\underline{a})T_1(\underline{b}) = T_1(\underline{a} \circ \underline{b}), \tag{5.8}$$

where $\underline{a} \circ \underline{b}$ denotes group composition. Let $\underline{z} = \underline{a} \circ \underline{b}$. It follows that

$$T_1(\underline{a})T_1(\underline{b}) = T_1(\underline{z}) = e^{a^1+b^1}\begin{pmatrix} e^{-(1/2)(a^2a^3+b^2b^3)} - a^2b^3 & a^2e^{(1/2)b^2b^3} + b^2e^{-(1/2)a^2a^3} \\ a^3e^{-(1/2)b^2b^3} + b^3e^{(1/2)a^2a^3} & e^{(1/2)(a^2a^3+b^2b^3)} - a^3b^2 \end{pmatrix} = e^{z^1}\begin{pmatrix} e^{-z^2z^3/2} & z^3 \\ z^3 & e^{z^2z^3/2} \end{pmatrix}. \tag{5.9}$$

We find

$$z^1 = K^1(\underline{a},\underline{b}) = a^1 + b^1 - \tfrac{1}{2}(a^2b^3 + a^3b^2), \quad z^2 = K^2(\underline{a},\underline{b}) = a^2 + b^2, \quad z^3 = K^3(\underline{a},\underline{b}) = a^3 + b^3. \tag{5.10}$$

Therefore, a matrix representation of the supergroup in terms of canonical coordinates of the first kind is (5.7), where

$$T_1(\underline{a})T_1(\underline{b}) = T_1[a^1 + b^1 - \tfrac{1}{2}(a^2b^3 + a^3b^2), a^2 + b^2, a^3 + b^3]. \tag{5.11}$$

The supergroup composition law is

$$\underline{a} \circ \underline{b} = (a^1 + b^1 - \tfrac{1}{2}(a^2b^3 + a^3b^2), a^2 + b^2, a^3 + b^3). \tag{5.12}$$

Let us next turn to a representation using canonical coordinates of the *third* kind. This scheme is defined in Eq. (4.24). For this superalgebra, canonical coordinates of the second and third kinds are equivalent, due to the simple form of the relations (5.2).

We need the subgroup coordinates

$$\exp(p^1X_1) = e^{p^1}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad p^1 \in {}^0B_L, \quad \exp(p^2X_2) = \begin{pmatrix} 1 & p^2 \\ 0 & 1 \end{pmatrix}, \quad p^2 \in {}^1B_L, \quad \exp(p^3X_3) = \begin{pmatrix} 1 & 0 \\ p^3 & 1 \end{pmatrix}, \quad p^3 \in {}^1B_L. \tag{5.13}$$

A representation $T_3(\underline{p})$ can be written

$$T_3(\underline{p}) = \exp(p^1X_1)\exp(p^2X_2)\exp(p^3X_3),$$

$$= e^{p^1}\begin{pmatrix} e^{-p^2p^3} & p^2 \\ p^3 & 1 \end{pmatrix}. \tag{5.14}$$

Note the difference between supergroup elements in terms of canonical coordinates of the first kind, Eq. (5.7), and those in terms of canonical coordinates of the third kind, Eq. (5.14). These two schemes are connected by a BCH relation.[20] Due to the difference in parametrizations, the supergroup composition laws will be different.

By the homomorphism property, the representation T_3 satisfies

$$T_3(\underline{p})T_3(\underline{q}) = T_3(\underline{p} \circ \underline{q}). \tag{5.15}$$

Let $\underline{z} = \underline{p} \circ \underline{q}$. We find

$$T_3(\underline{p})T_3(\underline{q}) = T_3(\underline{z}) = e^{p^1+q^1}\begin{pmatrix} e^{-(p^2p^3+q^2q^3)} - p^2q^3 & p^2e^{-q^2q^3} + q^2e^{-p^2p^3} \\ p^3e^{-q^2q^3} + q^3e^{-p^2p^3} & e^{-p^3q^2} \end{pmatrix} = e^{z^1}\begin{pmatrix} e^{-z^2z^3} & z^2 \\ z^3 & 1 \end{pmatrix}. \tag{5.16}$$

Solving the implied equations for z^1, z^2, and z^3 we have

$$z^1 = K^1(\underline{p},\underline{q}) = p^1 + q^1 - p^3q^2,$$
$$z^2 = K^2(\underline{p},\underline{q}) = p^2 + q^2, \quad z^3 = K^3(\underline{p},\underline{q}) = p^3 + q^3. \tag{5.17}$$

Therefore,

$$T_3(\underline{p})T_3(\underline{q}) = T(p^1 + q^1 - p^3q^2, p^2 + q^2, p^3 + q^3), \tag{5.18}$$

with supergroup composition law

$$\underline{p} \circ \underline{q} = (p^1 + q^1 - p^3q^2, p^2 + q^2, p^3 + q^3), \tag{5.19}$$

in canonical coordinates of the third kind.

Let us now turn to our second example: the (3,2)-dimensional supergroup associated with the five-dimensional superalgebra osp(1/2). This superalgebra arises[26] in the treatment of spin-orbit coupling for the harmonic oscillator, for example. In fact, a supergroup for it has previously been constructed,[29] but the method lacked the superanalytic supermanifold structure of Refs. 9 and 12.

The superalgebra has three even generators X_1, X_2, and X_3 and two odd generators X_4 and X_5. They satisfy the graded commutation relations

$$\begin{aligned} &[X_1,X_2] = -2X_3, \quad [X_3,X_1] = X_1, \\ &[X_3,X_2] = -X_2, \quad \{X_4,X_4\} = X_1, \\ &\{X_5,X_5\} = X_2, \quad \{X_4,X_5\} = X_3, \\ &[X_1,X_4] = 0, \quad [X_2,X_4] = X_5, \\ &[X_3,X_4] = \tfrac{1}{2}X_4, \quad [X_1,X_5] = -X_4, \\ &[X_2,X_5] = 0, \quad [X_3,X_5] = -\tfrac{1}{2}X_5. \end{aligned} \tag{5.20}$$

In this case, we shall be satisfied with the construction of an element of the supergroup in $B_L^{3,2}$ using canonical coordinates of the *third* kind, including the associated supergroup composition law. The calculation is somewhat tedious, but presents illuminating examples of the application of simple special superfunctions, i.e., functions of Grassmann variables.

The superalgebra has[3,30] a faithful 3×3 matrix representation[27]

$$X_1=\begin{pmatrix}0&0&0\\0&0&1\\0&0&0\end{pmatrix},\quad X_2=\begin{pmatrix}0&0&0\\0&0&0\\0&-1&0\end{pmatrix},$$

$$X_3=\begin{pmatrix}0&0&0\\0&\frac{1}{2}&0\\0&0&-\frac{1}{2}\end{pmatrix},\quad X_4=\begin{pmatrix}0&0&\frac{1}{\sqrt{2}}\\ \\ \frac{1}{\sqrt{2}}&0&0\\0&0&0\end{pmatrix},$$

$$X_5=\begin{pmatrix}0&\frac{1}{\sqrt{2}}&0\\ \\ 0&0&0\\ \\ -\frac{1}{\sqrt{2}}&0&0\end{pmatrix}. \tag{5.21}$$

The subgroup coordinates take the form

$$\exp(p^1X_1)=\begin{pmatrix}1&0&0\\0&1&p^1\\0&0&1\end{pmatrix},$$

$$\exp(p^2X_2)=\begin{pmatrix}1&0&0\\0&1&0\\0&-p^2&1\end{pmatrix},$$

$$\exp(p^3X_3)=\begin{pmatrix}1&0&0\\0&e^{p^3/2}&0\\0&0&e^{-p^3/2}\end{pmatrix}, \tag{5.22}$$

$$\exp(p^4X_4)=\begin{pmatrix}1&0&p^4/\sqrt{2}\\p^4/\sqrt{2}&1&0\\0&0&0\end{pmatrix},$$

$$\exp(p^5X_5)=\begin{pmatrix}1&p^5/\sqrt{2}&0\\0&1&0\\-p^5/\sqrt{2}&0&1\end{pmatrix}.$$

A representation $T_3(\underset{\sim}{p})$ can be defined with canonical coordinates $\underset{\sim}{p}$ of the third kind:

$$T_3(\underset{\sim}{p})=\exp(p^1X_1)\exp(p^2X_2)\exp(p^3X^3)\times\exp(p^4X_4)\exp(p^5X_5). \tag{5.23}$$

Computing the matrix product, we obtain the representation

$$T_3(\underset{\sim}{p})=\begin{pmatrix}e^{p^4p^5/2}&p^5/\sqrt{2}&p^4/\sqrt{2}\\(1-p^1p^2)e^{p^3/2}p^4/\sqrt{2}-p^1e^{-p^3/2}p^5/\sqrt{2}&(1-p^1p^2)e^{p^3/2}e^{-p^4p^5/2}&p^1e^{-p^3/2}\\-p^2e^{p^3/2}p^4/\sqrt{2}-e^{-p^3/2}p^5/\sqrt{2}&-p^2e^{p^3/2}e^{-p^4p^5/2}&e^{-p^3/2}\end{pmatrix}. \tag{5.24}$$

From the homomorphism property,

$$T_3(\underset{\sim}{p})T_3(\underset{\sim}{q})=T_3(\underset{\sim}{p}\circ\underset{\sim}{q}), \tag{5.25}$$

we can compute the composition rule. We follow the same procedure as in the previous example. Some details of the general method are given in Appendix C. Also, Appendix B contains our expressions for reciprocals and natural logarithms of Grassmann variables.

Let us define

$$Q=1-p^2q^1e^{p^3},\quad P=p^2e^{p^3}+q^2Q. \tag{5.26}$$

The results are

$$K^1(\underset{\sim}{p},\underset{\sim}{q})=p^1+\frac{q^1e^{p^3}}{Q}-\frac{\frac{1}{2}e^{p^3}}{Q^2}\times\{q^1p^4p^5+e^{q^3/2}p^4q^4+q^1e^{q^3/2}p^5q^4\}, \tag{5.27}$$

$$\begin{aligned}K^2(\underset{\sim}{p},\underset{\sim}{q})=&PQe^{-p^3}+\tfrac{1}{2}[q^2-p^2(1-q^1q^2)(Q-1)]\,p^4p^5e^{-p^3}\\&+\tfrac{1}{2}\{P^2e^{-p^3}e^{q^3/2}-p^2Qe^{-q^3/2}\}\,p^4q^4\\&+\tfrac{1}{2}P[1-(1-q^1q^2)Q]\,e^{-p^3}e^{q^3/2}p^5q^4\\&+\tfrac{1}{2}PQe^{-p^3}e^{-q^3/2}p^4q^5\\&+\tfrac{1}{2}[q^1PQe^{-p^3}e^{-q^3/2}-Qe^{-p^3}e^{-q^3/2}]\,p^5q^5\\&+\tfrac{1}{4}[P(Q+1)e^{-p^3}+p^2q^1Qe^{-q^3}]\,p^4p^5q^4q^5,\end{aligned} \tag{5.28}$$

$$K^3(\underset{\sim}{p},\underset{\sim}{q})=p^3+q^3-2\ln Q-\frac{(p^2q^1e^{p^3}p^4p^5+p^2e^{p^3}e^{q^3/2}p^4q^4+e^{q^3/2}p^5q^4)}{Q}, \tag{5.29}$$

$$K^4(\underset{\sim}{p},\underset{\sim}{q})=e^{p^4p^5/2}q^4+e^{-q^3/2}p^4+q^1e^{-q^3/2}p^5, \tag{5.30}$$

$$\begin{aligned}K^5(\underset{\sim}{p},\underset{\sim}{q})=&e^{p^4p^5/2}q^5-q^2e^{q^3/2}e^{-q^4q^5/2}p^4\\&+(1-q^1q^2)e^{q^3/2}e^{-q^4q^5/2}p^5.\end{aligned} \tag{5.31}$$

The correct structure constants follow directly from Eqs. (3.14) and (3.18).

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APPENDIX A: GLOSSARY OF FREQUENTLY USED SYMBOLS

Here, we give a glossary of frequently used symbols. We adhere as closely as possible to the conventions of Rogers.[9,12]

B_L	real Grassmann algebra with L generators
M_L	set of integer sequences, with $\mu=(\mu_1,\ldots,\mu_k)$, $1\leqslant\mu_1<\mu_2<\cdots<\mu_k\leqslant L$, $1\leqslant k\leqslant L$; Ω is the null sequence
β_μ	basis element in B_L; $\beta_\Omega=1$

$s(a)$	the "soul" of $a \in B_L$, i.e., the nilpotent part of a
$\epsilon(a)$	the "body" of $a \in B_L$, given by $\epsilon(a)\cdot 1 = a - s(a)$
$M_{L,0}(M_{L,1})$	the subset of M_L with an even (odd) number of elements
$B_L^{m,n}$	"flat superspace": the Cartesian product of m copies of the even part, ${}^0B_L$, of B_L with n copies of the odd part, ${}^1B_L$
$d = 2^{L-1}(m+n)$	dimension of $B_L^{m,n}$ viewed as a vector space over $\mathbb{R}$
ι	homeomorphism $\iota: B_L^{m,n} \to \mathbb{R}^d$
H	supergroup; also, supergroup viewed as a Lie group
W	left B_L supermodule
$\mathbf{h}$	Lie algebra with Lie group H
W_0	even part of W, isomorphic to h
$\underset{\sim}{x}$	element in $B_L^{m,n}$
$\vec{x}$	element in $\mathbb{R}^d$
$K(\underset{\sim}{x}, \underset{\sim}{y})$	composition mapping for supergroups
$\kappa(\vec{x}, \vec{y})$	composition mapping for Lie groups
$\chi_p^j(\underset{\sim}{x})$	transformation function for supergroups
$\chi_{p\sigma}^{j\mu}(\vec{x})$	transformation function for Lie groups

APPENDIX B: LEMMAS CONCERNING SUPERFUNCTIONS

In this Appendix, we prove several lemmas concerning the properties of superfunctions, i.e., functions of Grassmann variables. These lemmas are of great help in the technical calculations of Sec. V.

Lemma B1: Let $x_1, x_2 \in {}^1B_L$. Then

$$\exp(x_1x_2) = 1 + x_1x_2, \tag{B1}$$

$$x_j \exp(x_1x_2) = x_j, \quad j = 1,2, \tag{B2}$$

$$\exp(\lambda x_1x_2) + \mu x_1x_2 = \exp(\lambda + \mu)x_1x_2, \quad \lambda, \mu \in \mathbb{R}. \tag{B3}$$

Proof: Expanding $\exp(x_1x_2)$, we have

$$\exp(x_1x_2) = 1 + x_1x_2 + (1/2!)(x_1x_2)^2 + \cdots, \tag{B4}$$

The series terminates after the second term since $x_j^2 = 0$ for $x_j \in {}^1B_L$.

From (B1), for $j = 1,2$,

$$x_j \exp(x_1x_2) = x_j(1 + x_1x_2) = x_j. \tag{B5}$$

Expanding the exponential in Eq. (B3), we get

$$\begin{aligned}\exp(\lambda x_1x_2) + \mu x_1x_2 &= 1 + \lambda x_1x_2 + \mu x_1x_2 \\ &= 1 + (\lambda + \mu)x_1x_2 \\ &= \exp(\lambda + \mu)x_1x_2.\end{aligned} \tag{B6}$$

Lemma B2: Let $a \in B_L$, $\epsilon(a) \neq 0$. Then,

$$1/a = [1/\epsilon(a)](1 - \hat{a} + \hat{a}^2 - \cdots + (-\hat{a})^n), \tag{B7}$$

for $n \leqslant L$, where

$$\hat{a} = \sum_{\mu \in M_L}{}' \hat{a}^\mu \beta_\mu. \tag{B8}$$

The prime on the summation indicates that $\mu = \Omega$ is excluded, and $a^\mu = a^\mu/\epsilon(a)$.

Proof: For $\epsilon(a) \neq 0$,

$$1/a = 1/[\epsilon(a)\cdot 1 + s(a)] = 1/\epsilon(a)(1 + \hat{a}). \tag{B9}$$

Let $f(\hat{a}) = 1/(1 + \hat{a})$. Now, expand $f(\hat{a})$ in a Taylor series about $\hat{a} = 0$:

$$\begin{aligned} &f(0) = 1, \\ &\left.\frac{\partial f}{\partial \hat{a}^\mu}\right|_0 = -\beta_\mu, \\ &\left.\frac{\partial^2 f}{\partial \hat{a}^\mu \partial \hat{a}^\nu}\right|_0 = 2\beta_\nu \beta_\mu, \end{aligned} \tag{B10}$$

and so on. Thus,

$$\begin{aligned} f(\hat{a}) &= 1 - \sum_{\mu \in M_L}{}' \hat{a}^\mu \beta_\mu + \sum_{\mu \in M_L}{}' \sum_{\nu \in M_L}{}' \hat{a}^\nu \beta_\nu \hat{a}^\mu \beta_\mu - \cdots \\ &= 1 - \hat{a} + \hat{a}^2 - \cdots. \end{aligned} \tag{B11}$$

However, $\hat{a}$ is nilpotent,[9] i.e., $(\hat{a})^n \neq 0$ but $(\hat{a})^{n+1} = 0$ for some $n \leqslant L$. This means that the series converges for all finite values of $\hat{a}^\mu$. Hence, the lemma is proved.

Lemma B3: Let $a \in B_L$, $\epsilon(a) \neq 0$. Then, $1/a$ is the inverse of a, i.e.,

$$(1/a)a = a(1/a) = 1. \tag{B12}$$

Proof: We have

$$\begin{aligned} a(1/a) &= \epsilon(a)(1 + \hat{a})[(1/\epsilon(a))(1 - \hat{a} + \hat{a}^2 - \cdots + (-\hat{a})^n)] \\ &= (1 + \hat{a})(1 - \hat{a} + \hat{a}^2 - \cdots + (-\hat{a})^n) \\ &= 1 - \hat{a} + \hat{a}^2 - \cdots + (-\hat{a})^n \\ &\quad + \hat{a} - \hat{a}^2 + \cdots - (-\hat{a})^n + (-\hat{a})^{n+1} \\ &= 1. \end{aligned} \tag{B13}$$

The proof for $(1/a)a$ is analogous.

Lemma B4: Let $a \in {}^0B_L$ such that $\epsilon(a) \neq 0$. Then,

$$ba/a = ab/a = b, \tag{B14}$$

for any $b \in {}^0B_L$.

Proof: Since $a,b \in {}^0B_L$, $ab = ba$. The rest follows from Lemma B3.

Lemma B5: Let $a \in {}^0B_L$ such that $\epsilon(a) > 0$. Then,

$$\ln a = \ln \epsilon(a) + \hat{a} - \hat{a}^2/2 + \cdots - (-)^n(a^n/n), \tag{B15}$$

where $n \leqslant L$ and $\hat{a}$ is defined in Eq. (B8).

Proof: It may be shown that the definition (B15) for $\ln a$, $a \in {}^0B_L$, $\epsilon(a) > 0$, is the inverse of exponentiation, i.e., $\exp(\ln a) = a$. It follows that

$$\ln a = \ln \epsilon(a)(1 + \hat{a}) = \ln \epsilon(a) + \ln(1 + \hat{a}), \tag{B16}$$

where the second equality is obtained by noting that for any $a \in {}^0B_L$, $\epsilon(a) \neq 0$, there exists a unique $b \in {}^0B_L$ such that $e^b = a$.

Let $f(\hat{a}) = \ln(1 + \hat{a})$ and expand $f(\hat{a})$ in a Taylor series about $\hat{a} = 0$. Then,

$$f(0) = 0, \quad \left.\frac{\partial f}{\partial \hat{a}^\mu}\right|_0 = \beta_\mu, \quad \left.\frac{\partial^2 f}{\partial \hat{a}^\mu \partial \hat{a}^\nu}\right|_0 = -\beta_\nu \beta_\mu \tag{B17}$$

and so on. Thus,

$$f(\hat{a}) = \hat{a} - \hat{a}^2/2 + \cdots, \tag{B18}$$

which terminates for some $n \leqslant L$, since $\hat{a}$ is nilpotent. Hence,

$$\ln(1 + \hat{a}) = \hat{a} - \hat{a}^2/2 + \cdots - (-)^n(\hat{a}^n/n), \tag{B19}$$

which is valid for any finite $\hat{a}$.

APPENDIX C: SOME DETAILS OF TECHNICAL CALCULATIONS

Here, we provide some details of the technical calculations of Sec. V. Let us repeat the steps in Eq. (5.5). From Eq. (5.4), we have

$$\exp(tX) = \exp\left\{t\left[a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}+a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}\right]\right\}$$

$$=\begin{pmatrix}1&0\\0&1\end{pmatrix}+t\left[a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}+a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}\right]+\frac{t^2}{2!}\left[a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}+a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}\right]^2+\cdots. \quad \text{(C1)}$$

We adopt the *convention* that matrices with Grassmann variable entries are linear combinations of the generators and their products, multiplied from the *left* by Grassmann parameters. For example, in this convention,

$$\begin{pmatrix}a^1&a^2\\a^3&a^1\end{pmatrix} := a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}+a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}. \quad \text{(C2)}$$

Expression (C1) may be simplified by performing the matrix multiplications, being careful to recall that an odd generator must *anticommute* with an odd Grassmann variable. Thus,

$$\begin{pmatrix}0&1\\0&0\end{pmatrix}a^3 = -a^3\begin{pmatrix}0&1\\0&0\end{pmatrix}. \quad \text{(C3)}$$

This strange-seeming result arises because the faithful matrix representation that we are using for sqm(2) cannot incorporate the effects of the odd Grassmann variables. For example,

$$\left[a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^2\begin{pmatrix}0&1\\0&1\end{pmatrix}+a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}\right]^2$$

$$=a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}+a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}$$

$$+a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}+a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}a^1\begin{pmatrix}1&0\\0&1\end{pmatrix}+a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}, \quad \text{(C4)}$$

$$=(a^1)^2\begin{pmatrix}1&0\\0&1\end{pmatrix}+2a^1a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}+2a^1a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}-a^2a^3\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}0&0\\1&0\end{pmatrix}-a^3a^2\begin{pmatrix}0&0\\1&0\end{pmatrix}\begin{pmatrix}0&1\\0&0\end{pmatrix}, \quad \text{(C5)}$$

$$=(a^1)^2\begin{pmatrix}1&0\\0&1\end{pmatrix}+2a^1a^2\begin{pmatrix}0&1\\0&0\end{pmatrix}+2a^1a^3\begin{pmatrix}0&0\\1&0\end{pmatrix}-a^2a^3\begin{pmatrix}1&0\\0&0\end{pmatrix}+a^2a^3\begin{pmatrix}0&0\\0&1\end{pmatrix}, \quad \text{(C6)}$$

where we have used Eq. (C3) to go from Eq. (C4) to Eq. (C5). The final step follows because the Grassmann variables a^2 and a^3 are odd. We treat the matrices multiplying the product a^2a^3 in Eq. (C6) as even.

The expression (C1) then reduces to

$$\exp(tX) = e^{a^1 t}\begin{pmatrix}1-t^2a^2a^3/2 & ta^2\\ ta^3 & 1+t^2a^2a^3/2\end{pmatrix}. \quad \text{(C7)}$$

Using Lemma B1, we find the desired result, Eq. (5.5).

As a second example, we provide an explanation of the solution (5.10) of Eq. (5.9) for $\underline{z}$ in terms of $\underline{a}$ and $\underline{b}$. To compute an expression for z^1, take a product of the diagonal elements:

$$e^{2z^1} = e^{2(a^1+b^1)}(e^{-a^2a^3/2}e^{-b^2b^3/2} - a^2b^3)$$

$$\times(e^{a^2a^3/2}e^{b^2b^3/2} - a^3b^2),$$

$$= \exp(2(a^1+b^1) - a^2b^3 - a^3b^2), \quad \text{(C8)}$$

by Lemma B1. This implies the solution for z^1 given in Eq. (5.10).

Next, note that

$$e^{z^1}z^2 = e^{a^1+b^1}(a^2e^{b^2b^3/2} + b^2e^{-a^2a^3/2}). \quad \text{(C9)}$$

Substituting for $\exp(z^1)$ from (5.10) and applying Lemma B1 again, we find the result for z^2 given in (5.10). The solution for z^3 is similar.

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[27]In the following equation, the equalities hold up to a homomorphism.
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[30]We remark that the supergroup obtained from this 3×3 matrix representation, or any finite-dimensional representation for that matter, will not be unitary. This is due to the presence of the su(1,1) noncompact Lie algebra, embedded in osp($\frac{1}{2}$).

A new method of constructing the symmetry-adapted linear combinations based on the correspondence theorem and induced representations

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The theory of induced representations is incorporated into the method of constructing symmetry-adapted linear combinations for a symmetry group based on the correspondence theorem developed previously. The theory is effective for a highly symmetric molecule with a set of equivalent radicals, each of which again consists of a number of equivalent atoms. An illustrative example is given to construct the internal symmetry coordinates of molecular vibrations of $C(CH_3)_4$ with the frozen configuration belonging to the point group T_d.

I. INTRODUCTION

In previous papers[1,2] (hereafter referred to as I and II), the author has introduced a general method of constructing the symmetry-adapted linear combinations (or simply SALC's) of equivalent atomic orbitals of a molecule belonging to a symmetry group G. This method has been extended to construct the symmetry coordinates of molecular vibrations[3] (referred to as III). It is based on the correspondence theorem, which describes the parallelism between the SALC's and the elementary basis functions[1,4] of the space variables belonging to the same irreducible representations (or simply irreps) of G. More specifically, let $S^{(s)}$ be a set of s equivalent points in space with respect to G. Then the SALC's of s equivalent basis functions located at $S^{(s)}$ are described by the elementary basis vectors defined on the s-dimensional vector space $S^{(s)}$. The method is direct and general. It is effective for degenerate as well as for nondegenerate irreps. It requires neither additional symmetry consideration of the equivalent basis functions nor the actual matrix representations of the irreps. It simply requires the knowledge of elementary basis sets. This is quite a contrast to the conventional method of the projection operators.

Let $\Delta^{(s)}$ be the principal induced representation of G relative to the subgroup H which leaves a point in $S^{(s)}$ invariant. Hereafter, it will simply be called the permutation representation of G by H. Now, if $\Delta^{(s)}$ is not simply reducible, the method of the correspondence theorem becomes laborious since then it is necessary to introduce more than one set of mutually orthogonal elementary basis vectors on $S^{(s)}$ for some irreps. This kind of undesirable situation arises when $S^{(s)}$ consists of a number of equivalent subsets, each of which again consists of a number of equivalent points. Such a set may conveniently be said to be doubly equivalent. A molecular example can be seen in the cyclopropane $(CH_2)_3$ belonging to D_{3h}. In such a case, a similar difficulty also arises in the ordinary method of the projection operators. A way out of this difficulty was introduced through examples by Wilson, Decius, and Cross[5] in their treatise on molecular vibrations. It is based on the induced representation[6–8] of G via the irreps of an intermediate subgroup K $(H < K < G)$ that leaves one of the equivalent subsets invariant. Their treatment was, however, limited to the case where the intermediate subgroup K has only nondegenerate irreps.

The purpose of the present work is to incorporate the theory of induced representation into the method of the correspondence theorem in its full generality. For this purpose, we shall first reformulate the induced representation of a group G based on a simple algebraic identity that follows from the coset decomposition of G. It effectively eliminates the complicated arguments encountered in the conventional heuristic approach.[6] With a minimum presentation of the general theory we shall then express the permutation representation $\Delta^{(s)}$ of G by H in terms of the permutation representation $\Delta^{(n)}$ of G by K with index n using the transitivity of induction. This may avoid the aforementioned difficulty since $\Delta^{(n)}$ may simply be reducible even if $\Delta^{(s)}$ is not (Sec. II). We shall then construct the general expressions for the SALC's of the equivalent basis functions on $S^{(s)}$ via those on $S^{(n)}$, which provides the basis of $\Delta^{(n)}$ (Sec. III). As an illustrative example we shall apply the formalism to construct the internal symmetry coordinates of vibration for the tetramethyl methane molecule $C(CH_3)_4$ with the frozen configuration belonging to T_d.

II. BASIC THEORY

Let $G = \{A\}$ be a finite group and $K = \{B\}$ be a subgroup of G with index n. The left coset decomposition of G by K may be written as

$$G = A_1K + A_2K + \cdots + A_nK, \tag{2.1}$$

where the A_ν's are the coset representatives. It means that any element of G can be expressed as a product of a coset representative and an element of K. Thus, we obtain an identity

$$AA_\nu = \sum_{\mu,\, B\in K} \delta(B, A_\mu^{-1}AA_\nu)A_\mu B, \quad A \in G, \tag{2.2}$$

where $\delta(X, Y)$ is Kronecker's delta. This is the basic identity for the induced representations of G via the representations of K. To see this, let $\{\Psi^\beta{}_i; i = 1,2,\ldots,d_\beta\}$ be the basis belonging to a representation $D^\beta(B)$ of K. Then operating the both sides of (2.2) on this basis we arrive at the induced representations $D^{(\beta\uparrow)}(A)$ of G via $D^{(\beta)}(B)$ of K,

$$D^{(\beta\uparrow)}(A)_{\mu j,\,\nu i} = \sum_{B\in K} \delta(B, A_\mu^{-1}AA_\nu)D^{(\beta)}(B)_{ji}, \tag{2.3a}$$

through the induced basis

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$$\Psi^{(\beta\uparrow)}{}_{\nu i} = A_\nu \Psi^\beta{}_i, \quad \nu = 1,...,n, \quad i = 1,...,d_\beta. \tag{2.3b}$$

Let $H = \{C\}$ be a subgroup of K with index m and let the left coset decomposition of K by H be

$$K = \sum_{\sigma=1}^{m} B_\sigma H. \tag{2.4}$$

Then, from (2.1) and (2.4) we obtain the left coset decomposition of G by H,

$$G = \sum_{\nu,\sigma} A_\nu B_\sigma H. \tag{2.5}$$

This leads to the transitivity of induction[9]

$$(\hat{H} \uparrow K) \uparrow G = \hat{H} \uparrow G \tag{2.6}$$

written in terms of the notations due to Robinson.[6,7] Here $\hat{H}$ denotes a representation of H and $(\hat{H} \uparrow K)$ the induced representation of K via $\hat{H}$.

In a simple special case where $D^{(\beta)}$ is the identity representation of K we have from (2.3a) the permutation representation of G by K:

$$\Delta^{(n)}(A)_{\nu\mu} = \sum_B \delta(B, A_\mu{}^{-1} A A_\nu). \tag{2.7}$$

It describes the permutations of the cosets of K by the elements of G. Analogously, one obtains the permutation representations $\Delta^{(m)}(B)$ of K by H from (2.4) and $\Delta^{(s)}(A)$ of G by H from (2.5). Then the transitivity of induction (2.6) yields

$$\Delta^{(s)}(A) = \Delta^{(m\uparrow)}(A), \quad \forall A \in G. \tag{2.8}$$

For the present purpose we need the relation between $\Delta^{(s)}(A)$ and $\Delta^{(n)}(A)$ of G. To obtain this we shall first express $\Delta^{(m)}(B)$ of K by a representation subduced by a representation of G. Obviously, $\Delta^{(s)}(A)$ of G subduces a representation of K but it is not equal to $\Delta^{(m)}(B)$ in general. One way to find such a subduced representation is through decomposition of $\Delta^{(m)}(B)$ into its irreducible components,

$$\Delta^{(m)}(B) \sim \sum_\beta D^{(\beta)}(B), \quad \forall B \in K, \tag{2.9}$$

where $\sim$ denotes the equivalence and $D^{(\beta)}(B)$ is an irrep of K. Using the group and subgroup compatibility tables[10] one obtains

$$\sum_\beta D^{(\beta)}(B) \sim \sum_\alpha D^{(\alpha\downarrow)}(B), \quad \forall B \in K, \tag{2.10}$$

where $D^{(\alpha\downarrow)}(B)$ is the representation of K subduced by $D^{(\alpha)}(A)$ of G. In general, there exist more than one choice of the set $\{D^{(\alpha)}(A)\}$ that are compatible with the set $\{D^{(\beta)}(B)\}$, as will be discussed later.

Now, let $D^{(\alpha\downarrow\uparrow)}(A)$ be the induced representation of G via the subduced representation $D^{(\alpha\downarrow)}(B)$ of K. Then we have from (2.3a) the following equivalence:

$$D^{(\alpha\downarrow\uparrow)}(A) \sim \Delta^{(n)}(A) \times D^{(\alpha)}(A). \tag{2.11}$$

Combining (2.7)–(2.11) we obtain the desired relation in a factorized form:

$$\Delta^{(s)}(A) \sim \Delta^{(n)}(A) \times \sum_\alpha D^{(\alpha)}(A). \tag{2.12}$$

This reduces the problem of constructing the SALC's of the equivalent basis sets belonging to $\Delta^{(s)}(A)$ of G to those belonging to $\Delta^{(n)}(A) \times D^{(\alpha)}(A)$ of G. Note that the basis sets belonging to two different $\Delta^{(n)}(A) \times D^{(\alpha)}(A)$'s are orthogonal provided that the overlap integrals are neglected. Obviously, one can extend the above result to construct the SALC's of those belonging to $\Delta^{(s)}(A) \times D^{(\lambda)}(A)$ of G through those of $\Delta^{(n)}(A) \times D^{(\alpha)}(A) \times D^{(\lambda)}(A)$, as will be formulated explicitly in the next section.

We shall next discuss the nonuniqueness of the factorization (2.12). Let $\chi^{(s)}(A)$, $\chi^{(n)}(A)$, $\chi^{(\alpha)}(A)$ be the characters of $\Delta^{(s)}(A)$, $\Delta^{(n)}(A)$, and $D^{(\alpha)}(A)$, respectively. Then we have from (2.12)

$$\chi^{(s)}(A) = \chi^{(n)}(A) \sum \chi^{(\alpha)}(A). \tag{2.13}$$

If K is a proper subgroup of G, then any coset representative of K that is not an element of K permutes all the cosets of K as well as those of $H\,(<K)$. Accordingly, $\chi^{(s)}(A)/\chi^{(n)}(A)$ becomes indefinite for such an element of G. This establishes the nonuniqueness of (2.12) and hence of (2.10). Since this nonuniqueness should not affect the final result we can choose the set $\{D^{(\alpha)}\}$ in (2.10) such that it has the most convenient elementary basis sets.

In particular, if one can choose $D^{(\alpha)}(A)$ of G such that

$$D^{(\alpha)}(A_\nu)_{ij} = \delta_{ij} \tag{2.14}$$

for all the coset representatives A_ν of K, then we have

$$D^{(\alpha\downarrow\uparrow)}(A) = \Delta^{(n)}(A) \times D^{(\alpha)}(A), \tag{2.15}$$

where both sides are truly equal (not within a similarity transformation). This is possible, however, if and only if the set of coset representatives $\{A_\nu\}$ of K forms an invariant subgroup N of G. In such a case G is called the semidirect product of N by K and is denoted by[8]

$$G = N \circledS K, \quad N = \{A_\nu\}. \tag{2.16}$$

For such a G, every irrep $D^{(\beta)}(B)$ of K engenders an irrep $D^{(\alpha)}(A)$ of G that contains N in its kernel so that

$$D^{(\alpha\downarrow)}(B) = D^{(\beta)}(B), \quad \forall B \in K. \tag{2.17}$$

This choice is particularly convenient for constructing SALC's since then one can use the induced basis for the basis of $\Delta^{(n)}(A) \times D^{(\alpha)}(A)$ (see 3.12).

The semidirect groups occur quite frequently for highly symmetrical molecules or crystals. For example, in the case of cyclic conjugate double bond system of hydrocarbons, $(CH)_n$, belonging to D_{nh}, we have $D_{nh} = C_n \circledS C_{2v}$. For the tetramethyl methane $C(CH_3)_4$ with the frozen configuration belonging to T_d, we have $T_d = D_2 \circledS C_{3v}$. For a symmorphic space group G, we have $G = T \circledS G_0$, where T is the translational group and G_0 is a point group that describes the rotational symmetry of the crystal.

III. CONSTRUCTION OF SALC's

We shall first introduce a set of equivalent points in space that provides the basis of the permutation representation $\Delta^{(s)}$ of G introduced in Sec. II. Let r^0_{11} be a point in space that is invariant with respect to $H\,(<K<G)$. Then from (2.5) the basis of $\Delta^{(s)}$ is given by the set $S^{(s)}$ defined by

$$r^0_{\nu\sigma} = A_\nu B_\sigma r^0_{11}, \tag{3.1}$$
$$\nu = 1,2,...,n, \quad \sigma = 1,2,...,m.$$

Here both A_1 and B_1 represent the identity element. Analogously, the subset $s^{(m)} = \{r^0_{1\sigma}\}$ provides the basis of $\Delta^{(m)}$ of K by H. The basis set $S^{(n)} = \{r^0_\nu\}$ belonging to $\Delta^{(n)}$ of G by K is given by

$$r^0_\nu = \sum_\sigma \frac{r^0_{\nu\sigma}}{m}, \quad \nu = 1,2,...,n, \tag{3.2}$$

where r^0_1 is invariant with respect to K.

The above system of numbering the equivalent points in space is quite natural for a doubly equivalent set. The subset $S^{(m)} = \{r^0_{1\sigma}\}$ merely permutes itself under $B \in K$ while it transforms to another subset $S^{(m)}{}_\nu = \{r^0_{\nu\sigma}\}$ under $A_\nu \in G$. In terms of these equivalent points, the permutation representations take more explicit forms. For example,

$$\Delta^{(n)}(A)_{\mu\nu} = \delta(r^0_\mu, Ar^0_\nu). \tag{3.3}$$

Now, following (2.12) we shall construct the SALC's of the equivalent basis functions defined on $S^{(s)}$ through those on $S^{(n)}$. Let us consider the simplest special case of the equivalent scalar functions defined by

$$\phi_{\nu\sigma}(r) = \phi(|r - r^0_{\nu\sigma}|) \in \Delta^{(s)}. \tag{3.4}$$

Extension from this simple case to the general case is rather trivial. Let $\{u^\alpha{}_i(r)\}$ be an elementary basis set belonging to $D^{(\alpha)}(A)$ of G contained in (2.12). It follows from the correspondence theorem developed in I and II that the basis belonging to $\Delta^{(n)}(A)\times D^{(\alpha)}(A)$ of G is given by

$$\phi^\alpha{}_i(r, r^0_\nu) = \sum_\sigma u^\alpha{}_i(r^0_{\nu\sigma} - r^0_\nu)\phi_{\nu\sigma}(r). \tag{3.5}$$

Here, r^0_ν on the right-hand-side is inserted for convenience. If $D^{(\gamma)}(A)$ is an irrep contained in $\Delta^{(n)}(A)\times D^{(\alpha)}(A)$, then its basis is given by

$$\psi^\gamma{}_{j,\alpha}(r) = \sum_{\nu,i} [\mathring{T}^\gamma{}_j(r')g^\alpha{}_i(r')^*]_{r=r^0_\nu}\phi^\alpha{}_i(r, r^0_\nu), \tag{3.6}$$

where $\{\mathring{T}^\gamma{}_j(r')\}$ is an operator basis of $D^\gamma(A)$ and $\{g^\alpha{}_i(r')\}$ is an elementary basis set of $D^{(\alpha)}(A)$ [see Sec. II (2.6)]. Combining (3.5) and (3.6) we simply write

$$\psi^\gamma{}_{j\alpha}(r) = \sum_{\nu,\sigma} (\gamma j\alpha|\nu\sigma)\phi_{\nu\sigma}(r), \tag{3.7}$$

where the linear coefficients are defined by (3.5) and (3.6).

We shall next extend the above result for the general case. Let $\{f^\lambda{}_p(r - r^0_{\nu\sigma})\}$ be an equivalent basis functions belonging to $\Delta^{(s)}(A)\times D^{(\lambda)}(A)$ of G. Then simple replacement of $\phi_{\nu\sigma}(r)$ in (3.7) by $f^\lambda{}_p(r - r^0_{\nu\sigma})$ yields, for the basis belonging to $D^{(\gamma)}(A)\times D^{(\lambda)}(A)$ of G,

$$\psi^{\gamma\lambda}{}_{jp\alpha}(r) = \sum_{\nu,\sigma} (\gamma j\alpha|\nu\sigma) f^\lambda{}_p(r - r^0_{\nu\sigma}). \tag{3.8}$$

Accordingly the basis of $D^{(\delta)}(A)$ of G contained in the direct product $D^{(\gamma)}(A)\times D^{(\lambda)}(A)$ of G is given by

$$\psi^\delta{}_{t\alpha}(r) = \sum_{\gamma\lambda jp} \Gamma^{\delta\gamma\lambda}_{tjp}\psi^{\gamma\lambda}{}_{jp\alpha}(r), \tag{3.9}$$

where the linear coefficients are the coupling coefficients for the direct product $D^{(\alpha)}(A)\times D^{(\lambda)}(A)$. These are tabulated by Koster *et al.*[10] for the 32 point groups. A method of their construction has also been discussed in II based on the correspondence theorem. The above two equations (3.8) and (3.9) describe all the SALC's of $f^\lambda{}_p(r - r^0_{\nu\sigma})$ defined on $S^{(s)}$ through the decomposition (2.12) in the following steps:

$$D^{(\delta)} \in D^{(\gamma)}\times D^{(\lambda)} \in (\Delta^{(n)}\times D^{(\alpha)})\times D^{(\lambda)} \in \Delta^{(s)}\times D^{(\lambda)}. \tag{3.10}$$

Finally, we shall discuss the subtle difference between the basis of $\Delta^{(n)}(A)\times D^{(\alpha)}(A)$ given by (3.5) and the basis of $D^{(\alpha\downarrow\uparrow)}(A)$ given by

$$\phi^{(\alpha\downarrow\uparrow)}{}_{vi}(r) = \sum_{\sigma=1}^{n} u^\alpha{}_i(r^0_{1\sigma} - r^0_1)\phi_{\nu\sigma}(r). \tag{3.11}$$

Here, the linear coefficients are independent of ν while those of $\phi^\alpha{}_i(r, r^0_\nu)$ are dependent on ν in general. These two bases are connected by

$$\phi^\alpha{}_i(r, r^0_\nu) = \sum_j \phi^{(\alpha\downarrow\uparrow)}{}_{vj}(r)D^{(\alpha)}(A_\nu)^*{}_{ij}. \tag{3.12}$$

As is discussed in (2.14) and (2.15), both bases become identical in the case when $D^{(\alpha)}(A)$ is an engendered irrep of G. This will be explicitly shown by the illustrative example given in the next section.

IV. ILLUSTRATIVE EXAMPLE

To show the effectiveness of the present formalism we shall first construct the SALC's of the s-orbitals of the 12 H atoms in the tetramethyl methane molecule $C(CH_3)_4$ with the frozen configuration belonging to the point group T_d. The subgroup H that leaves an H atom invariant is C_s while the subgroup K that leaves a (CH_3) radical invariant is C_{3v}. Since $T_d = D_2 \otimes C_{3v}$, we can use the engendered irreps of T_d from the irreps of C_{3v} in constructing the SALC's. The result is then applied to construct the internal symmetry coordinates of the molecule under small vibrations.

A. The SALC's of $C(CH_3)_4$

Let us define the set of coordinates of 12 equivalent H atoms, $S^{(12)} = \{r^0_{\nu\sigma}, \ \nu = 1,...,4, \ \sigma = 1,2,3\}$ following (3.1). We place the coordinate origin at the central carbon atom, and define the set of the coordinates of the four equivalent carbon atoms $S^{(4)} = \{r^0_\nu\}$ in the order as follows:

$$(1, 1, 1), \quad (-1, -1, 1,), \quad (-1, 1, -1), \quad (1, -1, -1). \tag{4.1}$$

These are given in a relative scale. This is sufficient to determine the SALC's since the elementary basis functions are homogeneous with respect to the space variables. Let r^0_1 be the invariant point with respect to the subgroup C_{3v} and the coordinates of the three H atoms bonded to the carbon at r^0_1 be

$$r^0_{1\sigma} - r^0_1 = (1, 0, 0), \quad (0, 1, 0), \quad (0, 0, 1). \tag{4.2}$$

Then the remaining coordinates of $S^{(12)}$ are automatically defined by three C_2 operations belonging to D_2 according to (3.1).

For later use we may classify the irreps of T_d by their elementary bases,

$$\begin{aligned} &\Gamma_1; \quad 1, \qquad \Gamma_2; \quad \tilde{x}\tilde{y}\tilde{z}, \\ &\Gamma_3; \quad (u, v), \quad \Gamma_4; \quad (\tilde{x}, \tilde{y}, \tilde{z}), \\ &\Gamma_5; \quad (x, y, z), \end{aligned} \tag{4.3}$$

where $u = 2z^2 - x^2 - y^2$, $v = 3^{1/2}(x^2 - y^2)$, and $\tilde{x} = yz' - zy'$, etc. The above notations Γ_ν are in accordance with those of KDWS (see Ref. 10).

The primary problem is to construct the SALC's of the 12 scalar functions $\phi_{\nu\sigma}(r)$ located at the H atoms of $C(CH_3)_4$. Following (2.9) we first decompose the permutation representation $\Delta^{(3)}(B)$ of C_{3v} into its irreducible components,

$$\Delta^{(3)} \sim \Gamma_1 + \Gamma_3 \in C_{3v}. \tag{4.4}$$

From the compatibility table[10] of irreps between T_d and C_{3v}, we find that the engendered irreps corresponding to the above are given by[11]

$$\Gamma_1 + \Gamma_3 \in T_d. \tag{4.5}$$

Thus, from (2.12) we have

$$\Delta^{(12)} \sim \Delta^{(4)} + \Delta^{(4)} \times \Gamma_3 \in T_d. \tag{4.6}$$

From (3.5) the equivalent basis functions belonging to $\Delta^{(4)}$ are given by

$$\phi_\nu(r) = 3^{-1/2}(\phi_{\nu 1} + \phi_{\nu 2} + \phi_{\nu 3}), \quad \nu = 1,...,4, \tag{4.7a}$$

and those belonging to $\Delta^{(4)} \times \Gamma_3$ are

$$\begin{aligned} &\phi_u(r, r_\nu^0) = 6^{-1/2}(2\phi_{\nu 3} - \phi_{\nu 1} - \phi_{\nu 2}), \\ &\phi_v(r, r_\nu^0) = 2^{-1/2}(\phi_{\nu 1} - \phi_{\nu 2}). \end{aligned} \tag{4.7b}$$

Note that the linear coefficients in (4.7) are independent of ν since we have chosen the engendered irreps of T_d in (4.5).

The rest of calculation is almost routine now with the use of (3.6). For the later application, however, we write down the final expressions of the SALC's of 12 s-orbitals of H atoms.

(i) The SALC's $\in \Delta^{(4)} = \Gamma_1 + \Gamma_5$:

$$\Gamma_1; \quad \psi(r) = \frac{1}{4}\sum_\nu \phi_\nu, \tag{4.8a}$$

$$\Gamma_5; \quad \psi_x(r) = \frac{1}{2}\sum_\nu x_\nu^0 \phi_\nu(r), \quad \psi_y(r) = \frac{1}{2}\sum y_\nu^0 \phi_\nu(r), \quad \psi_z = \frac{1}{2}\sum_\nu z_\nu^0 \phi_\nu(r), \tag{4.8b}$$

where the coordinates $(x_\nu^0, y_\nu^0, z_\nu^0)$ are given by (4.1).

(ii) The SALC's $\in \Delta^{(4)} \times \Gamma_3 = \Gamma_3 + \Gamma_4 + \Gamma_5$:

$$\begin{aligned} &\Gamma_3; \ \psi_u(r) = \frac{1}{2}\sum_\nu \phi_u(r, r_\nu^0), \\ &\qquad \phi_v(r) = \frac{1}{2}\sum_\nu \phi_v(r, r_\nu^0), \\ &\Gamma_4; \ \psi_{\tilde{x}}(r) = 8^{-1/2}\sum_\nu x_\nu^0(\phi_{\nu 2} - \phi_{\nu 3}), \\ &\qquad \psi_{\tilde{y}}(r) = 8^{-1/2}\sum_\nu y_\nu^0(\phi_{\nu 3} - \phi_{\nu 1}), \\ &\qquad \psi_{\tilde{z}}(r) = 8^{-1/2}\sum_\nu z_\nu^0(\phi_{\nu 1} - \phi_{\nu 2}), \end{aligned} \tag{4.9a, 4.9b}$$

$$\begin{aligned} &\Gamma_5; \ \psi'_x = (24)^{-1/2}\sum_\nu x_\nu^0(2\phi_{\nu 1} - \phi_{\nu 2} - \phi_{\nu 3}), \\ &\qquad \psi'_y = (24)^{-1/2}\sum_\nu y_\nu^0(2\phi_{\nu 2} - \phi_{\nu 1} - \phi_{\nu 3}), \\ &\qquad \psi'_z = (24)^{-1/2}\sum_\nu z_\nu^0(2\phi_{\nu 1} + \phi_{\nu 2} - \phi_{\nu 3}). \end{aligned} \tag{4.9c}$$

Here we have used the operator basis $\tilde{x} = y\partial/\partial z - z\partial/\partial y$,... for (4.9b) and $\partial/\partial x$, $\partial/\partial y$, $\partial/\partial z$ for the (4.9c).

As is expected, two basis sets (ψ_x, ψ_y, ψ_z) and $(\psi'_x, \psi'_y, \psi'_z)$ belonging to Γ_5 of T_d are orthogonal provided that the overlap integrals are neglected. The results given above provide the starting point for the calculation LCAOMO or the internal symmetry coordinates of $C(CH_3)_4$, which will be discussed next.

B. The internal symmetry coordinates of $C(CH_3)_4$

There exists a total of 45 internal coordinates of small vibrations for the molecule $C(CH_3)_4 \in T_d$. Their symmetry coordinates may be constructed from the results given in Sec. IV A for the most part by mere correspondence between the internal coordinates and the equivalent basis functions through the rules given in III.

1. The bond stretching coordinates

There exist 12 C–H bond stretching $(s_{\nu\sigma}; \ \nu = 1,...,4, \ \sigma = 1,2,3) \in \Delta^{(12)}$ and 4 C–C bond stretchings $\{t_\nu\} \in \Delta^{(4)}$. Since $\{s_{\nu\sigma}\}$ transforms like the set of equivalent scalar functions $\{\phi_{\nu\sigma}\}$, by replacing $\phi_{\nu\sigma}$ in (4.7) with $s_{\nu\sigma}$ and using (4.8) and (4.9) we obtain their symmetry coordinates written as follows:

$$\begin{aligned} &s, \ (s_u, s_v), \quad (s_{\tilde{x}}, s_{\tilde{y}}, s_{\tilde{z}}), \\ &(s_x, s_y, s_z), \quad (s'_x, s'_y, s'_z). \end{aligned} \tag{4.10}$$

Analogously, replacing ϕ_ν in (4.8) with t_ν we obtain the symmetry coordinates of the C–C stretchings written as

$$t, \ (t_x, t_y, t_z). \tag{4.11}$$

2. The valence angle bending coordinates

There exist 12 H–C–H bendings $\{\alpha_{\nu\sigma}\}$, 12 C–C–H bendings $\{\beta_{\nu\sigma}\}$, and 6 C–C–C bendings $\{\gamma_{\nu\mu}; \ \nu > \mu, \ 1,2,3,4\}$. All these coordinates transform like scalar functions. More specifically the former two sets transform like the stretchings $\{s_{\nu\sigma}\}$ and thus their symmetry coordinates are given by replacing s in (4.10) with α or β. Among these 24 angle bendings, however, only 20 of them are independent because of redundancy conditions[5]:

$$\sum_{\sigma=1}^{3}(\alpha_{\nu\sigma} + \beta_{\nu\sigma}) = 0, \quad \nu = 1, 2, 3, 4. \tag{4.12}$$

The remaining 6 C–C–C bendings $\{\gamma_{\nu\mu}\}$ belong to the permutation representation $\Delta^{(6)}$ based on $S^{(6)} = \{(r_\nu^0 + r_\mu^0)/2, \ \nu < \mu, \ 1,2,3,4\}$ given by

$$(0, 0, 1), \quad (0, 1, 0), \quad (1, 0, 0), \quad (-1, 0, 0), \quad (0, -1, 0), \quad (0, 0, -1). \tag{4.13}$$

The irreps contained in $\Delta^{(6)}$ are

$$\Delta^{(6)} = \Gamma_1 + \Gamma_3 + \Gamma_5, \tag{4.14}$$

and their symmetry coordinates are, using the correspondence theorem,

$$\Gamma_1; \ \gamma = 6^{-1/2}\sum_{\nu<\mu}\gamma_{\nu\mu} = 0, \tag{4.15a}$$

$$\begin{aligned} &\Gamma_3; \ \gamma_u = (12)^{-1/2}(2\gamma_{12} - \gamma_{13} - \gamma_{14} - \gamma_{23} - \gamma_{24} + 2\gamma_{34}), \\ &\qquad \gamma_v = \tfrac{1}{2}(-\gamma_{13} + \gamma_{14} + \gamma_{23} - \gamma_{24}), \end{aligned} \tag{4.15b}$$

Γ_5; $\gamma_x = 2^{-1/2}(\gamma_{14} - \gamma_{23})$, $\gamma_y = 2^{-1/2}(\gamma_{13} - \gamma_{24})$,

$$\gamma_z = 2^{-1/2}(\gamma_{12} - \gamma_{34}). \tag{4.15c}$$

Note that only five of them are independent since $\gamma = 0$.

3. The hindered rotations of the 4 CH_3 radicals about the respective C–C bond, $\{\tau_\nu\}$

According to the correspondence rules given in III, the hindered rotation transforms like a pseudoscalar $\tilde{x}\tilde{y}\tilde{z} \in \Gamma_2$ of T_d analogous to a torsion. Thus, the set $\{\tau_\nu\}$ belongs to $\Delta^{(4)} \times \Gamma_2$. The irreducible components are

$$\Delta^{(4)} \times \Gamma_2 = \Gamma_2 + \Gamma_4. \tag{4.16}$$

Since Γ_2 is one dimensional their bases are given by, replacing ϕ_ν in (4.8) with τ_ν,

$$\Gamma_2;\quad \tau, \tag{4.17a}$$

$$\Gamma_4;\quad (\tau_{\tilde{x}}, \tau_{\tilde{y}}, \tau_{\tilde{z}}). \tag{4.17b}$$

These four modes will turn into free rotations as the temperature rises.

In the above, we have obtained a total of 45 symmetry coordinates for the molecule $C(CH_3)_4$ under small vibrations; there exist 16 stretchings, 25 bendings, and four hindered rotations. It is noted that the completely symmetrical hindered rotation τ is the only vibrational mode belonging to Γ_2. Summarizing these we have

$$\begin{aligned}
&\Gamma_1;\quad s, t, \alpha, \beta,\\
&\Gamma_2;\quad \tau,\\
&\Gamma_3;\quad (s_u, s_v),\ (\alpha_u, \alpha_v),\ (\beta_u, \beta_v),\ (\gamma_u, \gamma_v),\\
&\Gamma_4;\quad (s_{\tilde{x}}, s_{\tilde{y}}, s_{\tilde{z}}),\ (\alpha_{\tilde{x}}, \alpha_{\tilde{y}}, \alpha_{\tilde{z}}),\ (\beta_{\tilde{x}}, \beta_{\tilde{y}}, \beta_{\tilde{z}}),\\
&\qquad (\tau_{\tilde{x}}, \tau_{\tilde{y}}, \tau_{\tilde{z}}),\\
&\Gamma_5;\quad (s_x, s_y, s_z),\ (t_x, t_y, t_z),\ (\alpha_x, \alpha_y, \alpha_z),\\
&\qquad (\beta_x, \beta_y, \beta_z),\ (\gamma_x, \gamma_y, \gamma_z),\ (s'_x, s'_y, s'_z),\\
&\qquad (\alpha'_x, \alpha'_y, \alpha'_z),\ (\beta'_x, \beta'_y, \beta'_z).
\end{aligned} \tag{4.18}$$

The redundancy conditions for the valence angle bendings are given by (4.12).

V. CONCLUSION

By incorporating the theory of induced representation into the correspondence theory we have formulated a systematic method of constructing the SALC's of equivalent atomic orbitals for a molecule with a doubly equivalent structure. It requires only the knowledge of the elementary basis functions belonging to the irreps of the symmetry group of the molecule. The general expressions of the SALC's are given by (3.7)–(3.9). To show its effectiveness we have applied them to construct the SALC's of 12 equivalent H atoms of $C(CH_3)_4$ molecule in (4.7)–(4.9). This is then applied to construct 45 symmetry coordinates of vibration for the molecule as summarized in (4.18). In principle, the method can easily be extened for a molecule with a triply equivalent structure. The present formalism is particularly effective for the space groups since almost all crystals have doubly equivalent structure. This will be discussed in a forthcoming paper.

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Propagation of electromagnetic plane waves in random media

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In the frame of the spinor formalism of the electromagnetic field, the propagation of a plane wave in a random medium with a view to obtaining the moments of the energy density is considered. Using two different approximations to the solution of the spinor wave equation, it is shown that the energy conservation requires, on the statistics of the refractive index, some extra conditions difficult (eventually impossible) to satisfy. For the variance of the light intensity, a result valid for weakly scattering media is given. It is concluded that "dishonest" methods (in Keller's terminology) have to be used.

I. INTRODUCTION

In a well-known paper, Keller[1] discerns "honest" and "dishonest" methods of solving problems of wave propagation in random media. In an honest method, the solution u is first defined, most often by an approximation process, and then the statistics of u are computed from the explicit expression.

In a dishonest method, randomness is first used and if the moment $\langle u^n \rangle$ of u is sought, where the symbol $\langle\ \rangle$ denotes an ensemble average, the original equations after multiplication by u^{n-1} have to be averaged. Then dishonesty enters through an unproven assumption about some statistical property of the random wave function (for instance, $\langle \eta u \rangle = \langle \eta \rangle \langle u \rangle$, where η is the refractive index) in order to obtain the equation for $\langle u^n \rangle$. This assumption in general makes the problem solvable.

As a consequence, for a problem depending on a parameter, the dishonest solution is applicable for all values of the relevant parameter while the honest solution, obtained through a perturbation method, is valid only for small values. This explains why many important results in the theory of wave propagation in random media have been obtained by dishonest methods. Moreover most of these results agree with experiments.

In this paper, we discuss these problems in the frame of the spinor formalism of the electromagnetic field that we recently developed and that we start with.[2]

In a medium with the refractive index $\eta(\bar{x}) = 1 + \epsilon\nu(\bar{x})$, $|\epsilon| \ll 1$ the stationary spinor equation for the spinor field $\Psi(\bar{x})$ is

$$(i\sigma^j \partial_j + k_0)\Psi(\bar{x}) = -\epsilon k_0 \nu(\bar{x})\Psi(\bar{x}), \quad i = \sqrt{-1}. \tag{1}$$

In this equation $\Psi(\bar{x})$ is a spinor with two complex components $\psi_1(\bar{x})$ and $\psi_2(\bar{x})$, k_0 is the wave number, σ^j are the three Pauli matrices, ∂_j the derivatives with respect to $x_j, j = 1, 2, 3$, and we use the usual summation convention $\sigma^j \partial_j = \sigma_2 \partial_1 + \sigma_2 \partial_2 + \sigma_3 \partial_3$, and $\bar{x}$ denotes a point in $\mathbb{R}^3$.

The connection between the electromagnetic field (E, H), and the spinor field Ψ is given by the relation

$$\sqrt{\epsilon_0} E_j(\bar{x},t) + i\sqrt{\mu} H_j(\bar{x},t) = e^{2ik_0 ct}[\eta/|\Psi(\bar{x})|]\Psi^T(\bar{x})\tau_j\Psi(\bar{x}), \quad j = 1,2,3, \tag{2}$$

where ϵ_0, μ, and η are, respectively, the dielectric constant, the magnetic permability, and the refractive index; Ψ^T is the transpose spinor, and $|\Psi(\bar{x})| = (\Psi^+(\bar{x})\Psi(\bar{x}))^{1/2}$, where $\Psi^+(\bar{x})$ is the Hermitian conjugate spinor. The matrices τ_j are defined by the relations $\tau_j = -i\sigma_2\sigma_j$.

Eq. (1) can be put in an integral form:

$$\Psi(\bar{x}) = \Psi_0(\bar{x}) + \epsilon k_0 \int_V \nu(\bar{x}')\gamma(\bar{x},\bar{x}')\Psi(\bar{x}')d\bar{x}', \tag{3}$$

where $\Psi_0(\bar{x})$ is a solution of the homogeneous equation $(i\sigma^j\partial_j + k_0)\Psi_0(\bar{x}) = 0$, and $\gamma(\bar{x},\bar{x}')$ is the 2×2 Green's matrix[3] satisfying

$$(i\sigma^j \partial_j + k_0)\gamma(\bar{x},\bar{x}') = -\sigma_0 \delta(\bar{x} - \bar{x}'). \tag{4}$$

In this equation, σ_0 is the 2×2 identity matrix and $\delta(\bar{x} - \bar{x}')$ the Dirac distribution. Because of the identity $(i\sigma^j \partial_j + k_0)(-i\sigma^k \partial_k + k_0) = \Delta + k_0^2$, where Δ is the Laplacian operator, one has[3]

$$\gamma(\bar{x}, \bar{x}') = (-i\sigma^j\partial_j + k_0)G(\bar{x},\bar{x}') \tag{5}$$

where $G(\bar{x},\bar{x}')$ is the Green's function of the wave equation

$$(\Delta + k_0^2)G(\bar{x},\bar{x}') = -\delta(\bar{x} - \bar{x}').$$

We then consider the propagation along Oz of a light plane wave so that k_0 is very large which will allow some approximations. When there is no perturbation ($\epsilon = 0$) one has, in agreement with Eqs. (1) and (2),

$$\psi_{1,0}(\bar{x}) = ae^{ik_0 z}, \quad \psi_{2,0}(\bar{x}) = 0, \tag{6}$$

in which a denotes the amplitude of the plane wave, while the zero index corresponds to $\epsilon = 0$.

We further assume that $\nu(\bar{x})$ is a random field and that we look for the moments of the light intensity $I(\bar{x}) = \Psi^T(\bar{x})\Psi(\bar{x})$. So, in the frame of honest methods, we first have to obtain approximate solutions of $\Psi(\bar{x})$ either using Eq. (1) or Eq. (3). We start with this last equation.

II. PARAXIAL APPROXIMATION TO THE SPINOR FIELD

Using the Born method and the zero-order approximation (6), the first term of the perturbation series deduced from Eq. (3) is

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$$\psi_{1,1}(\bar{x}) + a(e^{ik_0 z} + \epsilon k_0 \int_V \nu(\bar{x}')\gamma_{11}(\bar{x},\bar{x}')e^{ik_0 z'}\, d\bar{x}'),$$

$$\psi_{21}(\bar{x}) = a\epsilon k_0 \int_V \nu(\bar{x}')\gamma_{21}(\bar{x},\bar{x}')e^{ik_0 z'}\, d\bar{x}', \tag{7}$$

where γ_{11} and γ_{21} are two elements in the first column of the Green's matrix γ. We are then facing the following two difficulties: (i) the higher terms in the perturbation are unmanageable; and (ii) the approximation (7) is not good enough to obtain the statistical properties of the intensity $I(\bar{x})$. But let us assume that $\gamma_{21}(\bar{x},\bar{x}')$ is negligible, and let us apply the Rayleigh renormalization technique[4] to $\psi_{1,1}(\bar{x})$; then we get from (7)

$$\psi_1(\bar{x}) = ae^{ik_0 z}e^{u(\bar{x})},$$
$$u(\bar{x}) = k_0\epsilon \int_V \nu(\bar{x},\bar{x}')\gamma_{11}(\bar{x},\bar{x}')e^{ik_0(z'-z)}\, d\bar{x}', \tag{8}$$
$$\psi_2(\bar{x}) = 0.$$

Using (4), it is easy to show that (8) is a solution of Eq. (1) so that we have to discuss when $\gamma_{21}(\bar{x},\bar{x}')$ can be neglected. We shall prove that this is possible at the paraxial approximation

$$[(\bar{x}-\bar{x}')^2 + (y-y')^2]/(z-z')^2 \ll 1. \tag{9}$$

In fact the Green's function

$$G(\bar{x},\bar{x}') = (1/4\pi)[e^{i\gamma(\bar{x}-\bar{x}')}/r(\bar{x},\bar{x}')]$$

of the wave equation in free space $[r^2(\bar{x},\bar{x}') = (x-x')^2 + (y-y')^2 + (z-z')^2]$ can be written when Eq. (9) is taken into account:

$$G(\bar{x},\bar{x}') \cong \frac{1}{4\pi}\frac{e^{ik_0(z-z')}}{z-z'}e^{i\theta(\bar{x},\bar{x}')},$$
$$\theta(\bar{x},\bar{x}') = [k_0/2(z-z')][(\bar{x}-\bar{x}')^2 + (y-y')^2]. \tag{10}$$

Therefore, according to (5), we get

$$\gamma_{21}(\bar{x},\bar{x}') = (1/k_0)(\partial_x + i\,\partial_y)G(\bar{x},\bar{x}')$$
$$\cong \frac{1}{4\pi}\frac{(\bar{x}-\bar{x}') + i(y-y')}{(z-z')^2}$$
$$\times \exp\{ik_0(z-z') + i\theta(\bar{x},\bar{x}')\},$$

which gives

$$|\gamma_{21}(\bar{x}-\bar{x}')| \cong \frac{1}{4\pi}\frac{\sqrt{(\bar{x}-\bar{x}')^2 + (y-y')^2}}{(z-z')^2},$$

which is using (9)

$$|\gamma_{21}(\bar{x},\bar{x}')| \leqslant \frac{1}{4\pi(z-z')},$$

so we may neglect γ_{21} in the far field and as long as relation (9) holds true.

Let us now consider γ_{11}; using (5) and (10), we obtain

$$\gamma_{11}(\bar{x},\bar{x}') \cong 2k_0\left(1 + \frac{i}{2k_0(z-z')} - \frac{\theta(\bar{x},\bar{x}')}{2k_0(z-z')}\right)G(\bar{x},\bar{x}').$$

Using (9), the last term on the right-hand side of the previous equation may be neglected and one has

$$\gamma_{11}(\bar{x},\bar{x}') = 2k_0(1 + [i/2k_0(z-z')])G(\bar{x},\bar{x}'). \tag{11}$$

This result together with (8) completes the determination of $\hat{\psi}_1(\bar{x})$.

Using (8) the light intensity becomes

$$I(\bar{x}) = a^2 e^{2v(\bar{x})}, \quad v(\bar{x}) = \tfrac{1}{2}(u(\bar{x}) + u^*(\bar{x})), \tag{12}$$

where the asterisk denotes the complex conjugation.

Remark: The wave equation

$$(\Delta + k_0^2)\varphi(\bar{x}) = -2k_0^2\epsilon\nu(\bar{x})\varphi(\bar{x})$$

is generally used to discuss the electromagnetic wave propagation in random media together with Rytov's perturbation method.[4] One gets for a plane wave[5]

$$I(\bar{x}) = a^2 e^{\epsilon v_1(\bar{x})}, \quad v_1(\bar{x}) = \tfrac{1}{2}(u_1(\bar{x}) + u_1^*(\bar{x})), \tag{13}$$

with

$$u_1(\bar{x}) = 2\epsilon k_0^2 \int_V \nu(\bar{x},\bar{x}')G(\bar{x},\bar{x}')e^{ik_0(z'-z)}\, d\bar{x}', \tag{13'}$$

so that according to (11) the expressions (8) and (13) are similar except for the existence of the term $[i/2k_0(z-z')]G(\bar{x},\bar{x}')$ (negligible in the far field) in (8). The slight difference is not surprising since Eq. (1) is exact while the wave equation assumes that the term $-2\nabla(\nabla\eta/\eta)\cdot E$), where ∇ is the nabla symbol and E the electromagnetic field, is dropped.

We may now discuss the statistics of the light intensity $I(\bar{x})$. Using (12), we get for the mean intensity

$$\langle I(\bar{x})\rangle = a^2\langle\exp(2v(\bar{x}))\rangle,$$

and using a well known result,[6] we get

$$\langle I(\bar{x})\rangle = a^2 \exp\left\{\sum_{k=1}^{\infty}\frac{\chi_k/2v)}{k!}\right\}, \tag{14}$$

where $\chi_k(2v)$ denotes the k th cumulant of the random field $2v(\bar{x})$. But because energy must be conserved and refractive index variations do not dissipate optical energy in the propagation of an infinite plane wave, we must have

$$\sum_1^{\infty}\frac{1}{k!}\chi_k(2v) = 0. \tag{15}$$

We conjecture that this relation is only possible [provided that $v(\bar{x})$ has a genuine continuous probability distribution (see Appendix E)] if $\chi_k(2v) = 0$, for $k > k_0$. (In Appendix A, we give some reasons to support this conjecture.) But using a theorem from Marcinkiewicz,[6] one can then show that all the cumulants are zero for $k > 2$, so that the random field $2v(\bar{x})$ has a Gaussian distribution. As a consequence, Eq. (15) reduces to

$$\chi_1(2v) + \tfrac{1}{2}\chi_2(2v) = 0,$$

that is, from the definition[6] of cumulants,

$$\langle v(\bar{x})\rangle + \langle v^2(\bar{x})\rangle - (\langle v(\bar{x})\rangle)^2 = 0. \tag{16}$$

To sum up, if the previous conjecture is true, the random field $2v(\bar{x})$ has a Gaussian distribution whose mean and variance are bound by the relation (16). Of course, had we used (13) instead of (12), we should have still obtained the relation (16) with $v_1(\bar{x})$ instead of $v(\bar{x})$.

Let us now discuss the consequences of (16). From (8), (10), and (11), we get

$$u(\bar{x}) = \frac{2k_0^2\epsilon}{4\pi}\int_V \nu(\bar{x}')\left(1 + \frac{i}{2k_0(z-z')}\right)\exp(i\theta(\bar{x},\bar{x}'))\, dx'\, dy'.$$

For a source in the plane $z' = 0$ and the volume V in the half space $z' > 0$, asuming the back scattering negligible, the integral over the region V in the last expression can be replaced by an integral on the part of ν which lies inside the plane layer $0 \leqslant z' \leqslant z$

$$\int_\nu d\bar{x}' = \int_0^z dz' \int\int_{-\infty}^{+\infty} dx'\, dy',$$

so, using (12) together with the last two relations, we get

$$v(\bar{x}) = \frac{k_0^2}{2\pi} \int_0^z \frac{dz'}{(z-z')} \int\int_{-\infty}^{+\infty} \nu(\bar{x}') \times \left(\cos\theta(\bar{x},\bar{x}') - \frac{\sin\theta(\bar{x},\bar{x}')}{2k_0(z-z')}\right) dx'\, dy',$$

which gives

$$\langle v(\bar{x})\rangle = \frac{k_0^2}{2\pi} \int_0^z \frac{dz'}{(z-z')} \int\int_{-\infty}^{+\infty} \langle \nu(\bar{x}')\rangle \times \left(\cos\theta(\bar{x},\bar{x}') - \frac{\sin\theta(\bar{x},\bar{x}')}{2k_0(z-z')}\right) dx'\, dy'. \tag{17}$$

With (13'), one obtains similarly

$$\langle v_1(\bar{x})\rangle = \frac{k_0^2}{2\pi} \int_0^z \frac{dz'}{(z-z')} \int\int_{-\infty}^{+\infty} \langle \nu(\bar{x}')\rangle \cos\theta(\bar{x},\bar{x}') dx'\, dy'. \tag{17'}$$

Of course $\langle \nu(\bar{x})\rangle$ is constant in the transverse planes $z = \text{const}$, but we may assume that this constant depends on z so that we get

$$\langle \nu(\bar{x})\rangle = \nu f(z). \tag{18}$$

Then in Appendix B, using (17), (17'), and (18), we prove the following results:

$$\langle v(\bar{x})\rangle = \frac{\nu}{2} \int_0^z \frac{f(z')dz'}{z-z'}, \quad \langle v_1(\bar{x})\rangle = 0. \tag{19}$$

Of course $\langle v_1(\bar{x})\rangle = 0$ is nonsense, since with (16) it implies that $I(\bar{x})$ has no fluctuation, but the result on $\langle v(\bar{x})\rangle$ is no more satisfactory. On one hand $\langle v(\bar{x})\rangle$ has a logarithmic singularity, and on the other hand, Eq. (16) leads to a functional relation for the correlation function $B(\bar{x},\bar{x}') = \langle \nu(\bar{x})\nu(\bar{x}')\rangle$ with no simple solution.

To sum up, the honest methods leading to expressions of $I(\bar{x})$ such as (12) or (13) fail to supply the statistics of the light intensity. Using (13) and assuming that $v_1(\bar{x})$ is a Gaussian random field, many authors[7,8] obtained the relation (16) but failed to note (19) (a noticeable exception is Ref. 9). The remedies proposed to cure these difficulties are not always very convincing.[7,9,10]

III. THE BORN APPROXIMATION TO THE SPINOR FIELD

With

$$\sigma_1 = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \quad \sigma_2 = \begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix}, \quad \sigma_3 = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix},$$

as a representation of the Pauli matrices, we get from Eq. (1)

$$\begin{aligned} &(i\,\partial_z + k_0)\psi_1(\bar{x}) + i(\partial_x - i\,\partial_y)\psi_2(\bar{x}) = k_0\epsilon\nu\psi_1(\bar{x}), \\ &i(\partial_x + i\,\partial_y)\psi_1(\bar{x}) - (i\,\partial_z - k_0)\psi_2(\bar{x}) = -k_0\epsilon\nu\psi_2(\bar{x}), \end{aligned} \tag{20}$$

and we look for solutions of (20) in the form

$$\begin{aligned} \psi_1(\bar{x}) &= ae^{ik_0z}(1 + \epsilon u_1(\bar{x}) + \epsilon^2 u_2(\bar{x}) + O(\epsilon^3)), \\ \psi_2(\bar{x}) &= ae^{ik_0z}(\epsilon v_1(\bar{x}) + \epsilon^2 v_2(\bar{x}) + O(\epsilon^3)), \end{aligned} \tag{21}$$

which for $\epsilon = 0$ reduces to the plane wave (6). (We hope that no confusion is possible with the functions u, v, of the previous section.)

From (21) we get

$$\begin{aligned} |\psi_1|^2 &= a^2\{1 + \epsilon(u_1 + u_1^*) + \epsilon^2(u_2 + u_2' + u_1u_1^*) + O(\epsilon^3)\}, \\ |\psi_2|^2 &= a^2(\epsilon^2 v_1 v_1^* + O(\epsilon^3)), \end{aligned}$$

which gives

$$I(\bar{x}) = a^2\{1 + \epsilon(u_1(\bar{x}) + u_1^*(\bar{x})) + \epsilon^2(u_2(\bar{x}) + u_2^*(\bar{x}) + u_1(\bar{x})u_1^*(\bar{x}) + v_1(\bar{x})v_1^*(\bar{x})) + O(\epsilon^3)\}. \tag{22}$$

The energy conservation implies

$$\langle I(\bar{x})\rangle = a^2, \tag{23a}$$

$$\langle u_1(\bar{x}) + u_1^*(\bar{x})\rangle = 0, \tag{23b}$$

$$\langle u_2(\bar{x}) + u_2^*(\bar{x}) + u_1(\bar{x})u_1^*(\bar{x}) + v_1(\bar{x})v_1^*(\bar{x})\rangle = 0. \tag{23c}$$

Now according to (22), one has

$$I^2(\bar{x}) = a^4\{1 + 2\epsilon(u_1(\bar{x}) + u_1^*(\bar{x})) + 2\epsilon^2(u_2(\bar{x}) + u_2^*(\bar{x}) + u_1(\bar{x})u_1^*(\bar{x}) + v_1(\bar{x})v_1^*(\bar{x})) + \epsilon^2(u_1(\bar{x}) + u_1^*(\bar{x}))^2 + O(\epsilon^3)\},$$

and using (23) we get

$$\langle I^2(\bar{x})\rangle = a^4(1 + \epsilon^2\langle(u_1(\bar{x}) + u_1^*(\bar{x}))^2\rangle + O(\epsilon^3)), \tag{24}$$

so that the variance of the light intensity is

$$\sigma_I^2 = a^4\{\epsilon^2\langle(u_1(\bar{x}) + u_1^*(\bar{x}))^2\rangle + O(\epsilon^3)\}. \tag{24'}$$

This is a rather simple result but we still have to obtain $u_1(\bar{x})$ and check whether the conditions (23b), and (23c) hold true.

Substituting (21) into (20) leads to the following equations:

$$\frac{\partial u_1(\bar{x})}{\partial z} + (\partial_x - i\,\partial_y)v_1(\bar{x}) = ik_0\nu(\bar{x}), \tag{25a}$$

$$(\partial_x + i\,\partial_y)u_1(\bar{x}) - 2ik_0v_1(\bar{x}) - \frac{\partial v_1(\bar{x})}{\partial z} = 0,$$

$$\frac{\partial u_2(\bar{x})}{\partial z} + (\partial_x - i\,\partial_y)v_2(\bar{x}) = ik_0\nu(\bar{x})u_1(\bar{x}), \tag{25b}$$

$$(\partial_x + i\,\partial_y)u_2(\bar{x}) - 2ik_0v_2(\bar{x}) - \frac{\partial v_2(\bar{x})}{\partial z} = k_0\nu(\bar{x})v_1(\bar{x}).$$

Assuming $\partial_z v_1$, and $\partial_z v_2$ negligible with respect to k_0v_1, and k_0v_2, the previous systems become, after elimination of v_1 and v_2 in the first equations

$$2ik_0\,\partial_z u_1(\bar{x}) + \Delta_\perp(\bar{x}) = -2k_0^2\nu(\bar{x}), \tag{26a}$$

$$\begin{aligned} v_1(\bar{x}) &= (-i/2k_0)(\partial_x + i\,\partial_y)u_1(\bar{x}), \\ 2ik_0\,\partial_z u_2(\bar{x}) + \Delta_\perp u_2(\bar{x}) &= k_0(\partial_x - i\partial_y)\nu(\bar{x})v_1(\bar{x}) - 2k_0^2\nu(\bar{x})u_1(\bar{x}), \end{aligned} \tag{26b}$$

$$v_2(\bar{x}) = (-i/2k_0)(\partial_x + i\,\partial_y)u_2(\bar{x}) + (i/2)\nu(\bar{x})v_1(\bar{x}),$$

where $\Delta_\perp$ denotes the transverse Laplacian $\partial^2/\partial x^2 + \partial^2/\partial y^2$.

Since k_0 is very large, we make the further assumption that $v_1(\bar{x})$ and $v_2(\bar{x})$ are negligible, respectively, with respect to $u_1(\bar{x})$ and $u_2(\bar{x})$, so we get from (26a) [we have no need of the second equation (26b)]

$$\begin{aligned} 2ik_0\,\partial_z u_1(\bar{x}) + \Delta_\perp u_1(\bar{x}) &= -2k_0^2 v(\bar{x}), \\ 2ik_0\,\partial_z u_2(\bar{x}) + \Delta_\perp u_2(\bar{x}) &= -2k_0^2 v(\bar{x}) u_1(\bar{x}). \end{aligned} \tag{27}$$

But the Green's function $G_1(\bar{x},\bar{x}')$ of the equation $2ik_0\,\partial_z u(\bar{x}) + \Delta_\perp u(\bar{x}) = -\delta(\bar{x}-\bar{x}')$ is

$$G_1(\bar{x},\bar{x}') = [1/4\pi(z-z')]\exp(i\theta(\bar{x},\bar{x}')),$$

with $\theta(\bar{x},\bar{x}')$ given in (10). So, we obtain at once

$$u_1(\bar{x}) = \frac{k_0^2}{2\pi}\int_0^z \frac{dz'}{z-z'} \int\int_{-\infty}^{+\infty} dx'\,dy'\, v(\bar{x}') e^{i\theta(\bar{x},\bar{x}')}, \tag{28a}$$

$$u_2(\bar{x}) = \frac{k_0^2}{2\pi}\int_0^z \frac{dz'}{z-z'} \int\int_{-\infty}^{+\infty} dx'\,dy'\, v(\bar{x}') u_1(\bar{x}') e^{i\theta(\bar{x},\bar{x}')}. \tag{28b}$$

We now have to discuss (23b) and (23c). It is clear from (28a) that if $\langle v(\bar{x})\rangle = 0$ then the condition (23b) holds true. Now, since v_1 is negligible, the condition (23c) becomes

$$\langle u_2(\bar{x}) + u_2^*(\bar{x}) + u_1^*(\bar{x}) u_1(\bar{x})\rangle = 0. \tag{29}$$

But according to (28) we get

$$\begin{aligned} &u_1(\bar{x}) u_1^*(\bar{x}) \\ &\quad = \frac{k_0^4}{4\pi^2}\int_0^z\int_0^z \frac{dz'\,dz''}{(z-z')(z-z'')} \int\int_{-\infty}^{+\infty}\int\int_{-\infty}^{+\infty} dx'\,dx''\,dy'\,dy'' \\ &\qquad \times v(\bar{x}') v(\bar{x}'') e^{(\theta(\bar{x},\bar{x}') - \theta(\bar{x},\bar{x}''))}, \\ &u_2(\bar{x}) \\ &\quad = \frac{k_0^4}{4\pi^2}\int_0^z\int_0^{z'} \frac{dz'\,dz''}{(z-z')(z'-z'')} \int\int_{-\infty}^{+\infty}\int\int_{-\infty}^{+\infty} dx'\,dx''\,dy'\,dy'' \\ &\qquad \times v(\bar{x}') v(\bar{x}'') e^{i(\theta(\bar{x},\bar{x}') + \theta(\bar{x}',\bar{x}''))}, \end{aligned}$$

which gives

$$\begin{aligned} &\langle u_1(\bar{x}) u_1^*(\bar{x})\rangle \\ &\quad = \frac{k_0^4}{4\pi^2}\int_0^z\int_0^z \frac{dz'\,dz''}{(z-z')(z-z'')} \int\int_{-\infty}^{+\infty}\int\int_{-\infty}^{+\infty} dx'\,dx''\,dy'\,dy'' \\ &\qquad \times B(\bar{x}',\bar{x}'') e^{i(\theta(\bar{x},\bar{x}') - \theta(\bar{x}',\bar{x}''))}, \end{aligned} \tag{30a}$$

$$\begin{aligned} &\langle u_2(\bar{x})\rangle \\ &\quad = \frac{k_0^4}{4\pi^2}\int_0^z\int_0^{z'} \frac{dz'\,dz''}{(z-z')(z'-z'')} \int\int_{-\infty}^{+\infty}\int\int_{-\infty}^{+\infty} dx'\,dx''\,dy'\,dy'' \\ &\qquad \times B(\bar{x}',\bar{x}'') e^{i(\theta(\bar{x},\bar{x}') + \theta(\bar{x}',\bar{x}''))}, \end{aligned} \tag{30b}$$

where $B(\bar{x},\bar{x}')$ is the correlation function

$$B(\bar{x}',\bar{x}'') = \langle u(\bar{x}') u(\bar{x}'')\rangle.$$

Let us assume that $B(\bar{x}',\bar{x}'')$ is the Gaussian function

$$\begin{aligned} B(\bar{x}',\bar{x}'') &= \frac{l_0}{2\sqrt{\pi}}\langle v^2\rangle \delta(z'-z'') \\ &\quad \times \exp\left\{ -\frac{(\bar{x}'-\bar{x}'')^2 + (y'-y'')^2}{l_0^2}\right\}, \end{aligned} \tag{31}$$

where l_0 is the transverse correlation length, $\delta(z)$ the Dirac distribution, and $\langle v^2\rangle$ the variance of the index of refraction fluctuations; then in Appendix C we prove the following relations in agreement with (29):

$$\langle u_1(\bar{x}) u_1^*(\bar{x})\rangle = -\langle u_2(\bar{x}) + u_2^*(\bar{x})\rangle = k_0^2 l_0 \langle v^2\rangle z/2\sqrt{\pi}.$$

We may now compute σ_I^2. Using (24'), (28a), (28b), and (31), one obtains in Appendix D

$$\frac{\sigma_I^2}{\langle I\rangle^2} = 2\beta z\left(1 - \frac{\arctan Z}{Z}\right), \quad Z = \frac{z}{z_f}, \quad z_f = \frac{k_0 l_0^2}{4}, \tag{32}$$

with

$$\beta = \epsilon^2\langle v^2\rangle\, k_0^2\, l_0/2\sqrt{\pi}. \tag{32'}$$

This result, valid for a weakly scattering medium ($\beta z \ll 1$), was previously obtained by Uscinski[11] using a "dishonest" method. This agreement can be considered as an *a posteriori* justification of this method.

Let us note that for the coherent intensity $\langle \psi_1\rangle\langle \psi_1^*\rangle$, one obtains according to (32') and (C8)

$$\begin{aligned} \langle \psi_1\rangle\langle \psi_1^*\rangle &= a^2\{1 + \epsilon^2\langle u_2(\bar{x}) + u_2^*(\bar{x})\rangle + O(\epsilon^3)\} \\ &= a^2\{1 - \beta z + O(\epsilon^3)\}, \end{aligned}$$

which is an approximation valid for $\beta z \ll 1$ of the exact value $e^{-\beta z}$.

IV. CONCLUSIONS

Let us start with a discussion of Eqs. (27) which could also have been obtained from the so-called parabolic approximation of the wave equation (see Ref. 5, for instance). Two kinds of assumptions are needed to deduce (27) from (26).

(i) First, $v_1(\bar{x})$ and $v_2(\bar{x})$ should be slowly varying functions so that one has

$$|\partial_z v_1(\bar{x})| \ll |k_0 v_1(\bar{x})|, \quad |\partial_z v_2(\bar{x})| \ll |k_0 v_2(\bar{x})|.$$

Some similar assumptions are necessary to obtain the parabolic equation whose validity is discussed in Ref. 12.

(ii) Second, $u_1(\bar{x})$ should be a slowly varying function of x,y to have

$$|v_1(\bar{x})| \ll \frac{1}{2k_0}\,|(\partial_x + i\partial y) u_1(\bar{x})|.$$

From Eq. (2) one easily sees that the electromagnetic waves corresponding to the spinor field are circularly polarized transverse waves. Since, for $z = 0$, one has $\psi_2 = 0$, neglecting $v_1(\bar{x})$ with respect to $u_1(\bar{x})$ is equivalent to assuming that polarization does not change along propagation.

If we now assume that all the conditions are fulfilled to make Eqs. (27) valid, we still have to ask why the "honest" methods fail to describe electromagnetic wave propagation in random media. First, at least for plane waves, we get into trouble since the energy conservation is not satisfied for each term of the perturbation series so that we have to impose on the random field some drastic conditions that are difficult and even impossible to satisfy. Second, the convergence of

the perturbation series to the exact solution of the wave equation does not guarantee the uniform convergence of the averaged series to the mean value of the solution. Moreover only the first two or three terms in the series can be computed.

These reasons explain why one has to look at "dishonest" methods, which, leaving aside some unproven statistical assumptions, have two important advantages: (i) the energy conservation is automatically fulfilled; and (ii) if one needs, for instance, only the first two moments of the light intensity $I(\bar{x})$ (the determination of the probability distribution is a rather difficult problem[13]), then we just have to solve the equations corresponding to these moments, a nontrivial task, but not as difficult as looking for solutions of equations like Eq. (1).

We discussed elsewhere[14] "dishonest" methods in the frame of the spinor formalism of the electromagnetic field.

The "dishonest" methods were thoroughly discussed by Van Kampen[15] in an outstanding paper. Let us transpose his discussion in spinor terms for wave propagation with random refractive index.

We start with the integral equation (3). To first order in the Born approximation $\Psi(\bar{x}')$ is replaced under the integral by $\Psi_0(\bar{x}')$,

$$\Psi(\bar{x}) = \Psi_0(\bar{x}) + \epsilon k_0 \int \nu(\bar{x}')\gamma(\bar{x},\bar{x}')\Psi_0(\bar{x}')d\bar{x}',$$

which gives $\langle\Psi(\bar{x})\rangle = \Psi_0(\bar{x})$ and

$$\langle|\Psi(\bar{x})|^2\rangle = |\Psi_0(\bar{x})|^2 + \epsilon^2 k_0^2 \iint \gamma^+(\bar{x},\bar{x}'')\gamma(\bar{x},\bar{x}') \times \langle\nu(\bar{x}')\nu(\bar{x}'')\rangle\, \Psi_0^+(\bar{x}')\Psi_0(\bar{x}'')d\bar{x}'\, dx'',$$

and we have proven here that these formulas lead to unsatisfactory results. Let us now iterate Eq. (3):

$$\Psi(\bar{x}) = \Psi_0(\bar{x}) + \epsilon k_0 \int \gamma(\bar{x},\bar{x}')\nu(\bar{x}')\Psi_0(\bar{x}')d\bar{x}' + \epsilon^2 k_0^2 \int \gamma(\bar{x},\bar{x}')\nu(\bar{x}')d\bar{x}' \int \gamma(\bar{x}',\bar{x}'')\nu(\bar{x}'')\Psi(\bar{x}'')d\bar{x}''.$$

Replacing $\Psi(\bar{x}'')$ in the last integral with $\langle\Psi(\bar{x}'')\rangle$, rather than $\Psi_0(\bar{x}'')$, we get

$$\langle\Psi(\bar{x})\rangle = \Psi_0(\bar{x}) + \epsilon^2 k_0^2 \int \gamma(\bar{x},\bar{x}')d\bar{x}' \times \int \gamma(\bar{x}',\bar{x}'')\langle\nu(\bar{x}')\nu(\bar{x}'')\rangle\langle\Psi(\bar{x}'')\rangle d\bar{x}''.$$

Applying the differential operator $i\sigma^j\partial_j + k_0$ and using (4) we get

$$(i\sigma^j\partial_j + k_0)\langle\Psi(\bar{x})\rangle = -\epsilon^2 k_0^2 \int \gamma(\bar{x},\bar{x}')\langle\nu(\bar{x}')\nu(\bar{x}'')\rangle\langle\Psi(\bar{x}')\rangle d\bar{x}', \tag{33}$$

which we may call Bourret's spinor integral equation for the average.

The longitudinal correction length l_c plays here the part of the correlation time τ_c in Van Kampen, so we may translate his result. On a course-gained level determined by Δz (we assume propagation along Oz) such that $\epsilon k_0 \Delta z \ll 1$ and $\Delta z \gg l_c$ the process is approximately Markovian, and in (33) the terms of order $(\epsilon k_0 l_c)^3$ are neglected. Thus as long as $\epsilon k_0 l_c \ll 1$ one obtains satisfactory results with "dishonest" methods.

APPENDIX A: HINT FOR CONJECTURE (15)

When the moment-generating function $\varphi(t)$ exists,[16] one has

$$\varphi(t) = \exp\left\{\sum_1^\infty (-1)^k \chi_k \frac{t^k}{k!}\right\},$$

so that Eq. (15) is equivalent to $\varphi(-1) = 1$. But for $t > 0$, $\varphi(t)$ possesses derivatives $\varphi^{(n)}$ of all orders[16] and $(-1)^n \varphi^{(n)}(t) > 0$. In particular $\varphi'(t)$ has a constant sign for $t > 0$. If $\varphi'(t)$ also has a constant sign for $-1 \leqslant t \leqslant 0$, then the conjecture is proved since one has $\varphi(0) = 1$, because in this case, Eq. (15) is only possible if there exists a relation between cumulants which requires that the series (15) reduce to a polynomial.

In fact all the checks we made with known generating functions showed that $\varphi(t)$ is an increasing function for $t < 0$.

APPENDIX B: PROOF OF EQ. (19)

From (17) and (18), we get

$$\langle v(\bar{x})\rangle = \frac{k_0^2}{2\pi}\langle\nu\rangle \int_0^3 \frac{f(z')dz'}{z-z'} \times \iint_{-\infty}^{+\infty} \left(\cos\theta(\bar{x},\bar{x}') - \frac{\sin\theta(\bar{x},\bar{x}')}{2k_0(z-z')}\right) dx'\, dy'. \tag{B1}$$

Using the Fresnel integrals $c(x)$ and $s(x)$ and their limit values $c(\infty) = s(\infty) = \frac{1}{2}$,

$$\int_{-\infty}^{+\infty} \cos\left(\frac{k_0(x-x')^2}{2(z-z')}\right)dx' = \int_{-\infty}^{+\infty} \sin\left(k_0\frac{(x-x')^2}{2(z-z')}\right)dx' = \sqrt{\frac{\pi(z-z')}{k_0}}. \tag{B2}$$

From the definition (10) of $\theta(\bar{x},\bar{x}')$, and using the relation

$$\cos\theta(\bar{x},\bar{x}') = \cos\left(\frac{k_0(x-x')^2}{2(z-z')}\right)\cos\left(\frac{k_0(y-y')^2}{2(z-z')}\right) - \sin\left(\frac{k_0(x-x')^2}{2(z-z')}\right)\sin\left(\frac{k_0(y-y')^2}{2(z-z')}\right)$$

and the similar relation for $\sin\theta(\bar{x},\bar{x}')$, we deduce at once from (B2)

$$\iint_{-\infty}^{+\infty} \cos\theta(\bar{x},\bar{x}')dx'\, dy' = 0, \qquad \iint_{-\infty}^{+\infty} \sin\theta(\bar{x},\bar{x}')dx'\, dy' = \frac{2\pi}{k_0}(z-z'), \tag{B3}$$

which leads to the relations (19) in the main text.

APPENDIX C: PROOF OF EQ. (29)

From (30a) and (31) and after integration on z'' we get

$$\langle u_1(\bar{x})\, u_1^*(\bar{x})\rangle = \frac{k_0^4}{4\pi^2} l_0 \frac{\langle\nu^2\rangle}{2\sqrt{\pi}} \int_0^z \frac{dz'}{(z-z')^2} I_1(z,z')I_2(z,z') \tag{C1}$$

with

$$I_1(z,z') = \iint_{-\infty}^{+\infty} dx'\,dx'' \exp\left\{ -\frac{(x'-x'')^2}{l_0^2} + \frac{ik_0(x-x')^2}{2(z-z')} - \frac{ik_0(x-x'')^2}{2(z-z')} \right\}, \quad \text{(C2)}$$

and $I_2(z,z')$ is the same expression with y's instead of x's.

With $u = x - x'$, $v = x - x''$, and p^2, q^2 such that

$$\frac{1}{p^2} = \frac{1}{l_0^2}\left(1 - \frac{ik_0 l_0^2}{2(z-z')}\right), \quad \frac{1}{q^2} = \frac{1}{p^{*2}} - \frac{p^2}{l_0^4}, \quad \text{(C3)}$$

$I_1(z,z')$ becomes

$$I_1(z,z') = \int_{-\infty}^{+\infty} dv\, e^{-v^2/p^{*2}} \int_{-\infty}^{+\infty} du \exp\left(-\frac{u^2}{p^2} + \frac{2uv}{l_0}\right)$$

$$= \sqrt{\pi}\, p \int_{-\infty}^{+\infty} e^{-v^2/q^2}\, dv$$

$$= \pi\, p\, q,$$

and since $I_1(z,z') = I_2(z,z')$, we get

$$I_1(z,z')I_2(z,z') = \pi^2 p^2 q^2 = (4\pi^2/k_0^2)(z-z')^2. \quad \text{(C4)}$$

Substituting (C4) into (C1) gives

$$\langle u_1(\bar{x})\, u_1^*(\bar{x})\rangle = k_0^2\, l_0 \langle \nu^2\rangle (3/2\sqrt{\pi}). \quad \text{(C5)}$$

In the same way, from (30b) and (31), we get

$$\langle u_2(\bar{x})\rangle = \frac{k_0^4}{4\pi^2}\frac{l_0}{2\sqrt{\pi}}\langle \nu^2\rangle \int_0^z \frac{dz'}{z-z'} \iint_{-\infty}^{+\infty} dx'\,dy'$$

$$\times \exp\left\{ik_0 \frac{(x-x')^2 + (y-y')^2}{2(z-z')}\right\} F(\bar{x}'), \quad \text{(C6)}$$

with

$$F(\bar{x}') = \int_0^{z'} \frac{dz'\,\delta(z'-z'')}{z'-z''}\left(\int_{-\infty}^{+\infty} du\, e^{-u^2/p_1^2}\right)^2, \quad \text{(C7)}$$

where $u = x' - x''$, $(1/p_1^2) = (1/l_0^2)(1 - ik_0 l_0^2/2(z'-z''))$, and where we used the fact that both integrals on x'' and y'' are equal. So, taking into account the relation

$$\int_a^b f(\xi)\delta(\xi - x)d\xi = \frac{1}{2}f(x-0), \quad \text{for } x = b,$$

we get

$$F(\bar{x}') = \pi \int_0^{z'} p_1^2 \frac{\delta(z'-z'')}{z'-z''}\, dz'' = \frac{i\pi}{k_0}.$$

With this last result, (C6) becomes

$$\langle u_2(\bar{x})\rangle = \frac{ik_0^3}{4\pi}\frac{l_c}{2\sqrt{\pi}}\langle \nu^2\rangle \int_0^z \frac{dz'}{z-z'} \iint_{-\infty}^{+\infty} dx'\,dy'$$

$$\times \exp\left(ik_0[(x-x')^2 + (y-y')^2]/2(z-z')\right).$$

Still using the Fresnel integrals, we get

$$\iint_{-\infty}^{+\infty} dx'\,dy' \exp\left(ik_0 \frac{(x-x')^2 + (y-y')^2}{2(z-z')}\right) = 2i\pi \frac{(z-z')}{k_0},$$

and finally

$$\langle u_2(\bar{x})\rangle = -(k_0^2\, l_0 z/2)(\langle \nu^2\rangle/2\sqrt{\pi}),$$

which gives

$$\langle u_2(\bar{x}) + u_2^*(\bar{x})\rangle = -(k_0^2\, l_0 z\langle \nu^2\rangle/2\sqrt{\pi}). \quad \text{(C8)}$$

APPENDIX D: COMPUTATION OF σ_I^2

According to (28a) and (31) and after integration on z'', we get

$$\langle u_1^2(\bar{x})\rangle = \frac{k_0^4}{4\pi^2}\frac{l_0\langle \nu^2\rangle}{2\sqrt{\pi}} \int_o^z \frac{dz'}{(z-z')^2}\, \mathcal{J}_1(z,z')\mathcal{J}_2(z,z'), \quad \text{(D1)}$$

where

$$\mathcal{J}_1(z,z') = \iint_{-\infty}^{+\infty} dx'\,dx'' \exp\left\{ -\frac{(x'-x'')^2}{l_0^2} + \frac{ik_0(x-x')^2}{2(z-z')} + ik_0\frac{(x-x'')^2}{2(z-z'')}\right\}, \quad \text{(D2)}$$

and $\mathcal{J}_2(z,z')$ is the same expression with y's instead of x's. With the expression (C3) of p^2 and with

$$1/r^2 = p^2(1/(p^2)^2 - 1/l_0^4), \quad \text{(D3)}$$

a computation similar to the computation made in Appendix B gives

$$\langle u_1^2(\bar{x})\rangle = \frac{k_0^4\, l_0}{4}\frac{\langle \nu^2\rangle}{2\sqrt{\pi}} \int_0^z \frac{p^2 r^2\, dz'}{(z-z')^2}. \quad \text{(D4)}$$

Now, according to (C3) and (D3), one has

$$p^2 r^2 = -\frac{4\, l_0^2\,(z-z')^2}{k_0(k_0\, l_0^2 + 4i(z-z'))},$$

which gives

$$p^2 r^2 + (p^2 r^2)^* = -\frac{8(z-z')^2}{k_0^2}\frac{1}{1 + 16(z-z')^2/k_0^2\, l_0^4},$$

and, using (D4)

$$\langle u_1^2(\bar{x}) + u_1^{*2}(\bar{x})\rangle = -\frac{k_0^2\, l_0}{\sqrt{\pi}}\langle \nu^2\rangle \int_o^z \frac{dz'}{1 + 16(z-z')^2/k_0^2\, l_0^4}$$

$$= -\frac{k_0^3\, l_0^3}{4\sqrt{\pi}}\langle \nu^2\rangle \arctan\frac{4z}{k_0 l_0^2}. \quad \text{(D5)}$$

From (C5) and (D5), we get

$$\langle (u_1(\bar{x}) + u_1^*(\bar{x}))^2\rangle = \langle \nu^2\rangle \frac{k_0^2\, l_0 z}{\sqrt{\pi}}\left(1 - \frac{\arctan(4z/k_0 l_0^2)}{4z/k_0 l_0^2}\right). \quad \text{(D6)}$$

APPENDIX E: COMMENT ON CONJECTURE (15)

The conjecture (15) is equivalent to assuming the existence of a random variable X with a genuine continuous probability density $f(x)$ such that $\langle e^x\rangle = 1$. By genuine, we mean that one discards any random variable $y = x - l_0 g\langle e^x\rangle$. Moreover when $f(x)$ is not a continuous function the conjecture need not be valid. For instance, let us consider $f(x) = \Sigma\, a_i \delta(x - x_i)$ with $\Sigma a_i = 1$ and $\Sigma a_i e^{xi} = 1$; then one has $\langle e^x\rangle = 1$.

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Relation between the connected diagram and smoothing methods for rough surface scattering

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In previous work by the author on connected diagram expansion methods for the problem of scattering from a random rough surface a stochastic Lippmann–Schwinger integral equation in Fourier transform space for the scattered part of the Green's function was derived. Averaging techniques using homogeneous statistics and a statistical cluster decomposition on the surface interaction function yielded a connected diagram expansion for the coherent and incoherent Green's functions. Here it is demonstrated that the smoothing method applied to this stochastic integral equation yields a result that agrees with the connected diagram expansion only to second order in the surface interaction. For third- and higher-order interactions, the smoothing method does not yield connected terms.

I. INTRODUCTION

In previous work,[1] summarized in Ref. 2, we derived a stochastic Lippmann–Schwinger integral equation in Fourier transform space for Γ, the scattered part of the Green's function describing scattering from a random rough surface $z = h(x_t)$, where $x_t = (x,y)$. The equation is in three-dimensional Fourier transform space off the energy shell. For a perfectly reflecting acoustically hard (Neumann boundary condition) surface it is given by

$$\Gamma(\mathbf{k}',\mathbf{k}'') = V(\mathbf{k}',\mathbf{k}'')\,A(\mathbf{k}'-\mathbf{k}'') + \int V(\mathbf{k}',\mathbf{k})\,A(\mathbf{k}'-\mathbf{k})G^0(k)\Gamma(\mathbf{k},\mathbf{k}'')\,d\mathbf{k}, \tag{1.1}$$

where V is called the vertex function (and is kinematic),

$$V(\mathbf{k}',\mathbf{k}) = \frac{-2i}{(2\pi)^3}\left[\frac{k_t'\cdot(k_t'-k_t)}{k_z'-k_z} + P\frac{K'^2}{k_z'}\right], \tag{1.2}$$

with P representing the Cauchy principal value, $K' = (K_0^2 - k_t'^2)^{1/2}$, k_0 is the free-space wave number, and G^0 the Fourier transform of the free-space Green's function. In addition, A is called the interaction function,

$$A(\mathbf{k}) = \int \exp\{-ik_t\cdot x_t - ik_z h(x_t)\}dx_t, \tag{1.3}$$

which is the phase modulation amplitude spectrum induced by the roughness element. Since A contains h explicitly (dynamics), if h is a stochastic variable, so is A, and hence so is Γ. The equation for Γ can also be viewed quantum mechanically[3] as scattering from a noncentral potential VA. Here Γ has actually been stripped of incident and exiting free-space Green's functions, and the scattering amplitude T is related to the on-shell value of Γ as

$$T(k_t',k_t) = \{(\pi i/k_z')\Gamma(\mathbf{k}',\mathbf{k})\}|_{k_z=-K;\,k_z'=K'}. \tag{1.4}$$

The equation for Γ describes the transition from incident wave number (or propagation vector) state $\mathbf{k}''$ to final state $\mathbf{k}'$ either through a single interaction given by the Born term VA, or through multiple interactions through a continuum of (generally off-shell) intermediate states $\mathbf{k}$. If we express the solution of Eq. (1.1) as a Born series expansion in powers of the interaction A, then, for a stochastic surface, the ensemble average of any power of Γ is in principle known once the ensemble average of any power of A is known. Analogous coupled equations for vector (electromagnetic) fields[4] and tensor (elastic) fields[5] have also been derived. An interpretation of Eq. (1) using (stochastic) Feynman diagram methods is also available[2] similar to the diagram expansions in random volume scattering theory.[6]

Here we restrict our attention to the first or coherent moment of Γ represented by $\langle\Gamma\rangle$. The bracket represents the average over the ensemble of surface realizations. The random surface h is assumed to be Gaussian distributed and to be a homogeneous statistical process. The ensemble averages of powers of the interaction are cluster decomposed to yield the "connected" terms of the diagram expansion, again analogous to the random volume problem.[6] Explicitly the first three moments are

$$\langle A(\mathbf{k})\rangle = A_1(\mathbf{k}) = (2\pi)^2\delta(k_t)\exp(-k_z^2\sigma^2/2), \tag{1.5}$$

$$\langle A(\mathbf{k}_1)A(\mathbf{k}_2)\rangle = A_1(\mathbf{k}_1)A_1(\mathbf{k}_2) + A_2(\mathbf{k}_1,\mathbf{k}_2), \tag{1.6}$$

and

$$\langle A(\mathbf{k}_1)A(\mathbf{k}_2)A(\mathbf{k}_3)\rangle = A_1(\mathbf{k}_1)A_1(\mathbf{k}_2)A_1(\mathbf{k}_3) + A_1(\mathbf{k}_1)A_2(\mathbf{k}_2,\mathbf{k}_3) + A_1(\mathbf{k}_2)A_2(\mathbf{k}_1,\mathbf{k}_3) + A_1(\mathbf{k}_3)A_2(\mathbf{k}_1,\mathbf{k}_2) + A_3(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3), \tag{1.7}$$

where σ is the root-mean-square height. The general connected term A_n is also available.[2]

The equation for the ensemble average of Γ can be written using these connected terms as

$$\langle\Gamma(\mathbf{k}',\mathbf{k}'')\rangle = M(\mathbf{k}',\mathbf{k}'') + \int M(\mathbf{k}',\mathbf{k})G^0(k)\langle\Gamma(\mathbf{k},\mathbf{k}'')\rangle\,d\mathbf{k}, \tag{1.8}$$

where the mass operator[6] M is the infinite sum

$$M(\mathbf{k}',\mathbf{k}'') = \sum_{j=1}^{\infty} M_j(\mathbf{k}',\mathbf{k}'') \tag{1.9}$$

and each M_j term contains only the connected term A_j. For

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example, the first three are given by

$$M_1(\mathbf{k}',\mathbf{k}'') = V(\mathbf{k}',\mathbf{k}'')\,A_1(\mathbf{k}'-\mathbf{k}''), \tag{1.10}$$

$$M_2(\mathbf{k}',\mathbf{k}'') = \int V(\mathbf{k}',\mathbf{k})G^0(k)V(\mathbf{k},\mathbf{k}'')A_2(\mathbf{k}'-\mathbf{k},\mathbf{k}-\mathbf{k}'')d\,\mathbf{k}, \tag{1.11}$$

and

$$M_3(\mathbf{k}',\mathbf{k}'') = \int V(\mathbf{k}',\mathbf{k}_1)G^0(k_1)V(\mathbf{k}_1,\mathbf{k}_2)G^0(k_2)V(\mathbf{k}_2,\mathbf{k}'') \times A_3(\mathbf{k}'-\mathbf{k}_1,\mathbf{k}_1-\mathbf{k}_2,\mathbf{k}_2-\mathbf{k}'')d\,\mathbf{k}_1\,d\,\mathbf{k}_2. \tag{1.12}$$

All the disconnected terms can be found from an iterate in the solution of Eq. (1.8). The two-dimensional delta function in Eq. (1.5) expressing overall horizontal momentum conservation can be shown to be characteristic of each A_j and hence each M_j. Thus Eq. (1.8) can be reduced to a one-dimensional equation and has been solved numerically when M is truncated at the first term.[7] The delta function arises due to the statistical translational invariance of the problem itself resulting from the assumption of homogeneous statistics. The description of the result in terms of only connected diagrams is an example of a partial summation technique.[6]

II. SMOOTHING

We now apply the smoothing method to Eq. (1.1). Originally developed by Keller[8] for wave propagation problems it has been applied most recently to the surface scattering problem for scalar waves by Watson and Keller[9] and to the electromagnetic problem by Brown.[10] Both applied the method in coordinate space whereas here we apply it in the transform domain.

Define the integral operator symbolically as

$$L = \int VG^0\,d\,\mathbf{k}, \tag{2.1}$$

so that Eq. (1.1) can be written symbolically as

$$\Gamma = VA + LA\Gamma. \tag{2.2}$$

Since A is stochastic, so is Γ. Write it as the sum of a mean and fluctuating part. It is also convenient since multiple averaging is required to replace the bracket average notation by the averaging operator E, i.e.,

$$\langle\Gamma\rangle = E\Gamma, \tag{2.3}$$

where E operates on any random variable occurring to its right. We thus have

$$\Gamma = E\Gamma + \Gamma', \tag{2.4}$$

where $E\Gamma' = 0$. Next substitute Eq. (2.4) in Eq. (2.2) to yield

$$E\Gamma + \Gamma' = VA + LA\,[E\Gamma + \Gamma']. \tag{2.5}$$

Take the ensemble average of Eq. (2.5). This is

$$E\Gamma = VEA + LEAE\Gamma + LEA\Gamma'. \tag{2.6}$$

Subtract Eq. (2.6) from Eq. (2.5) to give

$$\Gamma' = \overline{\Gamma} + L\,[A - EA\,]\Gamma', \tag{2.7}$$

where $\overline{\Gamma}$ is

$$\overline{\Gamma} = V\,[A - EA\,] + L\,[A - EA\,]E\Gamma \tag{2.8}$$

and is independent of the fluctuating part.

A formal solution by iteration of Eq. (2.7) is

$$\Gamma' = \sum_{n=0}^{\infty}\,[LA - LEA\,]^n\overline{\Gamma}, \tag{2.9}$$

which yields the fluctuating part solely in terms of the mean field through $\overline{\Gamma}$. Next substitute Eq. (2.9) in Eq. (2.6) and use Eq. (2.8). Combine the second term on the right-hand side of Eq. (2.6) with the second term contribution from $\overline{\Gamma}$ to get

$$E\Gamma = M^S + LEA\sum_{n=0}^{\infty}\,[LA - LEA\,]^nE\Gamma, \tag{2.10}$$

which is the smoothing integral equation on the mean field with the smoothing mass operator defined by

$$M^S = VEA + LEA\sum_{n=0}^{\infty}\,[LA - LEA\,]^nV\,[A - EA\,]. \tag{2.11}$$

III. COMPARISON OF DIAGRAM AND SMOOTHING TERMS

We compare the first three mass operator terms in the Born expansion for the smoothing method defined by M_j^s, $j = 1,2,3$, with the corresponding terms in the connected diagram expansion given by Eqs. (1.10)–(1.12). The first term is from Eq. (2.11),

$$M_1^S = VEA, \tag{3.1}$$

which, in Fourier transform space and using Eq. (1.5), is

$$M_1^S(\mathbf{k}',\mathbf{k}'') = V(\mathbf{k}',\mathbf{k}'')\,A_1(\mathbf{k}'-\mathbf{k}'') \tag{3.2}$$

and is the same as the connected diagram result.

The second term is for $n = 0$ in Eq. (2.11)

$$M_2^S = LEAV\,[A - EA\,] = LV\,[EAA - EAEA\,], \tag{3.3}$$

which in Fourier transform and bracket notation is

$$M_2^S(\mathbf{k}',\mathbf{k}'') = \int d\,\mathbf{k}\,V(\mathbf{k}',\mathbf{k})G^0(k)V(\mathbf{k},\mathbf{k}'') \times\{\langle A(\mathbf{k}'-\mathbf{k})\,A(\mathbf{k}-\mathbf{k}'')\rangle - A_1(\mathbf{k}'-\mathbf{k})\,A_1(\mathbf{k}-\mathbf{k}'')\}. \tag{3.4}$$

Using Eq. (1.6) we see that this again is the same as the connected diagram expansion term Eq. (1.11).

The third term, $n = 1$ in Eq. (2.11) is

$$M_3^S = LEA\,[LA - LEA\,]V\,[A - EA\,], \tag{3.5}$$

which in Fourier transform notation can be written as

$$M_3^S(\mathbf{k}',\mathbf{k}'') = \int\int V(\mathbf{k}',\mathbf{k}_1)G^0(k_1)V(\mathbf{k}_1,\mathbf{k}_2)G^0(k_2)V(\mathbf{k}_2,\mathbf{k}'') \times A_3^S(\mathbf{k}'-\mathbf{k}_1,\mathbf{k}_1-\mathbf{k}_2,\mathbf{k}_2-\mathbf{k}'')d\,\mathbf{k}_1\,d\,\mathbf{k}_2, \tag{3.6}$$

where A_3^S is given by four terms

$$\begin{aligned}A_3^S(\mathbf{k}'-\mathbf{k}_1,\mathbf{k}_1-\mathbf{k}_2,\mathbf{k}_2-\mathbf{k}'') &= \langle A(\mathbf{k}'-\mathbf{k}_1)\,A(\mathbf{k}_1-\mathbf{k}_2)\,A(\mathbf{k}_2-\mathbf{k}'')\rangle \\ &\quad - \langle A(\mathbf{k}'-\mathbf{k}_1)\,A(\mathbf{k}_1-\mathbf{k}_2)\rangle A_1(\mathbf{k}_2-\mathbf{k}'') \\ &\quad - A_1(\mathbf{k}'-\mathbf{k}_1)\langle A(\mathbf{k}_1-\mathbf{k}_2)\,A(\mathbf{k}_2-\mathbf{k}'')\rangle \\ &\quad + A_1(\mathbf{k}'-\mathbf{k}_1)\,A_1(\mathbf{k}_1-\mathbf{k}_2)\,A_1(\mathbf{k}_2-\mathbf{k}'').\end{aligned} \tag{3.7}$$

Comparison with Eq. (1.7) illustrates that Eq. (3.7) differs from the connected diagram result A_3 in two respects. It neglects the initial–final state two interaction correlation term

$$\langle A(\mathbf{k}' - \mathbf{k}_1) A(\mathbf{k}_2 - \mathbf{k}'')\rangle A_1(\mathbf{k}_1 - \mathbf{k}_2)$$

and has a different sign for the product of the three single interaction correlations. Higher-order terms can also be computed and they also differ.

Thus we have our conclusion. The connected diagram and smoothing methods agree to the first two orders of approximation and differ beyond that. For third- and higher-order terms the smoothing method does not produce connected terms. In order for it to do so some sort of renormalization in the method would appear to be necessary.

Finally, note that in this comparison, it makes sense to *only* compare the respective Born terms of the two methods. If we were to include the integral terms in an interaction expansion, both methods would fully resum to the same result to any given interaction order.

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A Hamiltonian approach to normal mode coupling in a Coulomb plasma

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A Hamiltonian approach is used to treat the nonlinear problem of normal mode coupling in an unmagnetized homogeneous Coulomb plasma. It is shown that this method yields results consistent with well-known equations of plasma physics.

I. INTRODUCTION

In a previous paper[1] we showed how the Hamiltonian structure for two-fluid plasma dynamics presented in Ref. 2 could be used to obtain the electrostatic normal mode frequencies in an unmagnetized homogeneous Coulomb plasma. The purpose of this paper is to show how the formalism of Ref. 1 can be extended to the much more difficult problem of mode coupling in an unmagnetized homogeneous Coulomb plasma.

For simplicity, we restrict our analysis to the one-dimensional problem. The results of Ref. 1 may be summarized as follows.

For the system under consideration, the state vector of dynamical variables is $\psi(x) = (\delta\rho_e, \delta u_e, \delta\rho_i, \delta u_i)$. Here, with the subscript s labeling the two species present, electrons and singly charged positive ions, $\delta\rho_s$ and δu_s represent density and velocity-field perturbations on a homogeneous stationary equilibrium. The Hamiltonian may be expanded as

$$H = H_0 + H_1 + H_2 + H_3, \tag{1}$$

where H_2 is the term which gives the linear behavior of the plasma, while H_3 determines the nonlinear behavior.

After Fourier transformation from x space to k space, the normal modes were obtained in the following way. H_2 was expressed in the form

$$H_2 = \int \frac{d^3k}{(2\pi)^3}\frac{1}{2}\tilde{\psi}(k)C(k)\psi(k)^*, \tag{2}$$

where

$$C = \begin{bmatrix} v_e + a_e^2/k^2 & 0 & a_e a_i/k^2 & 0 \\ 0 & \rho_{e0} & 0 & 0 \\ a_e a_i/k^2 & 0 & v_i + a_i^2/k^2 & 0 \\ 0 & 0 & 0 & \rho_{i0} \end{bmatrix} \tag{3}$$

and the tilde denotes transpose, while the fundamental Poisson bracket was written as

$$\{\psi(k), \psi(k')^*\} = -i(2\pi)^3 B(k)\delta(k - k'), \tag{4}$$

where

$$B = \begin{bmatrix} 0 & k & 0 & 0 \\ k & 0 & 0 & 0 \\ 0 & 0 & 0 & k \\ 0 & 0 & k & 0 \end{bmatrix}. \tag{5}$$

In Eq. (3) and in the following, we have abbreviated $v_s = [\partial^2(\rho_s U_s)/\partial\rho_s^2]|_{\rho_{s0}}$, where $U_s(\rho_s)$ is the specific internal energy of species s, a_s is the charge-to-mass ratio $a_s = q_s/m_s$, and ρ_{s0} denotes the equilibrium density of species s.

Equations (2) and (4) were then combined to obtain the linear equation of motion in the form

$$\dot{\psi} = A\psi, \tag{6}$$

where

$$A \equiv -iBC = -ik \begin{bmatrix} 0 & \rho_{e0} & 0 & 0 \\ v_e + a_e^2/k^2 & 0 & a_e a_i/k^2 & 0 \\ 0 & 0 & 0 & \rho_{i0} \\ a_e a_i/k^2 & 0 & v_i + a_i^2/k^2 & 0 \end{bmatrix}. \tag{7}$$

In order to proceed, we must now analyze the linear problem in more detail.

II. LINEAR THEORY

Although we are considering a dissipationless system, the matrix A is non-Hermitian. Thus, there are two separate eigenvalue problems which may be considered: the "right" problem, defined by

$$A\mathbf{u}^\alpha = -i\omega^\alpha \mathbf{u}^\alpha, \tag{8}$$

and the "left" problem,

$${}^\alpha\mathbf{u}A = -i\,{}^\alpha\omega\,{}^\alpha\mathbf{u}. \tag{9}$$

Although the set of right eigenvectors $\{\mathbf{u}^\alpha\}$ is not expected to be equal to the set of left eigenvectors $\{{}^\alpha\mathbf{u}\}$ (after transposition), the two sets of eigenvalues $\{\omega^\alpha\}$ and $\{{}^\alpha\omega\}$ must be identical. They were found in Ref. 1 to be the solutions of the equation

$$(\omega_e^2 + c_e^2 k^2 - \omega^2)(\omega_i^2 + c_i^2 k^2 - \omega^2) = \omega_e^2 \omega_i^2, \tag{10}$$

where $\omega_s^2 = \rho_{s0} a_s^2$ and $c_s = T_s/m_s$, with T_s denoting the temperature of species s. A straightforward calculation shows that the inverse transpose of the matrix of left eigenvectors is equal to the matrix of right eigenvectors (up to normalization).

Upon solving Eq. (8) for the $\mathbf{u}^\alpha$, we find the usual solutions to the linearized equations of motion

$$\begin{aligned} u_2^\alpha &= (\omega^\alpha/k\rho_{e0})\,u_1^\alpha, \\ u_3^\alpha &= \{\omega_e^2/[\omega_i^2 + c_i^2 k^2 - (\omega^\alpha)^2]\}\,u_1^\alpha, \\ u_4^\alpha &= \frac{\omega^\alpha}{k\rho_{e0}}\frac{\omega_e^2}{\omega_i^2 + c_i^2 k^2 - (\omega^\alpha)^2}\,u_1^\alpha. \end{aligned} \tag{11}$$

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Solving Eq. (9) for the left eigenvectors ${}^{\alpha}\mathbf{u}$, one finds

$$
\begin{aligned}
{}^{\alpha}u_2 &= (k\rho_{e0}/\omega^{\alpha})^{\alpha}u_1, \\
{}^{\alpha}u_3 &= \{[\omega_e^2 + c_e^2 k^2 - (\omega^{\alpha})^2]/\omega_i^2\}^{\alpha}u_1, \\
{}^{\alpha}u_4 &= \frac{k\rho_{i0}}{\omega^{\alpha}} \frac{\omega_e^2 + c_e^2 k^2 - (\omega^{\alpha})^2}{\omega_i^2} {}^{\alpha}u_1.
\end{aligned} \tag{12}
$$

We now consider the normalization of the eigenvectors.

Proposition: $\mathbf{u}^{\alpha} = \kappa({}^{\alpha}\mathbf{u}B)$, where κ is a constant.

Proof: Equations (7)–(9) imply

$$BC\mathbf{u}^{\alpha} = \omega^{\alpha}\mathbf{u}^{\alpha} \tag{13}$$

and

$${}^{\beta}\mathbf{u}BC = {}^{\beta}\omega\,{}^{\beta}\mathbf{u}. \tag{14}$$

Using the fact that B and C are symmetric, and taking the transpose of Eq. (14), we obtain ${}^{\beta}\omega\,\widetilde{{}^{\beta}\mathbf{u}} = CB\,\widetilde{{}^{\beta}\mathbf{u}} = C\,\widetilde{{}^{\beta}\mathbf{u}B}$. This leads to $\omega^{\beta}(\widetilde{{}^{\beta}\mathbf{u}B}) = \omega^{\beta}B\,\widetilde{{}^{\beta}\mathbf{u}} = BC\tilde{B}\,\widetilde{{}^{\beta}\mathbf{u}} = BC\,\widetilde{{}^{\beta}\mathbf{u}B}$, which, upon comparison with (13), proves the claim. □

The above proposition may also be verified explicitly from Eqs. (5), (11), and (12).

We now define normalized right and left eigenvectors $\mathbf{v}^{\alpha}$ and ${}^{\alpha}\mathbf{v}$ in terms of normalization coefficients c^{α} and ${}^{\alpha}c$, according to

$$\mathbf{v}^{\alpha} = c^{\alpha}\mathbf{u}^{\alpha} \quad \text{and} \quad {}^{\alpha}\mathbf{v} = {}^{\alpha}c\,{}^{\alpha}\mathbf{u}. \tag{15}$$

It follows from (8), (9), and (13) that ${}^{\beta}\mathbf{v}\cdot(\mathbf{v}^{\alpha})^* = 0$ for $\alpha \neq \beta$, and now impose the condition

$${}^{\beta}\mathbf{v}\cdot(\mathbf{v}^{\alpha})^* = \delta_{\alpha\beta}. \tag{16}$$

This requires the normalization coefficients to satisfy

$${}^{\beta}c\cdot(c^{\beta})^* = ({}^{\beta}u\cdot u^{\beta})^{-1}. \tag{17}$$

In addition, consistent with the above proposition, we impose the condition

$${}^{\alpha}\mathbf{v} = \widetilde{{}^{\alpha}\mathbf{v}B} = B\,\widetilde{{}^{\alpha}\mathbf{v}}. \tag{18}$$

Combining with (16), this implies ${}^{\beta}\mathbf{v}\cdot B\,\widetilde{{}^{\alpha}\mathbf{v}}^* = \delta_{\alpha\beta}$, or

$$|{}^{\alpha}c|^2 = [{}^{\alpha}\mathbf{u}B\,\widetilde{{}^{\alpha}\mathbf{u}}]^{-1}. \tag{19}$$

Similarly, we get

$$|c^{\alpha}|^2 = [\widetilde{\mathbf{u}^{\alpha}}B^{-1}\mathbf{u}^{\alpha}]^{-1}. \tag{20}$$

Of course, Eqs. (17), (19), and (20) are consistent with each other, and any one of them is implied by the other two. Thus these eight independent equations suffice to determine the eight normalization coefficients $\{c^{\alpha}\}$ and $\{{}^{\alpha}c\}$.

We are now ready to change variables to normal coordinates. First, we observe the following. Form the linear combination

$$a^{\alpha} = {}^{\alpha}\mathbf{v}\cdot\psi. \tag{21}$$

Then $\dot{a}^{\alpha} = {}^{\alpha}\mathbf{v}\cdot\dot{\psi} = {}^{\alpha}\mathbf{v}\cdot A\psi = -i\omega^{\alpha}\,{}^{\alpha}\mathbf{v}\cdot\psi = -i\omega^{\alpha}a^{\alpha}$. Hence a^{α} is a normal mode, a linear combination of state vectors which evolves sinusoidally, according to

$$\dot{a}^{\alpha} = -i\omega^{\alpha}a^{\alpha}, \quad a^{\alpha}(t) = a_0^{\alpha}e^{-i\omega^{\alpha}t}. \tag{22}$$

Indeed, using Eqs (21), (12), and (15), one finds

$$
\begin{aligned}
a^{\alpha} \propto \delta\rho_e &+ \frac{k\rho_{e0}}{\omega^{\alpha}}\delta u_e + \frac{\omega_e^2 + k^2c_e^2 - (\omega^{\alpha})^2}{\omega_e^2}\delta\rho_i \\
&+ \frac{k\rho_{e0}}{\omega^{\alpha}} \frac{\omega_e^2 + k^2c_e^2 - (\omega^{\alpha})^2}{\omega_i^2}\delta u_i,
\end{aligned}
$$

and it can be verified explicity from the equations of motion that $\dot{a}^{\alpha} = -i\omega^{\alpha}a^{\alpha}$.

Although A is not Hermitian, we assume that its sets of right and left eigenvectors form complete sets. Then, for an arbitrary state vector ψ, we write

$$\psi(t) = \sum_{\alpha} A^{\alpha}(\mathbf{v}^{\alpha})^* e^{-i\omega^{\alpha}t}. \tag{23}$$

The expansion coefficients A^{α} are just the a_0^{α} defined in (22), as may be seen by forming the inner product of Eq. (23) with ${}^{\beta}\mathbf{v}$ and using (16). Thus

$$\psi(t) = \sum_{\alpha} a^{\alpha}(t)(\mathbf{v}^{\alpha})^* = \sum_{\alpha} a_0^{\alpha}(\mathbf{v}^{\alpha})^* e^{-i\omega^{\alpha}t}, \tag{24}$$

and the a^{α} are in fact the amplitude coefficients in the normal mode expansion of ψ. Reality of the physical fields implies $\psi(k)^* = \psi(-k)$, so that $a_0^{\alpha}(-k) = a_0^{\alpha}(k)^*$, $\mathbf{v}^{\alpha}(-k) = \mathbf{v}^{\alpha}(k)^*$, and $\omega^{\alpha}(-k) = -\omega^{\alpha}(k)$.

Proposition: The change of variables from ψ to $\{a^{\alpha}\}$ diagonalizes H_2.

Proof: Inserting (24) into (2), we find

$$H_2 = \sum_{\alpha,\beta}\int \frac{d^3k}{(2\pi)^3}\tfrac{1}{2}a^{\beta}(t)(\widetilde{\mathbf{v}^{\beta}})^* C a^{\alpha}(t)^*\mathbf{v}^{\alpha},$$

which, after some manipulations, becomes

$$H_2 = \sum_{\alpha}\int \frac{d^3k}{(2\pi)^3}\frac{1}{2}a^{\alpha}(t)a^{\alpha}(t)^*\omega^{\alpha}, \tag{25}$$

or

$$H_2 = \sum_{\alpha}\int \frac{d^3k}{(2\pi)^3}\frac{1}{2}a_0^{\alpha}(a_0^{\alpha})^*\omega^{\alpha}. \tag{26}$$

It is instructive to take another view of the diagonalization procedure, as follows.

Defining $\Omega = BC$, we have $\Omega\mathbf{v}^{\alpha} = \omega^{\alpha}\mathbf{v}^{\alpha}$. Let T be the matrix of right eigenvectors of A, so that $T_{\nu\alpha} = v_{\nu}^{\alpha}$. One shows in the usual way that T diagonalizes Ω: $\Omega_{\mu\lambda}T_{\lambda\alpha} = \omega^{(\alpha)}T_{\mu\alpha} = T_{\mu\gamma}\omega^{(\alpha)}\delta_{\gamma\alpha}$, so that, defining Ω' to be the diagonalized form of Ω, $\Omega'_{\gamma\alpha} = \omega^{(\alpha)}\delta_{\gamma\alpha}$, that is, $\Omega T = T\Omega'$ or $T^{-1}\Omega T = \Omega'$.

We now write Eq. (8) in the form

$$\dot{a}^{\alpha}\cdot(\mathbf{v}^{\alpha})^* = -i\Omega a^{\beta}\cdot(\mathbf{v}^{\beta})^*.$$

Then

$$\dot{a}^{\alpha}\,T^*_{\nu\alpha} = -ia^{\beta}\,\Omega_{\mu\lambda}\,T^*_{\lambda\beta},$$

from which $\dot{a}^{\alpha} = -i\Omega^*_{\alpha\beta}\,a^{\beta} = -i\omega^{(\alpha)}\delta_{\alpha\beta}a^{\beta} = -i\omega^{\alpha}a^{\alpha}$, consistent with (22).

We now consider the transformation of the Hamiltonian H_2 and the Poisson tensor B.

In H_2 there appears

$$
\begin{aligned}
\tilde{\psi}C\psi^* &= a^{\beta}\mathbf{v}^{\beta}\,C(a^{\alpha})^*\mathbf{v}^{\alpha} \\
&= a^{\beta}(a^{\alpha})^*\,T^*_{\nu\beta}c_{\nu\mu}T_{\mu\alpha} \\
&= a^{\beta}(a^{\alpha})^*\,T^{\dagger}_{\beta\nu}c_{\nu\mu}T_{\mu\alpha},
\end{aligned}
$$

where † denotes the Hermitian conjugate. We define

$$C' = T^{\dagger}CT. \tag{27}$$

Therefore,

$$H_2 = \sum_{\alpha,\beta} \int \frac{d^3k}{(2\pi)^3} \frac{1}{2} a^\alpha(t) a^\beta(t)^* c'_{\alpha\beta}. \tag{28}$$

From Eqs. (4) and (24),

$$T_{\mu\alpha}(k)^*[a^\alpha(k), a^\beta(k')] T_{\nu\beta}(k')^* = -i(2\pi)^3 B(k)\delta(k+k'),$$

so that, using $T(-k) = T^*(k)$, and defining

$$B' = T^{-1} B (T^{-1})^\dagger, \tag{29}$$

we have

$$[a^\alpha(k), a^\beta(k')] = -i(2\pi)^3 B'(k)\delta(k+k'). \tag{30}$$

To recapitulate, we define a change of basis from ψ to the a^α, defined by $\psi_\mu = a^\alpha (v^\alpha_\mu)^* = T^*_{\mu\alpha} a^\alpha$, i.e.,

$$\psi = T\mathbf{a}, \tag{31}$$

where $\mathbf{a}$ denotes the vector of normal mode amplitudes; $\Omega' = T^{-1}BCT$, diagonal, implies $\dot{a}^\alpha = -i\omega^\alpha a^\alpha$; $C' = T^\dagger C T$ implies

$$H_2 = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2} a^\alpha(t) a^\beta(t)^* c'_{\alpha\beta};$$

and $B' = T^{-1}B(T^{-1})^\dagger$ implies $[a^\alpha(k), a^\beta(k')] = -i(2\pi) b'_{\alpha\beta}(k)\delta(k+k')$.

We obtain the equations of motion for the a^α by first computing that $\delta H_2/\delta a^\alpha = (2\pi)^{-1}(a^\alpha)^* \omega^{(\alpha)}$. Then by the chain rule,

$$\begin{aligned}\dot{a}^\alpha(k) &= [a^\alpha(k), H_2] = \int d^3k' [a^\alpha(k), a^\beta(k')] \frac{\delta H_2}{\delta a^\beta(k')} \\ &= -i \int d^3k' (2\pi)\, b'_{\alpha\beta}(k)\delta(k+k') \\ &\quad \times \frac{1}{2\pi} (a^\beta)^*(k') \omega^{(\beta)}(k') \\ &= i\, b'_{\alpha\beta}(k) a^\beta(k) \omega^{(\beta)}.\end{aligned}$$

We see then that we require, in addition to

$$\Omega'_{\alpha\beta} = (T^{-1}BCT)_{\alpha\beta} = \omega^{(\alpha)}\delta_{\alpha\beta}, \tag{32}$$

that

$$b'_{\alpha\beta} = (T^{-1}B(T^{-1})^\dagger)_{\alpha\beta} = \delta_{\alpha\beta}, \tag{33}$$

and, so that H_2 appears in normal form,

$$c'_{\alpha\beta} = (T^\dagger C T)_{\alpha\beta} = \omega^{(\alpha)}\delta_{\alpha\beta}. \tag{34}$$

Of course, $B'C' = \Omega'$.

We denote the two branches of the dispersion relation by subscripts for Bohm–Gross (bg) and ion acoustic (ia). Then, with the requirement $\omega^\alpha(-k) = -\omega^\alpha(k)$, the choices we make are, for the four ω^α,

$$\begin{aligned}\omega^1(k) &= \begin{cases} \omega_{\rm bg}(k), & k>0, \\ -\omega_{\rm bg}(k), & k<0, \end{cases} \\ \omega^2(k) &= \begin{cases} -\omega_{\rm bg}(k), & k>0, \\ \omega_{\rm bg}(k), & k<0, \end{cases} \\ \omega^3(k) &= \begin{cases} \omega_{\rm ia}(k), & k>0, \\ -\omega_{\rm ia}(k), & k<0, \end{cases} \\ \omega^4(k) &= \begin{cases} -\omega_{\rm ia}(k), & k>0, \\ \omega_{\rm ia}(k), & k<0. \end{cases}\end{aligned} \tag{35}$$

Diagonalizing the matrices Ω', B', and C' according to the requirements of Eqs. (32)–(34), one obtains

$$\Omega' = \begin{bmatrix} \omega_{\rm bg} & 0 & 0 & 0 \\ 0 & \omega_{\rm ia} & 0 & 0 \\ 0 & 0 & -\omega_{\rm bg} & 0 \\ 0 & 0 & 0 & -\omega_{\rm ia} \end{bmatrix}, \tag{36}$$

$$C' = \begin{bmatrix} \omega_{\rm bg} & 0 & 0 & 0 \\ 0 & \omega_{\rm ia} & 0 & 0 \\ 0 & 0 & \omega_{\rm bg} & 0 \\ 0 & 0 & 0 & \omega_{\rm ia} \end{bmatrix}, \tag{37}$$

$$B' = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{38}$$

III. NONLINEAR THEORY

We first write the expression for H_3, Eq. (7d) in Ref. 1, in terms of Fourier transformed dynamical variables. Using the relations

$$\begin{aligned}\int dx\, f(x)^2 g(x) &= \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \hat{f}(k)\hat{f}(k')\hat{g}(k+k')^* \\ &= \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \int \frac{dk''}{2\pi} \hat{f}(k)\hat{f}(k') \\ &\quad \times \hat{g}(k'')\delta(k+k'+k''),\end{aligned}$$

one obtains

$$\begin{aligned}H_3 = \sum_s \frac{1}{2} \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \int \frac{dk''}{2\pi} \hat{u}_s(k)\hat{u}_s(k')\hat{\rho}_s(k'') \\ \times \delta(k+k'+k'') + \sum_s \frac{1}{6} \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \int \frac{dk''}{2\pi} \\ \times \frac{\partial^3(\rho_s U_s)}{\partial \rho_s^3}\bigg|_{\rho_\infty} \hat{\rho}_s(k)\hat{\rho}_s(k')\hat{\rho}_s(k'')\delta(k+k'+k'').\end{aligned} \tag{39}$$

It can be verified that the equations of motion, Eqs. (1) in Ref. 1, are given to second order in perturbation quantities by

$$\begin{aligned}\dot{\chi}_s(k) &= [\chi_s(k), H_2 + H_3] \\ &= \int dk' [\chi_s(k), \chi_t(k')] \frac{\delta(H_2+H_3)}{\delta\chi_t(k')},\end{aligned} \tag{40}$$

where χ_s and χ_t represent the fields.

In terms of the state vectors $\psi(k)$, (39) may be written as

$$\begin{aligned}H_3 = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} \int \frac{dk''}{2\pi} \\ \times G_{\mu\nu\lambda} \psi_\mu(k)\psi_\nu(k')\psi_\lambda(k'')\delta(k+k'+k''),\end{aligned} \tag{41}$$

where the only nonzero components of $G_{\mu\nu\lambda}$ are

$$G_{111}=\frac{1}{6}\frac{\partial^3(\rho_e U_e)}{\partial\rho_e^3}\bigg|_{\rho_{e0}},\quad G_{221}=\frac{1}{2},$$
$$G_{333}=\frac{1}{6}\frac{\partial^3(\rho_i U_i)}{\partial\rho_i^3}\bigg|_{\rho_{i0}},\quad G_{443}=\frac{1}{2}. \tag{42}$$

Inserting the expansion (24) into (41), we obtain finally the normal mode form of H_3:

$$H_3=\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}\int\frac{dk''}{2\pi}a^\alpha(k,t)a^\beta(k',t)a^\gamma(k''',t)$$
$$\times g_{\alpha\beta\gamma}(k,k',k'')\delta(k+k'+k'')$$
$$=\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}\int\frac{dk''}{2\pi}a_0^\alpha(k)\,a_0^\beta(k')\,a_0^\gamma(k'')$$
$$\times g_{\alpha\beta\gamma}(k,k',k'')e^{-i(\omega^\alpha+\omega^\beta+\omega^\gamma)t}\delta(k+k'+k''), \tag{43}$$

where

$$g_{\alpha\beta\gamma}(k,k',k'')=G_{\mu\nu\lambda}\,v_\mu^\alpha(k)^*\,v_\nu^\beta(k')^*\,v_\lambda^\gamma(k'')^*. \tag{44}$$

To relate the $g_{\alpha\beta\gamma}(k,k',k'')$ to the mode coupling coefficients, we first calculate the functional derivatives of H_3. We have

$$\int\frac{\delta H_3}{\delta a^\lambda(s)}\bar a^\lambda(s)ds=\frac{d}{d\epsilon}\bigg|_{\epsilon=0}H_3(\{a^\alpha\}_{\alpha\neq\lambda},a^\lambda+\epsilon\bar a^\lambda)$$
$$=\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}\int\frac{dk''}{2\pi}\bar a^\lambda(k)\sum_{\beta,\gamma}a^\beta(k')a^\gamma(k'')g_{\lambda\beta\gamma}(k,k',k'')\delta(k+k'+k'')$$
$$+\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}\int\frac{dk''}{2\pi}\bar a^\lambda(k')\sum_{\alpha,\gamma}a^\alpha(k)a^\gamma(k'')g_{\alpha\lambda\gamma}(k,k',k'')\delta(k+k'+k'')$$
$$+\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}\int\frac{dk''}{2\pi}\bar a^\lambda(k'')\sum_{\alpha,\beta}a^\alpha(k)a^\beta(k')g_{\alpha\beta\lambda}(k,k',k'')\delta(k+k'+k''). \tag{45}$$

Performing the k', k'', and k integration in (45), one finds

$$\int\frac{\delta H_3}{\delta a^\lambda(s)}\bar a^\lambda(s)ds=\int\frac{ds}{2\pi}\bar a^\lambda(s)\left\{\int\frac{dk''}{2\pi}a^\beta(-s-k'')a^\gamma(k'')g_{\lambda\beta\gamma}(s,-s-k'',k'')\right\}$$
$$+\int\frac{ds}{2\pi}\bar a^\lambda(s)\left\{\int\frac{dk}{2\pi}a^\alpha(k)a^\gamma(-k-s)g_{\alpha\lambda\gamma}(k,s,-k-s)\right\}$$
$$+\int\frac{ds}{2\pi}\bar a^\lambda(s)\left\{\int\frac{dk'}{2\pi}a^\alpha(-k'-s)\,a^\beta(k')g_{\alpha\beta\lambda}(-k'-s,k',s)\right\}. \tag{46}$$

Finally then,

$$\frac{\delta H_3}{\delta a^\lambda(k)}=\frac{1}{(2\pi)^2}\int ds\{a^\beta(-k-s)a^\gamma(s)g_{\lambda\beta\gamma}(k,-k-s,s)+a^\alpha(s)a^\gamma(-s-k)g_{\alpha\lambda\gamma}(s,k,-s-k)$$
$$+a^\alpha(-s-k)a^\beta(s)g_{\alpha\beta\lambda}(-s-k,s,k)\}. \tag{47}$$

Now

$$\dot a^\alpha(k')=[a^\alpha(k'),H_2+H_3]=[a^\alpha(k'),H_2]+[a^\alpha(k'),H_3], \tag{48}$$

where the linear term, involving H_2, has been given in (22) as $[a^\alpha(k'),H_2]=-i\omega^\alpha(k')a^\alpha(k')$. For the nonlinear term involving H_3, we use Eq. (30) and the fact that B' is diagonal to write

$$[a^\alpha(k'),a^\lambda(k)]=-i(2\pi)b'_{\alpha\alpha}\,\delta_{\alpha\lambda}\delta(k+k').$$

Then

$$[a^\alpha(k'),H_3]=\int dk\left\{-i(2\pi)b'_{\alpha\alpha}\frac{\delta H_3}{\delta a^\alpha(k)}\delta(k+k')\right\}$$
$$=-2\pi i b'_{\alpha\alpha}\frac{\delta H_3}{\delta a^\alpha(-k')}. \tag{49}$$

Using (47), we get for the nonlinear time evolution of a^α

$$\dot a^\alpha(k)=\int c_{\alpha\beta\gamma}(k,k',k-k')a^\beta(k')a^\gamma(k-k')dk', \tag{50}$$

where

$$c_{\alpha\beta\gamma}(k,k')=-(i/2\pi)\,b'_{\alpha,\alpha}\{g_{\alpha\gamma\beta}(-k,k-k',k')$$
$$+g_{\beta\alpha\gamma}(k',-k,k-k')$$
$$+g_{\gamma\beta\alpha}(k-k',k',-k)\} \tag{51}$$

are the desired coupling coefficients.

Equation (50) may also be written as

$$\dot a^\alpha(k)=\int\int c_{\alpha\beta\gamma}(k,k',k'')a^\beta(k')$$
$$\times a^\gamma(k'')\delta(k-k'-k'')dk'\,dk'' \tag{52}$$

or

$$\dot{a}_0^\alpha(k) = \int\int c_{\alpha\beta\gamma}(k,k',k'')\, a_0^\beta(k')\, a_0^\gamma(k'') \times e^{+i(\omega^\alpha(k) - \omega^\beta(k') - \omega^\gamma(k''))t} \times \delta(k - k' - k'')dk'\,dk''. \quad (53)$$

This is the form given by Davidson,[3] Eq. (19) on p. 105.

ACKNOWLEDGMENT

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The Fermi surface for point interactions

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Using a computer, the Fermi surface for the one-electron model of an infinite crystal in three dimensions with zero range interactions, i.e., with so-called point interactions, is studied. A computer program is available which has, as input, the crystal structure, the scattering length of the solid considered, and the Fermi energy, and, as output, a drawing of the corresponding Fermi surface inside its Brillouin zone.

I. INTRODUCTION

The notion of Fermi surface is of great importance in solid state physics. Let us first recall what we mean by a Fermi surface.

In the one-electron model of an infinite three-dimensional crystal we consider the Schrödinger operator $H = -\Delta + V$ (in units where $\hbar = 1$, $m = \frac{1}{2}$) on $L^2(\mathbb{R}^3)$, where Δ is the Laplacian and V is periodic with periodicity Λ, where Λ is a three-dimensional lattice in $\mathbb{R}^3$. By standard techniques, this implies that

$$H = \int_{\hat{\Lambda}}^{\oplus} H(k)d^3k,$$

where the dual group $\hat{\Lambda} = \mathbb{R}^3/\Gamma$ can be identified with the Brillouin zone B, i.e., a Wigner–Seitz cell of the orthogonal (or dual) lattice Γ.

The band spectrum of H dissolves into discrete eigenvalues $E_1(k) \leq E_2(k) \leq \cdots$ of $H(k)$ and the Fermi surface is the set $\{k \in B \mid E_n(k) = E_F \text{ for } n \in \mathbb{N}\}$, where E_F is the Fermi energy that distinguishes the occupied states from the nonoccupied states at zero temperature in the Fermi–Dirac statistics.

Instead of considering the Fermi surface inside the Brillouin zone B, we can consider it on $\mathbb{R}^3$ by extending it periodically.

The actual computation of the Fermi surface for a specific solid is an impressive combination of theory and experiment. However, there is no unifying *rigorous* theory, and we always have to make a large number of approximations that are difficult to control *a priori*. See Ref. 1 for an extensive introduction to the subject.

In this paper we compute explicitly, with the aid of a computer, the Fermi surface from first principles for a particular interaction, namely a point interaction. Of course the point interaction represents an approximation to the real potential. However with this potential we do not make any further approximation.

The study of Schrödinger operators with point interactions, i.e., zero-range interactions or Fermi pseudopotentials, was started by, among others, Fermi, Peierls, Breit, and Thomas in the thirties in nuclear physics,[2] and continued in the fifties by Huang, Yang, Lee, Luttinger, and others in statistical mechanics.[3]

In addition, and in this connection more interesting, we have the celebrated Kronig–Penney model,[4] dating from 1933, which is a model of an infinite *one*-dimensional crystal with point interactions.

The nontrivial rigorous study of these operators especially in three dimensions was started in 1961 by Berezin, Faddeev, and others[5] and made into a systematic theory by Grossmann, Høegh-Krohn, and Mebkhout.[6,7] In particular, in Ref. 7, the periodic point interaction model is constructed, and its spectral properties are determined.

Thus the model we study here is a three-dimensional analog of the Kronig–Penney model.

More detailed properties of the spectrum when we remove some points with a point interaction and thus destroy the periodicity are studied in Ref. 8.

Starting from this there has been a thorough rigorous study of these operators and related operators with more realistic short-range potential. For an extensive exposition of all this we refer to Ref. 9.

We also note *en passant* that in the beginning of this rigorous study nonstandard analysis played an important part.[10]

One property of the point interactions is that the only parameter needed to specify the interaction completely is the scattering length.

Thus the equation we derive for the Fermi surface contains only the scattering length of the one-center problem, the Fermi energy, and the lattice.

This implies that the computer program[11] has, as input, the lattice, the scattering length, and the energy, and as output, the Fermi surface with the following four options: (i) the surface within the corresponding Brillouin zone, (ii) the surface over an arbitrary rectangle in the plane, (iii) contour maps of (i), and (iv) contour maps of (ii).

The Fermi surface is mathematically a multi-valued (actually infinite-valued) function.

The computer program is, however, only able to draw single-valued functions, so we can only see half the surface in (i) and a single sheet in (ii). In this short paper we can only give some examples of Fermi surfaces for a small number of different lattices and values of the parameters.

However, a specific Fermi surface with a particular lattice and values of the parameters can be obtained from the authors on request.

One may argue that a point interaction is not a realistic interaction. However, one virtue of the point interaction is that we can actually compute a nontrivial Fermi surface starting from a potential. In addition it is a possible starting point for a more general approach.

That is, we can show[12] (see Sec. II) that the Schrödinger

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operator with point interactions is very well approximated (actually in the norm resolvent sense) by Schrödinger operators with more general short-range interactions. We will return to this in connection with Fermi surfaces later.

II. POINT INTERACTIONS AND FERMI SURFACES

We study here the one-electron model of an infinite crystal in three dimensions with point interactions.

More precisely, let Λ be a Bravais lattice in $\mathbf{R}^3$, i.e.,

$$\Lambda = \{n_1a_1 + n_2a_2 + n_3a_3 | n_i \in \mathbf{Z}\}, \tag{1}$$

where $a_1, a_2, a_3 \in \mathbf{R}^3$ are three independent vectors. We consider here the case where we have exactly one atom for each Bravais lattice point.

The Schrödinger operator $-\Delta_\alpha$ corresponding to point interactions with strength α at each point in Λ has a resolvent with an integral kernel

$$\begin{aligned}(-\Delta_\alpha - E)^{-1}(p,q) &= (p^2 - E)^{-1}\delta(p-q) + (2\pi)^{-3} \\ &\times \sum_{\lambda,\lambda' \in \Lambda} \left[\left(\alpha - \frac{i\sqrt{E}}{4\pi}\right)\delta_{\lambda\lambda'} - \tilde{G}_E(\lambda - \lambda')\right]^{-1}_{\lambda\lambda'} \\ &\times e^{i(p\lambda - q\lambda')}/(p^2 - E)(q^2 - E),\end{aligned} \tag{2}$$

where $\operatorname{Im}\sqrt{E} > 0$ and

$$\tilde{G}_E(x) = \begin{cases} e^{i\sqrt{E}|x|}/4\pi|x|, & x \neq 0, \\ 0, & x = 0. \end{cases} \tag{3}$$

Recall that $e^{i\sqrt{E}|x-y|}/4\pi|x-y|$ is the integral kernel of $(-\Delta - E)^{-1}$ on $L^2(\mathbf{R}^3)$] and $[\ ]^{-1}_{\lambda\lambda'}$ denotes the (λ,λ')th element of the inverse of the matrix $[\ ]$ on $l^2(\Lambda)$.

We briefly digress here to give some insight into the definition of H_α. Formally, we are interested in the operator

$$H = -\Delta - \sum_{\lambda \in \Lambda} \nu\delta(\cdot - \lambda), \tag{4}$$

where δ is Dirac's delta function and $\nu > 0$ which is not a well-defined self-adjoint operator on $L^2(\mathbf{R}^3)$.

By making a Fourier transform we obtain the operator

$$H = p^2 - \sum_{\lambda \in \Lambda} \nu |\psi_\lambda\rangle\langle\overline{\psi_\lambda}|, \tag{5}$$

where

$$\psi_\lambda(p) = (2\pi)^{-3/2} e^{ip\lambda}, \tag{6}$$

and the operator $S = |f\rangle\langle g|$ is defined to be $Sh = f(g,h)$, [(g,h) is the inner product on $L^2(\mathbf{R}^3)$] and p^2 is considered as a multiplication operator, i.e., $H_0 = p^2$ means $(H_0 f)(p) = p^2 f(p)$.

To make this operator well defined we modify H in the following way: Replace ψ_λ with ψ^ω_λ, where

$$\psi^\omega_\lambda(p) = \chi_\omega(p)\psi_\lambda(p), \tag{7}$$

where χ_ω is the characteristic function of a ball with radius ω, i.e.,

$$\chi_\omega(p) = \begin{cases} 1, & |p| < \omega, \\ 0, & |p| > \omega, \end{cases} \tag{8}$$

and let ν be ω-dependent, $\nu = \nu(\omega)$.

By choosing

$$\nu(\omega) = (\omega/2\pi^2 + \alpha)^{-1}, \tag{9}$$

where $\alpha \in \mathbf{R}$ is arbitrary, one can show that H^ω, where

$$H^\omega = p^2 - \nu(\omega) \sum_{\lambda \in \Lambda} |\psi^\omega_\lambda\rangle\langle\overline{\psi^\omega_\lambda}|, \tag{10}$$

will converge in strong resolvent sense as $\omega \to \infty$ to the operator $-\Delta_\alpha$. Note that the coupling constant $\nu(\omega)$ tends to zero as $\omega \to \infty$. For more details see Refs. 6, 7, and 9.

The constant α can be interpreted as related to the scattering length in the sense that $a = 1/4\pi\alpha$ is the scattering length of the one-particle system with a single point interaction.

We now return to the operator $-\Delta_\alpha$. Using the invariance under Λ we can write

$$-\Delta_\alpha = \int_{\hat{\Lambda}}^{\oplus} -\Delta_\alpha(k)\, d^3k, \tag{11}$$

where the dual group $\hat{\Lambda} = \mathbf{R}^3/\Gamma$ (Γ is the orthogonal lattice, i.e., $\Gamma = \{n_1b_1 + n_2b_2 + n_3b_3 | n_i \in \mathbf{Z}\}$, where $a_i \cdot b_i = 2\pi\delta_{ij}$) can be identified with the Wigner–Seitz cell of the orthogonal lattice, i.e., the Brillouin zone B, and where $-\Delta_\alpha(k)$ is a self-adjoint operator on $l^2(\Gamma)$ with an integral kernel

$$\begin{aligned}(-\Delta_\alpha(k) - E)^{-1}_{(\gamma,\gamma')} &= (|\gamma + k|^2 - E)^{-1}\delta_{\gamma\gamma'} \\ &+ (2\pi)^{-3}\left[\alpha - i\sqrt{E}/4\pi - g_E(k)\right]^{-1} \\ &\times [(|\gamma + k|^2 - E)(|\gamma' + k|^2 - E)]^{-1},\end{aligned} \tag{12}$$

where $\operatorname{Im}\sqrt{E} > 0$ and

$$g_E(k) = \sum_{\lambda \in \Lambda} \tilde{G}_E(\lambda) e^{-i\lambda \cdot k}. \tag{13}$$

See Ref. 7 for more details.

We see from (12) that the negative part of the spectrum of $-\Delta_\alpha(k)$ consists of points where $\alpha - i\sqrt{E}/r\pi - g_E(k) = 0$.

Using this, we can[7] explicitly compute the spectrum of $-\Delta_\alpha$

$$\sigma(-\Delta_\alpha) = [E_0(\alpha), E_1(\alpha)] \cup [0, \infty), \tag{14}$$

where $E_1(\alpha) < 0$ provided $\alpha < \alpha_0 < 0$, where α_0 is a suitable constant. Here $E_0(\alpha)$, $E_1(\alpha)$ will also depend on the lattice.

The equation for the Fermi surface is then

$$\sum_{\lambda \in \Lambda} \tilde{G}_E(\lambda) e^{-i\lambda \cdot k} = \alpha - \frac{i\sqrt{E}}{4\pi}, \tag{15}$$

where Λ, α, and E are input and the implicit function in k is output and we recall that

$$\tilde{G}_E(\lambda) = \begin{cases} e^{i\sqrt{E}\lambda}/4\pi\lambda, & \lambda \neq 0, \\ 0, & \lambda = 0. \end{cases} \tag{16}$$

When we let $E < 0$ (15) can be written

$$\sum_{\substack{\lambda \in \Lambda \\ \lambda \neq 0}} \frac{e^{-\sqrt{|E|}|\lambda|}}{|\lambda|} \cos k \cdot \lambda = 4\pi\alpha - \sqrt{|E|}. \tag{17}$$

A few words may be appropriate here to indicate how we solve this equation.

We sum all the terms in the infinite series with $|\lambda| < R$ for some fixed R, use the symmetry of the lattice (which

implies that the program works for all Bravais lattices except for triclinic) to simplify and obtain a polynomial equation which can be solved by standard techniques.

In general an nth degree equation has n solutions. However, adding more and more terms in (17), which increases the degree of the equation, will not yield more and more different solutions, which is reasonable since Eq. (17) with a finite sum converges exponentially to the equation for a unique Fermi surface.

But as the computer is only able to draw single-valued functions, we usually end up with a small number of different drawings corresponding to *different* roots of the equation. To visualize the Fermi surface one has to superimpose visually the different drawings.

For example, in Fig. 1 we use an approximation which yields a third-degree equation, and we obtain three drawings that are all, however, identical to the one in Fig. 1.

However, in Fig. 2 we see an approximation which gives rise to a sixth-degree equation, and we obtain six drawings. In this case there are only two with major differences, Fig. 2(a) and 2(b).

In Sec. III we present some examples of Fermi surfaces with various values of the parameters and for some lattices.

As mentioned in the introduction, point interactions represent a first approximation to more realistic short-range interactions.

To be precise, let

$$H_\epsilon = -\Delta + \epsilon^{-2}\mu(\epsilon)\sum_{\lambda\in\Lambda} V\left[\frac{(\cdot - \lambda)}{\epsilon}\right], \tag{18}$$

where V is a real-valued potential that is Rollnik [i.e., $\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |V(x)V(y)||x-y|^{-2}\,dx\,dy < \infty$] with compact support and $\mu(\epsilon)$ is an analytic function with $\mu(0) = 1$.

We assume that $-\Delta + V$ has a simple zero-energy resonance, i.e., the equation

$$(-\Delta + V)\psi = 0 \tag{19}$$

has a simple solution ψ, which does not belong to $L^2(\mathbb{R}^3)$. To be more specific, using the standard decomposition ($E < 0$)

$$(-\Delta + V - E)^{-1} = G_E - G_E v(1 + uG_E v)^{-1}uG_E\,, \tag{20}$$

where

$$G_E = (-\Delta - E)^{-1} \tag{21}$$

and

$$u = |V|^{1/2}\,\mathrm{sgn}\,V\,, \quad v = |V|^{1/2}\,, \tag{22}$$

we see that eigenvalues of $-\Delta + V$ correspond to nontrivial solutions of

$$\phi + uG_E v\phi = 0\,. \tag{23}$$

We can show, see Ref. 14, that if ϕ is a solution of (23) then

$$\psi = G_E v\phi \tag{24}$$

is a solution of

$$(-\Delta + V)\psi = E\psi\,. \tag{25}$$

So we assume that

$$\phi + uG_0 v\phi = 0 \tag{26}$$

has a simple nontrivial solution $\phi \in L^2(\mathbb{R}^3)$. Then we can still prove that

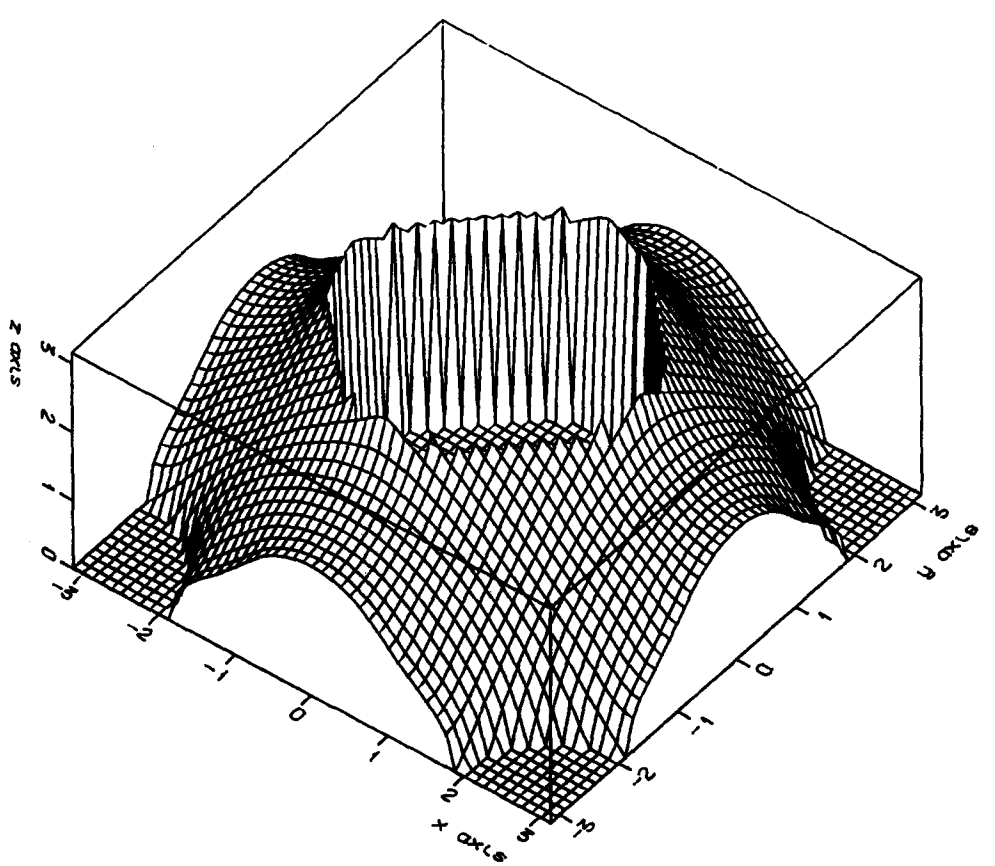


FIG. 1. The simplest Fermi surface we include here is for a simple cubic crystal (SC or cubic P) with $E = -1$, $\alpha = 0.12$, and $a = b = c = 1$ (for notation concerning the lattices, see Kittel[13]) inside the upper half of its Brillouin zone. Completely vertical or horizontal parts of the illustration are not parts of the Fermi surface.

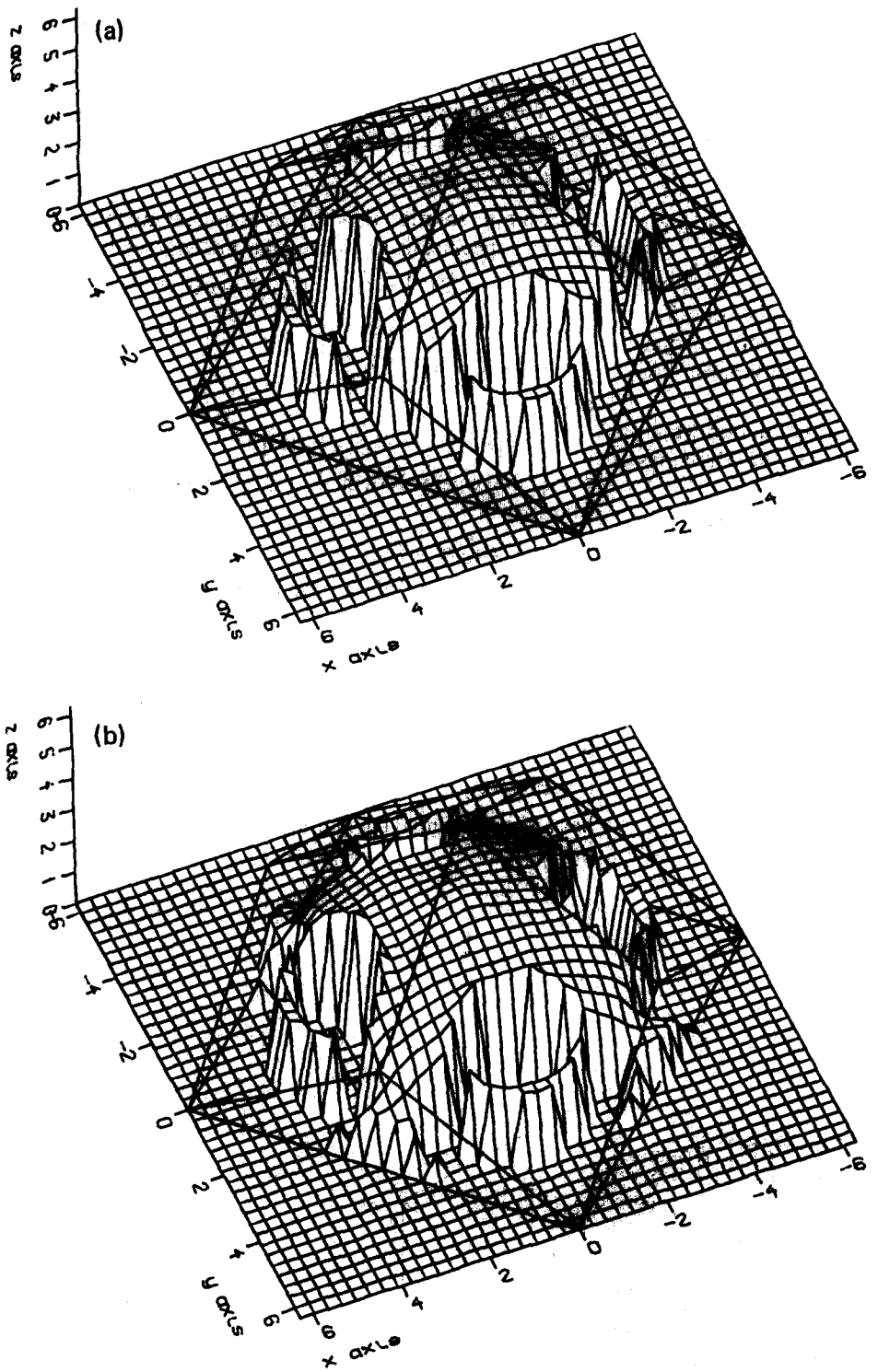


FIG. 2. The Fermi surface of a body-centered cubic (bbc or cubic I) crystal with $E = -1$ and $\alpha = -0.14$ inside the upper half of its Brillouin zone. The total surface within the upper half of the Brillouin zone is the union of the two surfaces depicted above.

$$\psi = G_0 v \phi \tag{27}$$

is a solution of

$$(-\Delta + V)\psi = 0 \tag{28}$$

in the sense of distributions, and what we assume is that this ψ is *not* in $L^2(\mathbb{R}^3)$.

From this assumption we can prove the following theorem.

Theorem 1: The operator H_ϵ converges in a norm resolvent sense to the operator $-\Delta_\alpha$ given by (2) where α is given according to

$$\alpha = \mu'(0)|(V\psi,\psi)|(V,\psi)|^{-2}. \tag{29}$$

Remark: The ψ in the definition of α is the ψ given by (27).

Proof: See Ref. 12.

Using the same decomposition for H_ϵ as for $-\Delta_\alpha$, i.e.,

$$H_\epsilon = \int_{\hat{\Lambda}}^{\oplus} H_\epsilon(k)\, d^3k, \tag{30}$$

we dissolve the bands of the spectrum into discrete eigenvalues.

We can then prove the following result.

Theorem 2: Let $E_0 < 0$ be an eigenvalue of $-\Delta_\alpha(k)$. Then there exists an eigenvalue E_ϵ for $H_\epsilon(k)$ such that $E_\epsilon \to E_0$ when $\epsilon \to 0$, and E_ϵ is analytic in ϵ. We have the following expansion:

$$E_\epsilon = E_0 + \epsilon E' + o(\epsilon), \tag{31}$$

where

$$E' = h^k_\Lambda (A + E_0 B) \tag{32}$$

and

$$h^k_\Lambda = (2\pi)^3 \left[|B| \sum_{\gamma \in \Gamma} \frac{1}{(|\Gamma + k|^2 - E)^2} \right]^{-1}. \tag{33}$$

Here $|B|$ is the Lebesgue measure of the Brillouin zone, and A,B are constants only depending on properties of $-\Delta + V$.

Remark: The explicit form of A and B are given in Ref. 12.

Proof: See Ref. 12.

Remark: This means that the Fermi surface computed with point interactions represents a first approximation to a Fermi surface with more general short-range interactions.

Using a scaling technique, point interactions can also be related to a limit other than the zero-range limit.

That is, let

$$H(\epsilon) = -\Delta + \mu(\epsilon) \sum_{\lambda \in \Lambda} V\left(\cdot - \frac{\lambda}{\epsilon} \right), \tag{34}$$

where V and μ are as before. Then, using the unitary operator U_ϵ defined by

$$(U_\epsilon f)(x) = \epsilon^{-3/2} f(x/\epsilon), \tag{35}$$

we see that

$$U_\epsilon^{-1} H_\epsilon U_\epsilon = \epsilon^{-2} H(\epsilon), \tag{36}$$

which implies that the eigenvalues E_ϵ and $E(\epsilon)$ of H_ϵ and $H(\epsilon)$, respectively, are related by

$$E_\epsilon = \epsilon^{-2} E(\epsilon). \tag{37}$$

Looking at the operator $H(\epsilon)$, we see that the limit $\epsilon \to 0$ represents a situation where the centers [i.e., the points where each potential $V(x - \lambda/\epsilon)$, $\lambda \in \Lambda$, is concentrated] move apart. As usual we decompose $H(\epsilon)$, i.e.,

$$H(\epsilon) = \int_{\hat{\Lambda}}^{\oplus} H(\epsilon, k) d^3k, \tag{38}$$

and we have the following theorem.

Theorem 3: Let $E(\epsilon,k) < 0$ be an eigenvalue of $H(\epsilon,k)$ such that

$$\lim_{\epsilon \to 0} \epsilon^{-2} E(\epsilon,k) < 0. \tag{39}$$

Then $E(\epsilon,k)$ is analytic and has the following expansion:

$$E(\epsilon,k) = \epsilon^2 E_0 + \epsilon^3 E' + o(\epsilon^3), \tag{40}$$

where E_0 is an eigenvalue of $-\Delta_\alpha(k)$ and E' is given by (32).

III. SOME FERMI SURFACES

In this section, we present some examples of Fermi surfaces with various values of the parameters and for some lattices.

Figures 3–12 show contour plots and periodic extensions of Fig. 2.

Figures 13–19 show how the Fermi surface inside the upper half of its Brillouin zone varies with E for an orthorhombic P crystal with axes $a = 3$, $b = 2$, $c = 1$, and with $\alpha = 0$.

Figures 20–22 show a similar series for a tetragonal P crystal with axes $a = b = 2$, $c = 1$, and with $\alpha = 0$.

Figures 23 and 24 show the Fermi surface inside the upper half of its Brillouin zone for a tetragonal P crystal with axes $a = b = 2$, $c = 3$, and with $\alpha = 0$ for two values of E.

Figures 25–27 show surfaces of a monoclinic C crystal, and a trigonal crystal.

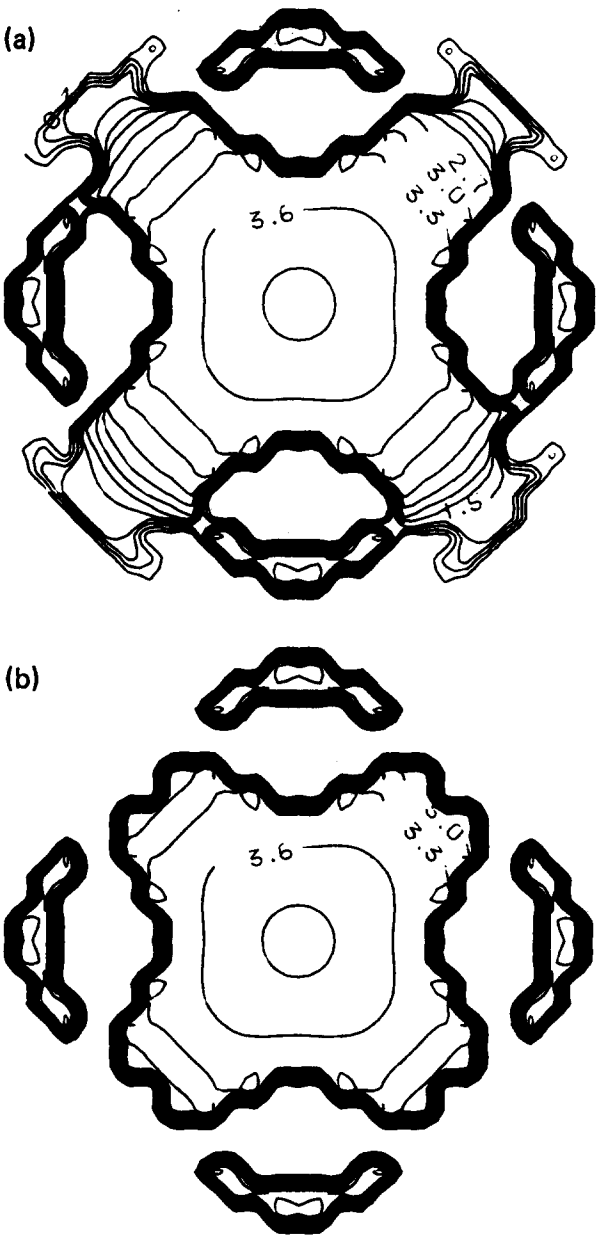
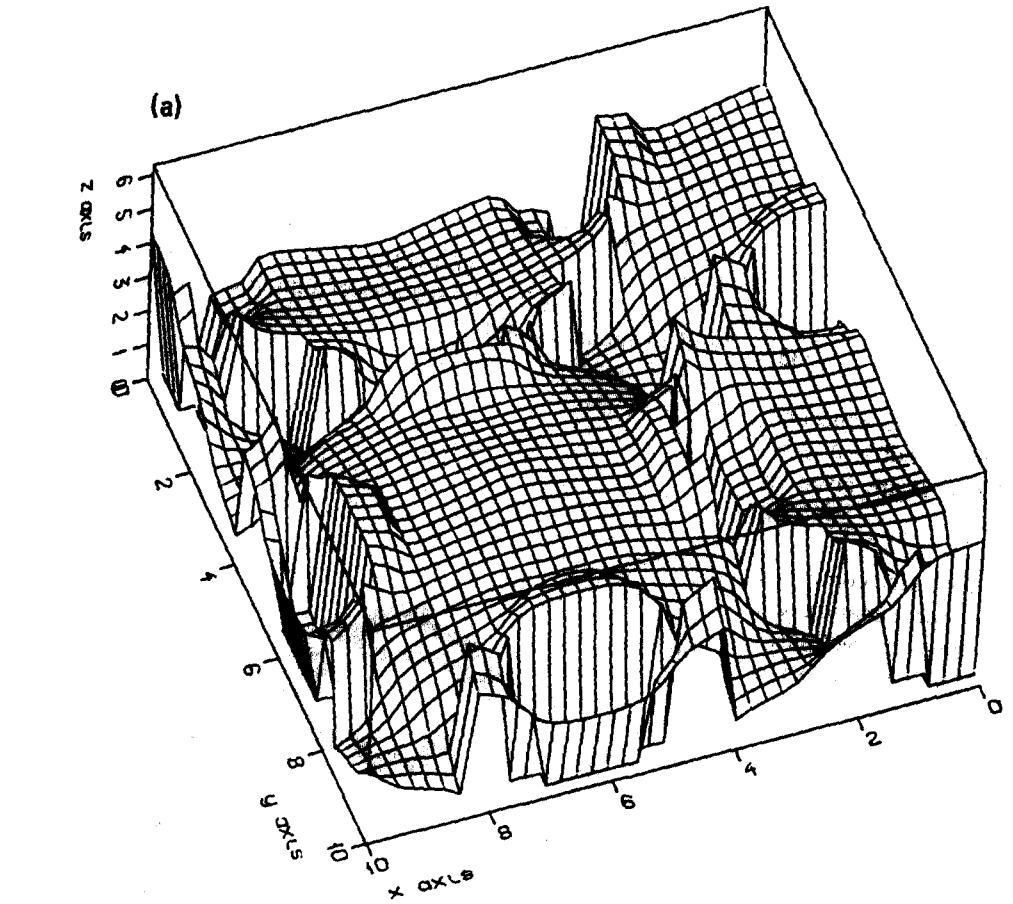


FIG. 3. A contour plot of Figs. 2(a) and 2(b).



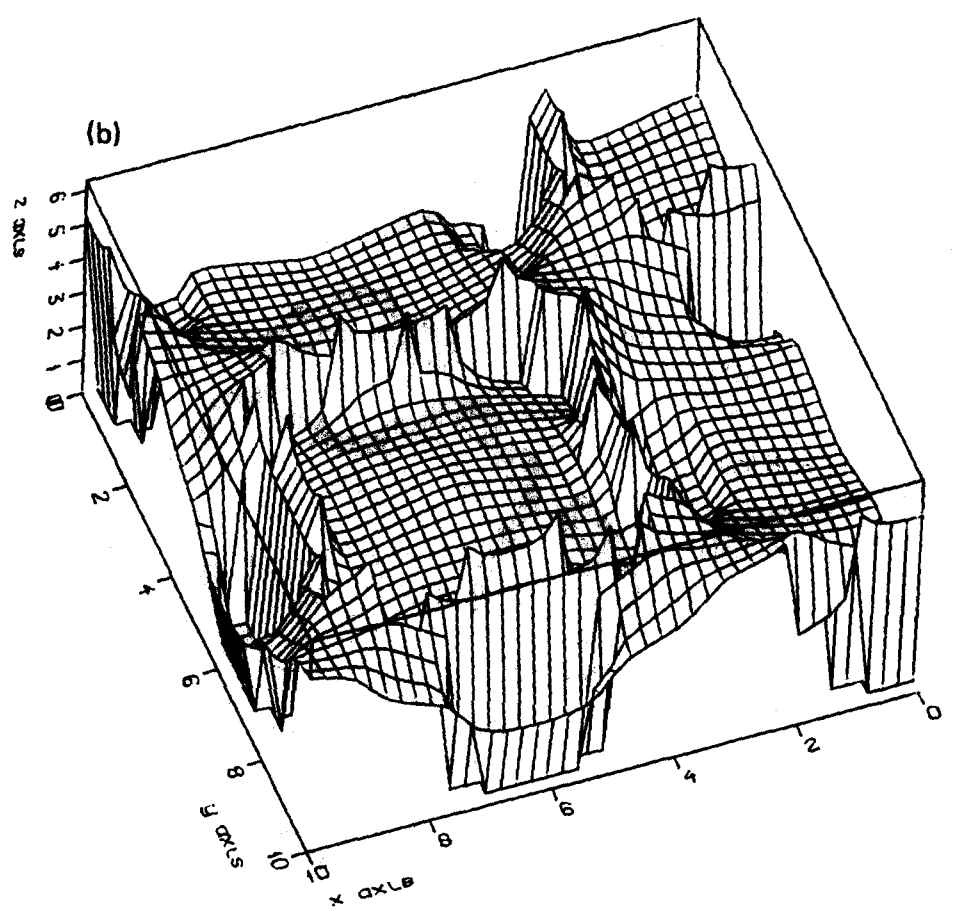


FIG. 4. The Fermi surface of Figs. 2(a) and 2(b) extended periodically. Again it is difficult to visualize the total surface in the sense that the total Fermi surface is the union of the two surfaces above extended periodically in the positive and negative z direction.

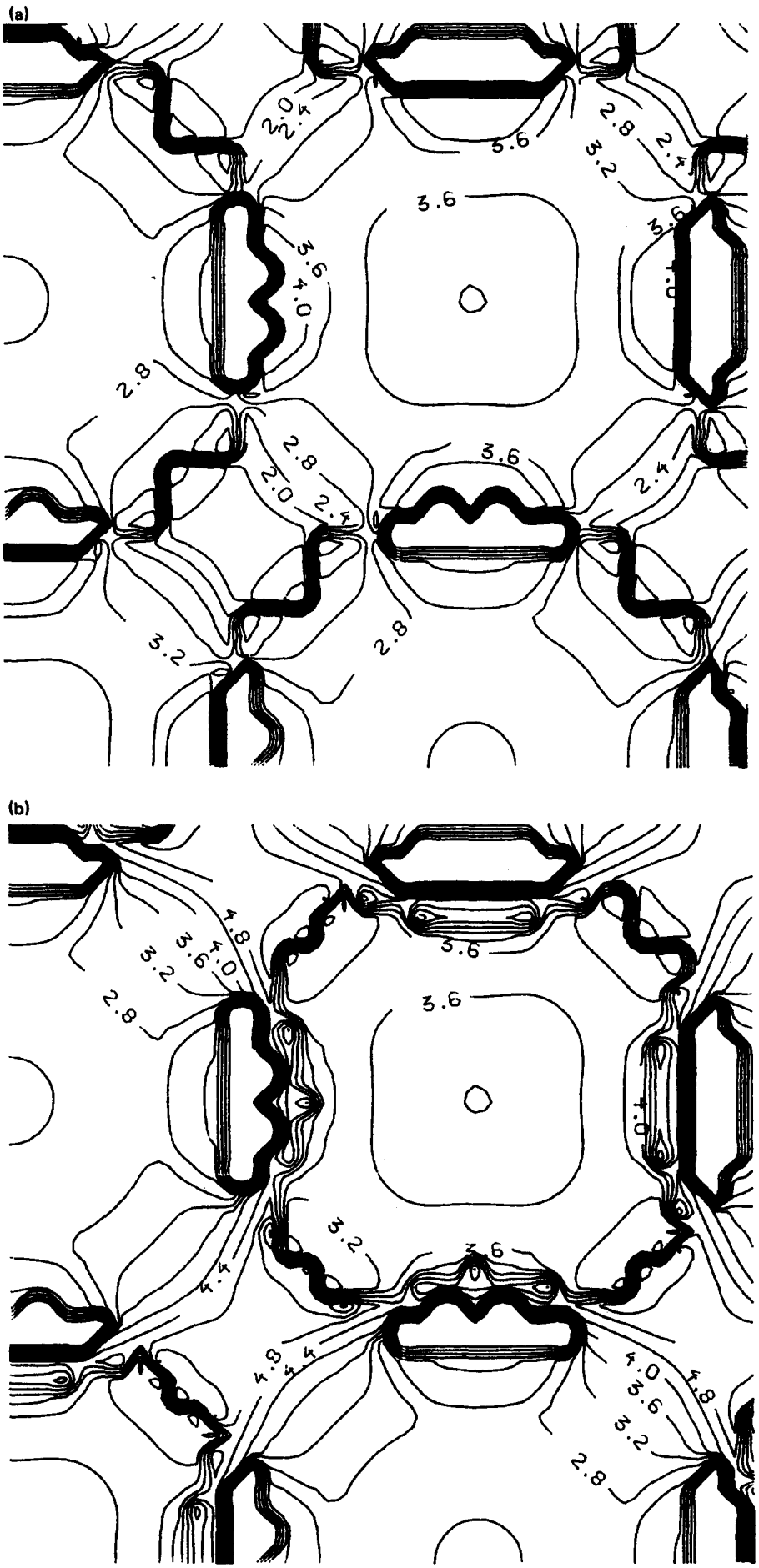


FIG. 5. A contour plot of Figs. 4(a) and 4(b).

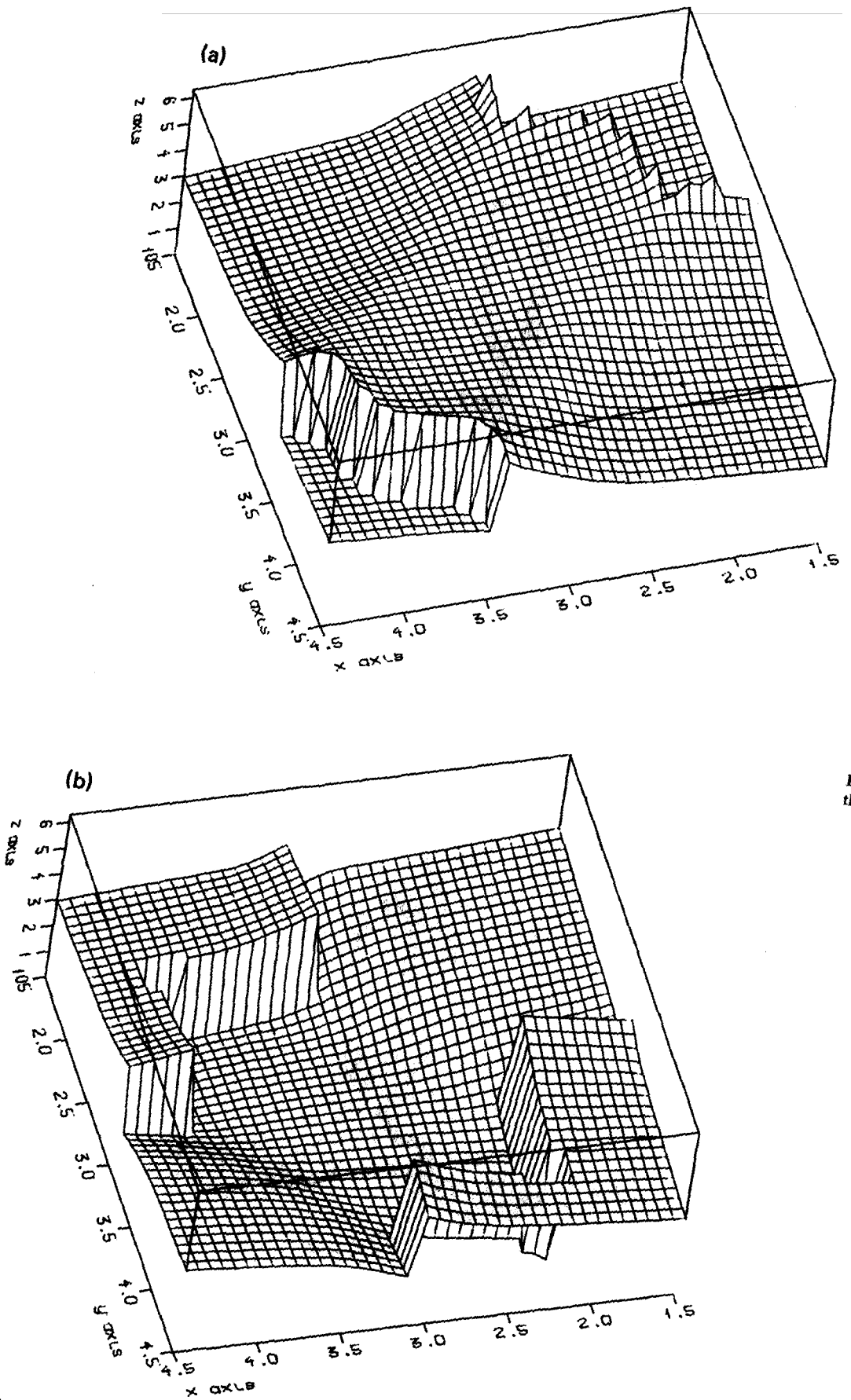
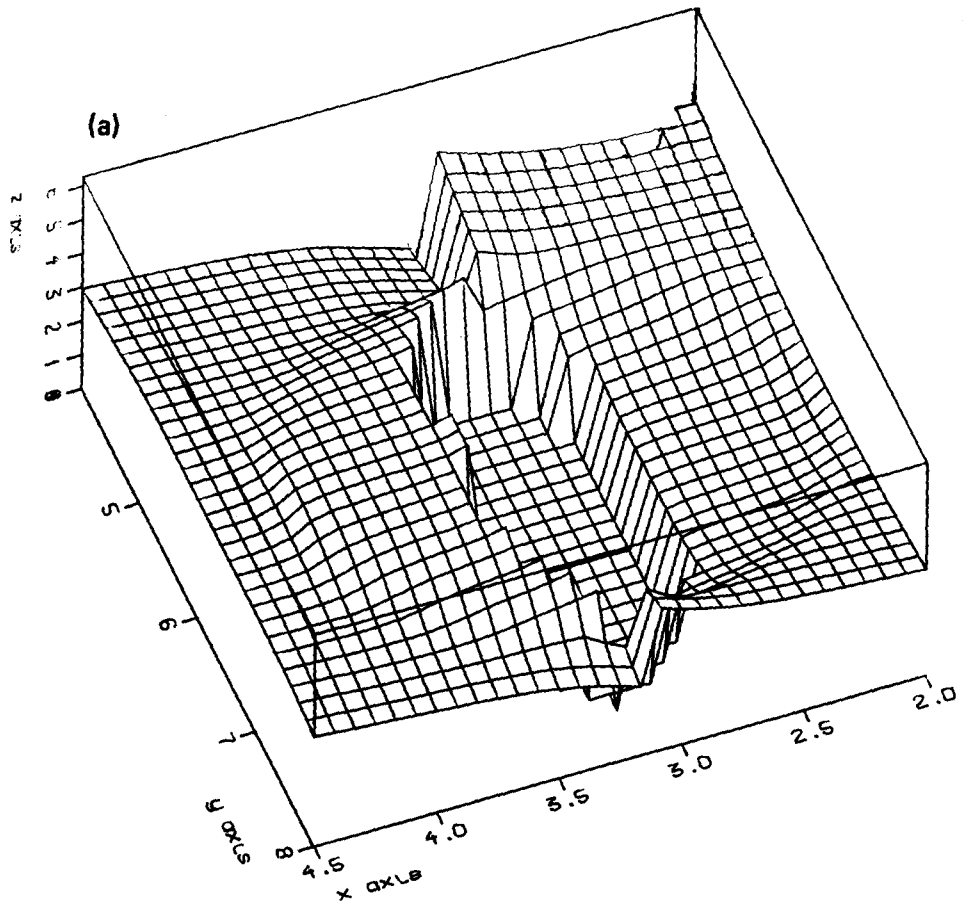


FIG. 6. A magnification of part of the surface in Figs. 4(a) and 4(b).



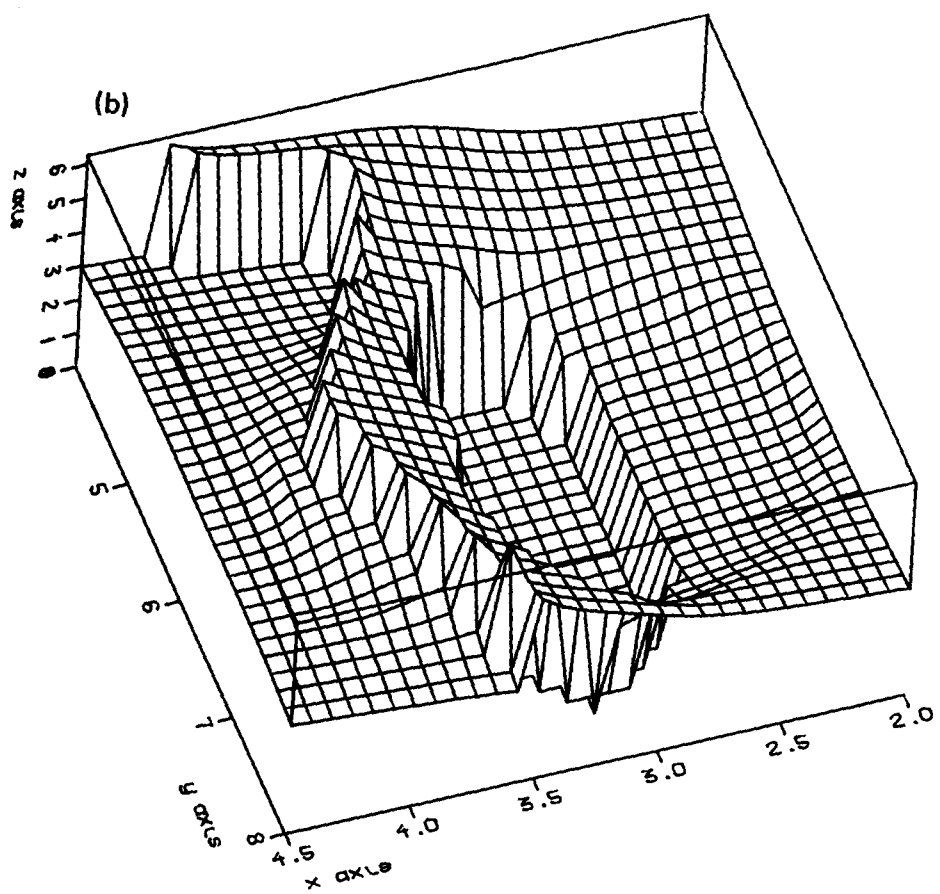


FIG. 7. A magnification of another part of the surface in Figs. 4(a) and 4(b).

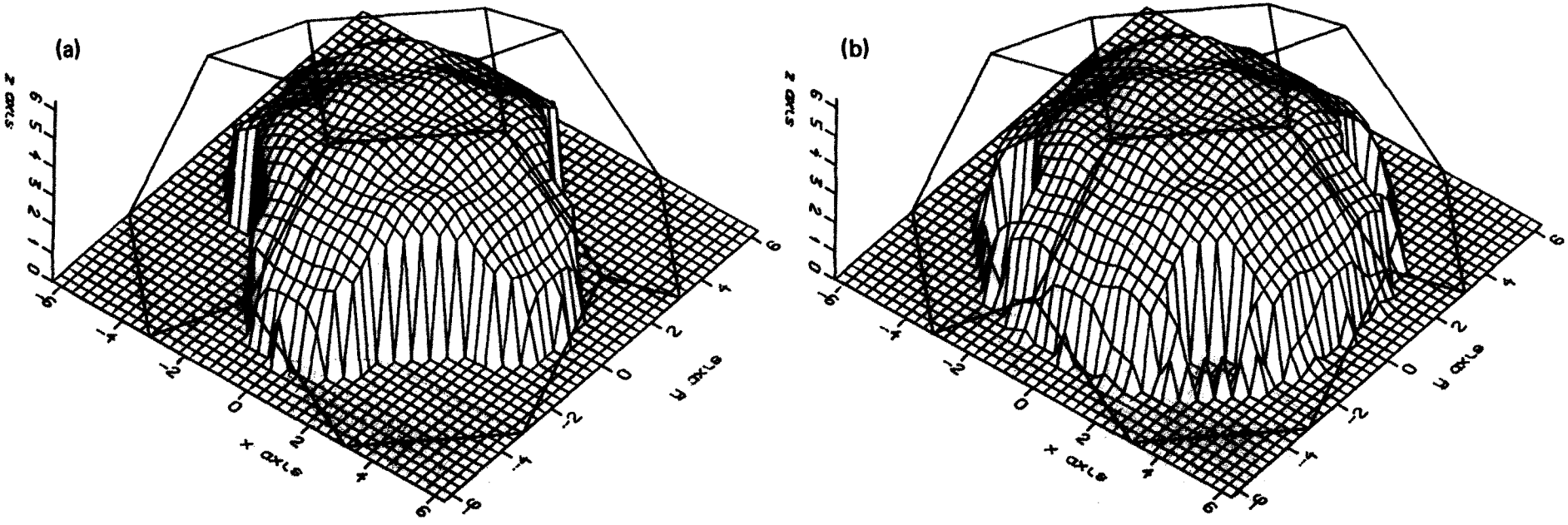


FIG. 8. The Fermi surface of a face-centered cubic (fcc or cubic F) crystal with $E = -1$ and $\alpha = -0.17$ inside the upper half of the Brillouin zone.

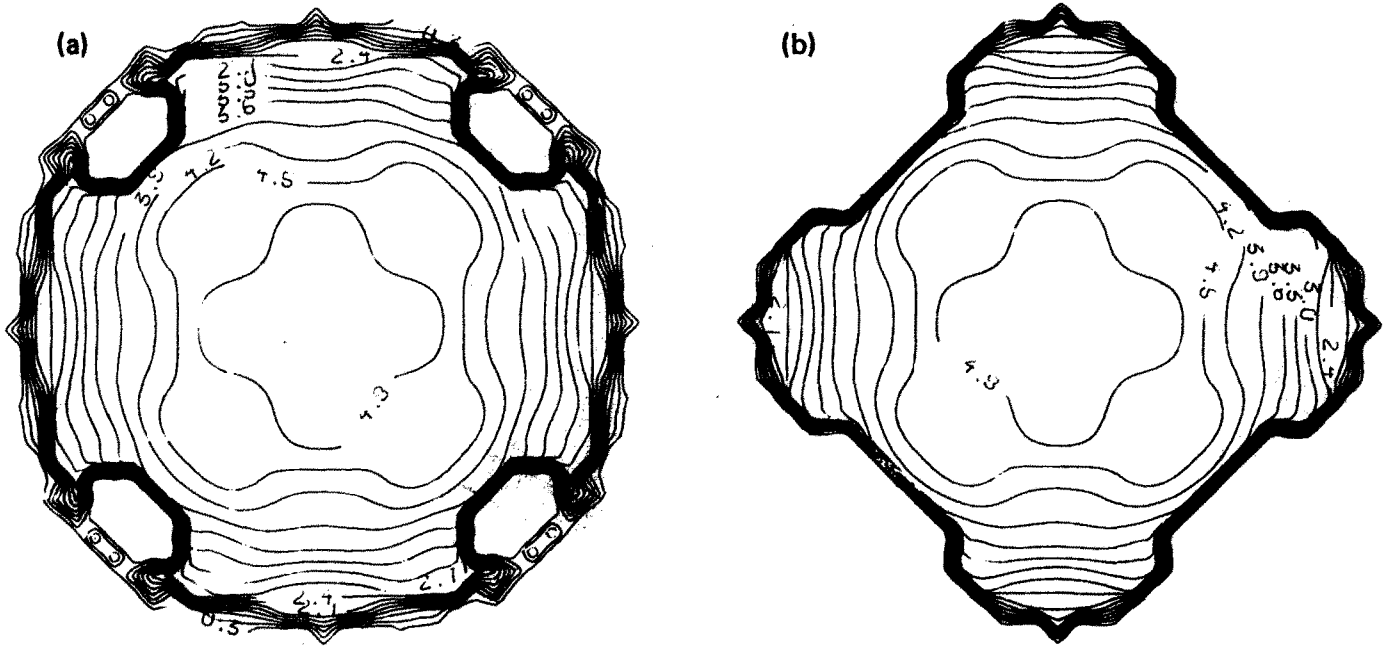


FIG. 9. Contour plot of Figs. 8(a) and 8(b).

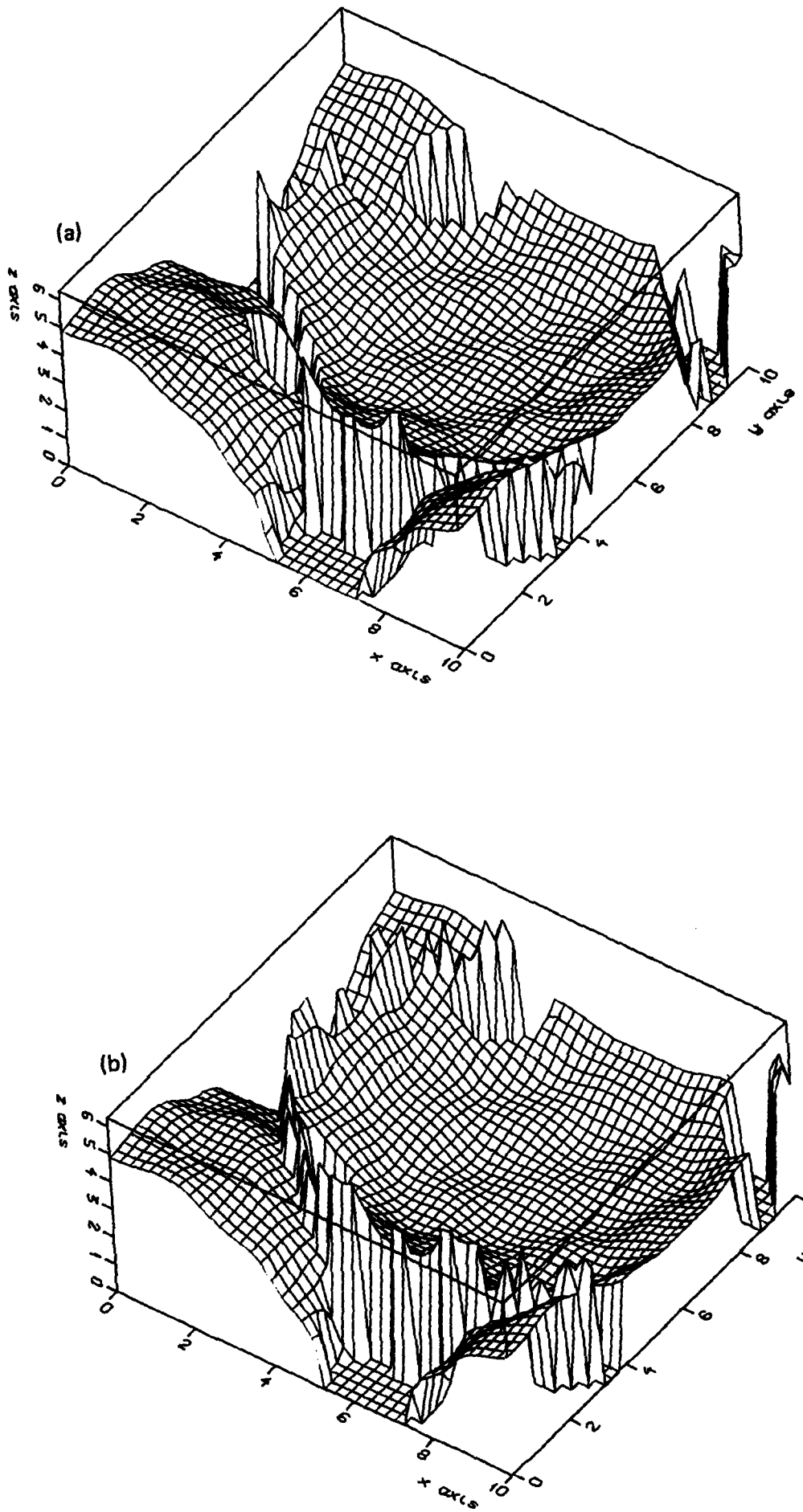
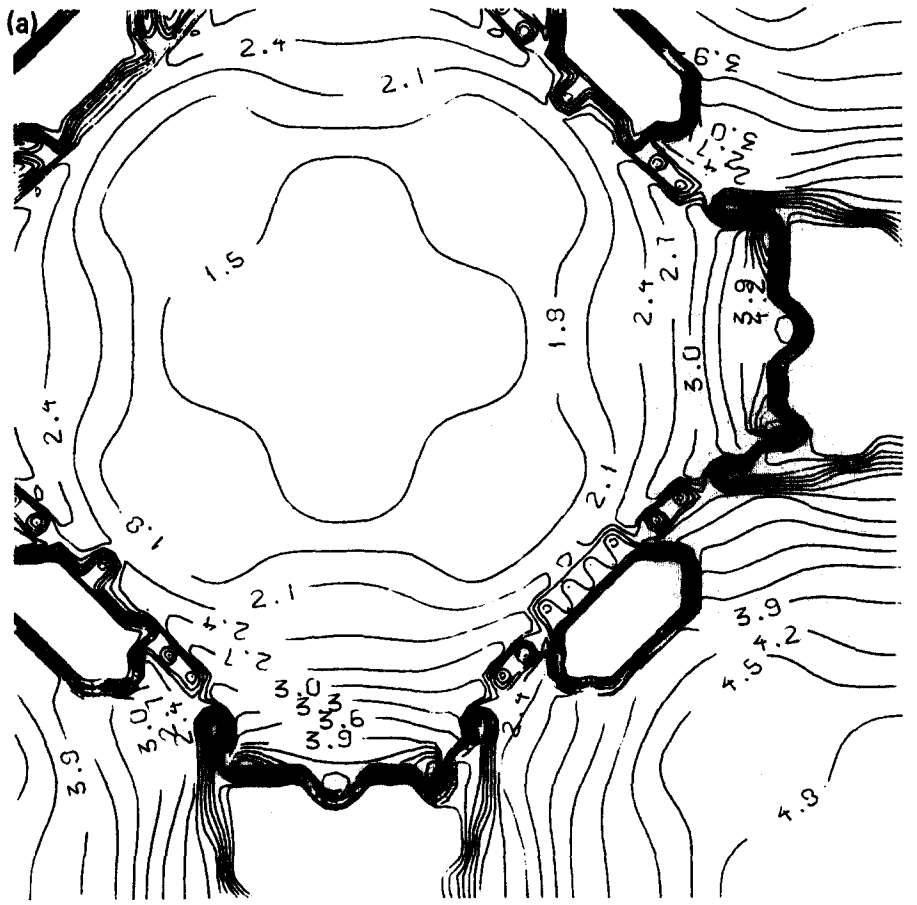


FIG. 10. The Fermi surface of Figs. 8(a) and 8(b) extended periodically.



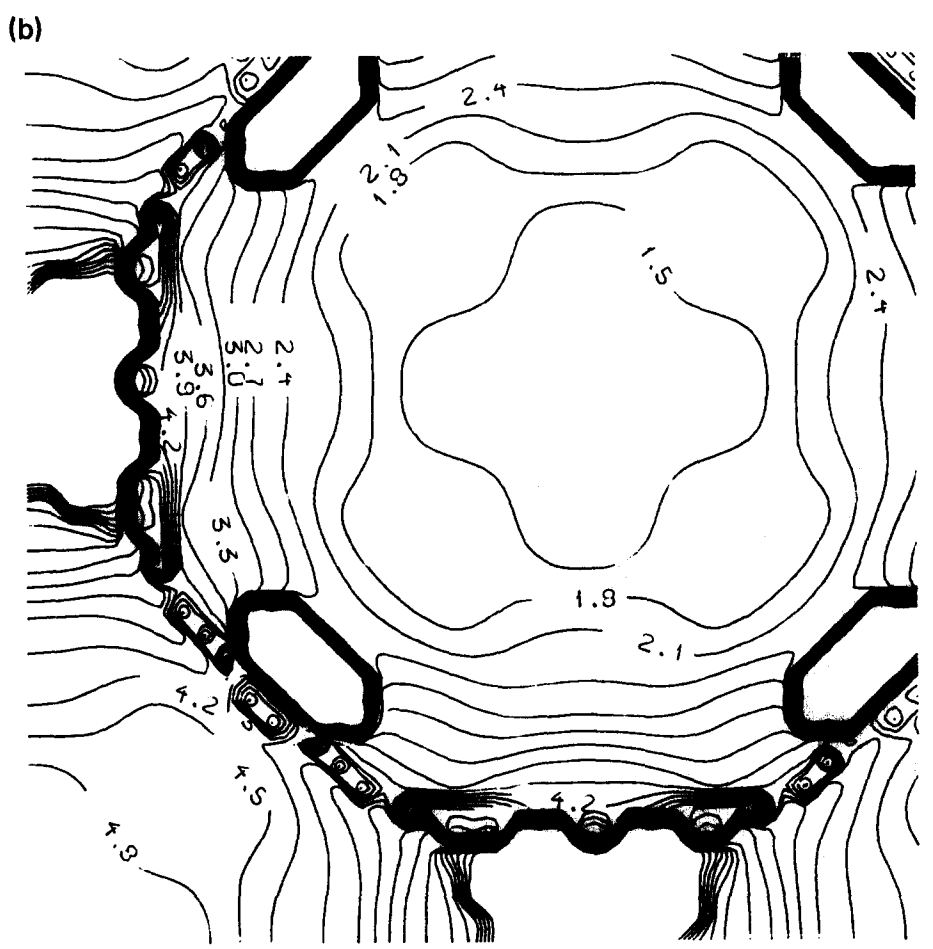
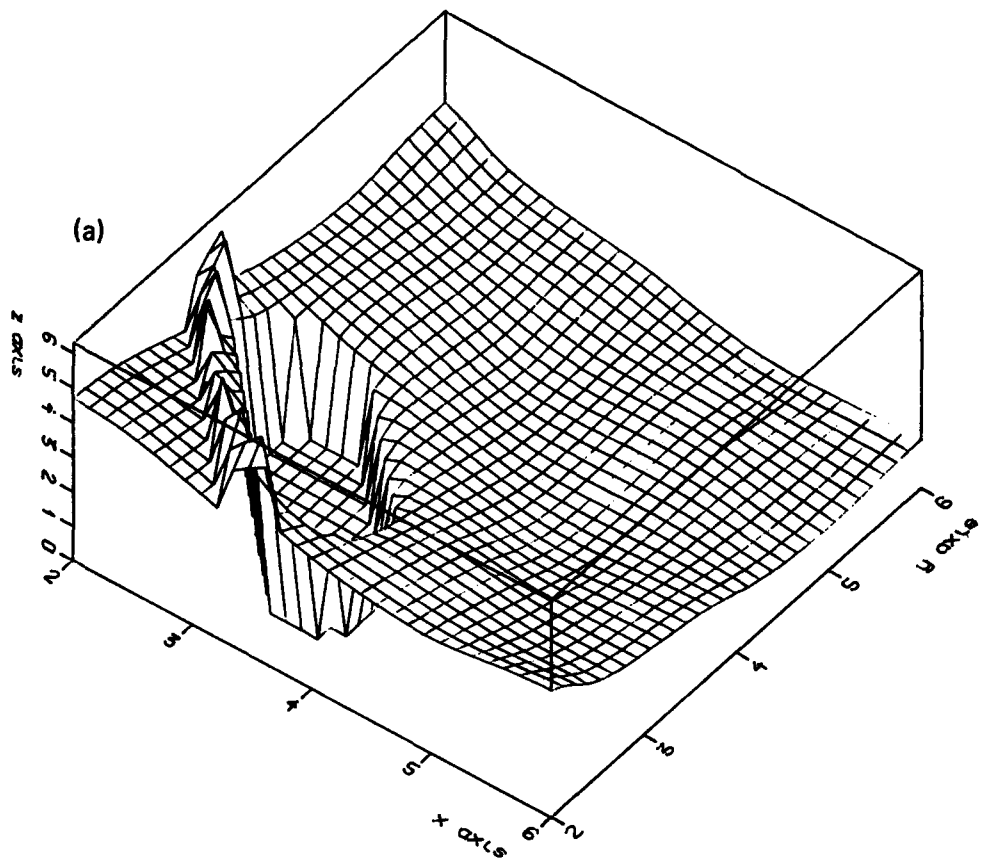


FIG. 11. Contour plot of Figs. 10(a) and 10(b).



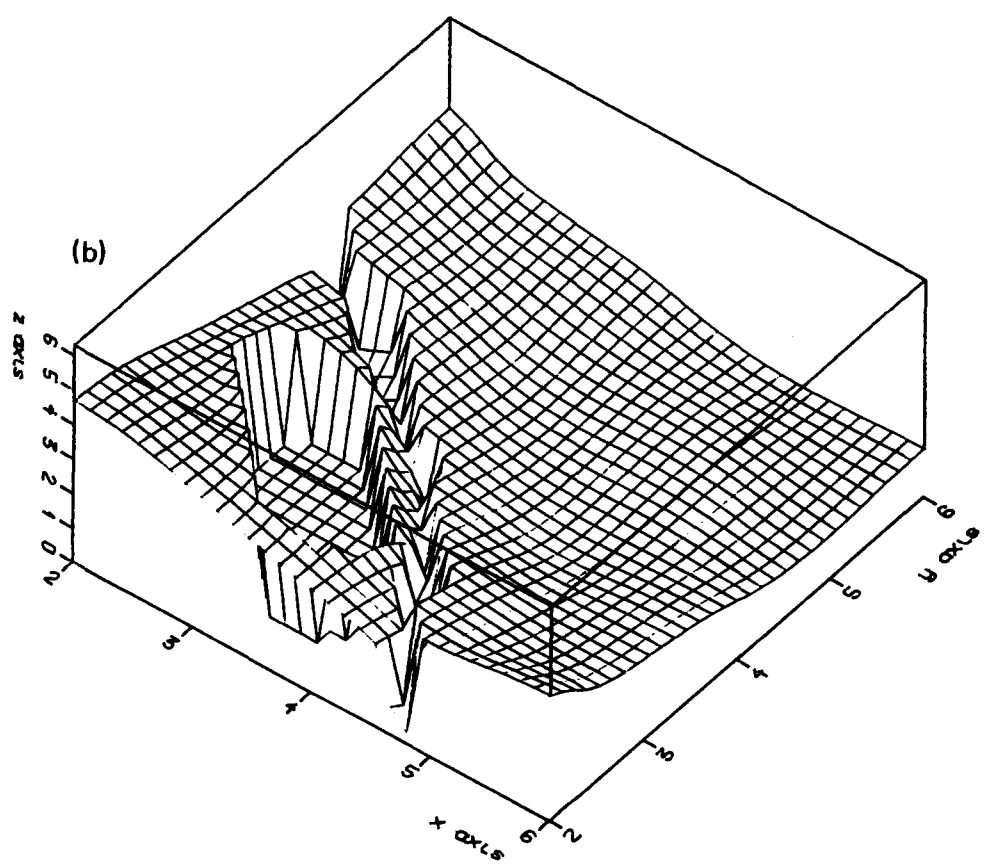


FIG. 12. A magnification of a part of Figs. 10(a) and 10(b).

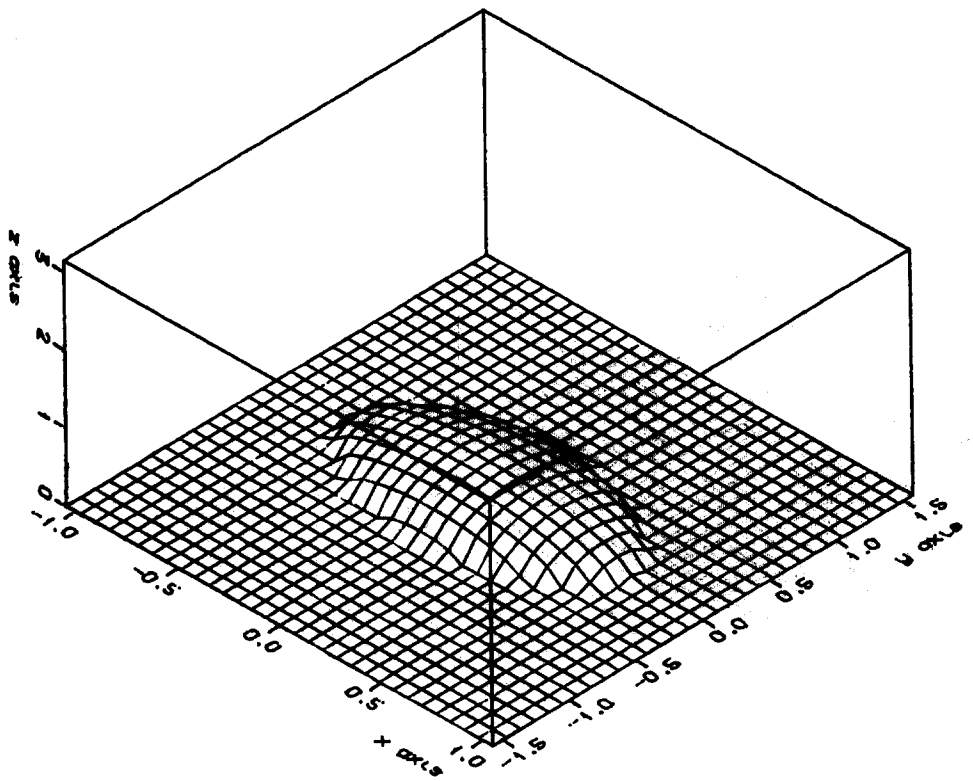


FIG. 13. $E = -1.2$. The Fermi surface is homeomorphic to a sphere around each print of the orthogonal lattice.

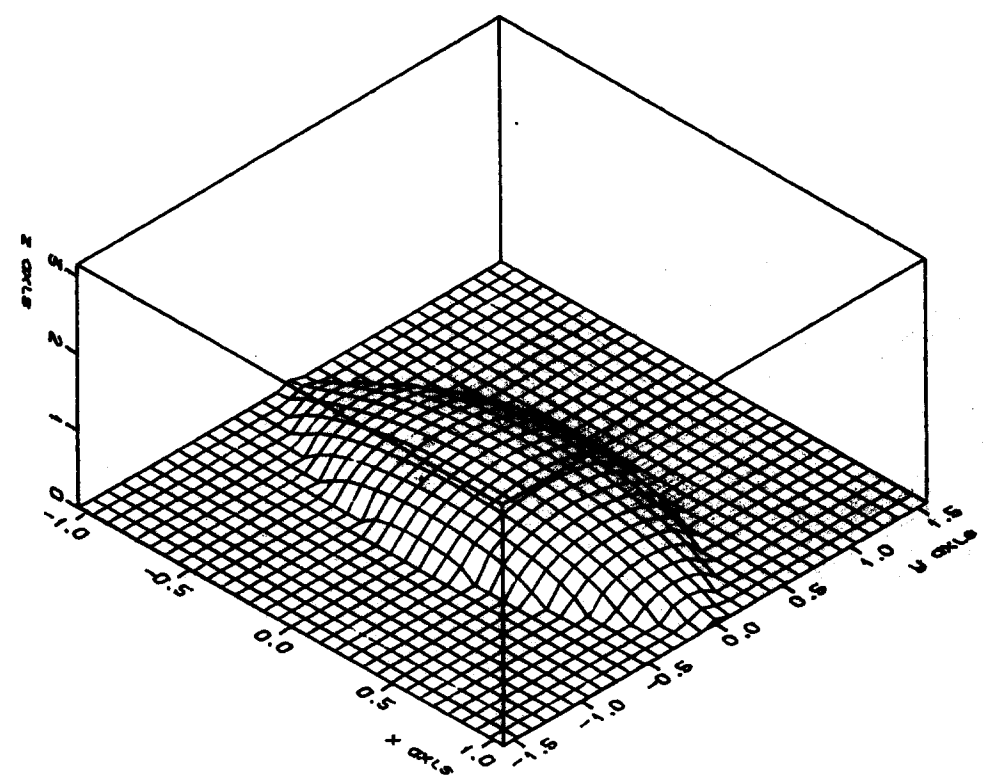


FIG. 14. $E = -1.1$.

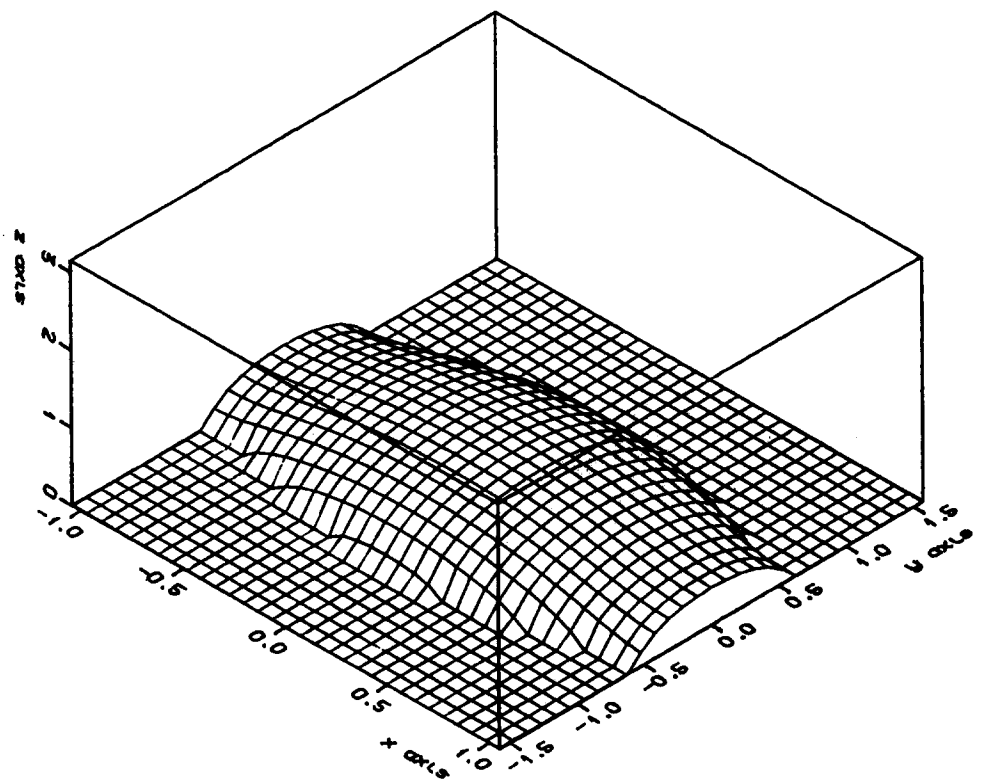


FIG. 15. $E = -0.9$. The Fermi surface is now connected in the x direction.

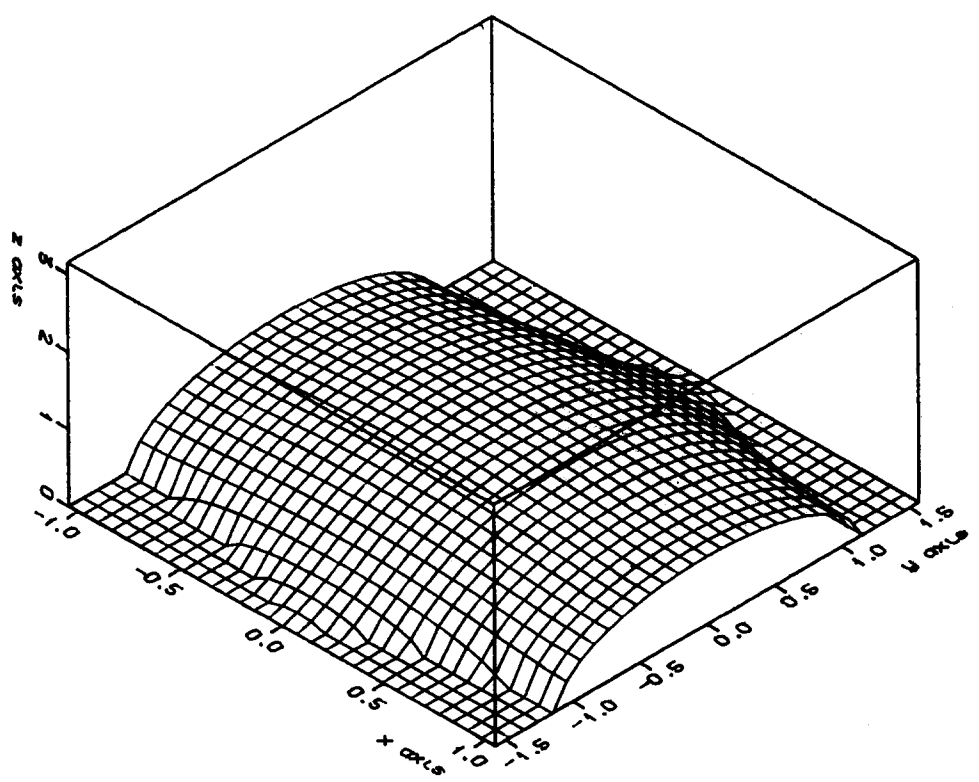


FIG. 16. $E = -0.425$.

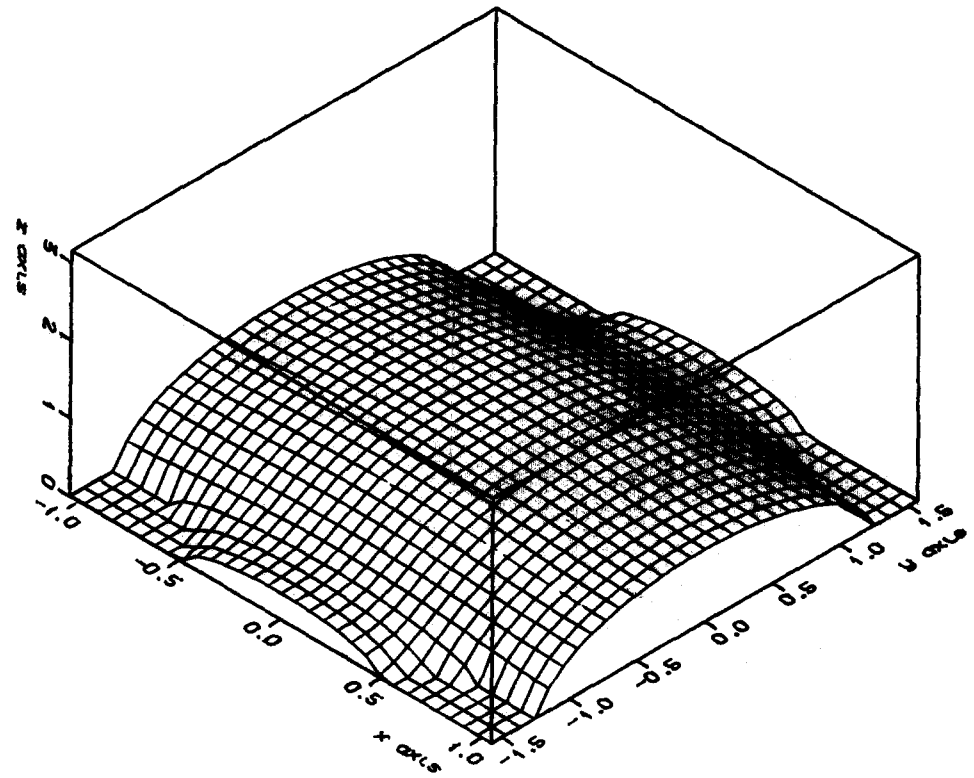


FIG. 17. $E = -0.35$. The Fermi surface is connected in the x and y directions.

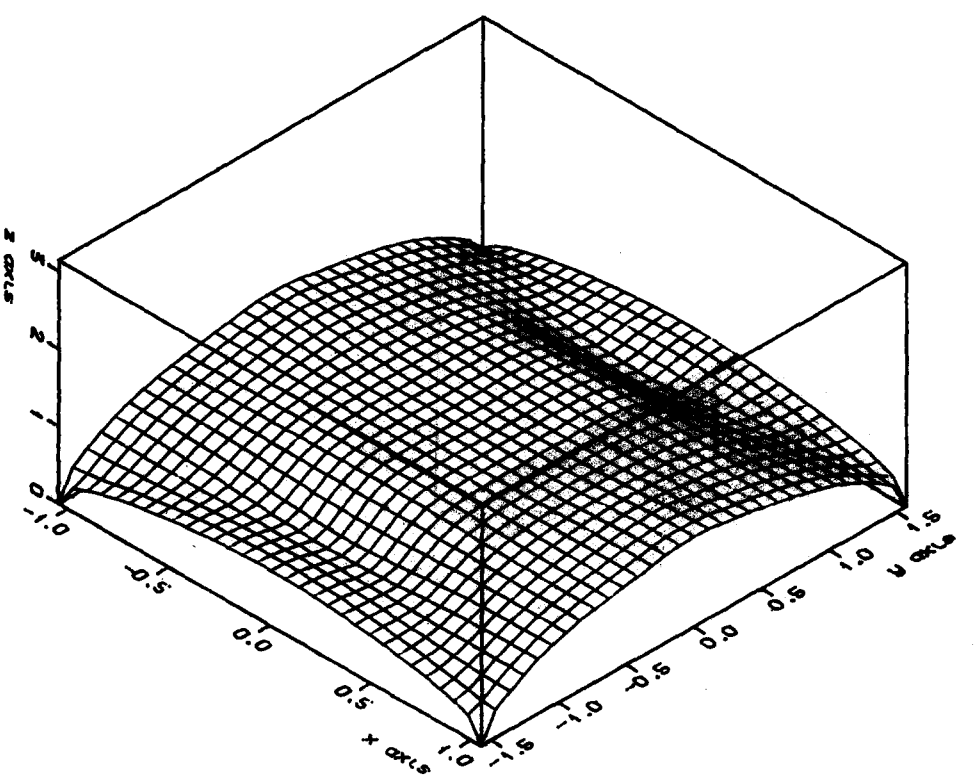


FIG. 18. $E = -0.13$.

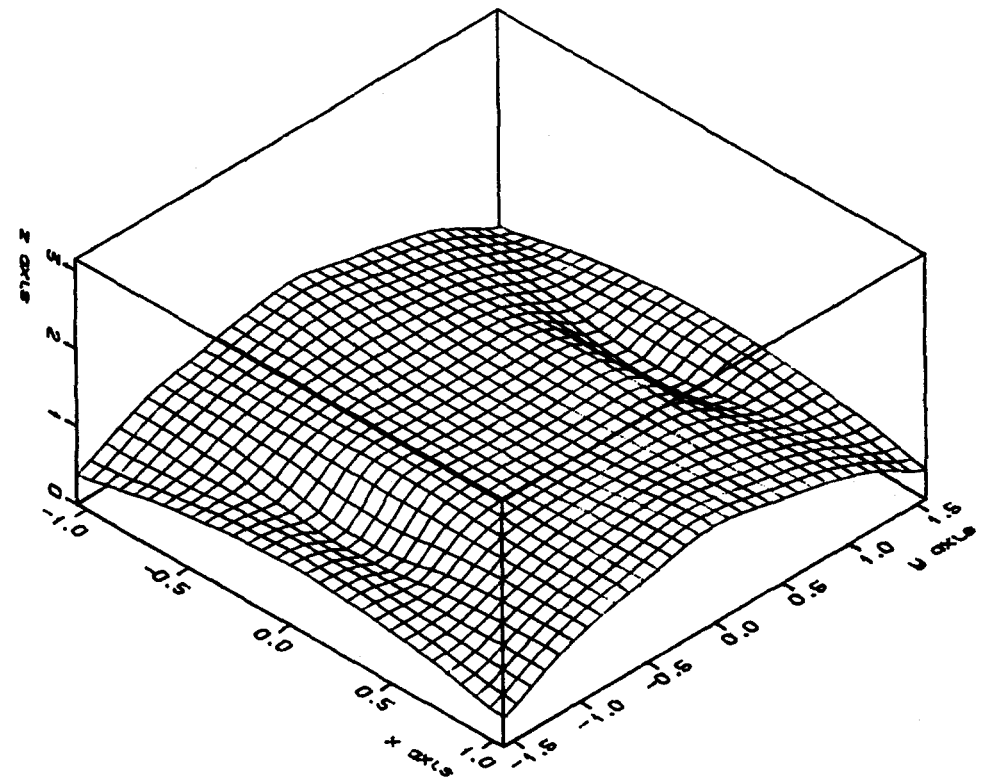


FIG. 19. $E = -0.1$.

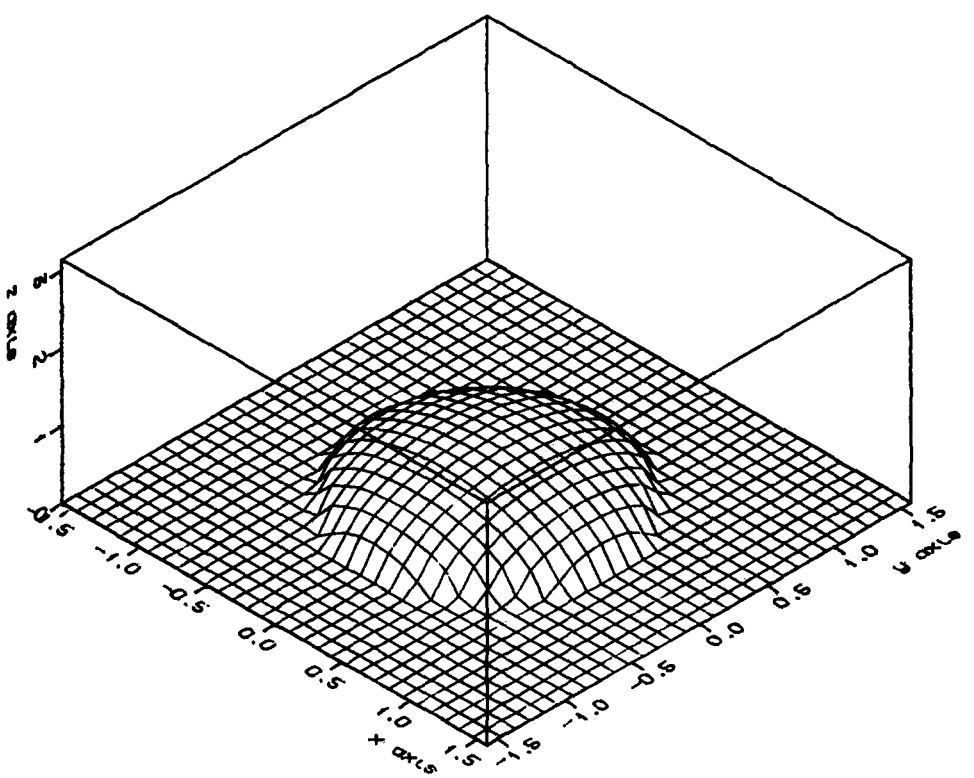


FIG. 20. $E = -1.1$.

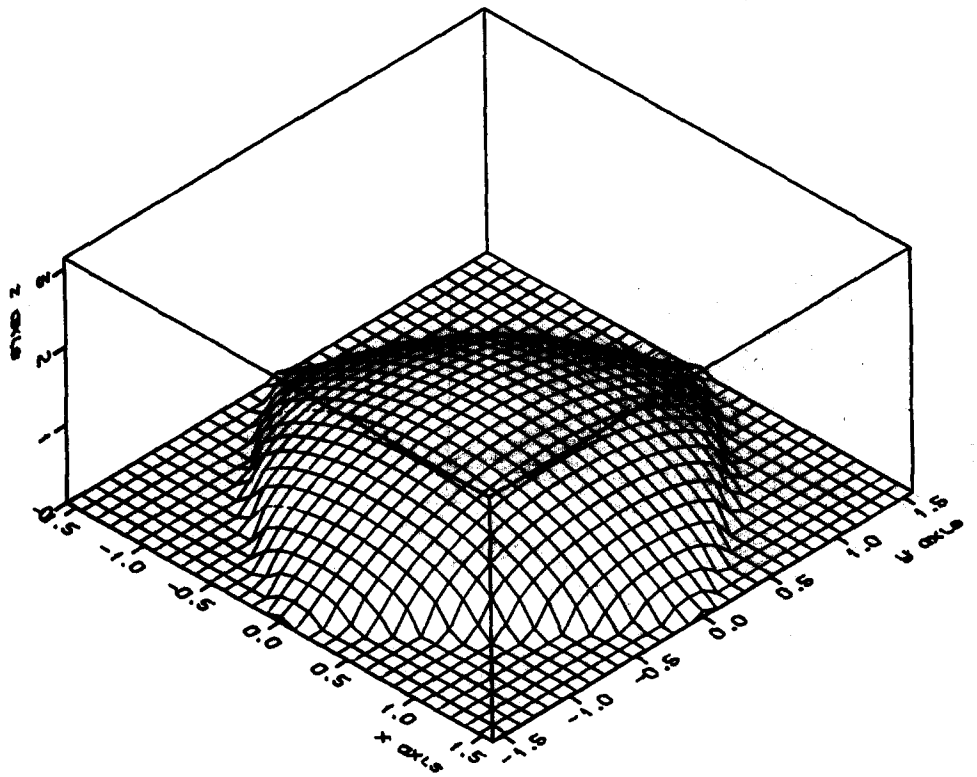


FIG. 21. $E = -0.6$.

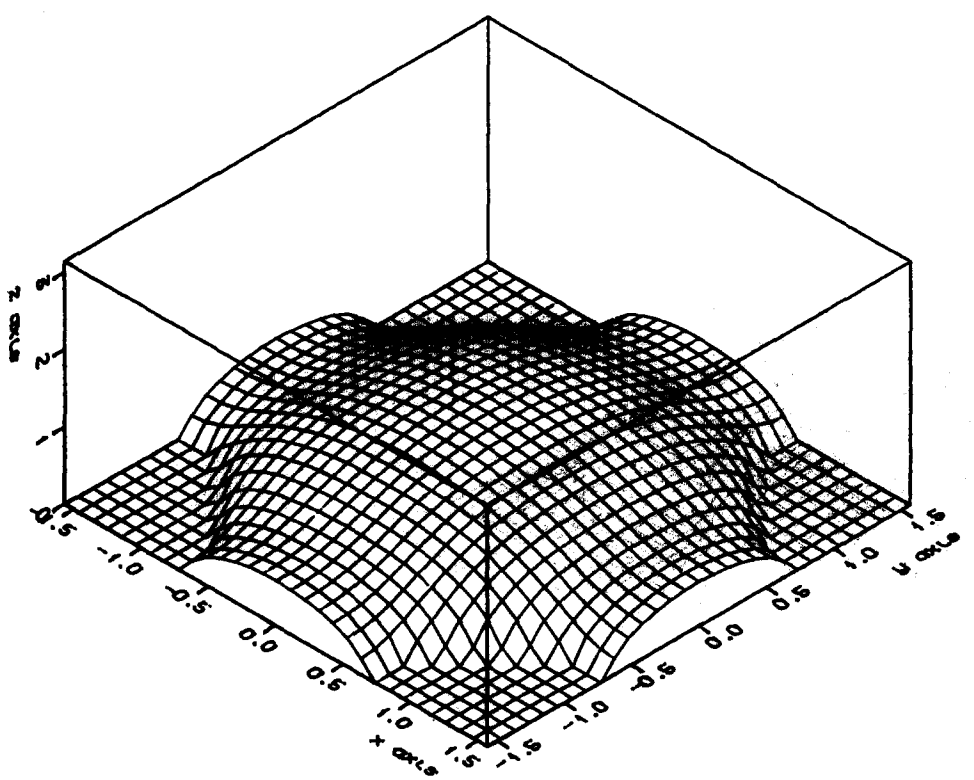


FIG. 22. $E = -0.4$.

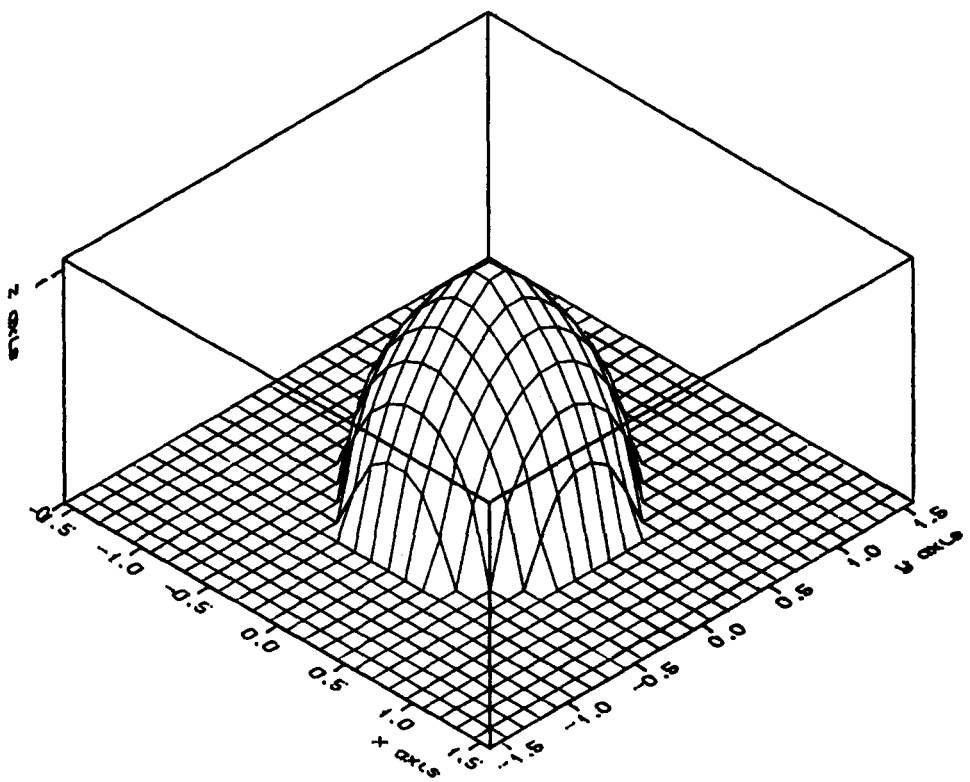


FIG. 23. $E = -0.2417$.

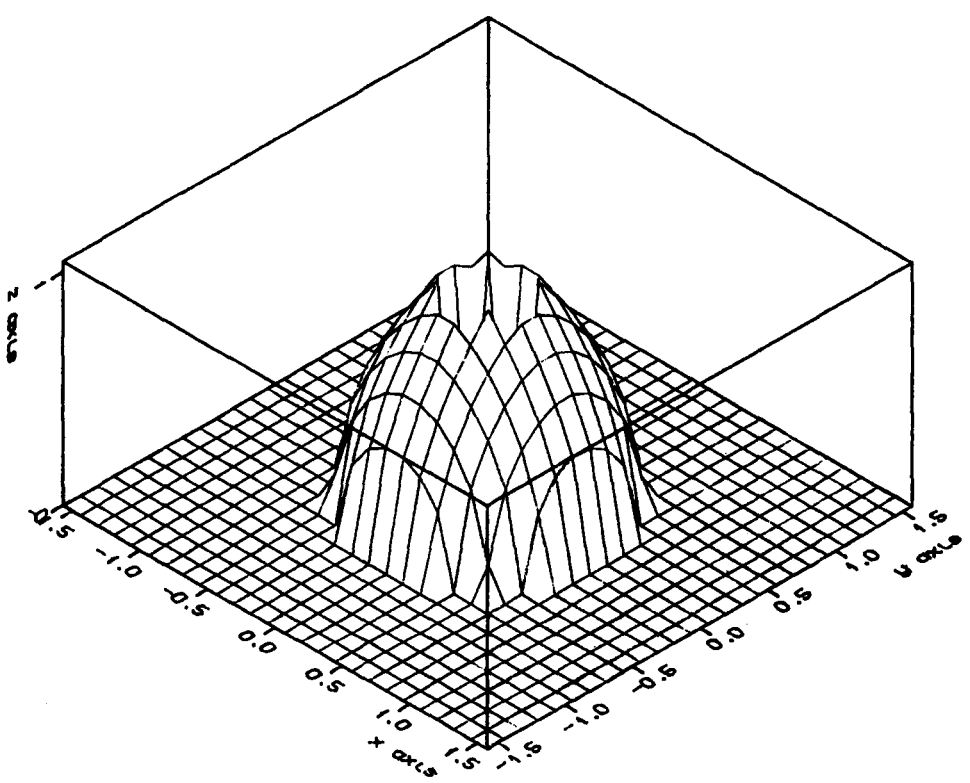


FIG. 24. $E = -0.2$. The Fermi surface is now connected in the z direction.

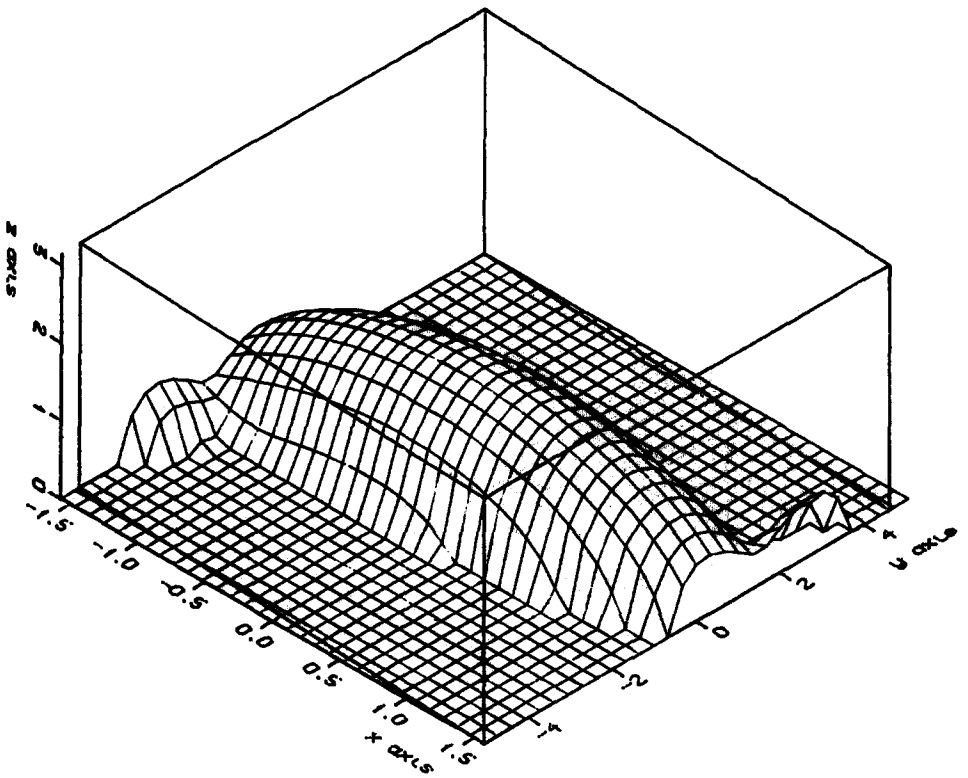


FIG. 25. The surface for a monoclinic C crystal with axes $a = 2$, $b = 1.5$, and $c = 1$ inside the upper half of its Brillouin zone. The angle between the axes a and c is 60°, $\alpha = 0$, and $E = -1$.

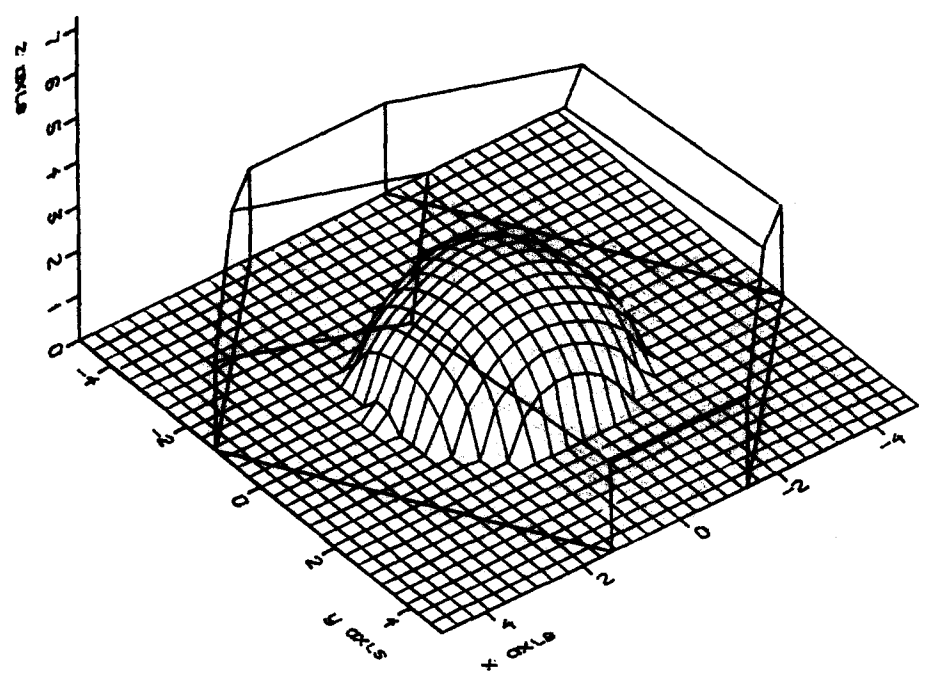


FIG. 26. The Fermi surfaces of a trigonal crystal with $\alpha = 0$ and $E = -1$ for an angle of 30° between the symmetry axis and each of the crystal axes.

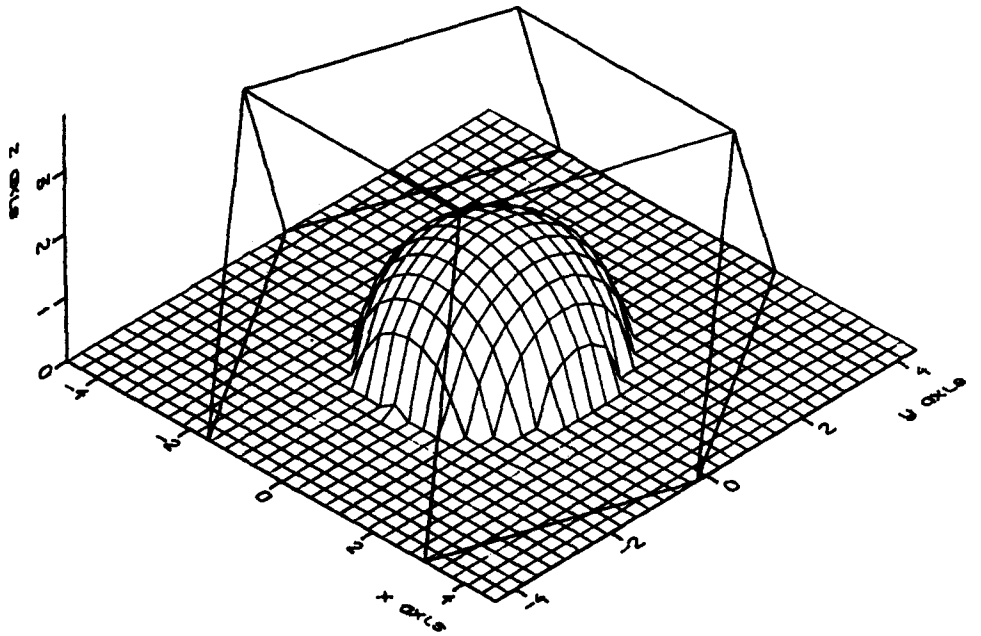


FIG. 27. The Fermi surfaces of a trigonal crystal with $\alpha = 0$ and $E = -1$ for an angle of 70° between the symmetry axis and each of the crystal axes.

ACKNOWLEDGMENT

We would like to thank the Computer Centre, Univeristy of Oslo, for its help with various computer technical problems.

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Two-fluid cosmological models

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Homogeneous and isotropic, relativistic two-fluid cosmological models are investigated. In these models two separate fluids act as the source of the gravitational field, as represented by the FRW line element. The general theory of two-fluid FRW models in which neither fluid need be comoving or perfect is developed. However, attention is focused on the physically interesting special class of flat FRW models in which one fluid is a comoving radiative perfect fluid and the second a noncomoving imperfect fluid. The first fluid is taken to model the cosmic microwave background and the second to model the observed material content of the universe. One of the motivations of the present work is to model the observed velocity of our galaxy relative to the cosmic microwave background that was recently discovered by G. F. Smoot, M. V. Gorenstein, and R. A. Muller [Phys. Rev. Lett. **39**, 898 (1977)]. Several models within this special class are found and analyzed. The models obtained are theoretically satisfactory in that they are represented by solutions of Einstein's field equations and the laws of thermodynamics in which all the physical quantities occurring in the solutions are suitably well behaved. In addition, the models are in agreement with current observations. Consequently it is believed that the models obtained are physically acceptable models of the universe.

I. INTRODUCTION

In this article we shall consider cosmological models that have two fluids (possibly imperfect) as the source of the gravitational field. In particular, we shall be dealing with isotropic and homogeneous models in which the metric is the general FRW line element given, in a "spherical polar coordinate system," by

$$ds^2 = -c^2\,dt^2 + R^2(t)\,\{dr^2/(1-kr^2) + r^2\,d\theta^2 + r^2\sin^2\theta\,d\phi^2\}\,, \tag{1.1}$$

where t is the cosmic time, R is the expansion factor, and k the normalized curvature constant (i.e., $k = -1, 0, +1$, depending on whether the model is open, flat, or closed). We shall also wish to study such models in "axial coordinates" in which the flat ($k = 0$) line element takes on the form

$$ds^2 = -c^2\,dt^2 + R^2(t)\{dx^2 + dy^2 + dz^2\}\,. \tag{1.2}$$

Although we shall be dealing with isotropic and homogeneous models, the analysis can, of course, be applied to general two-fluid cosmological models. In addition, we shall, for physical reasons that will be discussed below, focus our attention on models in which one of the two cosmological fluids is a comoving perfect fluid (black-body) radiation field.

The motivation behind this research is twofold. First, it has been established that cosmological models, in particular FRW models, can be interpreted as solutions of Einstein's field equations for a variety of different sources. In the earliest solutions the source was taken to be a comoving perfect fluid. Later, and mainly in the 1960's, authors interpreted the gravitational field to be due to two cosmological fluids, both perfect and comoving (see Sec. II). More recently,[1] FRW models have been investigated in which the source is a noncomoving imperfect fluid either (i) with or without heat conduction or (ii) with or without electromagnetic field. It is thus the aim to complete this mathematical analysis and investigate FRW models in which two-fluid sources are present, neither of which need be comoving or perfect.

It will be noted that models of this type are already implicitly available, for if we take a known two-fluid model, then we can "reinterpret" each of the two fluids separately using the techniques developed in Coley and Tupper.[1] However, in Secs. III and IV a general analysis of two-fluid cosmological fluids will be presented.

It will also be noted that this does not, strictly speaking, complete the general investigation of the interpretation of FRW models, since articles have been written in which n (comoving, perfect) fluids have constituted the source of the gravitational field (see Sec. II). Thus in a full analysis there would be n fluids, in general noncomoving and not necessarily perfect. However, such an analysis will not be undertaken here. First, an investigation involving n fluids (rather than two) would not introduce any new interesting or significant features from a mathematical point of view. Second, there is not such a strong physical motivation for studying n (>2) fluid models.

The second motivation for the present work is strictly physical. The presently accepted view of the evolution of the universe is that, except for very early times (when $T > 10^{10}$–10^{12} K, $T \sim 10^{10}$ K corresponds to $t \sim 10$ sec), the universe is reasonably described by "a FRW model." The conventional wisdom is that the universe evolved initially from a radiationlike state to a matterlike universe ("dust") at later times.

The first FRW models to appear had as sources either comoving radiation perfect fluids *or* comoving matter per-

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fect fluids; each model was supposedly applicable to different eras in the evolution of the universe. Later, attempts were made to take a known radiation model and a known matter model and smoothly (or, at least, continuously) match up the models at $\rho_r = \rho_m$ (where ρ denotes the energy density and the indices refer to the radiation and matter fluids) in order to obtain a qualitative description of the evolution of the universe in terms of a single model (see, for example, Refs. 2 and 3).

The discovery in 1965[4,5] of the 2.7 K isotropic cosmic microwave background, which was presumed to be a remnant of the "primeval fireball," stimulated renewed interest in the subject, and led many authors to investigate FRW models which included both matter and radiation fields (for all times). In these models the source of the gravitational field is assumed to be two comoving perfect fluids; a brief review of this approach will be given in Sec. II.

Recently it was discovered[6] that there is an observed motion of our galaxy relative to the microwave background radiation. This, in turn, stimulates our present interest in models in which there are two cosmological fluids, one representing the background radiation field and the second a matter field constituting the observed galaxies, and in which there is a relative motion between the two fields. We shall take the cosmic microwave background radiation field as comoving and thus seek models in which the matter field is noncomoving. Since the isotropy and homogeneity of both the cosmic microwave background and the observed matter is established to a reasonable experimental accuracy, we shall wish to study models in which isotropy and homogeneity is preserved, that is, FRW models. Thus we shall wish to investigate FRW models that have two fluids present, a comoving radiation field, and a tilting matter field. However, this is possibly only if one of the fluids (here assumed to be the matter field) is assumed to be imperfect.

There is one more aspect to this type of research worth mentioning here. There are two approaches possible. First, the expansion factor $R(t)$ in Eq. (1.1) can be specified and solutions are then sought in which two fluids constitute the source. The problem of finding such a model is essentially an algebraic mathematical problem; the outstanding problems that then need to be resolved require a determination of whether the resulting fluids are physically interesting. The second approach is to specify (physical) equations of state for the fluids present; seeking a model then consists of solving differential equations for the remaining unknown quantities in the model [for example, in the standard two-perfect-fluids case we have to solve an ordinary differential equation for $R(t)$]. Both approaches have been taken in the literature, and both will be discussed in this article.

As mentioned above, in Sec. III the theory of two general fluid sources in FRW models will be investigated. We shall discuss both "radial" and "axial" systems. In Sec. IV we shall restrict attention to the physically important case in which one fluid is comoving, perfect (black-body) radiation fluid and the second fluid a noncomoving imperfect fluid. Several acceptable models will be found, which will be discussed in Sec. V. The notation to be used in this article is similar to that found in Coley and Tupper[1] and McIntosh.[7-9]

II. THE STANDARD THEORY OF TWO-FLUID COSMOLOGIES

Einstein's field equations, with metric (1.1), and for a comoving perfect fluid source are (in cgs units)

$$8\pi G\rho = 3\left(\frac{\dot{R}^2}{R^2} + \frac{kc^2}{R^2}\right) - \Lambda c^2,$$
$$\frac{8\pi G p}{c^2} = -\left(\frac{2\ddot{R}}{R} + \frac{\dot{R}^2}{R^2} + \frac{kc^2}{R^2}\right) + \Lambda c^2, \tag{2.1}$$

where Λ is the cosmological constant and a dot denotes differentiation with respect to t. From these equations follow the conservation law

$$\frac{d}{dt}(\rho R^3) + \frac{p}{c^2}\frac{d}{dt}(R^3) = 0. \tag{2.2}$$

To complete the solution an equation of state relating ρ and p is needed. The dimensionless function $\epsilon(t)$ is introduced where

$$\epsilon(t) \equiv p/\rho c^2. \tag{2.3}$$

[If $\Lambda \neq 0$, $\epsilon(t) = (8\pi G p/c^2 - \Lambda c^2)/(8\pi G\rho + \Lambda c^2)$, and Λ will appear in all subsequent equations. For the rest of this section we shall not include the cosmological constant.]

Suppose that the model contains both matter (with density ρ_m, pressure p_m) and radiation (ρ_r, p_r, and temperature T_r), then we can write

$$\rho = \rho_r + \rho_m, \quad p = p_r + p_m. \tag{2.4}$$

Thus the universe consists of two (comoving) cosmological perfect fluids. The temperature in these models is usually taken to be that of the radiation of the cosmic microwave background (i.e., the temperature is taken to be T_r), since it is argued that the thermal balance is maintained by the radiation. Indeed, Szekeres and Barnes[10] argue that since the entropy of the universe is almost entirely carried by photons (the ratio of number densities of photons to baryons is 10^8 based on a background temperature of 2.7 K) the thermodynamics is almost entirely dictated by the photon field. If thermal equilibrium is assumed during the expansion all components consequently share the common temperature T_r.

If the radiation field is black body we also have that

$$\rho_r = aT_r^4, \quad p_r/c^2 = \tfrac{1}{3}\rho_r, \tag{2.5}$$

where $a = 7.57 \times 10^{-15}$ erg cm^{-3} deg^{-4} is Stefan's constant.

For the two-fluid model we can write the conservation law (2.2) as

$$E_r + E_m = 0, \tag{2.6}$$

where

$$E_r \equiv \frac{1}{R^3}\left\{c^2\frac{d}{dt}(\rho_r R^3) + p_r\frac{d}{dt}(R^3)\right\},$$
$$E_m = \frac{1}{R^3}\left\{c^2\frac{d}{dt}(\rho_m R^3) + p_m\frac{d}{dt}(R^3)\right\}, \tag{2.7}$$

where E_r is the rate of energy transfer per unit volume from matter to radiation and E_m that from radiation to matter. These expressions were first introduced by Davidson[11] and used by McIntosh.[7]

If the two fluids do not interact then the radiation and matter are both independently conserved, i.e.,

$$E_r = E_m = 0 . \tag{2.8}$$

Since we have five variables, ρ_m, ρ_r, p_m, p_r, and R, two field equations [two of Eqs. (2.1) or (2.2) or one of (2.8)] and essentially two equations of state [(2.5) and one of (2.8)], if we assume that the two fluids are separately conserved we only need one more equation of state to determine the model. This final assumption is usually taken to be that the pressure of the matter field p_m is zero; that is, the pressure from the random motions of galaxies and interstellar matter is negligible. Thus the matter is taken to be "dust" and consequently

$$p_m = 0 . \tag{2.9}$$

Indeed, the inclusion of radiation in the FRW models is only slightly affected by its interaction with matter and, in fact, such an effect is of about the same magnitude as that of including a nonzero p_m.[12]

As an illustration, with the above assumptions we obtain

$$\rho_r = c_1 R^{-4} , \quad \rho_m = c_2 R^{-3} , \tag{2.10}$$

and thus

$$\epsilon(t) = 1/3(1 + \bar{c}R) \quad \text{or} \quad R(t) = c^*(1 - 3\epsilon)/\epsilon \tag{2.11}$$

(where c_1, c_2, $\bar{c}$, and c^* are constants). There remains one ordinary differential equation to solve for $R(t)$. We note that $\bar{c}R \ll 1$ initially so that $\epsilon = \frac{1}{3}$, and that $\bar{c}R$ is large at later times (regardless of k) so that $\epsilon = 0$; hence the model expands out of a pure radiation state towards a final matter (dust) state. This is, in fact, a general feature of all such two-fluid models, and is regarded as a desirable feature.

Lemaitre[13] was the first to find a model of this type. Lemaitre only considered the case $k = 0$. Other early solutions were found by Alpher and Herman[14] (for the case $k = +1$) and by Chernin[15] (for general values of k, i.e., $k = -1, 0,$ or $+1$). Chernin's solutions were shown by McIntosh[8] to be equivalent to results obtained by Tolman.[16] Further models of this type, in which the universe consists of two noninteracting fluids, were found by Cohen,[17] McIntosh,[8] and more recently by Nowotny[18] (all three for general k). Payne[19] used models of this type to investigate the effect of a cosmic microwave background with present temperature greater than 3 K (increasing T_0 decreases the age of the universe). Harrison[12] argues that if $T_r > T_b \sim 5\times 10^9$ K the models above break down due to lepton and hadron pair production, and so developed a model in which a (quantum mechanical type) single-fluid FRW model with equation of state $\epsilon(t) = \text{const}$ is matched continuously at $T_r = T_b$ (at $t = t_b \sim 10$ sec) to a Lemaitre model.

A slightly different approach to the problem is to consider a particular functional form for $R(t)$ (although, traditionally, this approach is not usually taken). There are, of course, certain constraints that should be imposed from the outset. Let us consider a $k = 0$ FRW model here. For small t we wish the model to be approximated by radiation so that $R(t) \sim t^{1/2}$ and the equation of state is $\epsilon(t) \sim \frac{1}{3}$. For large t we wish the universe to be approximated by the Einstein–de Sitter dust universe so that $R(t) \sim t^{2/3}$ and $\epsilon(t) \sim 0$ [moreover, we wish $R(t)$ to be a monotonically increasing function of t]. Formally, we require that $R(t) \sim t^{1/2}$ and $\epsilon(t) \to \frac{1}{3}$ as $t \to 0$ and $R(t) \to t^{2/3}$ and $\epsilon(t) \to 0$ as $t \to \infty$. We note that the specification of $R(t)$ will give rise to an algebraic relationship between ρ and p [i.e., will give rise to an equation of state $\epsilon(t)$] that may or may not be physical. Other physical constraints to be imposed include $\rho \geqslant 0$, $p \geqslant 0$ (for all t), and possibly we should restrict $\epsilon(t)$ to be a monotonically decreasing function of t. Note that we are allowing the equation of state of the material content of the universe to change with time.

As a simple illustration of the above we consider the expression[20]

$$R(t) = t^{1/2}(1 + lt^{3/5})^{5/18} , \tag{2.12}$$

where l is a positive constant such that $lt^{3/5}$ is dimensionless. With this choice of $R(t)$ we note that all the constraints outlined in the previous paragraph are satisfied, since $\dot{\epsilon} < 0$ for all t where the time varying equation of state $\epsilon(t)$, obtained from Einstein's field equations (2.1), is given by

$$3\epsilon(t) = (1 + \tfrac{8}{15} lt^{3/5})/(1 + \tfrac{8}{3} t^{3/5} + \tfrac{16}{9} l^2 t^{6/5}) . \tag{2.13}$$

With $R(t)$ specified we can calculate the forms of ρ and p explicitly. If we write $\rho = \rho_r + \rho_m$ and $p = p_r + p_m$ we cannot find ρ_r, ρ_m, p_r, and p_m independently unless we specify equations of state between ρ_r and p_r and between ρ_m and p_m. Suppose we again put $p_r = (c^2/3)\rho_r$, and, for simplicity, $p_m = 0$, then we obtain

$$\rho_r = (3/32\pi G)(t^{-2})(1 + lt^{3/5})^{-2}(1 + \tfrac{8}{15} lt^{3/5}) , \tag{2.14}$$

$$\rho_m = (l/5\pi G)(t^{-7/5})(1 + lt^{3/5})^{-2}(1 + \tfrac{5}{6} lt^{3/5}) . \tag{2.15}$$

We note that in this model $E_m \neq 0$. In fact, we find that

$$E_m = (c^2 l/50\pi G)(t^{-12/5})(1 + lt^{3/5})^{-3}(1 - \tfrac{1}{6} lt^{3/5}) , \tag{2.16}$$

so that E_m is positive for small t and will become negative for sufficiently large t.

With $l = 1.06\times 10^{-7}$ we find that the model described above is in very good agreement with actual observations (see Ref. 20, Sec. V, and Table I).

This approach was in fact taken by McIntosh[9] in which he considered a $k = 0$ model of the above kind. In this model a particular functional form was taken for $R(t)$ and McIntosh attempted to show that this produced a model that was physically viable. Unfortunately, as pointed out by Jacobs,[3] in this particular model $\rho_m = \rho_r$ at $t_e \sim 8\times 10^{15}$ sec, whereas conventional wisdom[14] suggests that $t_e \sim 10^{12}$–10^{14} sec. The time t_e is when the universe enters the matter dominated stage and Gamow[21] has suggested that this is when galaxy formation begins.

This defect is not present in McIntosh's later models nor in the other models mentioned here. Nor is this defect necessarily present in models in which $R(t)$ is specified *a priori*, as can be seen from the model represented by Eqs. (2.12)–(2.16) and the models in Ref. 20 (see Secs. IV and V and Ref. 20). However, it is a general feature of two-fluid models that the including of radiation in a matter universe will tend to decrease t_0 and the inclusion of matter in a radiation universe will tend to decrease T_0.

The above comments serve to illustrate that not all models should be restricted by the severe constraints satisfied by

TABLE I. The observed or theoretical values of quantities appearing in this article are given below together with their sources where appropriate. We recall that a zero subscript denotes a quantity's current value.

Quantity	Numerical value	Refs./sources
Hubble constant H_0	55–100 km sec^{-1} Mpc^{-1}	various
Age of universe t_0	$2–6\times10^{17}$ sec	various
	2.5×10^{17} sec	Age of uranium and thorium isotopes
	5×10^{17} sec	Age determined for globular clusters
Temperature of cosmic microwave background T_0	2.5–3 K	Refs. 4, 5
ρ_0(total energy)	10^{-30}–5×10^{-29} g cm^{-3}	Ref. 24
$\rho_{r,0}$	10^{-34}–10^{-33} g cm^{-3}	(based on T_0 between 2.5 and 3 K)
$\rho_{m,0}$	5×10^{-31}–10^{-29} g cm^{-3}	Refs. 14, 24, 29
$p_{m,0}$	$1–5\times10^{-15}$ dyn cm^{-2}	
Within galaxy ρ_g	$1–3\times10^{-24}$ g cm^{-3}	Ref. 30
p_g	$5–7\times10^{-12}$ dyn cm^{-2}	
Time t_e at which $\rho_r = \rho_m$	10^{12}–10^{14} sec	Refs. 3, 14
Time at which elements form	10^2–10^3 sec	
Critical values of T	$T>10^{10}$ K	Radiation plus matter model breaks down due to lepton and hadron production (Ref. 12)
	$T>10^{12}$ K	p_m no longer negligible (Ref. 25)
	$T>2\times10^{12}$ K	Models break down
E_m (early times)	positive	Ref. 22
$E_{m,0}$	$-(10^{-30}$–$10^{-31})$ erg cm^{-3} sec^{-1}	Ref. 24
The velocity of the galaxy relative to the cosmic microwave background	200–600 km sec^{-1}	Ref. 6

the standard noninteracting two-fluid models discussed at the beginning of the section. Indeed, very soon after the noninteracting models were developed models were sought in which there was some energy transfer between the radiation and matter fields (i.e., $E_m \neq 0$) and (correspondingly) models were sought in which $p_m \neq 0$. Generically it is thought that at present there is a conversion or net rate of gain of energy per unit volume from radiation to matter (i.e., $E_{m,0} < 0$) due to the nuclear burning of stars in galaxies, and that $E_m \to 0$ as $t \to \infty$. It is believed that a reliable estimate for $E_{m,0}$ at present is $E_{m,0} \simeq -(10^{-31}$–$10^{-30})$ erg cm^{-3} sec^{-1}. It is also speculated[22] that $E_m > 0$ for small t (in the radiation dominated era) due to pair production and annihilation. It should be stressed that the above are only speculations and other forms for E_m may be acceptable.

Models in which the two fluids interact and consequently the energies of each are not separately conserved were investigated by many authors. McIntosh[7] developed general k models that exhibit the above generic behavior of E_m and include absorption and emission. Models with $k = 0$ were investigated in detail with equations of state of the form (i) $\epsilon(t) = \frac{1}{3}e^{-\beta t}$ and (ii) $\epsilon(t) = \frac{1}{3}(1+\mu t)^{-\lambda}$ (where β, μ, λ are positive constants chosen so that E_m is of the "correct" sign in the appropriate time periods). As in the models discussed earlier, these models generally evolve from an $\epsilon = \frac{1}{3}$ radiation dominated universe to an $\epsilon = 0$ dustlike final state.

Other interacting two-fluid models were found by May and McVittie[23] and Sistero.[24] In May and McVittie p_m is defined as an arbitrary function of t but is later restricted by $\epsilon(t)=\frac{1}{3}(1+\mu t)^{-\lambda}$ (and it is shown that McIntosh's solutions are the only ones possible in terms of elementary functions). The behavior of E_m is investigated in all models. Sistero also assumes p_m is an arbitrary function of t through $p_m=f(R)\rho_m$, where f is a non-negative function, and examines for general k the cases $\epsilon(t)=\frac{1}{3}(1+\mu t)^{-1}$ and $f(R)=(\alpha-\beta R+\gamma R^3)^{-1}$ in detail.

Other models in the literature that are variations on the above theme include (a) models with multifluids including those proposed by Vajk[25] [up to four noninteracting (possibly relativistic) fluids for general k], McIntosh[26] [n non-interacting fluids with equations of state $p_i=(\gamma_i-1)\rho_i$ and general k], Szekeres and Barnes[10] (radiation plus multicomponent Synge gas for general k), and Sistero[27] (three interacting fluids including two radiation fields—photons and neutrinos—for general k); (b) models with a nonzero cosmological constant including those proposed by May[22] (generalization of May and McVittie[23]) and McIntosh[26] (in which a nonzero cosmological constant is treated in terms of an additional fluid in an n–fluid model); and (c) other two-fluid models in which neither fluid is a radiation field (McIntosh[26]).

III. GENERAL TWO-FLUID MODELS

Einstein's field equations for two general viscous fluids are

$$\begin{aligned}(c^4/8\pi G)G^{ij}&=(\rho_r+c^{-2}p_r)v^iv^j+p_rg^{ij}-2\eta_r\sigma_r^{ij}+q_r^iv^j+q_r^jv^i\\&\quad+(\rho_m+c^{-2}p_m)u^iu^j+p_mg^{ij}-2\eta_m\sigma_m^{ij}\\&\quad+q_m^iu^j+q_m^ju^i,\end{aligned}\tag{3.1}$$

where $\sigma_{r,m}^{ij}$ is the shear tensor, $\eta_{r,m}$ the shear viscosity coefficient, $q_{r,m}^j$ the heat conduction vector, and v^i and u^i are the velocities of the r and m (radiation and matter) fields, respectively. We could investigate models in which these velocities are radially or axially directed. For illustration, in this section we shall consider the case when v^i and u^i both have nonzero components in the radial direction and can be written

$$v^i=(\alpha_r,\beta_rR^{-1},0,0),\quad u^i=(\alpha_m,\beta_mR^{-1},0,0),\tag{3.2}$$

where

$$\alpha_r^2-\beta_r^2=c^2,\quad \alpha_m^2-\beta_m^2=c^2.\tag{3.3}$$

Corresponding to (3.2) we also assume that the $q_{r,m}^j$ are of the form

$$\begin{aligned}q_i^r&=(Q_r/c)(\beta_r,-\alpha_rR,0,0),\\q_i^m&=(Q_m/c)(\beta_m,-\alpha_mR,0,0),\end{aligned}\tag{3.4}$$

so that $q_i^rv^i=q_i^mu^i=0$ and $Q_{r,m}^2\equiv(q_iq^i)_{r,m}$. In addition, there will be an appropriate set of thermodynamic laws governing the two fields (see Sec. IV).

With the metric taken in the form given by Eq. (1.1), Einstein's field equations become

$$\begin{aligned}3(\dot R^2+kc^2)/c^2R^2&=\frac{8\pi G}{c^4}\left\{\rho_r\alpha_r^2+\frac{1}{c^2}p_r\beta_r^2-\frac{4}{3c^2}\beta_r^2\eta_rX_r\right.\\&\quad-\frac{2}{c}Q_r\alpha_r\beta_r+\rho_m\alpha_m^2+\frac{1}{c^2}p_m\beta_m^2\\&\quad\left.-\frac{4}{3c^2}\beta_m^2\eta_mX_m-\frac{2}{c}Q_m\alpha_m\beta_m\right\},\\-(\dot R^2+2R\ddot R+kc^2)/c^2R^2&=\frac{8\pi G}{c^4}\left\{\rho_r\beta_r^2+\frac{1}{c^2}p_r\alpha_r^2-\frac{4}{3c^2}\alpha_r^2\eta_rX_r\right.\\&\quad-\frac{2}{c}Q_r\alpha_r\beta_r+\rho_m\beta_m^2+\frac{1}{c^2}p_m\alpha_r^2\\&\quad\left.-\frac{4}{3c^2}\alpha_m^2\eta_mX_m-\frac{2}{c}Q_m\alpha_m\beta_m\right\},\end{aligned}\tag{3.5}$$

$$\begin{aligned}-(\dot R^2+2R\ddot R+kc^2)/c^2R^2&=\frac{8\pi G}{c^4}\left\{p_r+\frac{2}{3}\eta_rX_r+p_m+\frac{2}{3}\eta_mX_m\right\},\\0&=\left\{\rho_r+\frac{1}{c^2}p_r-\frac{4}{3c^2}\eta_rX_r\right\}\alpha_r\beta_r-\frac{Q_r}{c}(\alpha_r^2+\beta_r^2)\\&\quad+\left\{\rho_m+\frac{1}{c^2}p_m-\frac{4}{3c^2}\eta_mX_m\right\}\alpha_m\beta_m\\&\quad-\frac{Q_m}{c}(\alpha_m^2+\beta_m^2),\end{aligned}$$

where

$$\begin{aligned}X_r&=(\dot\alpha_r/c+\beta_r'R^{-1}-\beta_rR^{-1}r^{-1})(1-kr^2)^{1/2},\\X_m&=(\dot\alpha_m/c+\beta_m'R^{-1}-\beta_mR^{-1}r^{-1})(1-kr^2)^{1/2},\end{aligned}\tag{3.6}$$

where a prime denotes differentiation with respect to r. All quantities are assumed to depend on r and t only.

Solutions of Eqs. (3.5) are already known in certain special cases. If we have one comoving perfect fluid (for example, $\rho_r\neq0$, $\alpha_r=c$, $\eta_r=Q_r=0$, $\rho_m=p_m=\eta_m=Q_m=0$) we have the standard one-fluid FRW models. If we have one noncomoving viscous fluid (for example, $\rho_r=p_r=\eta_r=Q_r=0$) we obtain the models of Ref. 1. If we have two comoving perfect fluids ($\alpha_r=\alpha_m=c$, $\eta_r=\eta_m=Q_r=Q_m=0$) we recover the solutions outlined in Sec. II. We can use the above solutions to obtain more general solutions in the following manner: We take a solution in which there are two comoving perfect fluids; each of the "perfect fluids" in this model is "equated" with a noncomoving viscous fluid according to the prescription in Ref. 1; thus we obtain a solution containing two noncomoving viscous fluids. As mentioned in Sec. I there will exist general solutions to Eqs. (3.5). However, in Sec. IV and the remainder of this article we shall seek solutions of Eqs. (3.5) in a particular configuration of physical interest.

IV. RADIATION AND VISCOUS FLUID MODELS

Motivated by the arguments outlined in Sec. I, we shall look for two-fluid models of the following description. We shall assume that the first fluid is a comoving, perfect fluid with radiative equations of state [Eq. (2.5)]. This fluid will

model the observed cosmic microwave background. The second fluid will be taken to be a noncomoving, imperfect fluid modeling the observed matter in the universe. We shall focus our attention on $k=0$ FRW models with line element given by Eq. (1.2) and will assume that the matter is moving axially relative to the comoving radiation, thus modeling the observed relative velocity between the center of our galaxy and the cosmic microwave background.

In this physical configuration Einstein's equations are

$$\frac{c^4}{8\pi G}G_{ij} = \frac{\rho_r}{3}(4v_iv_j + c^2g_{ij}) + \left(\rho_m + \frac{1}{c^2}p_m\right)u_iu_j + p_m g_{ij} - 2\eta_m\sigma^m_{ij} + q^m_i u_j + q^m_j u_i\,, \tag{4.1}$$

where $v_i = (-c,0,0,0)$. We shall assume u_i has an axial component and is of the form

$$u_i = (-\alpha,0,0,\beta R)\,, \tag{4.2}$$

where $\alpha^2 - \beta^2 = c^2$, and α and β are functions of z and t. We also assume that

$$q^m_i = (Q_m/c)(\beta,0,0,-\alpha R)\,, \tag{4.3}$$

so that $q^m_i u^i = 0$ and $Q^2_m \equiv q^m_i q^i_m$.

Using Eqs. (4.1)–(4.3), Einstein's field equations for $k=0$ become ($\beta \neq 0$)

$$\left(\frac{3c^2}{8\pi G}\right)\frac{\dot R^2}{R^2} = c^2\rho_r + \alpha^2\rho_m + \beta^2\frac{p_m}{c^2} - \frac{4}{3}\beta^2\frac{\eta_m}{c^2}\left(\frac{\dot\alpha}{c}+\frac{\beta'}{R}\right) - \frac{2\alpha\beta Q_m}{c}\,, \tag{4.4a}$$

$$\left(\frac{-c^2}{8\pi G}\right)\left(\frac{\dot R^2 + 2R\ddot R}{R^2}\right) = c^2\frac{\rho_r}{3} + \beta^2\rho_m + \alpha^2\frac{p_m}{c^2} - \frac{4}{3}\alpha^2\frac{\eta_m}{c^2}\left(\frac{\dot\alpha}{c}+\frac{\beta'}{R}\right) - \frac{2\alpha\beta Q_m}{c}\,, \tag{4.4b}$$

$$\left(\frac{-c^2}{8\pi G}\right)\left(\frac{\dot R^2 + 2R\ddot R}{R^2}\right) = c^2\frac{\rho_r}{3} + p_m + \frac{2c^2}{3}\frac{\eta_m}{c^2}\left(\frac{\dot\alpha}{c}+\frac{\beta'}{R}\right), \tag{4.4c}$$

$$0 = \rho_m + \frac{1}{c^2}p_m - \frac{4}{3}\frac{\eta_m}{c^2}\left(\frac{\dot\alpha}{c}+\frac{\beta'}{R}\right) - \frac{1}{c}\frac{(\alpha^2+\beta^2)}{\alpha\beta}Q_m\,, \tag{4.4d}$$

where a prime denotes differentiation with respect to z.

The temperature T_r associated with the radiation field satisfies $\rho_r = aT_r^4$. The physical quantities associated with the imperfect fluid will satisfy the set of thermodynamic laws set out below. Henceforward we shall drop the suffix m (pertaining to the matter field) on all physical quantities in the imperfect fluid (i.e., η, Q, n, S, T, κ) since there should be no confusion, retaining the m suffices on ρ_m and p_m only. In general we shall not take T_r and T equal in the models. This means that the two fluids will not be in thermal equilibrium throughout the history of the universe, which is what we expect for imperfect fluid solutions with nonzero heat conduction vector. However, we shall assume that the following set of thermodynamic laws, based on the assumption that deviations from thermodynamic equilibrium are not too large, are valid.

The thermodynamic laws are[1] the baryon conservation law,

$$(nu^\mu)_{;\mu} = 0\,; \tag{4.5}$$

Gibb's relation,

$$Td\left(\frac{S}{n}\right) = d\left(\frac{\rho_m}{n}\right) + p_m\, d\left(\frac{1}{n}\right); \tag{4.6}$$

positive entropy production,

$$(Su^\mu + T^{-1}q^\mu)_{;\mu} \geqslant 0\,; \tag{4.7}$$

and the temperature gradient law,

$$q^\mu = (-\kappa h^{\mu\nu}/c^2)(T_{,\nu} + Ta_\nu/c^2)\,, \quad \kappa \geqslant 0\,. \tag{4.8}$$

In the above n is the particle density (of the matter field), T the temperature, S the entropy density, $h^{\mu\nu} = g^{\mu\nu} + u^\mu u^\nu/c^2$ the projection tensor, $a_\nu = u_{\nu;\alpha}u^\alpha$ the acceleration vector, and κ the thermal conductivity. We note that Eq. (4.7) is automatically satisfied in the models under consideration if Eq. (4.8) holds.

In addition, we insist that the energy conditions $\rho_r > 0$, $\rho_m > 0$, $\rho_m - p_m/c^2 \geqslant 0$, $p_m \geqslant 0$ are all satisfied and we impose the "boundary conditions" (I) $\alpha \to c$ as $t \to \infty$, (IIa) $\alpha \to \infty$ as $t \to 0$, or (IIb) $\alpha \to Ac$ as $t \to 0$, where $A > 1$.

Solving Eqs. (4.4), we obtain

$$\rho_m = \frac{1}{c^2}\left\{\frac{1}{8\pi G}\left[\frac{\dot R^2}{R^2}(3\alpha^2 - \beta^2) - \frac{2\beta^2\ddot R}{R}\right] - \frac{\rho_r}{3}(3\alpha^2+\beta^2)\right\}, \tag{4.9a}$$

$$3p_m = \frac{1}{8\pi G}\left\{\frac{\dot R^2}{R^2}(5\beta^2 - 3\alpha^2) - \frac{2\ddot R}{R}(3\alpha^2 - 2\beta^2)\right\} - \frac{\rho_r}{3}(3\alpha^2+\beta^2)\,, \tag{4.9b}$$

$$\frac{\eta}{c^2}\left(\frac{\dot\alpha}{c}+\frac{\beta'}{R}\right) = \frac{-\beta^2}{2c^2}\left\{\frac{1}{8\pi G}\left[\frac{2\dot R^2}{R^2} - \frac{2\ddot R}{R}\right] - \frac{4}{3}\rho_r\right\}, \tag{4.9c}$$

$$Q = \frac{1}{c}\left\{\frac{1}{8\pi G}\left[\frac{2\dot R^2}{R^2} - \frac{2\ddot R}{R}\right] - \frac{4}{3}\rho_r\right\}\alpha\beta\,. \tag{4.9d}$$

The right-hand sides of Eqs. (4.9a) and (4.9b) are positive, which always ensures that the terms in braces on the right-hand sides of Eqs. (4.9c) and (4.9d) are positive, so that Q is the same sign as β and η is non-negative if and only if

$$\dot\alpha/c + \beta'/R \leqslant 0\,. \tag{4.10}$$

We note that Eq. (4.8) reduces to the single expression

$$Q=\frac{\kappa}{c^2}\left[\beta\dot{T}+\frac{\alpha T'}{cR}+T\dot{\beta}+\frac{T\alpha'}{cR}+\beta T\frac{\dot{R}}{R}\right]. \quad (4.11)$$

For $\kappa\geqslant 0$ we must have the expression in square brackets divided by β non-negative (since $Q\beta\geqslant 0$).

One final note concerning notation before the various models are established. The models set out below may also be solutions of Einstein's equations with a comoving perfect radiation fluid and a comoving perfect fluid matter field acting as the source; and in this sense the new models may be thought of as "reinterpretations" of standard-type two-fluid models. That is, the right-hand side of Eq. (4.1) may be formally equivalent to

$$(\rho_r^*/3)(4v_iv_j+c^2g_{ij})+(\rho_m^*+c^{-2}p_m^*)u_iu_j+p_m^*g_{ij}\,, \quad (4.12)$$

where $u_i=v_i=(-c,0,0,0)$ and $\rho_r^*=\rho_r$. The asterisk notation is being used to denote the pressure and density in the standard-type two-fluid FRW model. Using this notation, the left-hand side of Eq. (4.4a) can be written as $c^2\rho_r+c^2\rho_m^*$, and the left-hand sides of Eqs. (4.4b) and (4.4c) can be written as $(c^2/3)\rho_r+p_m^*$. In addition, Einstein's equations (4.9) can be written in the new notation as

$$\rho_m=(\alpha^2/c^2)\rho_m^*+(\beta^2/c^4)p_m^*\,, \quad (4.13a)$$

$$3p_m=\beta^2\rho_m^*+[(3\alpha^2-2\beta^2)/c^2]\,p_m^*\,, \quad (4.13a)$$

$$2\eta(\dot{\alpha}/c+\beta'/R)=-\beta^2(\rho_m^*+p_m^*/c^2)\,, \quad (4.13c)$$

$$cQ=\alpha\beta(\rho_m^*+p_m^*/c^2)\,. \quad (4.13d)$$

Note that if ρ_m^* and p_m^* are both non-negative, then so are ρ_m and p_m.

Models will exist in which the physical quantities occurring in the models depend upon both z and t. However, such models will not be explicitly sought here. Henceforward, we shall look for models in which the physical quantities are functions of t alone (i.e., α, β, and T are functions of t only). This is in keeping with the types of cosmological models that we seek, and is also a mathematical simplification that enables us to find solutions more easily. With this assumption the equations to be solved simplify as follows.

(a) Einstein's equations: Equations (4.9a), (4.9b), (4.9c), and (4.9d) determine ρ_m, p_m, η, and Q, respectively. Condition (4.10), which ensures η is non-negative, reduces to

$$\dot{\alpha}\leqslant 0\,. \quad (4.14)$$

(b) Thermodynamical laws: We can integrate the baryon conservation law (4.5) to obtain

$$n=n_0R^{-3}\alpha^{-1}\,, \quad (4.15)$$

where n_0 is a constant. If α, β, and n are functions of t alone, $T=T(t)$ guarantees that the Gibb's relation has a solution [T is the integrating factor that ensures that the right-hand side of Eq. (4.6) is an exact differential]. With $T=T(t)$, Eq. (4.6) determines S. The temperature gradient law (4.11) then determines κ. The condition for $\kappa\geqslant 0$ [ensuring Eq. (4.7)] reduces to

$$\dot{T}/T+\dot{\beta}/\beta+\dot{R}/R\geqslant 0\,. \quad (4.16)$$

(c) Other restrictions: We recall that all energies must be non-negative. We expect T to be a decreasing function of t. The conditions on α are

$$\text{(I)}\quad \alpha\to c \quad \text{as } t\to\infty\,,$$

$$\text{(IIa)}\quad \alpha\to\infty \quad \text{as } t\to 0\,, \quad (4.17)$$

or

$$\text{(IIb)}\quad \alpha\to\text{const}>c \quad \text{as } t\to 0\,.$$

A. Model I

We assume that

$$E_m=0 \quad \text{and} \quad p_m^*=0\,. \quad (4.18)$$

From Eqs. (2.7) we find that

$$\rho_r=c_1R^{-4} \quad \text{and} \quad \rho_m^*=c_2R^{-3}\,. \quad (4.19)$$

Einstein's equations now reduce to an ordinary differential equation for $R(t)$, whose solution is given by[8]

$$t+\text{const}=(2/3\lambda^2)(\lambda R-2\mu)(\lambda R+\mu)^{1/2}\,, \quad (4.20)$$

where $\lambda=(8\pi G/3)c^2$, $\mu=(8\pi G/3)c_1$. We note that $\rho_r=aT_r^4$ so that $T_r\sim R^{-1}$. From Eq. (4.14) $\dot{\alpha}<0$ so we observe that T_r and T cannot be equal, otherwise Eq. (4.16) is violated. Let us choose α, T in the following manner:

$$\rho_m^*=c_3T^{3/p}\,, \quad T=(c_2/c_3)^{p/3}R^{-p}\,, \quad (4.21)$$

and

$$\alpha=\frac{c(1+hR^{-q})}{(1+2hR^{-q})^{1/2}}\,, \quad \beta=\frac{chR^{-q}}{(1+2hR^{-q})^{1/2}}\,, \quad (4.22)$$

where $p(>\frac{3}{4})$, q, and h are positive constants. With this choice of α the conditions (4.17) are satisfied, and Eq. (4.14) is satisfied implying $\eta>0$, since

$$\dot{\alpha}/c=-qh^2R^{-2q-1}\dot{R}/(1+2hR^{-q})^{3/2}\,. \quad (4.23)$$

From Eqs. (4.21)–(4.23), Eq. (4.16) becomes

$$(1-p-q)+(2-2p-q)hR^{-q}>0\,, \quad (4.24)$$

which simply implies that $1-p-q\geqslant 0$ (providing $q\neq 0$). As an illustration let us choose $p=\frac{5}{6}$, $q=\frac{1}{7}$, whence from Eqs. (4.5), (4.6), (4.9), and (4.11) we obtain

$$\begin{aligned}
&\rho_m=c_2(1+hR^{-1/7})^2R^{-3}/(1+2hR^{-1/7})\,,\\
&3p_m/c^2=c_2h^2R^{-23/7}/(1+2hR^{-1/7})\,,\\
&\eta=(7c^2/2)c_2(1+2hR^{-1/7})R^{-3}(\mu+\lambda R)^{-1/2}\,,\\
&Q/c=c_2h(1+hR^{-1/7})R^{-22/7}/(1+2hR^{-1/7})\,,\\
&n=(n_0/c)(1+2hR^{-1/7})^{1/2}(1+hR^{-1/7})^{-1}R^{-3}\,,\\
&\kappa/c^2=\kappa_0(1+hR^{-1/2})(1+2hR^{-1/7})^{1/2}\\
&\qquad\times(\mu+\lambda R)^{-1/2}R^{-12/7}\,,
\end{aligned} \quad (4.25)$$

where $\kappa_0\equiv 7c_2^{9/7}c_3^{-2/7}h^{-1}$. We note that ρ_m and p_m are always positive with $(3p_m/c^2\rho_m)\to 1$ as $t\to 0$ and $(3p_m/c^2\rho_m)\to 0$ as $t\to\infty$.

B. Model II

We assume that

$$p_m^*=0\,, \quad E_m\neq 0\,, \quad 3\epsilon(t)=\rho_r/(\rho_r+\rho_m^*)\,. \quad (4.26)$$

In particular, we shall investigate

$$3\epsilon(t)=(1+\mu t)^{-\lambda}\,, \quad (4.27)$$

where μ and λ are positive constants. Standard two-fluid models of this type were investigated by McIntosh[7] and May and McVittie,[23] and the solutions (4.28) below are due to them. We note that with Eq. (4.27) $\epsilon\to\frac{1}{3}$ as $t\to 0$ and $\epsilon\to 0$ as $t\to\infty$. We also note that $E_m\neq 0$; indeed, $E_m>0$ for small t

and $E_m < 0$ for large t providing $\lambda < \frac{2}{3}$.

For illustrative purposes we shall investigate the model $\lambda = \frac{1}{2}$, $\mu = 3.5\times 10^{-9}$. The observational predictions of this model were studied by McIntosh.[7] Although the model is in reasonable agreement with actual observations, McIntosh showed that the model $\lambda = \frac{7}{11}$, $\mu = 4.4\times 10^{-11}$ is a better model in that it is in better agreement with observations. We shall consider the former model due to its simplicity, and since it serves to illustrate the general nature of such a class of models.

The model is characterized by[7]

$$\begin{aligned} &\epsilon(t) = \tfrac{1}{3}(1+\mu t)^{-1/2}, \quad \dot\epsilon = -\tfrac{9}{2}\mu\epsilon^3, \\ &R(t) = \frac{c_1(1+5\epsilon)^{5/6}(1-3\epsilon)^{1/2}}{\epsilon^{4/3}}, \\ &K \equiv \frac{\dot R}{R} = \frac{6\mu\epsilon^2}{(1+5\epsilon)(1-3\epsilon)}, \\ &\rho_r = (9/8\pi G)K^2\epsilon, \quad \rho_m^* = (3/8\pi G)K^2(1-3\epsilon), \end{aligned} \tag{4.28}$$

where c_1 is a positive constant.

We assume that α is of the form

$$\frac{\alpha}{c} = \frac{(1+h\epsilon^q)}{(1+2h\epsilon^q)^{1/2}}, \quad \frac{\beta}{c} = \frac{h\epsilon^q}{(1+2h\epsilon^q)^{1/2}}, \tag{4.29}$$

where h and q are positive constants. Note that as $t\to\infty$, $\alpha/c\to 1$ and as $t\to 0$ $(\epsilon\to\frac{1}{3})$, $\alpha/c\to(1+h3^{-q})(1+2h3^{-q})^{-1/2} > 1$. Also

$$\alpha\dot\alpha/\beta^2 = -\tfrac{9}{2}\mu q(1+h\epsilon^q)\epsilon^2(1+2h\epsilon^q)^{-1}, \tag{4.30}$$

so that $\dot\alpha < 0$, which implies that $\eta > 0$ in Eq. (4.9c). We also assume T is of the form

$$T = T_0 R^{-p}\epsilon^s, \tag{4.31}$$

where p and s are positive constants.

The condition for κ to be non-negative is $\dot T/T + \alpha\dot\alpha/\beta^2 + \dot R/R \geqslant 0$, which becomes

$$\begin{aligned} &\{4(1-p) - 3(s+q)(1+5\epsilon)(1-3\epsilon)\} \\ &\quad + 2h\epsilon^q\{4(1-p) - 3(s+q/2)(1+5\epsilon)(1-3\epsilon)\} \geqslant 0, \end{aligned} \tag{4.32}$$

which is certainly satisfied if the first term in the braces is positive for all ϵ. Since $(1+5\epsilon)(1-3\epsilon)$ is always positive and has a maximum value of $\frac{16}{15}$, Eq. (4.32) is (strictly) satisfied if

$$1 - p - \tfrac{4}{5}(s+q) \geqslant 0. \tag{4.33}$$

In this model we wish to relate the temperature of the radiation T_r and the temperature of the matter T. The temperatures T_r and T cannot be equal for all t otherwise Eq. (4.16) would be violated for particular eras. Nor would we necessarily expect that $T_r = T$ for all t, since the two fields would then always be in thermal equilibrium. However, as $t\to\infty$, E_m and E_r (and Q) tend to zero so that we might expect that there will be thermal equlibrium as $t\to\infty$. Therefore, in this model we shall add the restriction that

$$\text{as } t\to\infty, \quad T/T_r \to 1. \tag{4.34}$$

From (4.28), as $t\to\infty$ $(\epsilon\to 0)$, $K\to\epsilon^2$, $R\to\epsilon^{-4/3}$, $\rho_r\to\epsilon^5$, $T_r\to\epsilon^{5/4}$, $\rho_m^*\to\epsilon^4$, $T\to\epsilon^{(4p+3s)/3}$, so that Eq. (4.34) implies that

$$\tfrac{5}{4} = \tfrac{4}{3}p + s. \tag{4.35}$$

(Note that $\rho_m^* \sim T^{16/5}$ as $t\to\infty$ as a consequence.) Since $s \geqslant 0$ we have that $p \leqslant \frac{15}{16}$, and Eqs. (4.33) and (4.35) imply that $p - 12q \geqslant 0$.

As an illustration let us choose $p = \frac{3}{4}, s = \frac{1}{4}, q = \frac{1}{16}$. With these values $T/T_r\to 1$ as $t\to\infty$, and η and κ are always positive, so that the model is physically acceptable. From Eqs. (4.5), (4.9), and (4.11) the full solution becomes

$$\begin{aligned} \rho_m &= (27\mu^2/2\pi G)(1+h\epsilon^{1/16})^2(1+2h\epsilon^{1/16})^{-1} \\ &\quad\times\epsilon^4(1+5\epsilon)^{-2}(1-3\epsilon)^{-1}, \\ 3p_m/c^2 &= (27\mu^2h^2/2\pi G)(1+2h\epsilon^{1/16})^{-1} \\ &\quad\times\epsilon^{33/8}(1+5\epsilon)^{-2}(1-3\epsilon)^{-1}, \\ T &= T_0 c_1^{-3/4}(1+5\epsilon)^{-5/8}(1-3\epsilon)^{-3/8}\epsilon^{5/4}, \\ \eta &= (24c^2\mu/\pi G)(1+2h\epsilon^{1/16})^{1/2}\epsilon^2(1+5\epsilon)^{-2}(1-3\epsilon)^{-1}, \\ Q/c &= (27hq^2/2\pi G)(1+h\epsilon^{1/16})(1+2h\epsilon^{1/16})^{-1} \\ &\quad\times\epsilon^{65/16}(1+5\epsilon)^{-2}(1-3\epsilon)^{-1}, \\ n &= (n_0/cc_1^3)(1+2h\epsilon^{1/16})^{1/2}(1+h\epsilon^{1/16})^{-1} \\ &\quad\times\epsilon^4(1+5\epsilon)^{-5/2}(1-3\epsilon)^{-3/2}, \\ \kappa/c^2 &= \kappa_0(1+2h\epsilon^{1/16})^{1/2}(1+h\epsilon^{1/16})(1+5\epsilon)^{1/8} \\ &\quad\times(1-3\epsilon)^{3/8}\epsilon^{3/4}\big[\{2-\tfrac{15}{8}(1+5\epsilon)(1-3\epsilon)\} \\ &\quad + h\epsilon^{1/16}\{4-\tfrac{27}{8}(1+5\epsilon)(1-3\epsilon)\}\big]^{-1}, \end{aligned} \tag{4.36}$$

where $\kappa_0 = 9c_1^{3/4}/128\mu\pi GT_0$. We note that ρ_m and p_m are always positive and that

$$3p_m/c^2\rho_m \to 0 \quad \text{as } t\to\infty \ (\epsilon\to 0)$$

and

$$\frac{3p_m}{c^2\rho_m} \to \frac{h^2 3^{-1/8}}{(1+h3^{-1/16})^2} = \frac{0.872h^2}{(1+0.934h)^2},$$

as $t\to 0$ $(\epsilon\to\frac{1}{3})$. Note that this last expression continues increasing as h increases but is always less than 1.

C. Model III

We consider the model with

$$R(t) = t^{1/2}(1+lt^{3/5})^{5/18}, \tag{4.37}$$

as outlined in Sec. II. From Eqs. (2.14) and (2.15) we have that

$$\begin{aligned} \rho_r &= (3/32\pi G)(t^{-2})(1+lt^{3/5})^{-2}(1+\tfrac{8}{15}lt^{3/5}), \\ \rho_m^* &= (l/5\pi G)(t^{-7/5})(1+lt^{3/5})^{-2}(1+\tfrac{5}{6}lt^{3/5}), \\ p_m^* &= 0. \end{aligned} \tag{4.38}$$

We note that $\epsilon(t)$ and $E_m (\neq 0)$ are given by Eqs. (2.13) and (2.16), respectively.

We assume that α and β are of the form

$$\frac{\alpha}{c} = \frac{1+ht^{-q}}{(1+2ht^{-q})^{1/2}}, \quad \frac{\beta}{c} = \frac{ht^{-q}}{(1+2ht^{-q})^{1/2}}, \tag{4.39}$$

where h and q are positive constants. With this choice of α we note that as $t\to\infty$, $\alpha/c\to 1$ and as $t\to 0$, $\alpha/c\to\infty$. From Eq. (4.39) we have that

$$\frac{\alpha\dot\alpha}{\beta^2} = -qt^{-1}\frac{(1+ht^{-q})}{(1+2ht^{-q})}, \tag{4.40}$$

so that $\dot{\alpha}<0$ guaranteeing $\eta>0$ [Eq. (4.9c)]. We also assume T is of the form

$$T=T_0 t^{-b}R^{-p}\alpha^s, \tag{4.41}$$

where b, p, and s are positive constants.

Condition (4.16), ensuring κ is non-negative, becomes

$$\begin{aligned}&(\tfrac{1}{2}-\tfrac{1}{2}p-b-q)+(\tfrac{3}{2}-\tfrac{3}{2}p-3b-2q)ht^{-q}\\&\quad+(1-p-q-2b-sq)h^2t^{-2q}\\&\quad+(\tfrac{2}{3}-\tfrac{2}{3}p-b-q)lt^{3/5}\\&\quad+(2-2p-3b-2q)hlt^{-q}t^{3/5}\\&\quad+(\tfrac{4}{3}-\tfrac{4}{3}p-q-2b-sq)lh^2t^{-2q}t^{3/5}\geqslant 0\,.\end{aligned} \tag{4.42}$$

We note that this inequality is satisfied for all t (and all h and l) if (i) $s\leqslant 1$ and $\frac{1}{2}-p/2-b-q\geqslant 0$ or (ii) $s>1$ and $1-p-2b-q-sq\geqslant 0$. There will be various solutions depending on the desired behavior of physical quantities (such as T) as $t\to 0$ or $t\to\infty$. Here, we shall make the following assumptions. First, we shall find that as $t\to 0$, $\epsilon(t)\to\frac{1}{3}$, so that we shall assume that $\rho_m^{-1}T^4\to$const as $t\to 0$, which implies that $\frac{7}{5}+q-4b-2p-2qs=0$. Second, we shall assume that as $t\to\infty$, $\rho_m^{-1}T^a\to$const, where $a\leqslant 4$, which implies that $b/2+p/3\geqslant\frac{1}{4}$. Finally, for simplicity we shall assume that $b=0$ and $s\leqslant 1$ so that the conditions to be satisfied become

$$0\leqslant s\leqslant 1\,, \tag{4.43a}$$

$$p\geqslant\tfrac{3}{4}\,, \tag{4.43b}$$

$$\tfrac{7}{5}+q-2p-2qs=0\,, \tag{4.43c}$$

$$1-p-2q\geqslant 0\quad(\text{or } 0\leqslant q\leqslant\tfrac{1}{8})\,. \tag{4.43d}$$

Writing $q=\frac{1}{2}-p/2-\delta/2$ ($\delta\geqslant 0$), Eq. (4.43c) becomes

$$2s/5=(\tfrac{19}{25}-p-\delta/5)/(1-p-\delta)\,,$$

so that Eq. (4.43a) implies $\frac{19}{25}\geqslant p$. This suggests two straightforward solutions:

$$\text{(A)}\quad p=\tfrac{3}{4}\,,\quad q=\tfrac{1}{8}\,,\quad s=\tfrac{1}{10}\quad(b=0)\,, \tag{4.44a}$$

$$\text{(B)}\quad p=\tfrac{19}{25}\,,\quad q=\tfrac{3}{25}\,,\quad s=0\quad(b=0)\,. \tag{4.44b}$$

Note that in solution (A) $\rho_m\sim T^4$ for large t and in solution (B) $\rho_m\sim T^{75/19}$ for large t.

We shall concentrate on model (B) henceforward. In this case $T=T_0R^{-19/25}$, η and κ are always positive, and the model satisfies the end conditions outlined above. The model is consequently physically acceptable. Using Eqs. (4.5), (4.9), and (4.11) the solution becomes

$$\begin{aligned}\rho_m&=(l/5\pi G)(1+lt^{3/5})^{-2}(1+\tfrac{5}{6}lt^{3/5})\\&\quad\times(1+2ht^{-3/25})^{-1}(1+ht^{-3/25})^2t^{-7/5}\,,\\3p_m/c^2&=(lh^2/5\pi G)(1+lt^{3/5})^{-2}(1+\tfrac{5}{6}lt^{3/5})\\&\quad\times(1+2ht^{-3/25})^{-1}t^{-41/25}\,,\\\eta&=(5c^2l/6\pi G)(1+lt^{3/5})^{-2}(1+\tfrac{5}{6}lt^{3/5})\\&\quad\times(1+2ht^{-3/25})^{1/2}t^{-2/5}\,,\\Q/c&=(lh/5\pi G)(1+lt^{3/5})^{-2}(1+\tfrac{5}{6}lt^{3/5})\\&\quad\times(1+2ht^{-3/25})^{-1}(1+ht^{-3/25})\,t^{-38/25}\,,\\n&=(n_0/c)(1+lt^{3/5})^{-5/6}(1+2ht^{-3/25})^{1/2}\\&\quad\times(1+ht^{-3/25})t^{-3/2}\,,\end{aligned} \tag{4.45}$$

$$\begin{aligned}\kappa&=(5c^2/T_0\pi G)(1+lt^{3/5})^{-71/90}(1+\tfrac{5}{6}lt^{3/5})\\&\quad\times(1+2ht^{-3/25})^{1/2}(1+ht^{-3/25})\,t^{-31/50}\\&\quad\times[1+(3h/l)\,t^{-18/25}+5ht^{-3/25}]^{-1}\,.\end{aligned}$$

We note that ρ_m and p_m are always positive and monotonically decreasing and that $3p_m/c^2\rho_m\to 1$ as $t\to 0$ and $3p_m/c^2\rho_m\to 0$ as $t\to\infty$. The observational predictions of this model will be analyzed in Sec. V.

D. Model IV

In previous articles[1] we have considered imperfect fluid models for which the metric is that of a standard FRW model with a perfect fluid obeying the equation of state $p=\gamma\rho$. As a final example we consider a model based on the Einstein–de Sitter metric, i.e., we take $R=t^{2/3}$. In this case the field equations become

$$\begin{aligned}&\rho_m c^2-3p_m=c^2/6\pi Gt^2\,,\\&\tfrac{1}{3}\rho_r(3\alpha^2+\beta^2)+\rho_m c^2=\alpha^2/6\pi Gt^2\,.\end{aligned} \tag{4.46}$$

These equations imply that

$$\frac{3p_m}{c^2\rho_m}<\frac{\beta^2}{\alpha^2}\,,\quad\frac{\rho_r}{\rho_m}<\frac{3\beta^2}{3\alpha^2+\beta^2}\,, \tag{4.47}$$

and the second of these inequalities shows that $\rho_r/\rho_m<\frac{3}{4}$ always so that the model can describe only the later part of the matter-dominated era. Accordingly, there is little point in requiring $3p_m/c^2\rho_m\to 1$ as $t\to 0$ and $\alpha\to\infty$ as $t\to 0$, although we could do this and then assume that the model is applicable only for $t>10^{12}$ sec approximately.

Bearing in mind the inequalities (4.48) we shall assume that

$$\rho_r/\rho_m=3\beta^2/4\alpha^2\,, \tag{4.48}$$

which leads to

$$3p_m/c^2\rho_m=\beta^2c^2/4\alpha^4\,. \tag{4.49}$$

The field equations now yield

$$\begin{aligned}&6\pi G\rho_m=4\alpha^4(4\alpha^4-\beta^2c^2)^{-1}t^{-2}\,,\\&6\pi G\rho_r=3\alpha^2\beta^2(4\alpha^4-\beta^2c^2)^{-1}t^{-2}\,,\\&6\pi Gp_m=\tfrac{1}{3}\beta^2c^4(4\alpha^4-\beta^2c^2)^{-1}t^{-2}\,.\end{aligned} \tag{4.50}$$

As suitable functions for α and β we choose

$$\alpha=c[1+h^2(t+t_0)^{-2b}]^{1/2}\,,\quad\beta=ch\,(t+t_0)^{-b}\,, \tag{4.51}$$

where b, h, and t_0 are positive constants. We also choose T to be of the form

$$T=T_0(t+t_0)^{-m}\,, \tag{4.52}$$

where m is positive. The complete solution is

$$\begin{aligned}\rho_r&=(1/2\pi G)h^2(t+t_0)^{-2b}[1+h(1+t_0)^{-2b}]\\&\quad\times[4+7h^2(t+t_0)^{-2b}+4h^4(t+t_0)^{-4b}]^{-1}t^{-2}\,,\\\rho_m&=(2/3\pi G)[1+h^2(t+t_0)^{-2b}]^2[4+7h^2(t+t_0)^{-2b}\\&\quad+4h^4(t+t_0)^{-4b}]^{-1}t^{-2}\,,\\3p_m/c^2&=(c^2/6\pi G)h^2(t+t_0)^{-2b}[4+7h^2(t+t_0)^{-2b}\\&\quad+4h^4(t+t_0)^{-4b}]^{-1}t^{-2}\,,\end{aligned} \tag{4.53}$$

$$\eta = (c^2/12\pi Gb)[4 + 3h^2(t + t_0)^{-2b}]$$
$$\times [1 + h^2(t + t_0)^{-2b}]^{1/2}[4 + 7h^2(t + t_0)^{-2b}$$
$$+ 4h^4(t + t_0)^{-4b}]^{-1}(t + t_0)t^{-2},$$
$$Q/c = (1/6\pi G)h(t + t_0)^{-b}[4 + 3h^2(t + t_0)^{-2b}]$$
$$\times [1 + h^2(t + t_0)^{-2b}]^{1/2}$$
$$\times [4 + 7h^2(t + t_0)^{-2b} + 4h^4(t + t_0)^{-2b}]^{-1}t^{-2},$$
$$n = (n_0/c)[1 + h^2(t + t_0)^{-2b}]^{1/2}t^{-2},$$
$$\kappa = (1/18\pi G)c^3T_0^{-1}(1 + t_0)^{m+1}[4 + 3h^2(t + t_0)^{-2b}]$$
$$\times [1 + h^2(t + t_0)^{-2b}]^{1/2}[4 + 7h^2(t + t_0)^{-2b}$$
$$+ 4h^4(t + t_0)^{-4b}]^{-1}[2t_0 + (2 - 3m - 3b)t]^{-1}t^{-1},$$

where we require

$$2 - 3m - 3b \geqslant 0, \tag{4.54}$$

in order to ensure that $\kappa \geqslant 0$ at all times. Provided that this condition holds, all quantities are positive and ρ_r, ρ_m, and p_m are montonically decreasing functions such that $\rho_r/\rho_m \to 0$ and $3p_m/c^2\rho_m \to 0$ as $t \to \infty$. We note that the choice $m = \frac{33}{50}$, $b = \frac{1}{150}$, which satisfies the condition (4.54), results in $\rho_m \sim T^{3.03}$ for large t.

V. DISCUSSION

In the first three models discussed in Sec. IV, $R(t)$ is a monotonically increasing function of t, changing from $R(t) = t^{1/2}$ for early times, so that the universe was initially in a pure radiation state, to $R(t) = t^{2/3}$ for later times, so that the universe evolves towards a final dustlike state. In all the models ρ_r, ρ_m, and p_m are always positive, monotonically decreasing functions of time and all positive energy conditions are satisfied. Einstein's equations and the laws of thermodynamics (4.5) to (4.8) are satisfied. In addition, η and κ are always positive. We conclude that the models are physically acceptable from a theoretical point of view. In order to show that the models are acceptable in the sense that they agree with the actual nature of the universe, we need to investigate the observational predictions of the models.

In actual fact all of the models are in good agreement with observation, as can be seen from Refs. 7, 8, 20, and 23. As an illustration we shall present a detailed investigation of the observational predictions of model III.

We let the subscript zero denote the present time. All numerical values will be calculated to three significant places only. We shall assume that the value of the arbitrary positive constant l is given by $l = 1.06 \times 10^{-7}$ (see Ref. 20). Based upon a Hubble parameter $H_0 = 55$ km sec^{-1} Mpc^{-1} we find that $t_0^* \equiv H_0^{-1} = 5.67 \times 10^{17}$ sec, so that from the definition of H_0 and Eq. (4.37) we find that $t_0 = 3.78 \times 10^{17}$ sec (the age of the universe). Note that $lt_0^{3/5} \equiv 3.73 \times 10^3$.

We shall assume that the present velocity of our galaxy relative to the cosmic microwave background is three hundred kilometers per second,[6] so that from Eqs. (4.39) we find that $ht_0^{-3/25} = 1.00 \times 10^{-3}$, which fixes h as $h = 1.29 \times 10^{-1}$.

From Eq. (4.45) we find that $\rho_{m,0} = 5.57 \times 10^{-30}$ g cm^{-3}. From Eq. (4.38) we find that $\rho_{r,0} = 4.47 \times 10^{-34}$ g cm^{-3}. Consequently, we find that $T_{r,0} = 2.70$ K from the relationship $\rho_r = aT_r^4$. In addition, Eq. (4.45) yields $(1/c^2)p_{m,0} = 1.86 \times 10^{-36}$ g cm^{-3}. Therefore, from Eq. (2.3), $\epsilon_0 = 2.71 \times 10^{-5}$ and, finally, $p_{m,0}/c^2\rho_{m,0} = 3.33 \times 10^{-7}$.

Let t_e be the time when $\rho_r = \rho_m$. From Eqs. (4.38) and (4.45) we then obtain a quadratic equation in $lt_e^{3/5}$. Taking the positive root, and using the established value of l, we find that $t_e = 1.01 \times 10^{11}$ sec. As remarked earlier, E_m is positive for small t, and from Eq. (2.16) we find that $E_{m,0} = -7.16 \times 10^{-32}$ erg cm^{-3} sec^{-1}.

Comparing the above with the values indicated in Table I we see that the predictions of the model are in excellent agreement with actual observations. Indeed, it could be claimed that the model is in better agreement with observations than existing cosmological models since, in addition to comparing very favorably with regard to the standard observations, the model is also able to predict the relative velocity of the galaxy with respect to the cosmic microwave background. Regardless of such merits, it is clear that the model is a *bona fide* cosmological model. The same is true of the other models outlined in Sec. IV. We conclude that the models in Sec. IV are physically acceptable models of the universe.

In general the temperature of the radiation T_r and the temperature of the matter T need to be taken to be equal. In the models established in the previous section T_r and T are certainly not equivalent, although in model II the possibility that T_r and T are related as $t \to \infty$ was investigated. Indeed, it is important that T_r and T are not equivalent in two-fluid cosmologies in which (at least) one fluid is imperfect with a nonzero heat conduction vector. In such models the two fluids will not be in thermal equilibrium throughout the evolution of the universe. (It might be noted that it is presently believed that the current temperature of the "matter" in the universe is about four times higher than that of the cosmic microwave background.)

In Sec. IV we demanded that the models satisfy the set of thermodynamic laws represented by Eqs. (4.5)–(4.8). It should be noted that these laws are based on the assumption that deviations from thermodynamic equilibrium are not too large. In view of the comments made in the previous paragraph it might be argued that the models outlined here (and, in fact, all models of this type) deviate sufficiently from thermal equilibrium that more general laws of thermodynamics ought to be considered (see, for example, Israel and Stewart[28]). Indeed, it has been suggested before that a more general set of laws of thermodynamics is needed in the cosmological arena.[1] However, the issue of determining the "appropriate thermodynamics" of the universe is a very difficult and controversial question that is at present unanswered. We shall assume here that the laws of thermodynamics that have been used are adequate for our purposes. The fact of the matter is that for reasonable values of t the deviations from thermodynamic equilibrium are not sufficient to raise doubts about the validity of the laws of thermodynamics that have been used [so that Eqs. (4.5)–(4.8) do govern the evolution of the universe for most values of t]. Presumably, if the laws of thermodynamics do break down, they will break down for small values of t, where more gen-

eral laws will consequently be needed. However, the FRW description of the universe breaks down for very small values of t regardless.

We recall that the motivation for the present work was twofold. We wished to complete the work of Ref. 1 regarding the study of FRW cosmological models, in which the FRW models are interpreted as solutions of Einstein's field equations for a variety of different sources. In the present work we study FRW models in the most general case—that in which the source of the gravitational field is due to two (general) imperfect fluids (see Sec. III). The special cases studied previously can be listed as follows: The case in which there are two comoving perfect fluids was reviewed in Sec. II. The case in which there is one noncomoving imperfect fluid was studied in Ref. 1. The case in which there is one comoving perfect fluid gives rise to the so-called standard FRW models.

Although we have alluded to the general case (as set out in Sec. III), we have, in fact, focused our attention on the special case in which one fluid is a comoving (radiative) perfect fluid and the second a noncomoving (matter) imperfect fluid moving with an *axial* velocity relative to the comoving radiation (Sec. IV). This special case is one of particular physical interest. We shall assume that the comoving perfect fluid models the cosmic microwave background and the noncomoving imperfect fluid models the observed matter of the universe. The motivation behind the study of such models is to model the observed velocity of our galaxy relative to the cosmic microwave background.

There are several reasons why we have chosen to attempt to model this effect in the context of two-fluid FRW cosmological models, namely the following: (1) both the observed material content of the universe and the cosmic microwave background are observed to be (approximately) homogeneous and isotropic; (2) it is generally believed that the universe is described with reasonable accuracy by a FRW radiation model for early t and by the Einstein–de Sitter model for later t; and (3) with the discovery of the cosmic microwave background (which was presumed to be a remnant of the radiation era), it became desirable to model the universe as consisting of two fluids, each existing forever, and each "dominating" in the appropriate evolutionary phase of the universe.

We remark that the only way that our objective can be reconciled with the desire to remain within the context of a FRW model is for one of the fluids to be a noncomoving imperfect fluid. The models of Sec. IV are of this form. As mentioned previously, these models are theoretically reasonable and are in excellent agreement with observation. Moreover, through these models, we have achieved our objective of modeling the observed motion of our galaxy relative to the cosmic microwave background. We note that the assumption of a noncomoving imperfect fluid implies that there is a general motion of all matter relative to the cosmic microwave background.

The present work can be generalized somewhat. First, although we have concentrated on FRW models for the reasons given above, we could, of course, repeat the analysis in a more general setting. Indeed, it might be argued that such an analysis would be more appropriate in a nonisotropic and inhomogeneous model. Presumably one would investigate models that approximate FRW models (at least for later times) in order that agreement with present observations is retained. Second, in the actual models that have been described in Sec. IV we have assumed that $k = 0$ and that physical quantities appearing in the models depend on t only. Although both of these assumptions may be relaxed, they have been made here partly for simplicity, but mainly because they give rise to models that exhibit precisely the type of behavior we seek.

We have one final note. This present article represents a natural development of the work by the authors as set out in Ref. 1. In Ref. 1 the imperfect fluid moves relative to a "hypersurface orthogonal preferred observer"; however, such an observer has no physical role within the models. In the present article the imperfect fluid moves relative to the observed cosmic microwave background (and thus a physical interpretation is given to the hypersurface orthogonal preferred observer within the models). So, from a philosophical point of view, the present article presents a more suitable environment for the study of imperfect fluid FRW models.

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Imparting rotation to a Bianchi type II space-time

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A generalization of Batakis's procedure for imparting vorticity to a Bianchi type II space-time is considered. A Bianchi type II rotating model is presented. The limiting case of zero rotation is a known vacuum solution.

I. INTRODUCTION

The problem of obtaining solutions to Einstein's gravitational field equations in which the source of curvature of space-time possesses rotation is fairly old.[1] Nevertheless, as has been pointed out by Batakis,[2,3] the investigation of cosmological space-times with vorticity and, particularly, the search for exact rotating cosmological solutions has received less attention than the search for exact nonrotating models. This may be interpreted as a measure of the difficulties which vorticity introduces into Einstein's field equations rather than of the relative interest in those two subjects. A particular way of circumventing the difficulties introduced into Einstein's equations by the extra terms due to vorticity was first considered by Batakis.[2] He introduced a small vorticity into an empty spatially homogeneous Bianchi model. He was able to isolate a parameter ν directly responsible for the rotation and solved exactly the linearized field equations. In Batakis' paper the parameter ν was taken as a perturbation of the invariant one-forms σ^i $(i = 1, 2, 3)$ corresponding to Bianchi type VI_h.

In this paper, stimulated by Batakis' works,[2,3] we present an exact spatially homogeneous Bianchi type II cosmological solution of the Einstein–Maxwell field equations in which there is a rotating timelike congruence of geodesics. However, in a different manner from Batakis' approximation scheme, we shall consider an *exact perturbation* of our invariant one-forms, so that our treatment may be considered as a generalization of his procedure for a Bianchi type II space-time.

Most of the calculations in this paper were performed by using computer programs written in the symbolic manipulation language SHEEP.[4]

II. THE METRIC AND THE VORTICITY

Let us begin by considering our line element. The invariant one-forms ω^i $(i = 1, 2, 3)$ of Bianchi type II obey the Lie algebra

$$d\omega^1 = \omega^2 \wedge \omega^3, \quad d\omega^2 = 0, \quad d\omega^3 = 0, \tag{2.1}$$

and are given by

$$\omega^1 = dx + y\,dz, \quad \omega^2 = dy, \quad \omega^3 = dz. \tag{2.2}$$

We define the line element of our space-time by

$$ds^2 = dt^2 - 2A\,dt\,\omega^1 - C^2(\omega^1)^2 - B^2[(\omega^2)^2 + (\omega^3)^2], \tag{2.3}$$

where A, B, and $C^2 = B^2 - A^2$ depend only on the time coordinate t.

The metric (2.3) may be considered within Batakis' perturbation scheme by defining the new one-forms

$$\theta^0 = dt + A\omega^1, \quad \theta^1 = B\omega^1, \quad \theta^2 = B\omega^2, \quad \theta^3 = B\omega^3, \tag{2.4}$$

and requiring local Lorentzian character, viz.,

$$ds^2 = \eta_{AB}\theta^A\theta^B \quad (A, B = 0,1,2,3), \tag{2.5}$$

where

$$\eta_{AB} = \mathrm{diag}(+1, -1, -1, -1). \tag{2.6}$$

Thus from Eqs. (2.4)–(2.6) it is obvious that our metric is different from the standard diagonal Bianchi type II metrics. As a matter of fact, the term $A\omega^1$ which we have added to the standard Bianchi orthonormal basis may be thought of as a perturbation. However, contrary to Batakis' procedure, we will not linearize the field equations with respect to A, so as to have an *exact perturbation* scheme.

We shall now consider the existence of vorticity in the model. The presence of the eletromagnetic field together with the nondiagonal terms in (2.3) turns out to be the desired compromise for the existence of rotation in our space-time. It can be easily verified that the congruence of timelike curves, defined by

$$u_\alpha u^\alpha = 1, \quad u_1 = z^{-1}u_2, \quad u_2 = az, \quad u_3 = 0, \quad a = \mathrm{const} \neq 0, \tag{2.7}$$

is geodesic and has rotation vector field given by

$$\Omega^\alpha = (a/2B^3)[-a, (u_0 - zv), v, -(y/z)v], \tag{2.8}$$

where

$$v = a^2 z/(C^2 u_0 + aA). \tag{2.9}$$

Throughout this paper Greek letters are tensor indices and capital letters are tetrad indices. We shall also use a comma for partial derivative, a semicolon for covariant derivative, and a bar for the tetrad components of covariant derivatives.

It should be mentioned that the components of the vorticity vector field Ω^α can be easily checked by using the SHEEP[4] program package MATTER.[5] The SHEEP input should be the Lorentz frame together with the matrix ZUD and the vector UDC (in SHEEP-MATTER notation).

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III. FIELD EQUATIONS AND SOLUTIONS

Let us first consider the source-free Maxwell equations

$$F^{AB}{}_{|B} + \gamma^{A}{}_{MB}F^{MB} + \gamma^{C}{}_{MC}F^{AM} = 0, \tag{3.1}$$

$$F_{[AB|C]} + 2F_{M[C}\gamma^{M}{}_{AB]} = 0, \tag{3.2}$$

where the brackets mean total antisymmetrization and where $\gamma^{A}{}_{BC}$ are the Ricci coefficients of rotation.

From spatial homogeneity and due to the existence of a preferred direction, we choose the nonvanishing components of the electromagnetic field as

$$F_{01} = E(t), \quad F_{23} = -H(t). \tag{3.3}$$

According to Eqs. (3.1)–(3.3), Maxwell's equations reduce to

$$\frac{dE}{dt} - \frac{1}{B}H + 2\frac{\dot{B}}{B}E = 0, \tag{3.4}$$

$$\frac{dH}{dt} + \frac{1}{B}E + 2\frac{\dot{B}}{B}H = 0. \tag{3.5}$$

Introducing a new time coordinate and new measures for the electromagnetic field by

$$dt' = B^{-1}\,dt, \quad E' = EB^{2}, \quad H' = HB^{2}, \tag{3.6}$$

Maxwell's equations can be easily integrated to give the general solution

$$E' = a\cos(t' - t_0), \tag{3.7}$$

$$H' = a\sin(t' - t_0), \tag{3.8}$$

where t_0 is a new constant.

Now the SHEEP programs referred to in the Introduction can be used to display Einstein's field equations, which after some further reductions turn out to be

$$(\dot{B}/B) - (2B)^{-2} = 0, \tag{3.9}$$

$$A\ddot{A} + \dot{A}^{2} + 3A\dot{A}(\dot{B}/B) + \beta^{2}(A^{2} - 6B^{2}) + 1 = 0, \tag{3.10}$$

where the dot denotes the derivative with respect to the time coordinate and β and t_0 are constants which appear in the integrations of (3.9), viz.,

$$B = (1/2\beta)\cosh(t - t_0). \tag{3.11}$$

If one introduces a new time coordinate τ and a new function u by

$$u = A^{2}, \quad \tau = t - t_0, \tag{3.12}$$

Eq. (3.10) can be written as

$$(\xi^{2} - 1)\xi\frac{d^{2}u}{d\xi^{2}} + (4\xi^{2} - 3)\frac{du}{d\xi} + 2\xi u = \frac{3\xi}{\beta^{2}}\left(\xi^{2} - \frac{2}{3}\right), \tag{3.13}$$

where $\xi = \cosh(\tau)$. A solution of the remaining Einstein equation can be written as

$$u = \frac{a^{2}}{\cosh^{2}(\tau)}\left[\frac{1}{4a^{2}\beta^{2}}\cosh^{4}(\tau) - 1\right], \tag{3.14}$$

where the constant a^{2} must lie within the interval

$$0 \leqslant a^{2} \leqslant 1/4\beta^{2}, \tag{3.15}$$

so as to make A a real function. The constant a fixes the character (spacelike) for the hypersurface of homogeneity.

To conclude, we remark that when the electromagnetic field as well as the rotation tend to zero ($a \to 0$) we recover one of the Kinnersley vacuum solutions.[6]

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ERRATA

Erratum: On topological boundary characteristics in nonabelian gauge theory [J. Math. Phys. 24, 2528 (1983)]

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There is an arithmetic mistake in the proof of Eq. (28). The error is due to an incorrect binomial formula in Eq. (A10). The correct version of Eq. (28) is

$$C^{\mu}(U) = 3\,\partial_{\alpha} H^{\mu\alpha}(Z).$$

Correspondingly, Eq. (A11) should read as follows

$$C = -3dH.$$

The authors are grateful to Adam Bincer for calling their attention to the mistake in question.

Erratum: Hamiltonian operators with maximal eigenvalues [J. Math. Phys. 25, 48 (1984)]

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Egnell[1] has pointed out that it was not actually proved that the maximizer for the set $Q(1,c)$ remains in that set, and thus the truncation argument of the proof of Theorem 1 is not justified. If the maximizer does not remain in that set, then it need not be a multiple of a characteristic function. He has constructed an example (with mixed boundary conditions) where the maximizer is in fact a delta function.[1] For some improved existence results and related material, see Refs. 1 and 2.

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Erratum: Calculating resonances (natural frequencies) and extracting them from transient fields [J. Math. Phys. 26, 1012 (1985)]

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The last paragraph in Sec. II C should read as follows:

A similar idea was used in Ref. 11. Convergence of the methods given in Sec. II B and a study of their stability are given in the next subsection.

The line (3.3) should read as follows:

provided that $b_1 < b_2 < \cdots$.

