On the irreducibility of projective corepresentations—Application to double Shubnikov point groups

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An irreducibility criterion for projective corepresentations is stated and specified to projective corepresentations of double Shubnikov point groups, where the choice of the considered factor systems is influenced by the representation theory of double Shubnikov space groups.

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INTRODUCTION

Projective corepresentations and corresponding Clebsch–Gordan series for such representations of Shubnikov point or space groups are of importance for solid state physics.[1] The main objective of the present paper is firstly to generalize a well known irreducibility criterion[2] for corepresentations to projective ones and secondly to extend the usual definition of Shubnikov point groups to corresponding double groups. The reasons for considering this generalization are to avoid the cumbersome distinction between "vector" and "spinor" corepresentation of such groups and to prepare the discussion of double Shubnikov space groups, whose definition and representation theory will be investigated in a forthcoming paper.

The material of this article is organized as follows. In Sec. I we state some necessary definitions and notations concerning projective corepresentations of a given finite group G. In Sec. II we consider special induced projective corepresentations of G. In order to be able to decide which type of projective unitary irreducible corepresentation (counirrep) is realized, we state in Sec. III an irreducibility criterion which generalizes the theorem of Koster and Dimmock.[2,1] Simultaneously we construct for each type of projective counirrep unitary matrices which transform the previously mentioned induced corepresentations into "standard form."[1,3] Starting with the definition of double point groups, we define in Sec. IV corresponding double Shubnikov point groups of type II and type III. Influenced by the representation theory of double space groups, we discuss briefly in Sec. IV A projective unirreps of double point groups which belong to special factor systems. Extending these special factor systems to double Shubnikov point groups of type II and type III, we specify in Sec. IVB respectively Sec. IVC the irreducibility criteiron to these groups.

I. PRELIMINARIES

Let $G=\{H,sH\}$ be a finite group which contains a normal subgroup H of index 2. We call a matrix representation of G (over $\mathbb{C}$) a unitary projective corepresentation, if the matrices $\mathbb{R}(g)$; $g\in G$ satisfy the following equations:

$$\mathbb{R}(g_1)\mathbb{R}(g_2)^{g_1}=\sigma(g_1,g_2)\mathbb{R}(g_1g_2) \quad \text{for all } g_j\in G, \tag{I.1}$$

$$\mathbb{R}(g')^g=\begin{cases}\mathbb{R}(g') & \text{for all } g\in H,\\ \mathbb{R}(g')^* & \text{for all } g\in sH,\end{cases} \tag{I.2}$$

$$\mathbb{R}(s)^*\mathbb{R}(h)\mathbb{R}(s)=\sigma(h,s)\sigma^*(s,s^{-1}hs)\mathbb{R}(s^{-1}hs)^* \quad \text{for all } h\in H, \tag{I.3}$$

$$\mathbb{R}(s)\mathbb{R}(s)^*=\sigma(s,s)\mathbb{R}(s^2) \quad \text{with } s^2\in H, \tag{I.4}$$

$$\mathbb{R}(s)\mathbb{R}(h)^*=\sigma(s,h)\mathbb{R}(sh) \quad \text{for all } h\in H, \tag{I.5}$$

where some of them are redundant but written down for convenience. Since the matrices are assumed to be unitary, the factor system $\sigma: G\times G\to\mathbb{C}$ has the properties

$$\sigma(g_1,g_2)\sigma(g_1g_2,g_3)=\sigma(g_1,g_2g_3)\sigma(g_2,g_3)^{g_1} \quad \text{for all } g_j\in G, \tag{I.6}$$

$$\sigma(e,g)=\sigma(g,e)=1 \quad \text{for all } g\in G, \tag{I.7}$$

$$\sigma(g_1,g_2)^{-1}=\sigma(g_1,g_2)^* \quad \text{for all } g_j\in G, \tag{I.8}$$

$$\sigma(g,g^{-1})=\sigma(g^{-1},g)^g \quad \text{for all } g\in G. \tag{I.9}$$

Finally we call two unitary projective matrix corepresentations $\mathbb{R}$ and $\mathbb{R}'$ equivalent, if there exists a unitary matrix W which satisfies

$$W^*\mathbb{R}(g)W^g=\mathbb{R}'(g) \quad \text{for all } g\in G. \tag{I.10}$$

II. INDUCED PROJECTIVE COREPRESENTATIONS

Let us assume from the outset that a complete set of projective unirreps $\mathbb{D}^\delta(h)$, $h\in H$ ($\delta\in A_H$), are given, which belong to the considered standard factor system σ. A_H denotes the set of equivalence classes of the projective unirreps of H.

Obviously the matrices $\mathbb{P}^\delta(g)=(\mathbb{D}^\delta\uparrow G)(g)$, $g\in G$,

$$\mathbb{P}^\delta(h)=\begin{bmatrix}\mathbb{D}^\delta(h) & 0\\ 0 & \sigma(h,s)\sigma^*(s,s^{-1}hs)\mathbb{D}^\delta(s^{-1}hs)^*\end{bmatrix} \quad \text{for all } h\in H \tag{II.1}$$

$$\mathbb{P}^\delta(s)=\begin{bmatrix}0 & \sigma(s,s)\mathbb{D}^\delta(s^2)\\ \mathbf{1}_\delta & 0\end{bmatrix} \tag{II.2}$$

form a $2n_\delta$-dimensional (induced) corepresentation of G, if $\mathbb{D}^\delta(h)$; $h\in H$ is n_δ-dimensional (compare with results of Ref. 3). The remaining matrices $\mathbb{P}^\delta(sh)$; $h\in H$ are defined by (I.5). The properties (I.3) and (I.4) are readily verified with the aid of (I.6)–(I.9), where

$$\mathbb{P}^\delta(s)^+=\sigma^*(s,s^{-1})\mathbb{P}^\delta(s^{-1})^* \tag{II.3}$$

$$\mathbb{P}^\delta(s^{-1})=\begin{bmatrix}0 & \sigma(s^{-1},s)\mathbf{1}_\delta\\ \sigma^*(s,s^{-2})\mathbb{D}^\delta(s^{-2}) & 0\end{bmatrix} \tag{II.4}$$

have to be taken into account. Like in Eq. (II.2) the symbol $\mathbf{1}_\delta$ means the n_δ-dimensional unit matrix.

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III. PROJECTIVE COUNIRREPS OF G

By similar arguments as in Ref. 2 or Ref. 3, it is obvious to make an analogous character test for projective corepresentations, in order to be able to decide what type of projective counirrep is realized. The corresponding formula reads

$$\frac{1}{|H|}\sum_{h\in H}\sigma(sh,sh)\mathbb{X}^{\delta}((sh)^2)=C(\delta);\quad \delta\in A_H, \tag{III.1}$$

where $\mathbb{X}^{\delta}(h)=\mathrm{Tr}\mathbb{D}^{\delta}(h)$, $h\in H$. Thereby one has to note that $(sh)^2\in H$, since s^2, $s^{-1}hs\in H$. By transfering the arguments of Ref. 1 to projective corepresentations, i.e., by utilizing the orthogonality and representations properties of $\mathbb{D}^{\delta}$, respectively the properties (I.6)–(I.9) we arrive to the formula

$$C(\delta)=\begin{cases}+1 & \text{for } \delta=\alpha\in A_{\mathrm{I}} \quad \text{(type I)},\\ -1 & \text{for } \delta=\beta\in A_{\mathrm{II}} \quad \text{(type II)},\\ 0 & \text{for } \delta=\gamma\in A_{\mathrm{III}} \quad \text{(type III)}.\end{cases} \tag{III.2}$$

This classification divides A_H into three disjoint subsets, whose intersection yields A_H. Moreover, (III.2) represents an irreducibility criterion for projective corepresentations, containing the special case of ordinary corepresentations in a consistent way.

Now let us briefly discuss for the three different cases how the induced representations (II.1), (II.2) can be transferred by unitary transformations into their "standard form."[1,3]

Type I: Presupposed $C(\alpha)=+1$ is realized, there must exist a unitary n_α-dimensional matrix U^{α} which satisfies

$$U^{\alpha+}\mathbb{D}^{\alpha}(h)U^{\alpha}=\sigma(h,s)\sigma^{*}(s,s^{-1}hs)\mathbb{D}^{\alpha}(s^{-1}hs)^{*}\quad \text{for all } h\in H, \tag{III.3}$$

$$U^{\alpha}U^{\alpha *}=\sigma(s,s)\mathbb{D}^{\alpha}(s^2), \tag{III.4}$$

which implies that we can choose

$$\mathbb{B}^{\alpha}(h)=\mathbb{D}^{\alpha}(h)\ \text{for all } h\in H,\quad \mathbb{B}^{\alpha}(s)=U^{\alpha} \tag{III.5}$$

at which projective counirreps of type I of G are denoted by $\mathbb{B}^{\alpha}(g)$; $g\in G$. Now the problem is to find a unitary $2n_\alpha$-dimensional matrix W^{α} which decomposes the reducible projective corepresentation $\mathbb{P}^{\alpha}(g)$, $g\in G$ into a direct sum of its irreducible constituents,

$$W^{\alpha+}\mathbb{P}^{\alpha}(h)W^{\alpha}=(\oplus 2)\mathbb{D}^{\alpha}(h)\quad \text{for all } h\in H. \tag{III.6}$$

$$W^{\alpha+}\mathbb{P}^{\alpha}(s)W^{\alpha *}=(\oplus 2)U^{\alpha}. \tag{III.7}$$

Now it is easy to verify that the unitary matrix

$$W^{\alpha}=\frac{1}{\sqrt{2}}\begin{bmatrix} i\mathbb{1}_{\alpha} & \mathbb{1}_{\alpha}\\ -iU^{\alpha+} & U^{\alpha+}\end{bmatrix} \tag{III.8}$$

engenders the decompositions (III.6) and (III.7).

Type II: Provided $C(\beta)=-1$ is realized, there must exist a unitary n_β-dimensional matrix U^{β} with the properties

$$U^{\beta+}\mathbb{D}^{\beta}(h)U^{\beta}=\sigma(h,s)\sigma^{*}(s,s^{-1}hs)\mathbb{D}^{\beta}(s^{-1}hs)^{*}\quad \text{for all } h\in H \tag{III.9}$$

$$U^{\beta}U^{\beta *}=-\sigma(s,s)\mathbb{D}^{\beta}(s^2). \tag{III.10}$$

Now it is readily verified that there exists a unitary $2n_\beta$-dimensional matrix W^{β}, so that

$$W^{\beta+}\mathbb{P}^{\beta}(h)W^{\beta}=\mathbb{B}^{\beta}(h)=\begin{bmatrix}\mathbb{D}^{\beta}(h) & 0\\ 0 & \mathbb{D}^{\beta}(h)\end{bmatrix}\quad \text{for all } h\in H, \tag{III.11}$$

$$W^{\beta+}\mathbb{P}^{\beta}(s)W^{\beta *}=\mathbb{B}^{\beta}(s)=\begin{bmatrix}0 & U^{\beta}\\ -U^{\beta} & 0\end{bmatrix}. \tag{III.12}$$

(Of course the right hand side of (III.12) contains a further convention, namely the place of the minus sign.) A simple calculation shows that Eqs. (III.11) and (III.12) can be achieved, e.g., by

$$W^{\beta}=\begin{bmatrix}0 & \mathbb{1}_{\beta}\\ U^{\beta+} & 0\end{bmatrix}. \tag{III.13}$$

In this connection we have to note that the minus sign in Eq. (III.10) prevents that $\mathbb{B}^{\beta}(s)$ can be carried over in a direct sum.

Type III: The third and last case is characterized through the fact, that $\mathbb{D}^{\gamma}(h)$, $h\in H$, and $\sigma(h,s)\sigma^{*}(s,s^{-1}hs)\mathbb{D}^{\gamma}(s^{-1}hs)^{*}$ are inequivalent projective unirreps of the normal subgroup H. This implies that there must exist a unitary n_γ-dimensional matrix Z^{γ}, so that

$$Z^{\gamma+}\mathbb{D}^{\bar{\gamma}}(h)Z^{\gamma}=\sigma(h,s)\sigma^{*}(s,s^{-1}hs)\mathbb{D}^{\gamma}(s^{-1}hs)^{*}\quad \text{for all } h\in H,$$
$$\text{where } \gamma(\neq\bar{\gamma})\in A_{\mathrm{III}}. \tag{III.14}$$

Hence

$$\mathbb{B}^{\gamma}(h)=\mathbb{P}^{\gamma}(h),\ h\in H,\quad \text{and}\quad \mathbb{B}^{\gamma}(s)=\mathbb{P}^{\gamma}(s) \tag{III.15}$$

define already a projective counirrep in standard form of type III of G.

Concluding this section, we call projective counirreps to be in "standard form", if they are given by (III.5) for type I corepresentations, by (III.11), (III.12) for type II corepresentations and by (III.15) for type III corepresentations. Consequently projective counirreps in standard form are obtained as follows. First compute a complete set of projective unirreps of the normal subgroup H. Secondly inspect (III.1) in order to decide what type of counirrep is realized. Then depending on the three different cases, one has to determine unitary matrices U^{δ} satisfying either (III.3) with (III.4), or (III.9) with (III.10), or (III.14). Provided the respective matrices U^{δ} have been determined, type I corepresentations follow from (III.5), type II corepresentations from (III.11), (III.12) and finally type III corepresentations from (III.15).

IV. DOUBLE SHUBNIKOV POINT GROUPS

A. Double point groups

As usual we call the group P_h^{*},

$$P_h^{*}=P^{*}\times S_2,\quad S_2=\{E,I\} \tag{IV.1}$$

or any subgroup of this group a "double point group," if P^{*} is a finite subgroup of SU(2) and P_h^{*} itself a direct product group of P^{*} with S_2, where I represents the "inversion." Concerning the group elements of P_h^{*} (or any of its subgroups) we adopt the following notation:

$$R_0^{a}R_jI^{m}=g\in P_h^{*},\quad a=1,2,\quad m=1,2, \tag{IV.2}$$

$$R_0\in Z[\mathrm{SU}(2)]=Z[P^{*}]=\{E,R_0\}, \tag{IV.3}$$

$$R_j\in P^{*}:Z[P^{*}]. \tag{IV.4}$$

Thereby R_0 is the nontrivial element of the center $Z[P^*]$ of P^*, $P^*:Z[P^*]$ the set of left coset representatives of P^* (or of the considered subgroup of P_h^*) with respect to $Z[P^*]$. For notational convenience the elements of P_h^* are sometimes briefly written as g. Furthermore, we have

$$R_0^2 = I^2 = E, \tag{IV.5}$$

where E represents the identity element of P_h^*. The multiplication law of P_h^* reads

$$(R_0^a R_j I^m)(R_0^b R_k I^n) = gg' = R_0^{a+b} R_j R_k I^{m+n}, \tag{IV.6}$$

$$R_j R_k = Z(j,k) R_{jk},$$

$$Z(j,k) \in Z[P^*] \text{ and } R_{jk} \in P^*:Z[P^*]. \tag{IV.7}$$

In case of a subgroup F of P_h^*, which is not a direct product like (IV.1), one has to be more careful when establishing the corresponding multiplication law, even though the group elements of each subgroup of P_h^* can be factorized like in (IV.2). The difference between such a subgroup F and P_h^* arises therefrom that the indices of the left coset representatives $R_j I^{m(j)} \in F:Z[P^*]$ cannot be chosen independently as in Eq. (IV.2). Finally we assume that the factor group

$$P_h^*/Z[P^*] \simeq P_h, \tag{IV.8}$$

respectively the factor groups of the subgroups of P_h^* with respect to $Z[P^*]$, are isomorphic to one of the 32 point groups, which are of interest for physical applications.

In the following we want to discuss projective unirreps of P_h^* which belong to special factor systems. Motivated through the representation theory of "double space groups" we consider factor systems $\gamma: P_h^* \times P_h^* \to \mathbb{C}$ with the following properties:

$$\gamma(R_0^a R_j I^m, R_0^b R_k I^n) = \gamma(R_j I^m, R_k I^n)$$

$$\text{for all } a,b = 1,2,\ m,n = 1,2, \text{ and } R_j, R_k \in P^*:Z[P^*]. \tag{IV.9}$$

Assuming that a complete set of projective unirreps of P_h^* is known, we call in particular the set of matrices

$$\mathbb{D}^\delta = \{\mathbb{D}^\delta(g): g \in P_h^*\}, \quad \delta \in A_{P_h^*(\gamma)} \tag{IV.10}$$

a n_δ–dimensional projective unirrep of P_h^* and $A_{P_h^*(\gamma)}$ the set of all equivalence classes (which of course depends on the considered factor system γ). Due to Schurs Lemma (with respect to P_h^*) it follows from the group properties $R_0 g = g R_0$; $g \in P_h^*$ and the special factor system (IV.9) for each projective unirrep

$$\mathbb{D}^\delta(R_0)\mathbb{D}^\delta(g) = \mathbb{D}^\delta(g)\mathbb{D}^\delta(R_0) \quad \text{for all } g \in P_h^* \tag{IV.11}$$

that within each projective unirrep $\mathbb{D}^\delta$ the nontrivial element R_0 of the center of P^* must be represented by the multiple of the corresponding identity matrix $\mathbf{1}_\delta$. Since $\mathbb{D}^\delta$ is assumed to be unitary we have

$$\mathbb{D}^\delta(R_0) = \pm \mathbf{1}_\delta \tag{IV.12}$$

which remain valid, if restricting to any subgroup of P_h^* and considering factor systems which have analogous properties as (IV.9).

Concluding this subsection, we remark that for trivial factor systems [being equivalent to $\gamma(g,g') = 1, g,g' \in P_h^*$] unirreps of the factor group $P_h^*/Z[P^*]$ are called "vector" representations, if associated with the plus sign in (IV.12), respectively "spinor"-representations, if associated with the minus sign in (IV.12). Obviously such an artificial distinction of representations is meaningless, if considering from the outset double groups. As already mentioned, factor systems of the type (IV.9) may occur, when unirreps of nonsymmorphic "double space groups" are determined by means of induction. A discussion of such space groups and their extensions to "double Shubnikov space groups" will be given in a forthcoming paper, where the main objective will be directed to the computation of Clebsch–Gordan coefficients. In this connection we remark, that the results of Refs. 4 and 5 may only concern vector representations of the homomorphic image of such double Shubnikov space groups.

B. Double Shubnikov point groups of type II

We call a group G_h^* a double Shubnikov point group of type II, which is generated by the double point group P_h^*, if its structure is given through

$$G_h^* = P_h^* \cup \{\kappa\} P_h^*, \tag{IV.13}$$

in which

$$\kappa g = g\kappa \quad \text{for all } g \in P_h^*, \tag{IV.14}$$

$$\kappa^2 = R_0 \Leftrightarrow \kappa^{-1} = \kappa R_0. \tag{IV.15}$$

Consequently, double Shubnikov point groups of type II which are generated by any subgroup of P_h^* are correspondingly defined. Since κ commutes (per definition) with each element of P_h^*, it must belong to the center of G_h^*,

$$Z[G_h^*] = \{E, R_0, \kappa, \kappa R_0\}. \tag{IV.16}$$

(Note that $Z[G_h^*]$ is isomorphic to the "Kleinsche Vierergruppe".) Roughly speaking the group elements κg, $g \in P_h^*$ represents "antiunitary" group elements. (This is, of course, a somewhat misleading diction, since elements of an abstract group cannot be associated with additional properties, like antiunitarity, or something else). Apart from this we have

$$(\kappa g)g' = g(\kappa g') \quad \text{for all } g,g' \in P_h^* \tag{IV.17}$$

$$(\kappa g)(\kappa g') = R_0 gg' \quad \text{for all } g,g' \in P_h^*, \tag{IV.18}$$

which represents together with (IV.6) the multiplication law of G_h^*. Consequently G_h^* is neither a direct nor a semi-direct product group, although κ engenders only the identical automorphism of P_h^*, i.e.,

$$\kappa g \kappa^{-1} = g \quad \text{for all } g \in P_h^*, \tag{IV.19}$$

whereas the homomorphic image G_h of G_h^* being defined by

$$G_h \simeq G_h^*/Z[P^*] \tag{IV.20}$$

is a direct product group, namely $G_h = P_h \times \{E,\kappa\}$. (Note that the property of $Z[G_h^*]$ to be a normal subgroup of G_h^* also allows us to define the factor group $G_H^*/Z[G_h^*]$ which is isomorphic to the ordinary point $P_h \simeq P_h^*/Z[P^*]$ in question.)

Analogously to the foregoing subsection we want to discuss projective representations of G_h^*, which now have to be corepresentations. By similar arguments as previously we restrict our considerations to factor systems

$$\gamma(\kappa^p g,\kappa^q g') = \gamma(g,g')$$
$$\text{for all } g,g' \in P_h^* \text{ and } p,q = 1,2, \quad \text{(IV.21)}$$

which are trivially extended from a factor system of P_h^* [satisfying (IV.9)] to a factor system for G_h^*.

Specifying the general irreducibility criterion (III.1) to this case, we obtain

$$\frac{1}{|P_h^*|}\sum_{g\in P_h^*}\gamma(g,g)\mathbb{X}^\delta((\kappa g)^2) = C(\delta), \quad \text{(IV.22)}$$

where the property (IV.21) of the factor system γ has been already taken into account and the character $\mathbb{X}^\delta(g')$ is given by the trace of $\mathbb{D}^\delta(g')$, $g' \in P_h^*$. Utilizing furthermore

$$(\kappa g)^2 = (\kappa R_0^a R_j I^m)^2 = R_0 R_j^2 = R_0 Z(j,j) R_{jj}, \quad \text{(IV.23)}$$
$$\mathbb{X}^\delta(R_0 g) = \mathrm{sgn}\mathbb{X}^\delta(R_0)\mathbb{X}^\delta(g) \quad \text{for all } g \in P_h^*, \quad \text{(IV.24)}$$

Eq. (IV.22) simplifies to

$$\frac{1}{|P^*|}\sum_{\substack{m=1,2\\ R_j}}\gamma(R_j I^m, R_j I^m)\mathbb{X}^\delta(R_j^2) = \begin{cases} +\mathrm{sgn}\mathbb{X}^\delta(R_0), & \text{type I counirrep,} \\ -\mathrm{sgn}\mathbb{X}^\delta(R_0), & \text{type II counirrep,} \\ 0, & \text{type III counirrep.} \end{cases} \quad \text{(IV.25)}$$

Concluding this subsection we mentioned that the well known results concerning vector or spinor representations of $P_h^*/Z[P^*]$ with their corepresentations are contained in a consistent way in formula (IV.25). The advantage of the present considerations is that a distinction of vector and spinor representations is meaningless, since only "ordinary" representations of P_h^*, respectively corepresentations of G_h^* have to be discussed. Nevertheless these considerations should make clear, that already for corepresentations belonging to the identical factor system, it is reasonable to distinguish carefully between the reality of unirreps of P_h^* and the type of the corresponding counirreps of G_h^*.

C. Double Shubnikov point groups of type III

In order to be able to define a double Shubnikov point group M_h^* of type III, which is generated by a subgroup H^* of index 2 of the double point P_h^*, let us start with some definitions and notations:

$$P_h^* = H^* \cup \{B\} H^* \quad \text{(IV.26)}$$
$$Z[H^*] = Z[P^*]. \quad \text{(IV.27)}$$

Taking condition (IV.27) into account, we can choose without loss of generality the left coset representative B as follows:

$$B = R_t I^m; \quad t,m = \text{fixed} \quad \text{(IV.28)}$$
$$R_t \in P^* : Z[P^*]. \quad \text{(IV.29)}$$

This choice for B lead us to

$$B^2 = R_t^2 = Z(t,t) R_{tt} \in H^*,$$
$$Z(t,t) \in Z[P^*], \quad R_{tt} \in H^* : Z[H^*], \quad \text{(IV.30)}$$

where we now introduce for convenience the notation $R_0^a H_j = h \in H^*$, with $R_0^a \in Z[H^*]$ and $H_j \in H^* : Z[H^*]$. (Obviously similar considerations are necessary in order to be able to define for a subgroup of P_h^* a corresponding double Shubnikov point group of type III.)

We call the group M_h^*,

$$M_h^* = H^* \cup \{\kappa B\} H^*, \quad \text{(IV.31)}$$

a double Shubnikov point group of type III if

$$h(\kappa B h') = \kappa h B h' \in \{\kappa B\} H^* \quad \text{for all } h,h' \in H^*, \quad \text{(IV.32)}$$
$$(\kappa B h)(\kappa B h') = R_0 B h B h' \in H^* \text{ for all } h,h' \in H^*. \quad \text{(IV.33)}$$

Consequently,

$$(\kappa B)^2 = R_0 B^2 = R_0 R_t^2 = R_0 Z(t,t) R_{tt}, \quad \text{(IV.34)}$$

which implies that there can be realized two quite different situations, namely $Z(t,t) = E$ or $Z(t,t) = R_0$, depending on the considered subgroup H^* of P_h^*. Apart from this, we have, furthermore,

$$(\kappa B)^{-1} = \kappa R_0 B^{-1} = (\kappa B) R_0 Z(t,t) R_{tt}^{-1} = Z(t,t) R_{tt}^{-1} (\kappa B), \quad \text{(IV.35)}$$
$$B^{-1} = R_t^{-1} I^m = Z(t,t) R_{tt}^{-1} B = B Z(t,t) R_{tt}^{-1}, \quad \text{(IV.36)}$$
$$R_t^{-1} = Z(t,t) R_{tt}^{-1} R_t = Z(t,t) R_t R_{tt}^{-1}, \quad \text{(IV.37)}$$

which gives rise to a nontrivial automorphism of H^*,

$$(\kappa B) h (\kappa B)^{-1} = (\kappa B)(R_0^a H_j)(\kappa B)^{-1} = R_0^a B H_j B^{-1} = R_0^a R_t H_j R_t^{-1} \in H^*. \quad \text{(IV.38)}$$

Note that M_h^* is *not* isomorphic to P_h^*, but $M_h^*/Z[P^*] \simeq P_h$ holds.

Turning to the problem of constructing projective counirreps of M_h^*, we restrict our considerations to factor systems which satisfy the properties

$$\gamma(R_0^a H_j, R_0^b H_k) = \gamma(H_j, H_k)$$
$$\text{for all } H_j, H_k \in H^* : Z[H^*] \text{ and } a,b = 1,2, \quad \text{(IV.39)}$$
$$\gamma(R_0^a H_j, (\kappa B) R_0^b H_k) = \gamma(H_j, B H_k), \quad \text{(IV.40)}$$
$$\gamma((\kappa B) R_0^a H_j, R_0^b H_k) = \gamma(B H_j, H_k), \quad \text{(IV.41)}$$
$$\gamma((\kappa B) R_0^a H_j, (\kappa B) R_0^b H_k) = \gamma(B H_j, B H_k), \quad \text{(IV.42)}$$

and additional (I.6) and (I.9), which are, of course, nontrivial.

Provided a complete set of projective unirreps of H^* is known, where

$$\mathbb{D}^\omega = \{\mathbb{D}^\omega(h) : h \in H^*\}, \quad \omega \in A_{H^*(\gamma)} \quad \text{(IV.43)}$$

(is a n_ω-dimensional projective unirrep of H^*), there remains the task of deciding what type of projective corepresentation of M_h^* is induced due to (II.1), (II.2). Specifying the irreducibility criterion (III.1) to the present case, we have by virtue of

$$(\kappa B h)^2 = (\kappa B R_0^a H_j)^2 = R_0 (R_t H_j)^2, \quad \text{(IV.44)}$$
$$\mathbb{X}^\omega(R_0 h) = \mathrm{sgn}\mathbb{X}^\omega(R_0)\mathbb{X}^\omega(h) \quad \text{for all } h \in H^*, \quad \text{(IV.45)}$$

where $\mathbb{X}^\omega(R_0 H_j) = \mathrm{Tr}\mathbb{D}^\omega(R_0 H_j)$, the following final formula

$$\frac{2}{|H^*|}\sum_{H_j}\gamma(BH_j,BH_j)\,\mathrm{X}^{\omega}((R_tH_j)^2)$$
$$=\begin{cases}+\,\mathrm{sgn}\mathrm{X}^{\omega}(R_0), & \text{type I counirrep},\\ -\,\mathrm{sgn}\mathrm{X}^{\omega}(R_0), & \text{type II counirrep},\\ 0, & \text{type III counirrep}.\end{cases}\qquad\text{(IV.46)}$$

Analogous to the previous subsection one would be forced to consider vector and spinor representations, if restricting to the factor group $M_h \simeq M_h^*/Z\,[P^*]$ (and discussing representations which belong to the special trivial factor system $(\gamma.,.) = 1$). Consequently the present approach is more appropriated than the previous mentioned one, since a distinction of vector and spinor representations for M_h^* is now meaningless.

SUMMARY

It was the aim of the present article to generalize an irreducibility criterion for ordinary corepresentations to projective ones, to determine quite general unitary matrices transforming induced projective corepresentations into "standard form," to define double Shubnikov point groups (in order to avoid a somewhat cumbersome distinction of vector and spinor representations) and to specify the general irreducibility criterion to projective corepresentations of these groups. The choice of the (nontrivial) factor systems is influenced by the representation theory of double Shubnikov space groups (whose representation theory with application to Clebsch–Gordan series will be discussed in a forthcoming paper). Apart from this we have shown among others that double Shubnikov point groups of type II do not form a direct product group, although the special "antiunitary" group element engenders only the trivial automorphism of the normal subgroup of index 2.

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Objects for the symmetric group

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The permutations, group multiplication tables, decomposition of permutations into neighboring transpositions, representation matrix elements, basis states, and basis state operators have been constructed for the symmetric groups S(n), $n = 1,...,5$. Part of the results have been relegated to PAPS. The algorithm for generating the permutations of the symmetric groups is discussed.

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Though the symmetric groups and their representations are well understood, with properties worked out thoroughly, the results are often implicit. Clearly having these results made explicit should be useful.

Here we present, explicitly, various objects for the symmetric group and their representations, which have been generated by computer programs described elsewhere.[1,2] These programs, having been written, are now available, and can be used for any suitable application as well as for the construction of these objects for other symmetric groups than are considered here.

This work is a continuation of a project whose results have already been presented.[3-7] All terminology, notation, and concepts are based on these papers, which also have references to other work on the symmetric groups.

The results of this paper are in the tables, whose captions describe the methods for using them, as well as some conventions. Only parts of the tables are included, the remainder being in PAPS.[8]

For the group itself the objects are a list of generators (the permutations), the group multiplication tables, and the decomposition of permutations into products of neighboring transpositions.[9] The permutations are given in Table I (which thereby gives the indices by which they will be referred to elsewhere), the group tables are in Table II, and the decomposition into neighboring transpositions in Table III.

Representations are usually the aspect of group theory of most interest to physicists. The objects associated with them are given here for the orthogonal representations. The rules for converting these to the corresponding objects for the seminormal representations have been stated previously.[10] The frames and tableaus have already been given.[11] Here we present the representation matrices for all the permutations (Table IV), the basis vector operators (the ξ's for the orthogonal representations and the e's for the seminormal representations),[12] and the representation basis state vectors (Table V).

Each basis vector operator is a sum over all permutations, each times a matrix element and with an overall numerical factor. The permutations in this sum operate on indices (say, subscripts of functions) and permute them. The representation basis state vectors are found by having a basis vector operator act on a function with n indices [for S(n)], producing a sum over functions with different permutations of indices, each times the appropriate matrix element, times the overall numerical factor.

As written, with the stated overall factor, the basis vector operators are orthonormal.[13] Thus, the basis states are also orthonormal if the product of two of the functions is defined as 1 when the permutations of the indices are the same, and 0 if the permutations of the indices differ.

The specific functions are, of course, irrelevent here. All we are interested in is the value of the matrix element going with each ordering of the indices. Thus, the basis state vectors are presented as a set of numerals, which are the indices of any function we wish, paired with the corresponding matrix element, and with the value of the overall factor.

The results presented here are for the symmetric groups. However, any finite group is a subgroup of some symmetric group[14] (Cayley's theorem). Thus, once the inclusion rules and the decomposition into irreducible representations are known, all the objects presented are also available for any finite group (at least implicitly).

In Appendix A we discuss the algorithm used for generating the pemutations. In Appendix B we consider the maximum number of neighboring transpositions a permutation decomposes into.

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APPENDIX A: THE ALGORITHM FOR THE GENERATION OF THE PERMUTATIONS

Each permutation of the symmetric group S(n) is to be generated, and generated only once. This will produce $n!$ distinct permutations, each a product in the form of independent cycles, each cycle being a pair of parentheses enclosing a set of numerals.

The algorithm is iterative on n, starting from $n = 2$ and at each stage using the permutations generated for S($n - 1$).

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Start with the string of numerals $2\cdots n$, and produce from it, by the application of all the permutations of $S(n-1)$, the $(n-1)!$ different strings in the numerals $2,\cdots,n$, these being all the permutations of these numerals. Into each string insert the numeral 1, in every position. This then produces the $n!$ different strings in the numerals $1,\cdots,n$, which are the $n!$ permutations of these numerals. From these strings the permutation operators are generated.

Getting the permutations is now simply a matter of inserting parentheses in the strings. The set of cycle lengths is the same as the set of row lengths of the frames labeling the representations, since both consist of all the partitions of the integer n. Thus, the cycle lengths are known. So, into each of the above strings, parentheses can be inserted at such positions as to give all the possible set of cycles. Each string then will lead to several permutations, one for each set of cycles.

The problem is that while this will produce every permutation, it will produce each several times. So rules must be introduced to determine how each string is to be cut up into cycles (by insertion of parentheses) in order to generate each permutation, and only once.

A cycle is determined by the set of numerals it contains and by their order. But the numeral which appears first is irrelevant; every rotation of the numerals, keeping the order fixed, gives the same cycle. Also, the cycles commute since each numeral appears in only one cycle. Thus, the ordering of the cycles within the permutation is irrelevant.

Thus, the rules for the insertion of the parentheses are: each set of cycle (or frame) lengths is considered in turn, according to the previously given ordering.[15] For each set of cycle lengths, every one of the above strings of permutations of $1,\cdots,n$ is taken in turn. Then the set of numerals which would be the first in their cycles, if parentheses were inserted according to the current cycle lengths, is considered. Each of these numbers is required to be the smallest in its cycle, and the first numerals in every set of equal-length cycles are required to increase from left to right (cycle lengths are ordered to be nonincreasing from left to right).

Those strings, and only those, which pass both of these tests are used to form permutations by the insertion of parentheses according to the current set of cycle lengths.

Does this procedure give every permutation, and each only once?

Consider uniqueness first. A given string will lead to several permutations, but each will have a different set of cycle lengths, and so are all different. And a given set of cycle lengths will appear several times, giving permutations obtained from different strings. In any two of these, at least two numerals will be in different positions. The only way they can give the same permutation is if the numerals which differed between the two strings all belonged to the same cycle (or, more generally, broke up into several groups of corresponding sets of numerals, each corresponding set belonging to a single cycle). If the two sets of numerals in the two corresponding cycles were in different orders, they would give different permutations. For both cycles the first number must be the same, the smallest in the cycle. Since the first number is the same, and the order of the rest of the numerals is the same, then all numerals must be in the same positions. Thus, two different strings cannot give identical cycles. So each permutation is generated no more than once.

Is every permutation generated? Clearly, every possible permutation can be made to obey the rules. The numerals in every cycle can be rotated until the smallest one is at the left, and the cycles of equal length permuted until the left-most elements are in increasing order from left to right.

Consider any permutation. If its parentheses are removed, then it corresponds to one of the strings generated as discussed above (since all such strings are generated). Its parentheses form one of the allowed set of cycle lengths, which is, therefore, used in the above procedure. The permutation obeys the rules given above (or if not so written, can be brought to that form). Thus, when the corresponding set of cycle lengths and the string are considered, the parentheses will be inserted, and the permutation constructed.

So every permutation is constructed by the procedure.

APPENDIX B: THE MAXIMUM NUMBER OF NEIGHBORING TRANSPOSITIONS

Any permutation can be written as a product of neighboring transpositions.[9] The maximum number of neighboring transpositions, subject to a convention we use, into which any permutation can decompose (as a function of n) is needed in some computer calculations. We find it here.

Any permutation can be decomposed as $(i_1 i_2 \cdots i_n) = (i_1 i_2)(i_2 i_3)\cdots(i_{n-1} i_n)$. If this permutation consists of more than one cycle, the only effect will be that some of the transpositions do not appear in this decomposition. Since we are interested in the largest number of transpositions, we only consider single-cycle transpositions. Now each transposition, with the convention $i_s < i_b$, can be written as $(i_s i_b) = (1 i_s)(1 i_b)(1 i_s)$, unless $i_s = 1$. And $(1 i_w) = (i_w i_{w-1})(i_{w-1} i_{w-2})\cdots(21)(21)(21)\cdots(i_{w-1} i_w)$. In this last expression there are $2(i_w - 1) + 1$ terms. The number of terms resulting from $(i_s i_b)$ is $2[(2i_s - 1) + 1] + [2(i_b - 1) + 1] = 4i_s + 2i_b - 1$ (but when $i_s = 1$ this is $2i_b - 1$).

The permutation we consider is $(234\cdots n-1\ n1) = (23)(34)\cdots(n-1\ n)(n1)$. Each numeral from 3 to $n-1$ will appear in two neighboring transpositions, in one of which it will be the larger numeral, in the other the smaller. Thus, there are $6i$ transpositions contributed by each numeral i, from 3 to $n-1$. Summing we get $3n^2 - 3n - 18$. The numeral 2 contributes 8 transpositions. The numeral n contributes $2n$ from $(n-1\ n)$ and $2n-1$ from $(1n)$. There are $n-2$ transpositions so the -3 term contributes $-3(n-2)$.

Thus, the total number of neighboring transpositions is $3n^2 - 2n - 5$.

Does this permutation give the largest number of neighboring transpositions? All the numerals except two appear in two permutations. These two should be as small as possible (because the number of neighboring transpositions is proportional to the value of the numeral and is the sum of the values for each of the two transpositions, for those in two). This permutation has the two exceptional numerals 1 and 2, clearly the smallest possible.

The other way in which the total could be increased is if

larger numerals appeared as the smaller numeral in more tranpositions than in the above case, so their contribution would be $8i$ instead of $6i$. (This would mean some other numeral would be the larger one in more cases). In general, any permutation can be obtained from the above by applying to it some permutation, which is a product of transpositions. Consider a transposition which interchanges numerals s and b, with $s < b$. Before the interchange the contribution of these two was $6b + 6s$, and now it becomes $2b + 8s$, which is always smaller. So any other permutation gives fewer neighboring transpositions.

So the maximum number of neighboring transpositions is $3n^2 - 2n - 5$.

APPENDIX C: TABLE DESCRIPTIONS

The permutations for $S(n)$ are listed in Table I, and indexed, the index being enclosed in double parentheses. They will be referred by these indices. Each permutation is written as a product of cycles, and acts from right to left. Thus, (13)(254)(6) leaves the subscript in position 6 unchanged (not the number 6), replaces the subscript in position 2 by that in position 5, which is replaced by that in position 4, which is replaced by that in position 2. Finally, indices in positions 1 and 3 are interchanged. For this table, the ordering of the cycles is irrelevant, for they commute. But when products of permutations are considered there will be noncommuting cycles. In these products the right permutation acts first, and then the left permutation acts on the result. Thus $(134)(25)\times(15)(23)(4)$ means that the first and fifth indices of the original string are interchanged, the second and third indices are interchanged, and then (134)(25) acts on the resultant string of indices (interchanging the second and fifth indices of this new string and so on) to get the final string of indices. Thus, for example, $(13)(234)f(1234) = f(4312)$, not $f(3142)$. In the table the value of n is listed, followed by the $n!$ permutations for that n.

The product of every pair of permutations, the group multiplication table, is in Table II. The previous paragraph gives the conventions used, and Table I gives the indices for the permutations, which are used here to refer to them. In the intersection of row i and column j is the ordinal of the permutation obtained from the product of the permutation whose index is at the head of column j and the permutation whose index is at the left of row i. In writing this product the permutation at the head of the column is written to the right of the permutation labeling the row. Thus, the column-heading permutation acts on a string and then the row-labeling permutation acts on the resultant to give the final string. The final string is the same as would be obtained by having the resultant permutation (whose ordinal is at the intersection of row i and column j) act on the original string. The table is headed by the column indices, doubly underlined, at the top, in blocks of 24. The row indices, at the left followed by a right parenthesis, are repeated for each set of 24 columns.

Every permutation can be written as a product of neighboring transpositions (the proof and rule are given by Rutherford[9]). The actual decomposition is needed to find the representation matrices (which are known explicitly for only the neighboring transpositions[16]). The decomposition is given here explicitly, following the value of n. The convention for the ordering of the transpositions is given above.

The decomposition for each permutation is on the line following the permutations' index. To save space (12)(12)(12) has been replaced by (12), to which it is equal. The neighboring transpositions also decompose in this manner, and are included (only because it is simpler to keep them). All the permutations are given [except the identity and (12) permutations].

All the representation matrices, for all representations, for each S(n) are given in Table IV. These are for the orthogonal representations, but can be simply converted to those of the seminormal representations.[10] The ordering of the representations (the frames) and the states (the tableaux) is the same as that given previously.[15] For each value of n there is the ordinal of each representation, followed by the ordinals of the permutations and after each the representation matrix for that permutation. The rows and columns are labeled by tableaux,[3,4] which can be found from Table II of Ref. 4. The table does not include the first representation for each n (the one whose frame is a single column) or the last (whose frame is a single row). For the latter representation all matrices are 1, for the former the matrices are 1 for even permutations and -1 for odd ones. The parities of the permutations are clear from the results in Table III. Since S(2) has only one-dimensional representations it is not included.

The basis operators and vectors are labeled by three indices, giving the equivalence class, representation, and basis vector (the state). The equivalence class is labeled by a frame, specified by its row lengths, which have been given previously.[4] In Table V for each n are the operators and vectors, each preceded by a line giving explicitly the frame ordinal (which has been previously defined[11]), and the values of i and j which specify the state and representation respectively, and which are the indices on the basis state operators (the e's, or ξ's). The last number on this line is the value of θ, which is the number, which depends only on the frame, by which the vectors following should be divided for correct normalization.[13] The state vectors are obtained by having the basis state operators act on some function with n indices, and are sums of terms each with a different permutation of the indices, times the appropriate matrix element, divided by the overall numerical factor given in the previous line. Of course, only the indices are important. Thus, the state vectors are given as sums of matrix elements each times a function, labeled by a, with the appropriate permutation of indices. The basis state operator is the sum of matrix elements times the appropriate permutation, divided by the overall numerical factor. The states and operators differ in their appearance only in that one has a permutation, the other the permuted indices. Thus, under each set of permuted indices is the ordinal of the corresponding permutation, and substituting that permutation in the line above gives the operators. These operators and states are in the orthogonal representation and can easily be converted to the seminormal.[10]

TABLE II. The Group Multiplication Tables.

S(2)

	1	2
1)	1	2
2)	2	1

S(3)

	1	2	3	4	5	6
1)	1	2	3	4	5	6
2)	2	1	6	5	4	3
3)	3	5	1	6	2	4
4)	4	6	5	1	3	2
5)	5	3	4	2	6	1
6)	6	4	2	3	1	5

S(4)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2)	2	1	12	16	11	14	8	7	20	24	5	3	21	6	23	4	19	22	17	9	13	18	15	10
3)	3	11	1	13	12	9	15	19	6	21	2	5	4	22	7	24	23	20	8	18	10	14	17	16
4)	4	14	15	1	10	16	13	22	23	5	19	20	7	2	3	6	24	21	11	12	18	8	9	17
5)	5	12	11	10	1	18	17	23	22	4	3	2	24	20	19	21	7	6	15	14	16	9	8	13
6)	6	16	9	14	17	1	18	21	3	19	24	23	22	4	20	2	5	7	10	15	8	13	12	11
7)	7	8	13	15	18	17	1	2	24	20	22	21	3	19	4	23	6	5	14	10	12	11	16	9
8)	8	7	21	23	22	19	2	1	10	9	18	13	12	17	16	15	14	11	6	24	3	5	4	20
9)	9	24	6	22	23	3	20	10	1	8	16	17	14	13	18	11	12	15	21	7	19	4	5	2
10)	10	20	19	5	4	21	24	9	8	1	15	14	17	12	11	18	13	16	3	2	6	23	22	7
11)	11	3	5	24	2	22	19	15	18	16	12	1	10	9	17	13	8	14	23	6	4	20	7	21
12)	12	5	2	21	3	20	23	17	14	13	1	11	16	18	8	10	15	9	7	22	24	6	19	4
13)	13	22	7	3	21	24	4	14	17	12	8	18	15	11	1	9	16	10	2	5	20	19	6	23
14)	14	4	20	6	19	2	22	13	12	17	10	15	18	16	9	1	11	8	24	23	7	21	3	5
15)	15	19	4	7	20	23	3	11	16	18	14	10	1	8	13	17	9	12	22	21	5	2	24	6
16)	16	6	23	2	24	4	21	18	15	11	17	9	8	1	12	14	10	13	5	3	22	7	20	19
17)	17	23	24	19	6	7	5	12	13	14	9	16	11	15	10	8	18	1	20	4	2	3	21	22
18)	18	21	22	20	7	5	6	16	11	15	13	8	9	10	14	12	1	17	4	19	23	24	2	3
19)	19	15	10	17	14	8	11	3	21	6	20	4	5	23	24	7	22	2	9	16	1	12	13	18
20)	20	10	14	18	15	12	9	24	2	7	4	19	6	21	22	5	3	23	13	8	17	16	11	1
21)	21	18	8	12	13	10	16	6	19	3	7	22	23	5	2	20	4	24	1	11	9	17	14	15
22)	22	13	18	9	8	11	14	4	5	23	21	7	20	24	6	3	2	19	16	17	15	10	1	12
23)	23	17	16	8	9	15	12	5	4	22	6	24	2	7	21	19	20	3	18	13	11	1	10	14
24)	24	9	17	11	16	13	10	20	7	2	23	6	19	3	5	22	21	4	12	1	14	15	18	8

TABLE I. Permutations.

```
S(2)
((1))=(1)(2);  ((2))=(12);

S(3)
((1))=(1)(2)(3);  ((2))=(12)(3);  ((3))=(13)(2);  ((4))=(23)(1);  ((5))=(123);
((6))=(132);

S(4)
((1))=(1)(2)(3)(4);  ((2))=(12)(3)(4);  ((3))=(13)(2)(4);  ((4))=(14)(2)(3);  ((5))=(23)(1)(4);
((6))=(24)(1)(3);  ((7))=(34)(1)(2);  ((8))=(12)(34);  ((9))=(13)(24);  ((10))=(14)(23);
((11))=(123)(4);  ((12))=(132)(4);  ((13))=(143)(2);  ((14))=(124)(3);  ((15))=(134)(2);
((16))=(142)(3);  ((17))=(234)(1);  ((18))=(243)(1);  ((19))=(1234);  ((20))=(1324);
((21))=(1432);  ((22))=(1243);  ((23))=(1342);  ((24))=(1423);
```

TABLE III: Decomposition of permutations into neighboring transpositions.

```
S(3)
      3
(32)(21)(32)
      4
(21)(32)(21)(32)(21)
      5
(21)(21)(32)(21)(32)(21)
      6
(32)(21)(32)(21)(32)(21)(32)(21)
```

TABLE IV. Representation matrices.

S(3) FRAME: 2

```
     1
  1.00000E+00   0.00000E+00
  0.00000E+00   1.00000E+00
     2
  1.00000E+00   0.00000E+00
  0.00000E+00  -1.00000E+00
     3
 -5.00000E-01  -8.66025E-01
 -8.66025E-01   5.00000E-01
     4
 -5.00000E-01   8.66025E-01
  8.66025E-01   5.00000E-01
     5
 -5.00000E-01   8.66025E-01
 -8.66025E-01  -5.00000E-01
     6
 -5.00000E-01  -8.66025E-01
  8.66025E-01  -5.00000E-01
```

S(4) FRAME: 2

```
     1
  1.00000E+00   0.00000E+00   0.00000E+00
  0.00000E+00   1.00000E+00   0.00000E+00
  0.00000E+00   0.00000E+00   1.00000E+00
     2
  1.00000E+00   0.00000E+00   0.00000E+00
  0.00000E+00  -1.00000E+00   0.00000E+00
  0.00000E+00   0.00000E+00  -1.00000E+00
     3
 -5.00000E-01  -8.66025E-01   0.00000E+00
 -8.66025E-01   5.00000E-01   0.00000E+00
  0.00000E+00   0.00000E+00  -1.00000E+00
     4
 -5.00000E-01  -2.88675E-01   8.16497E-01
 -2.88675E-01  -8.33333E-01  -4.71404E-01
  8.16497E-01  -4.71404E-01   3.33333E-01
     5
 -5.00000E-01   8.66025E-01   0.00000E+00
  8.66025E-01   5.00000E-01   0.00000E+00
  0.00000E+00   0.00000E+00  -1.00000E+00
     6
 -5.00000E-01   2.88675E-01  -8.16497E-01
  2.88675E-01  -8.33333E-01  -4.71404E-01
 -8.16497E-01  -4.71404E-01   3.33333E-01
     7
 -1.00000E+00   0.00000E+00   0.00000E+00
  0.00000E+00  -3.33333E-01   9.42809E-01
  0.00000E+00   9.42809E-01   3.33333E-01
     8
 -1.00000E+00   0.00000E+00   0.00000E+00
  0.00000E+00   3.33333E-01  -9.42809E-01
  0.00000E+00  -9.42809E-01  -3.33333E-01
     9
  0.00000E+00   5.77350E-01   8.16497E-01
  5.77350E-01  -6.66667E-01   4.71404E-01
  8.16497E-01   4.71404E-01  -3.33333E-01
    10
  0.00000E+00  -5.77350E-01  -8.16497E-01
 -5.77350E-01  -6.66667E-01   4.71404E-01
 -8.16497E-01   4.71404E-01  -3.33333E-01
    11
 -5.00000E-01   8.66025E-01   0.00000E+00
 -8.66025E-01  -5.00000E-01   0.00000E+00
  0.00000E+00   0.00000E+00   1.00000E+00
    12
 -5.00000E-01  -8.66025E-01   0.00000E+00
  8.66025E-01  -5.00000E-01   0.00000E+00
  0.00000E+00   0.00000E+00   1.00000E+00
    13
  5.00000E-01   8.66025E-01   0.00000E+00
  2.88675E-01  -1.66667E-01  -9.42809E-01
 -8.16497E-01   4.71404E-01  -3.33333E-01
    14
 -5.00000E-01   2.88675E-01  -8.16497E-01
 -2.88675E-01   8.33333E-01   4.71404E-01
  8.16497E-01   4.71404E-01  -3.33333E-01
    15
  5.00000E-01   2.88675E-01  -8.16497E-01
  8.66025E-01  -1.66667E-01   4.71404E-01
  0.00000E+00  -9.42809E-01  -3.33333E-01
    16
 -5.00000E-01  -2.88675E-01   8.16497E-01
 -2.88675E-01   8.33333E-01   4.71404E-01
 -8.16497E-01   4.71404E-01  -3.33333E-01
    17
  5.00000E-01  -2.88675E-01   8.16497E-01
 -8.66025E-01  -1.66667E-01   4.71404E-01
  0.00000E+00  -9.42809E-01  -3.33333E-01
    18
  5.00000E-01  -8.66025E-01   0.00000E+00
 -2.88675E-01  -1.66667E-01  -9.42809E-01
  8.16497E-01   4.71404E-01  -3.33333E-01
    19
  5.00000E-01  -2.88675E-01   8.16497E-01
  8.66025E-01   1.66667E-01  -4.71404E-01
  0.00000E+00   9.42809E-01   3.33333E-01
    20
  0.00000E+00   5.77350E-01   8.16497E-01
 -5.77350E-01   6.66667E-01  -4.71404E-01
 -8.16497E-01   4.71404E-01   3.33333E-01
    21
  5.00000E-01   8.66025E-01   0.00000E+00
 -2.88675E-01   1.66667E-01   9.42809E-01
  8.16497E-01  -4.71404E-01   3.33333E-01
    22
  5.00000E-01  -8.66025E-01   0.00000E+00
  2.88675E-01   1.66667E-01   9.42809E-01
 -8.16497E-01  -4.71404E-01   3.33333E-01
    23
  5.00000E-01   2.88675E-01  -8.16497E-01
 -8.66025E-01   1.66667E-01  -4.71404E-01
  0.00000E+00   9.42809E-01   3.33333E-01
    24
  0.00000E+00  -5.77350E-01  -8.16497E-01
  5.77350E-01   6.66667E-01  -4.71404E-01
  8.16497E-01  -4.71404E-01   3.33333E-01
```

TABLE V. Basis Vector Operators and Basis State Vectors.

```
S(2)

FRAME:  1        J= 1     I= 1          2
 +( 1.000000000E+00)(A1A2)  +(-1.000000000E+00)(A2A1)
                    1                        2

FRAME:  2        J= 1     I= 1          2
 +( 1.000000000E+00)(A1A2)  +( 1.000000000E+00)(A2A1)
                    1                        2

S(3)

FRAME:  1        J= 1     I= 1          6
 +( 1.000000000E+00)(A1A2A3)  +(-1.000000000E+00)(A2A1A3)  +(-1.000000000E+00)(A3A2A1)
                    1                        2                        3
 +(-1.000000000E+00)(A1A3A2)  +( 1.000000000E+00)(A2A3A1)  +( 1.000000000E+00)(A3A1A2)
                    4                        5                        6
```

Table V continued

```
FRAME:  2        J= 1     I= 1              3
 +( 1.0000000000E+00)(A1A2A3)  +( 1.0000000000E+00)(A2A1A3)  +(-5.0000000000E-01)(A3A2A1)
                              1                             2                             3
 +(-5.0000000000E-01)(A1A3A2)  +(-5.0000000000E-01)(A2A3A1)  +(-5.0000000000E-01)(A3A1A2)
                              4                             5                             6

FRAME:  2        J= 2     I= 1              3
 +( 0.0000000000E+00)(A1A2A3)  +( 0.0000000000E+00)(A2A1A3)  +(-8.6602540378E-01)(A3A2A1)
                              1                             2                             3
 +( 8.6602540378E-01)(A1A3A2)  +(-8.6602540378E-01)(A2A3A1)  +( 8.6602540378E-01)(A3A1A2)
                              4                             5                             6

FRAME:  2        J= 1     I= 2              3
 +( 0.0000000000E+00)(A1A2A3)  +( 0.0000000000E+00)(A2A1A3)  +(-8.6602540378E-01)(A3A2A1)
                              1                             2                             3
 +( 8.6602540378E-01)(A1A3A2)  +( 8.6602540378E-01)(A2A3A1)  +(-8.6602540378E-01)(A3A1A2)
                              4                             5                             6

FRAME:  2        J= 2     I= 2              3
 +( 1.0000000000E+00)(A1A2A3)  +(-1.0000000000E+00)(A2A1A3)  +( 5.0000000000E-01)(A3A2A1)
                              1                             2                             3
 +( 5.0000000000E-01)(A1A3A2)  +(-5.0000000000E-01)(A2A3A1)  +(-5.0000000000E-01)(A3A1A2)
                              4                             5                             6

FRAME:  3        J= 1     I= 1              6
 +( 1.0000000000E+00)(A1A2A3)  +( 1.0000000000E+00)(A2A1A3)  +( 1.0000000000E+00)(A3A2A1)
                              1                             2                             3
 +( 1.0000000000E+00)(A1A3A2)  +( 1.0000000000E+00)(A2A3A1)  +( 1.0000000000E+00)(A3A1A2)
                              4                             5                             6

S(4)

FRAME:  3        J= 1     I= 1                       12
 +( 1.0000000000E+00)(A1A2A3A4)  +( 1.0000000000E+00)(A2A1A3A4)  +(-5.0000000000E-01)(A3A2A1A4)
                                 1                               2                               3
 +(-5.0000000000E-01)(A4A2A3A1)  +(-5.0000000000E-01)(A1A3A2A4)  +(-5.0000000000E-01)(A1A4A3A2)
                                 4                               5                               6
 +( 1.0000000000E+00)(A1A2A4A3)  +( 1.0000000000E+00)(A2A1A4A3)  +( 1.0000000000E+00)(A3A4A1A2)
                                 7                               8                               9
 +( 1.0000000000E+00)(A4A3A2A1)  +(-5.0000000000E-01)(A2A3A1A4)  +(-5.0000000000E-01)(A3A1A2A4)
                                10                              11                              12
 +(-5.0000000000E-01)(A4A2A1A3)  +(-5.0000000000E-01)(A2A4A3A1)  +(-5.0000000000E-01)(A3A2A4A1)
                                13                              14                              15
 +(-5.0000000000E-01)(A4A1A3A2)  +(-5.0000000000E-01)(A1A3A4A2)  +(-5.0000000000E-01)(A1A4A2A3)
                                16                              17                              18
 +(-5.0000000000E-01)(A2A3A4A1)  +( 1.0000000000E+00)(A3A4A2A1)  +(-5.0000000000E-01)(A4A1A2A3)
                                19                              20                              21
 +(-5.0000000000E-01)(A2A4A1A3)  +(-5.0000000000E-01)(A3A1A4A2)  +( 1.0000000000E+00)(A4A3A1A2)
                                22                              23                              24
FRAME:  3        J= 2     I= 1                       12
 +( 0.0000000000E+00)(A1A2A3A4)  +( 0.0000000000E+00)(A2A1A3A4)  +(-8.6602540378E-01)(A3A2A1A4)
                                 1                               2                               3
 +( 8.6602540378E-01)(A4A2A3A1)  +( 8.6602540378E-01)(A1A3A2A4)  +(-8.6602540378E-01)(A1A4A3A2)
                                 4                               5                               6
 +( 0.0000000000E+00)(A1A2A4A3)  +( 0.0000000000E+00)(A2A1A4A3)  +( 0.0000000000E+00)(A3A4A1A2)
                                 7                               8                               9
 +( 0.0000000000E+00)(A4A3A2A1)  +(-8.6602540378E-01)(A2A3A1A4)  +( 8.6602540378E-01)(A3A1A2A4)
                                10                              11                              12
 +( 8.6602540378E-01)(A4A2A1A3)  +( 8.6602540378E-01)(A2A4A3A1)  +(-8.6602540378E-01)(A3A2A4A1)
                                13                              14                              15
 +(-8.6602540378E-01)(A4A1A3A2)  +( 8.6602540378E-01)(A1A3A4A2)  +(-8.6602540378E-01)(A1A4A2A3)
                                16                              17                              18
 +(-8.6602540378E-01)(A2A3A4A1)  +( 0.0000000000E+00)(A3A4A2A1)  +(-8.6602540378E-01)(A4A1A2A3)
                                19                              20                              21
 +( 8.6602540378E-01)(A2A4A1A3)  +( 8.6602540378E-01)(A3A1A4A2)  +( 0.0000000000E+00)(A4A3A1A2)
                                22                              23                              24
FRAME:  3        J= 1     I= 2                       12
 +( 0.0000000000E+00)(A1A2A3A4)  +( 0.0000000000E+00)(A2A1A3A4)  +(-8.6602540378E-01)(A3A2A1A4)
                                 1                               2                               3
 +( 8.6602540378E-01)(A4A2A3A1)  +( 8.6602540378E-01)(A1A3A2A4)  +(-8.6602540378E-01)(A1A4A3A2)
                                 4                               5                               6
 +( 0.0000000000E+00)(A1A2A4A3)  +( 0.0000000000E+00)(A2A1A4A3)  +( 0.0000000000E+00)(A3A4A1A2)
                                 7                               8                               9
 +( 0.0000000000E+00)(A4A3A2A1)  +( 8.6602540378E-01)(A2A3A1A4)  +(-8.6602540378E-01)(A3A1A2A4)
                                10                              11                              12
 +(-8.6602540378E-01)(A4A2A1A3)  +(-8.6602540378E-01)(A2A4A3A1)  +( 8.6602540378E-01)(A3A2A4A1)
                                13                              14                              15
 +( 8.6602540378E-01)(A4A1A3A2)  +(-8.6602540378E-01)(A1A3A4A2)  +( 8.6602540378E-01)(A1A4A2A3)
                                16                              17                              18
 +(-8.6602540378E-01)(A2A3A4A1)  +( 0.0000000000E+00)(A3A4A2A1)  +(-8.6602540378E-01)(A4A1A2A3)
                                19                              20                              21
 +( 8.6602540378E-01)(A2A4A1A3)  +( 8.6602540378E-01)(A3A1A4A2)  +( 0.0000000000E+00)(A4A3A1A2)
                                22                              23                              24
FRAME:  3        J= 2     I= 2                       12
 +( 1.0000000000E+00)(A1A2A3A4)  +(-1.0000000000E+00)(A2A1A3A4)  +( 5.0000000000E-01)(A3A2A1A4)
                                 1                               2                               3
 +( 5.0000000000E-01)(A4A2A3A1)  +( 5.0000000000E-01)(A1A3A2A4)  +( 5.0000000000E-01)(A1A4A3A2)
                                 4                               5                               6
 +(-1.0000000000E+00)(A1A2A4A3)  +( 1.0000000000E+00)(A2A1A4A3)  +( 1.0000000000E+00)(A3A4A1A2)
                                 7                               8                               9
 +( 1.0000000000E+00)(A4A3A2A1)  +(-5.0000000000E-01)(A2A3A1A4)  +(-5.0000000000E-01)(A3A1A2A4)
                                10                              11                              12
 +(-5.0000000000E-01)(A4A2A1A3)  +(-5.0000000000E-01)(A2A4A3A1)  +(-5.0000000000E-01)(A3A2A4A1)
                                13                              14                              15
 +(-5.0000000000E-01)(A4A1A3A2)  +(-5.0000000000E-01)(A1A3A4A2)  +(-5.0000000000E-01)(A1A4A2A3)
                                16                              17                              18
 +( 5.0000000000E-01)(A2A3A4A1)  +(-1.0000000000E+00)(A3A4A2A1)  +( 5.0000000000E-01)(A4A1A2A3)
                                19                              20                              21
 +( 5.0000000000E-01)(A2A4A1A3)  +( 5.0000000000E-01)(A3A1A4A2)  +(-1.0000000000E+00)(A4A3A1A2)
                                22                              23                              24
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Dimension and character formulas for Lie supergroups [a)]

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A character formula is derived for Lie supergroups. The basic technique is that of symmetrization and antisymmetrization associated with Young tableaux generalized to supergroups. We rewrite the characters of the ordinary Lie groups $U(N)$, $O(N)$, and $Sp(2N)$ in terms of traces in the fundamental representation. It is then shown that by simply replacing traces with supertraces the characters of certain representations for $U(N/M)$ and $OSP(N/2M)$ are obtained. Dimension formulas are derived by calculating the characters of a special diagonal supergroup element with $(+1)$ and (-1) eigenvalues. Formulas for the eigenvalues of the quadratic Casimir operators are given. As applications, the decomposition of a representation into representations of subgroups is discussed. Examples are given for the Lie supergroup SU(6/4) which has physical applications as a dynamical supersymmetry in nuclei.

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I. INTRODUCTION

So far superalgebras have found some applications in physics[1] in the context of dual models,[2] supersymmetric field theories,[3] supergravity[4] and recently in nuclear physics as well.[5] There exists extensive papers on superalgebras.[6] The representation theory of superalgebras has been studied less extensively. Kac has given character and dimension formulas for "typical" finite dimensional representations in terms of weights.[7]

Lie supergroups are obtained by exponentiating Lie superalgebras where the even generators of the superalgebra are associated with commuting parameters and the odd generators with anticommuting parameters.[6,8] In this paper we show how certain finite-dimensional representations of Lie supergroups can be constructed using a symmetrization–antisymmetrization procedure associated with Young tableaux generalized to supergroups. The character and dimension formulas are obtained for these representations which include "typical" as well as "nontypical"[7] representations.

In Sec. II we describe our method and obtain the character and dimension formulas for the representations of $U(N/M)$ type supergroups. Formulas which give the number of bosonic and fermionic components are also included.

Our results are formalized in Sec. III. In this section we introduce graded "symmetric" functions which are invariants of the supergroups $U(N/M)$ and obtain some relationships between them.

An extension of the above results to the orthosymplectic groups $OSp(N/2M)$ is presented in Sec. IV. We show that characters of orthogonal and sympletic groups are the limiting cases of the characters of orthosympletic supergroups given in this paper.

In Sec. V we describe a technique to calculate the eigenvalues of Casimir operators for various representations. The quadratic Casimir invariants for $SU(N/M)$, $N \neq M$, type supergroups are explicitly calculated.

The decomposition of certain representations of $U(N/M)$ into representations of its Lie subgroups is discussed in Sec. VI. As examples, the decompositions of SU(6/4) and SU(7/6), which are potentially useful in nuclear physics, are worked out.

The last section contains a brief discussion of our results.

II. CONSTRUCTION OF HIGHER DIMENSIONAL REPRESENTATIONS FROM KRONECKER PRODUCTS

In this section we first review the construction of representations of $U(N)$, their characters, and their dimensions from Kronecker products of the fundamental representation. Next, we generalize this procedure to the supergroups $U(N/M)$. Our basic observations in this section will be further generalized to the supergroups $OSp(N/2M)$ in the coming sections.

It is a well-known fact that the higher dimensional irreducible representations of $U(N)$-type groups can be obtained from the fundamental representations of such groups employing a symmetrization–antisymmetrization procedure. A Young tableau is associated with any representation obtained in this way as explained in Ref. 9. For a given Young tableau one first performs the symmetrization for every row, then the antisymmetrization of the columns. Let us consider the basis states of any irreducible representation constructed as above, i.e., written in terms of tensor products of the basis states of the fundamental representation appropriately symmetrized or antisymmetrized. A transformation on these states gives an irreducible representation of the group. By taking the trace of this expression we obtain the characters for $U(N)$ written in terms of the traces of various powers of the fundamental representation as illustrated below. We denote the character by $\chi_{(n_1,n_2,n_3,\cdots)}$ where n_i is the number of the boxes in the ith row of the corresponding tableau.

To give some simple examples let us consider the basis ϕ_a, $a = 1, \ldots, N$ of the fundamental representation of $U(N)$.

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Under the group ϕ_a transform into $\phi'_a = U_{ab}\phi_b$, where the $N \times N$ matrix U is a group element in the fundamental representation. The symmetrized tensor product of two basis vectors $\phi_a^{(1)}$ and $\phi_b^{(2)}$ is defined as

$$\phi_{(ab)} = \phi_a^{(1)}\phi_b^{(2)} + \phi_a^{(2)}\phi_b^{(1)}, \tag{2.1}$$

which transforms into

$$\begin{aligned}\phi'_{(ab)} &= \phi'^{(1)}_a \phi'^{(2)}_b + \phi'^{(2)}_a \phi'^{(1)}_b \\ &= U_{aa'}\phi^{(1)}_{a'} U_{bb'}\phi^{(2)}_{b'} + U_{ab'}\phi^{(2)}_{b'} U_{ba'}\phi^{(1)}_{a'}.\end{aligned} \tag{2.2}$$

Since a' and b' are summed over, one can rewrite $\phi'_{(ab)}$, interchanging a' and b'. Adding these two expressions, we get

$$\phi'_{(ab)} = U_{(ab),(a'b')}\,\phi_{(a'b')}, \tag{2.3}$$

where

$$U_{(ab),(a'b')} = \tfrac{1}{2}(U_{aa'}U_{bb'} + U_{ba'}U_{ab'}) \tag{2.4}$$

is a group element in this irreducible representation.

To take the trace, we let $a = a'$, $b = b'$ and sum over a and b. We find the character to be

$$\chi_{(2,0,\ldots)} = \tfrac{1}{2}[(\mathrm{Tr}U)^2 + \mathrm{Tr}(U^2)]. \tag{2.5}$$

For the next example we consider the representation associated with the tableau with $n_1 = 2$ and $n_2 = 1$:

$$\begin{array}{|c|c|}\hline a & b \\ \hline c \\ \cline{1-1}\end{array}$$

The basis $\phi_{(ab,c)}$ of this representation is found by first symmetrizing with respect to the rows and then antisymmetrizing with respect to the columns as follows

$$\begin{aligned}\phi_{(ab,c)} &= \phi_a^{(1)}\phi_b^{(2)}\phi_c^{(3)} + \phi_a^{(2)}\phi_b^{(1)}\phi_c^{(3)} \\ &\quad - \phi_a^{(3)}\phi_b^{(2)}\phi_c^{(1)} - \phi_a^{(2)}\phi_b^{(3)}\phi_c^{(1)},\end{aligned} \tag{2.6}$$

which, under the group, transforms into

$$\phi'_{(ab,c)} = U_{(ab,c),(a'b',c')}\phi_{(a'b',c')}, \tag{2.7}$$

where

$$\begin{aligned}U_{(ab,c),(a'b',c')} &= \tfrac{1}{3}[U_{aa'}U_{bb'}U_{cc'} + U_{ba'}U_{ab'}U_{cc'} \\ &\quad - U_{ca'}U_{bb'}U_{ac'} - U_{ba'}U_{cb'}U_{ac'}]\end{aligned} \tag{2.8}$$

is a group element in this representation. Upon taking the trace we find the character

$$\chi_{(2,1,0,\ldots)} = \tfrac{1}{3}[(\mathrm{Tr}U)^3 - \mathrm{Tr}(U^3)]. \tag{2.9}$$

Characters of some low-dimensional representations calculated in this way are listed in the Appendix with their corresponding tableaux. We see from this list that the characters of the representations of type $(n, 0, 0, \cdots)$ corresponding to Young tableaux with a single row is given by $\chi_{(n,0,0\ldots)} \equiv \chi_n$, where

$$\begin{aligned}\chi_n = \frac{(\mathrm{Tr}U)^n}{n!} &+ \frac{(\mathrm{Tr}U)^{n-2}}{(n-2)!}\,\frac{\mathrm{Tr}(U^2)}{2} + \frac{(\mathrm{Tr}U)^{n-3}}{(n-3)!}\,\frac{\mathrm{Tr}(U^3)}{3} \\ &+ \cdots + \frac{\mathrm{Tr}(U^n)}{n}.\end{aligned} \tag{2.10}$$

Furthermore, we observe from the Appendix that the character of any representation can be written as follows:

$$\chi_{(n_1,n_2,n_3,\ldots)} = \begin{vmatrix} \chi_{n_1} & \chi_{n_2-1} & \chi_{n_3-2} & \cdots & \chi_{n_N-N+1} \\ \chi_{n_1+1} & \chi_{n_2} & \chi_{n_3-1} & \cdots & \chi_{n_N-N+2} \\ \chi_{n_1+2} & \chi_{n_2+1} & \chi_{n_3} & \cdots & \chi_{n_N-N+3} \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \chi_{n_1+N-1} & \chi_{n_2+N-2} & \chi_{n_3+N-3} & \cdots & \chi_{n_N} \end{vmatrix} \tag{2.11}$$

where we define $\chi_m = 1$ for $m = 0$ and $\chi_m = 0$ for $m < 0$. For example Eq. (2.9) can be rewritten in the form

$$\chi_{(2,1,0,0,\cdots)} = \begin{vmatrix} \chi_2 & 1 \\ \chi_3 & \chi_1 \end{vmatrix}.$$

In general the order of the determinant is equal to the number of rows in the Young tableau. These explicit forms are potentially useful for physical applications because they are given directly in terms of the matrix U. In the next section we will show that this form may be derived rigorously from Weyl's character formula,[10] which is written in terms of the eigenvalues of U rather than the matrix U.

A more compact form for χ_n can be derived from Eq. (2.10) which may be expressed as

$$\chi_n = \sum_{k_1,k_2,\ldots,k_n} \prod_{l=1}^{n} \frac{1}{k_l!}\left(\frac{\mathrm{Tr}U^l}{l}\right)^{k_l} \delta(n - k_1 - 2k_2 \cdots - nk_n), \tag{2.12}$$

where as indicated by the delta function the sum is over all possible partitions of the integers $(k_1,\ldots,k_n)$ which satisfy $n = k_1 + 2k_2 + \cdots + nk_n$. In other words, $k_l = 0$ for $l > n$. Therefore, the product over l can also be written from $l = 1$ to ∞. Expressing the delta function in integral form the sum over partitions becomes sums over various k_l's:

$$\begin{aligned}\chi_n &= \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-in\theta} \prod_{l=1}^{\infty} \sum_{k_l} \frac{1}{k_l!}\left[\frac{(\mathrm{Tr}U^l)e^{il\theta}}{l}\right]^{k_l} \\ &= \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-in\theta} \prod_{l=1}^{\infty} \exp\left[\frac{(\mathrm{Tr}U^l)e^{il\theta}}{l}\right] \\ &= \oint_c \frac{dz}{2\pi i} z^{-n-1} \exp\left[\sum_{l=1}^{\infty} \frac{z^l(\mathrm{Tr}U^l)}{l}\right],\end{aligned} \tag{2.13}$$

where c is a contour around the origin. We note that the expression (2.13) can be written in two alternative forms:

$$\chi_n = \oint_c \frac{dz}{2\pi i} z^{-n-1} \exp[\mathrm{Tr}\,\log(1 - zU)] \tag{2.14}$$

or

$$\chi_n = \oint_c \frac{dz}{2\pi i}\,\frac{z^{-n-1}}{\det(1 - zU)}. \tag{2.15}$$

To find the dimension $d_{(n_1,n_2,n_3,\cdots)}$ of any representation $(n_1,n_2,n_3,\cdots)$, we just calculate the character of the identity element in this representation. We let $U = I_N$, where I_N is the $N \times N$ unit matrix. Then $\mathrm{Tr}U^k = N$ for any power k. For example, the dimensions of the representations considered in Eqs. (2.4) and (2.8) are

$$d_{(2,0,0,\cdots)} = \tfrac{1}{2}(N^2 + N) = \tfrac{1}{2}N(N+1) \tag{2.16a}$$

and

$$d_{(2,1,0,\cdots)} = \tfrac{1}{3}(N^3 - N) = \tfrac{1}{3}(N-1)N(N+1). \tag{2.16b}$$

The same can be done for the characters listed in the Appendix or the general character of Eq. (2.11). We note that for the

single row (completely symmetric) one obtains, $d_{(n,0,0,\cdots)} = d_n$,

$$d_n = N(N+1)\cdots(N+n-1)/n!, \tag{2.16c}$$

as expected. Therefore, the general dimension formula will have the same determinantal form as Eq. (2.11) except for $\chi_n(U)$ replaced by d_n. Of course, this agrees with the standard result.

Now we show how the procedure described above generalizes to the supergroups of type SU(N/M). We have two different fundamental representations for supergroups. Let the basis for the fundamental representations be ξ_A and $\tilde{\xi}_A$, both of which are graded vectors. We take

$$\xi_A = \begin{pmatrix} \phi_a \\ \psi_\alpha \end{pmatrix}, \tag{2.17}$$

where the indices $A = a$ (Latin indices) $= 1, \ldots, N$ denote the SU(N) part and $A = \alpha$ (Greek indices) $= N+1, \ldots, N+M$ denote the SU(M) part. We take ϕ_a bosonic or a commuting wavefunction and ψ_α fermionic or an anticommuting wavefunction. The *degree* or *grade* of the index A, $g(A)$, is defined to be 0 for bosonic indices and 1 for fermionic indices. For the representation above $g(a) = 0$ and $g(\alpha) = 1$. The basis for the second fundamental representation space is taken as

$$\tilde{\xi}_A = \begin{pmatrix} \psi_a \\ \phi_\alpha \end{pmatrix}, \tag{2.18}$$

where this time the Latin SU(N) indices denote the odd part and the Greek SU(M) indices denote the even part, i.e., ψ_a is fermionic and ϕ_α is bosonic. For this representation we have $g(a) = 1$ and $g(\alpha) = 0$. In fact, one can define a tilde operation that changes the grade of the indices.[11] Under this tilde operation the basis vectors ξ_A and $\tilde{\xi}_A$ transform into each other. The tilde operation converts bosons into fermions and vice versa, but is not a generator of the SU(N/M) group. We call these basis vectors class I and class II fundamental representations, respectively. In addition to these there are the complex conjugate fundamental representations which, of course, have the same dimension.

Under the supergroup ξ_A transforms into $\xi'_A = \mathscr{U}_{AB}\xi_B$, where $\mathscr{U}$ is an element of the supergroup in the fundamental representation. If the matrix element $\mathscr{U}_{AB}$ has an odd number of fermionic indices, then it is an anticommuting parameter; otherwise it is a commuting parameter. In fact the matrix $\mathscr{U}$ can be written as

$$\mathscr{U} = \begin{pmatrix} \mathscr{A} & \mathscr{B} \\ \mathscr{C} & \mathscr{D} \end{pmatrix}, \tag{2.19}$$

where the elements of the $N \times N$ matrix $\mathscr{A}$ and $M \times M$ matrix $\mathscr{D}$ are bosonic and the elements of the $N \times M$ matrix $\mathscr{B}$ and $M \times N$ matrix $\mathscr{C}$ are fermionic. Under the supergroup $\tilde{\xi}_A$ also transforms with the same matrix: $\mathscr{U}:\tilde{\xi}'_A = \mathscr{U}_{AB}\tilde{\xi}_B$. We call the bases of the representations obtained by symmetrizing or antisymmetrizing ξ_A and $\tilde{\xi}_A$ as class I and class II bases respectively. The lowest dimensional representation of the group applied on class I and class II bases is the same: the graded matrix $\mathscr{U}$.

The *supertrace* is defined as

$$\mathrm{Str}\mathscr{U} = \sum_A (-1)^{g(A)}\mathscr{U}_{AA}. \tag{2.20}$$

Following this definition, one writes

$$\mathrm{Str}\mathscr{U} = \mathrm{Tr}\mathscr{A} - \mathrm{Tr}\mathscr{D} \tag{2.21}$$

for the class I fundamental representation and

$$\mathrm{Str}\mathscr{U} = -\mathrm{Tr}\mathscr{A} + \mathrm{Tr}\mathscr{D} \tag{2.22}$$

for the class II fundamental representation. The *superdeterminant* is defined as

$$\mathrm{Sdet}\mathscr{U} = \exp[\mathrm{Str}(\log\mathscr{U})]. \tag{2.23}$$

For example when $\mathscr{B} = 0 = \mathscr{C}$, Sdet$\mathscr{U}$ becomes det$\mathscr{A}$/det$\mathscr{D}$ or det$\mathscr{D}$/det$\mathscr{A}$ depending on class I or class II representations. For the supergroup SU(N/M) one has Sdet$\mathscr{U} = 1$.

The "symmetrized" and "antisymmetrized" tensor products of two basis vectors of class I, $\xi_A^{(1)}$ and $\xi_B^{(2)}$ (and also of class II, $\tilde{\xi}_A^{(1)}$ and $\tilde{\xi}_B^{(2)}$), form bases of irreducible representations for the supergroup SU(N/M). More generally we form the irreducible representations of SU(N/M) type supergroups using the same algorithm we used for U(N) type groups. That is, we associate a Young tableau with each irreducible representation and first perform the "symmetrization" of states corresponding to boxes at the same row, then "antisymmetrization" of states at the same column. Let us first analyze the "symmetrized" tensor product of two basis vectors belonging to the same class:

$$\xi_{(AB)} = \xi_A^{(1)}\xi_B^{(2)} + \xi_A^{(2)}\xi_B^{(1)}, \tag{2.24}$$

which can also we rewritten as

$$\xi_{(AB)} = \xi_A^{(1)}\xi_B^{(2)} + (-1)^{g(A)\cdot g(B)}\xi_B^{(1)}\xi_A^{(2)}, \tag{2.25}$$

where the order of the wavefunctions is changed in the second term. $\tilde{\xi}_{(AB)}$ is defined in the same way. We note that, for class I, when both indices are purely bosonic, $A = a$, $B = b$, the product is *symmetric* since $g(a) = g(b) = 0$. On the other hand, when both indices are fermionic, $A = \alpha$, $B = \beta$, the product is *antisymmetric* since $g(\alpha) = g(\beta) = 1$. Thus we have

$$\xi_{ab} = \phi_a^{(1)}\phi_b^{(2)} + \phi_b^{(1)}\phi_a^{(2)}, \tag{2.26a}$$

$$\xi_{\alpha\beta} = \psi_\alpha^{(1)}\psi_\beta^{(2)} - \psi_\beta^{(1)}\psi_\alpha^{(2)}. \tag{2.26b}$$

These products are bosonic. The fermionic components are given by

$$\xi_{a\beta} = \phi_a^{(1)}\psi_\beta^{(2)} + \psi_\beta^{(1)}\phi_a^{(2)} = \xi_{\beta a}. \tag{2.26c}$$

We see that the number of components of $(\xi_{ab}, \xi_{\alpha\beta}, \xi_{a\beta})$ are $[\frac{1}{2}N(N+1), \frac{1}{2}M(M-1), MN]$, respectively, so that the dimension of $\xi_{(AB)}$ is $\frac{1}{2}[(N+M)^2 + (N-M)]$.

The symmetrization of two class II basis vectors yields the tensors

$$\tilde{\xi}_{ab} = \psi_a^{(1)}\psi_b^{(2)} - \psi_b^{(1)}\psi_a^{(2)}, \tag{2.27a}$$

$$\tilde{\xi}_{\alpha\beta} = \phi_\alpha^{(1)}\phi_\beta^{(2)} + \phi_\beta^{(1)}\phi_\alpha^{(2)}, \tag{2.27b}$$

which are bosonic, and

$$\tilde{\xi}_{ab} = \phi_a^{(1)}\psi_b^{(2)} + \psi_b^{(1)}\phi_a^{(2)} = \tilde{\xi}_{ba}, \tag{2.27c}$$

which is fermionic. The number of components of $(\tilde{\xi}_{ab}, \tilde{\xi}_{ab}, \tilde{\xi}_{a\beta})$ are $[\frac{1}{2}N(N-1), NM, \frac{1}{2}M(M+1)]$, respectively, so that the dimension of $\tilde{\xi}_{(AB)}$ is $\frac{1}{2}[(N+M)^2 + (M-N)]$.

Under the supergroup $\xi_{\{AB\}}$ transforms into

$$\xi'_{\{AB\}} = \mathcal{U}_{AA'}\xi^{(1)}_{A'}\mathcal{U}_{BB'}\xi^{(2)}_{B'} + \mathcal{U}_{AA'}\xi^{(2)}_{A'}\mathcal{U}_{BB'}\xi^{(1)}_{B'}. \quad (2.28)$$

We note that the order of the factors is important since some of the parameters or wavefunctions are fermionic. After changing the orders this can be written as

$$\xi'_{\{AB\}} = \mathcal{U}_{(AB),(A'B')}\xi_{(A'B')}, \quad (2.29)$$

where

$$\mathcal{U}_{(AB),(A'B')} = \tfrac{1}{2}[(-1)^{g(A')\cdot[g(B)-g(B')]}\mathcal{U}_{AA'}\mathcal{U}_{BB'} + (-1)^{g(A)\cdot g(B)}(-1)^{g(A')\cdot[g(A)-g(B')]} \times \mathcal{U}_{BA'}\mathcal{U}_{AB'}]. \quad (2.30)$$

For class II, $\tilde{\xi}_{\{AB\}}$ also transforms with the matrix $\mathcal{U}$, but the degrees of the indices are interchanged. In arriving at Eq. (2.30) we used the following formulas for interchanging the orders of bosonic or fermionic quantities:

$$\xi^{(1)}_A\xi^{(2)}_B = (-1)^{g(A)\cdot g(B)}\xi^{(2)}_B\xi^{(1)}_A, \quad (2.31)$$

$$\xi_A\mathcal{U}_{BC} = (-1)^{g(A)\cdot[g(B)-g(C)]}\mathcal{U}_{BC}\xi_A, \quad (2.32)$$

$$\mathcal{U}_{AB}\mathcal{U}_{CD} = (-1)^{[g(A)-g(B)]\cdot[g(C)-g(D)]}\mathcal{U}_{CD}\mathcal{U}_{AB}. \quad (2.33)$$

Corresponding to the construction described in the previous paragraph we introduce the Young supertableau

whose meaning differs from the ordinary tableau: It indicates symmetrization of indices for the purely bosonic subspace, but antisymmetrization of indices for the purely fermionic subspace. Both of these possibilities are automatically taken into account in Eqs. (2.24), (2.25), (2.28), (2.30). To distinguish between two classes, we use white boxes for class I and black boxes for class II fundamental representations. Just as in the usual case we associate supertableaux with representations of the supergroup. For class I the supertableau is constructed from white boxes only and for class II from black boxes only. In this paper we do not discuss the representations that would result from taking direct products of class I with class II fundamental representations. Accordingly, we will not treat the supertableaux containing both white and black boxes. As in the usual case we first "symmetrize" the *wavefunctions* corresponding to each row, then "antisymmetrize" with respect to the columns. However, there is a major difference between SU(N)-type groups and SU(N/M)-type supergroups: For SU(N)-type groups Young tableaux can have at most $N-1$ rows since complete antisymmetrization of more than N indices for N bosonic numbers is impossible. On the other hand, for SU(N/M) type supergroups, since "antisymmetrization" of basis states implies antisymmetrization of bosonic *but* symmetrization of fermionic parts, one can continue the "antisymmetrization" process up to infinity. That is, Young supertableaux can have any number of rows. We denote a given representation by $(n_1,n_2,n_3,\cdots)$, where n_i is the number of the boxes in the ith row of the corresponding supertableaux.

The character, which is an invariant, can now be defined as the supertrace of the group element which is applied on this basis. For example, for both representations $\xi_{\{AB\}}$ and $\tilde{\xi}_{\{AB\}}$ discussed above we have

$$\mathcal{K}_{(2,0,\cdots)} = \sum_{A,B}(-1)^{g(A)}(-1)^{g(B)}\mathcal{U}_{(AB),(AB)} = \tfrac{1}{2}[(\mathrm{Str}\,\mathcal{U})^2 + \mathrm{Str}(\mathcal{U}^2)]. \quad (2.34)$$

We see that this is formally the same expression as Eq. (2.5) for the ordinary Lie groups, except for the fact that *traces are replaced by supertraces! This is our basic observation*, which allows us to generalize the character formulas of ordinary Lie groups to Lie supergroups. We observe that the meaning of the supertrace differs by a $(-)$ sign from class I to class II representations as in Eqs. (2.22), (2.23). Therefore, the expression for $\chi_{(2,0,0,\cdots)}$ given above yields different results for these two representations, since some of the supertraces are squared.

We perform similar calculations for other representations of U(N/M) just as we did for U(N). *For the representations whose supertableaux are formally the same as the ordinary Young tableaux the characters are expressed by the same formula except for traces replaced by supertraces.* A few such examples can be easily worked out and this general result can be explicitly verified, as we did for the representations listed in the Appendix. We conclude that the character equations (2.14), (2.15), for completely symmetric states of U(N)-type groups, is also valid for U(N/M)-type supergroups if we substitute supertraces for traces. Therefore the character of the representation $(n,0,0,\cdots)$ associated with the supertableau consisting of a single row of n boxes is given by

$$\mathcal{K}_{(n,0,0,\cdots)} = \mathcal{K}_n$$

$$\mathcal{K}_n = \sum_{k_1,k_2,\cdots,k_n}\prod_{l=1}^{n}\frac{1}{k_l!}\left(\frac{\mathrm{Str}U^l}{l}\right)^{k_l} \times\delta(n-k_1-2k_2-\cdots-nk_n). \quad (2.35)$$

Following the steps of Eqs. (2.13), (2.14), (2.15), we obtain

$$\mathcal{K}_n = \oint_c\frac{dz}{2\pi i}\frac{z^{-n-1}}{\mathrm{Sdet}(1-z\mathcal{U})} \quad (2.36)$$

which generalizes Eq. (2.15) to the supergroups. Here $\mathcal{U}$ is the supergroup element in the fundamental representation and c is a contour around the origin in the complex plane. Similarly the character of any representation denoted by $(n_1,n_2,\cdots)$ is given by the determinantal form:

$$\mathcal{K}_{(n_1,n_2,\cdots)} = \begin{vmatrix} \mathcal{K}_{n_1} & \mathcal{K}_{n_2+1} & \cdots \\ \mathcal{K}_{n_1-1} & \mathcal{K}_{n_2} & \cdots \\ \vdots & \vdots & \end{vmatrix}, \quad (2.37)$$

which is analogous to Eq. (2.11). The order of the above determinant is equal to the number of rows in the supertableau.

To conclude this section, we note that the dimension of any representation can be found by calculating the character of the matrix $\mathcal{J}$, with matrix elements

$$\mathcal{J}_{AB} = (-1)^{g(A)}\delta_{AB}, \quad (2.38)$$

in this representation. For class I representations $\mathcal{J}$ takes the form

$$\begin{pmatrix} I_N & 0 \\ 0 & -I_M \end{pmatrix}, \quad (2.39)$$

and for class II representations it takes the form

$$\begin{pmatrix} -I_N & 0 \\ 0 & I_M \end{pmatrix}, \tag{2.40}$$

where I_N and I_M are N- and M-dimensional unit matrices. Thus when we consider class I [class II] representations $\mathrm{Str}(\mathscr{J}^k)$ es equal to $(N+M)$ for odd k and $(N-M)$ $[(M-N)]$ for even k. We denote dimensions of class I and class II representations by $D_{(n_1,n_2,\cdots)}$ and $\tilde{D}_{(n_1,n_2,\cdots)}$ respectively. The dimensions of the representations $\xi_{(AB)}$ and $\tilde{\xi}_{(AB)}$ we discussed above can easily be calculated from the character formulas given in Eqs. (2.36), (2.37) by substituting $\mathscr{U} = \mathscr{J}$. This gives

$$D_{(2,0,\cdots)} = \tfrac{1}{2}[(N+M)^2 + (N-M)], \tag{2.41}$$

$$\tilde{D}_{(2,0,\cdots)} = \tfrac{1}{2}[(N+M)^2 + (M-N)], \tag{2.42}$$

which agree with the dimensions we found previously following Eqs. (2.26) and (2.27) by counting the number of the components of the wavefunctions. Dimensions of the other representations are calculated in the same way. In particular, the dimension $D_n = \mathscr{K}_n(\mathscr{J})$ of the class I representation with a single row follows from Eq. (2.36) and the definition of the superdeterminant, Eq. (2.23), as

$$\begin{aligned} D_n &= \oint \frac{dz}{2\pi i} z^{-n-1} \frac{(1+z)^M}{(1-z)^N} \\ &= \sum_{k=0}^{n} \binom{M}{k} \quad \binom{-N}{n-k} \\ &= \sum_{k=0}^{n} [d_{(1^k)}(M)] \ [d_{n-k}(N)], \end{aligned} \tag{2.43}$$

where we have identified $d_{n-k}(N) = \binom{-N}{n-k}$ with the dimension of the symmetric representation of $\mathrm{U}(N)$ containing $n-k$ boxes in a single row and $d_{(1^k)}(M) = \binom{M}{k}$ as the dimension of the completely antisymmetric representation of $\mathrm{U}(M)$ containing k boxes in a single column. Similarly, the dimension $\tilde{D}_n$ of the class II representation with a single row is

$$\tilde{D}_n = \sum_{k=0}^{n} [d_{(1^k)}(N)] \ [d_{n-k}(M)]. \tag{2.44}$$

The dimension of an arbitrary representation will have the form $D_{(n_1,n_2,\cdots)} = \mathscr{K}_{(n_1,n_2,\cdots)}(\mathscr{J})$. For class I representations we write

$$D_{(n_1,n_2,\cdots)} = \begin{vmatrix} D_{n_1} & D_{n_2-1} & \cdots \\ D_{n_1+1} & D_{n_2} & \cdots \\ \vdots & \vdots & \end{vmatrix}, \tag{2.45}$$

where the order of the determinant is equal to the number of the rows in the supertableau. $\tilde{D}_{(n_1,n_2,\cdots)}$ is also given by the same equation if we exchange D_n's with $\tilde{D}_n$'s.

Finally we can find the number of fermionic and bosonic components of a given representation by calculating the characters of the matrix

$$\mathscr{J} = \begin{pmatrix} I_N & 0 \\ 0 & -I_M \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} -I_N & 0 \\ 0 & I_M \end{pmatrix}$$

of Eq. (2.38) and the unit matrix

$$I = \begin{pmatrix} I_N & 0 \\ 0 & I_M \end{pmatrix}.$$

We denote the number of bosonic and fermionic components of the class I representation $(n_1,n_2,\cdots)$ by $B_{(n_1,n_2,\cdots)}$ and $F_{(n_1,n_2,\cdots)}$ respectively and those of the class II representation $(n_1,n_2,\cdots)$ by $\tilde{B}_{(n_1,n_2,\cdots)}$ and $\tilde{F}_{(n_1,n_2,\cdots)}$. We note that in Eq. (2.43)the terms with $k =$ odd ($n-k =$ odd) are associated with fermionic components of class I (class II) representations. This observation allows us to identify the total numbers of bosons and fermions by taking the following linear combination of characters:

$$B_{(n_1,n_2,\cdots)} = \tfrac{1}{2}[\mathscr{K}_{(n_1,n_2,\cdots)}(\mathscr{J}) + \mathscr{K}_{(n_1,n_2,\cdots)}(I)] \tag{2.46}$$

and

$$F_{(n_1,n_2,\cdots)} = \tfrac{1}{2}[\mathscr{K}_{(n_1,n_2,\cdots)}(\mathscr{J}) - \mathscr{K}_{(n_1,n_2,\cdots)}(I)]. \tag{2.47}$$

$\mathscr{K}_{(n_1,n_2,\cdots)}(I)$ is obtained from Eq. (2.37), in which we substitute $\mathscr{K}_n(I) = \binom{M-N}{n}(-1)^n$ as computed from Eq. (2.36). These expressions apply to both class I and class II representations except for the meanings of $\mathscr{J}$ and the supertrace as given in Eqs. (2.39), (2.40), (2.20). As an example, Eqs. (2.46) and (2.47) give the number of bosonic and fermionic components of the class I representation (2, 0, 0, ···) as $[\frac{1}{2}N(N+1) + \frac{1}{2}M(M-1)]$ and NM, respectively. The same result was obtained following Eq. (2.26) by directly counting the bosonic and fermionic components of the wavefunction ξ_{AB}.

III. FORMAL DEVELOPMENTS

In this section we review the relationship between Eqs. (2.11), (2.15) and Weyl's character formula[10] and generalize certain concepts to the supergroup case.

An irreducible representation of $\mathrm{U}(N)$ type groups is completely determined by its character. Let the eigenvalues of the group element U in the fundamental representation by $\epsilon_1, \epsilon_2, \ldots, \epsilon_N$. Weyl's formula gives the character of the representation $(n_1,n_2,\ldots,n_{N-1},n_N)$ as the ratio of two determinants[10]:

$$\chi_{(n_1,n_2,\ldots,n_N)} = \frac{\begin{vmatrix} \epsilon_1^{n_1+N-1} & \epsilon_1^{n_2+N-2} & \cdots & \epsilon_1^{n_N} \\ \epsilon_2^{n_1+N-1} & \epsilon_2^{n_2+N-2} & \cdots & \epsilon_2^{n_N} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \epsilon_N^{n_1+N-1} & \epsilon_N^{n_2+N-2} & \cdots & \epsilon_N^{n_N} \end{vmatrix}}{\begin{vmatrix} \epsilon_1^{N-1} & \epsilon_1^{N-2} & \cdots & \epsilon_1^{0} \\ \epsilon_2^{N-1} & \epsilon_2^{N-2} & \cdots & \epsilon_2^{0} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \epsilon_N^{N-1} & \epsilon_N^{N-2} & \cdots & \epsilon_N^{0} \end{vmatrix}} \tag{3.1}$$

To consider $\mathrm{SU}(N)$ instead of $\mathrm{U}(N)$, we simply take $n_N = 0$.

If we interchange ϵ_1 and ϵ_2 in the numerator (which corresponds to changing two consecutive rows of the determinant) its sign changes. On the other hand interchanging ϵ_1 and ϵ_3 keeps its sign the same: The numerator of the above

equation is an alternating function. The denominator, which is called the Vandermonde's determinant, is also an alternating function. Their ratio is a *symmetric function*: It remains unaltered when any two variables are interchanged.

One defines[12] the *complete homogeneous symmetric function* of degree n in the arguments x_i, $i = 1,...,N$, as the sum of the products of the variables x_i, taking n of them at a time. It is denoted by h_n. The sum of the products of the same variables again taking n of them at a time, but this time without repetition of any x_i in a product, is called the *elementary symmetric function* in the arguments x_i, $i = 1,...,N$, and is denoted by a_n. The following are some examples for three variables x_1,x_2,x_3:

$$a_1(x) = h_1(x) = x_1 + x_2 + x_3,$$
$$a_2(x) = x_1x_2 + x_1x_3 + x_2x_3,$$
$$a_3(x) = x_1x_2x_3,$$
$$h_2(x) = x_1^2 + x_2^2 + x_3^2 + x_1x_2 + x_1x_3 + x_2x_3,$$
$$h_3(x) = \sum_i x_i^3 + \sum_{i,k} x_i^2x_k + x_1x_2x_3.$$

We note that $a_n = 0$ if $n < N$. One writes a generating function for the elementary symmetric functions as

$$f(z,x) = \prod_{i=1}^{N}(1 - x_iz) = \sum_n (-1)^n a_n(x)z^n \tag{3.2}$$

and for the complete homogeneous symmetric functions as

$$F(z,x) = \prod_{i=1}^{N} \frac{1}{(1 - x_iz)} = \sum_n h_n(x)z^n. \tag{3.3}$$

One defines $h_0 = a_0 = 1$ and $h_n = a_n = 0$ for $n < 0$. Multiplying Eqs. (3.2) and (3.3), one gets the following relations:

$$\begin{aligned} &h_0a_k - h_1a_{k-1} + h_2a_{k-2} - \cdots + (-1)^k h_k a_0 = 0,\\ &h_0a_{k-1} - h_1a_{k-2} + \cdots + (-1)^{k-1}h_{k-1}a_0 = 0,\\ &h_0a_1 - h_1a_0 = 0, \end{aligned} \tag{3.4}$$

which are called Wronski's relations. We can consider (3.4) as a set of k equations with k unknowns $a_k, a_{k-1},...,a_0$ and coefficients $h_0, -h_1,...,(-1)^j h_j,\cdots$. Solving for a_k, one finds the determinant

$$a_k = \begin{vmatrix} h_1 & h_2 & \cdots & h_k \\ h_0 & h_1 & \cdots & h_{k-1} \\ 0 & h_0 & \cdots & h_{k-2} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & \cdots h_0 & h_1 \end{vmatrix}. \tag{3.5}$$

Reversing the roles of a_k and h_k, we can also write

$$h_k = \begin{vmatrix} a_1 & a_2 & \cdots & a_k \\ a_0 & a_1 & \cdots & a_{k-1} \\ 0 & a_0 & \cdots & a_{k-2} \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots a_0 & a_1 \end{vmatrix}. \tag{3.6}$$

Now let us write down the character, χ_m, of the representation $(m,0,...,0)$ corresponding to the Young tableau with a single row of m boxes. We recall that the general character formulas in the previous section were based on this representation. We now try to relate that form to Weyl's character formula. From Weyl's formula we can write

$$\chi_m = \frac{\begin{vmatrix} \epsilon_1^{m+N-1} & \epsilon_1^{N-2} & \cdots & 1 \\ \epsilon_2^{m+N-1} & \epsilon_2^{N-2} & \cdots & 1 \\ \vdots & \vdots & \cdots & \vdots \\ \epsilon_N^{m+N-1} & \epsilon_N^{N-2} & \cdots & 1 \end{vmatrix}}{\Delta(\epsilon_1,\epsilon_2,...,\epsilon_N)} \tag{3.7}$$

where $\Delta(\epsilon_1, \epsilon_2, ..., \epsilon_N)$ denotes the Vandermonde's determinant in the arguments $\epsilon_1, \epsilon_2, ..., \epsilon_N$. After some algebra[13] one finds that χ_m is equal to the symmetric function $h_m(\epsilon)$:

$$\chi_m = h_m(\epsilon) = \sum_{i=1}^{N} \epsilon_i^m + \sum_{i,k=1}^{N} \epsilon_i^{m-1}\epsilon_k + \cdots + \epsilon_1\epsilon_2\cdots\epsilon_N. \tag{3.8}$$

Similarly the character of any representation can be written as a single determinant (rather than a ratio) by manipulating the properties of determinants. Then it follows that Weyl's formula reduces to [14,15]

$$\chi_{(n_1,n_2,\cdots)} = \begin{vmatrix} h_{n_1} & h_{n_2-1} & \cdots & h_{n_N-N+1} \\ h_{n_1+1} & h_{n_2} & \cdots & h_{n_N-N+2} \\ \vdots & \vdots & & \vdots \\ h_{n_1+N-1} & h_{n_2+N-2} & \cdots & h_{n_N} \end{vmatrix}. \tag{3.9}$$

This is the form we noted in Sec. II on the basis of the examples in the Appendix which were arrived at by the method of symmetrization and antisymmetrization, and therefore it must also apply generally to supergroups, as we have shown in the previous section. There remains to make contact between the formulas for χ_m of the present section (3.8), (3.9), which are written in terms of eigenvalues ϵ_i, with the formulas of the previous section (2.11), (2.15) written in terms of the group element U. This is achieved through the generating function $F(z,\epsilon)$ of Eq. (3.3) if we identify ϵ_i with the eigenvalues of U and write

$$F(z,\epsilon) = \prod_{i=1}^{N} \frac{1}{(1 - z\epsilon_i)} = \frac{1}{\det(1 - zU)}. \tag{3.10}$$

On the other hand, $h_n(\epsilon)$ is the nth term of the Taylor expansion of $F(z,\epsilon)$:

$$h_n(\epsilon) = \frac{1}{n!}\left[\frac{d^n}{dz^n} F(z,\epsilon)\right]_{z=0} \tag{3.11}$$

Using Cauchy's theorem and substituting $F(z,\epsilon)$ from Eq. (3.10), this result is equivalent to

$$h_n(\epsilon) = \frac{1}{2\pi i}\oint_c \frac{dz}{z^{n+1}} \frac{1}{\det(1 - zU)}, \tag{3.12}$$

which is the form we noted in Sec. II, Eq. (2.15).

Finally we want to point out that Eq. (3.9) gives the character of the representation $(1, 1, ..., 1) = (1^k)$, associated with the tableau with a single column of k boxes, as

$$\chi_{(1^k)} = \begin{vmatrix} h_1 & 1 & \cdots & 0 \\ h_2 & h_1 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ h_{k-1} & h_{k-2} & \cdots & 1 \\ h_k & h_{k-1} & \cdots & h_1 \end{vmatrix}, \tag{3.13}$$

which is equivalent to $a_k(\epsilon)$ by Eq. (3.5):

$$\chi_{(1^k)} = a_k(\epsilon) \tag{3.14}$$

In the second part of this section we develop a formalism for the class of representations of U(N/M) type supergroups defined by Eqs. (2.17) and (2.18). The diagonalized form of the supergroup element $\mathscr{U}$ is

$$\mathscr{U} = \begin{pmatrix} \mathscr{A}' & o \\ 0 & \mathscr{D}' \end{pmatrix}, \tag{3.15}$$

where $\mathscr{A}'$ and $\mathscr{D}'$ are diagonal $N \times N$ and $M \times M$ matrices, respectively. We denote the eigenvalues of $\mathscr{A}'$ by ϵ_i, $i = 1, ...,N$, and those of $\mathscr{D}'$ by $\lambda_j, j = 1,...,M$. We introduce the *graded homogeneous symmetric function* of degree n in the arguments $\epsilon_1,...,\epsilon_N; \lambda_1,...,\lambda_M$ as

$$H_n(\epsilon,\lambda) = \oint_c \frac{dz}{2\pi i} \frac{z^{-n-1}}{\mathrm{Sdet}(1 - z\mathscr{U}')} = \oint_c \frac{dz}{2\pi i z^{n+1}} \frac{\Pi_{j=1}^{M}(1 - \lambda_j z)}{\Pi_{i=1}^{N}(1 - \epsilon_i z)}, \tag{3.16}$$

where c is a contour around the origin. This is the class I character corresponding to the representation with a single row in a supertableau as was given in the previous section. From this definition we can write the generating function for graded homogeneous symmetric functions as

$$G(z;\epsilon,\lambda) = \frac{\Pi_{j=1}^{M}(1 - \lambda_j z)}{\Pi_{i=1}^{N}(1 - \epsilon_i z)} = \sum_n H_n(\epsilon,\lambda) z^n. \tag{3.17}$$

Another set of invariant functions, denoted by $A_n(\epsilon,\lambda)$, can be introduced as in Eq. (3.2) by the generating function $g(z\epsilon,\lambda) = \mathrm{Sdet}(1 - z\mathscr{U}')$.

$$g(z;\epsilon,\lambda) = \frac{\Pi_{i=1}^{N}(1 - \epsilon_i z)}{\Pi_{j=1}^{M}(1 - \lambda_j z)} = \sum_n (-1)^n A_n(\epsilon,\lambda) z^n. \tag{3.18}$$

Clearly we should define $H_n = 0 = A_n$ for $n < 0$ and $H_0 = 1 = A_0$. Since their generating functions are inverses of each other, $H_n(\epsilon,\lambda)$ and $A_n(\epsilon,\lambda)$ also satisfy Wronski's relations. Therefore, following the same procedure which leads to Eqs. (3.5) and (3.6), we can express A_n as an $n \times n$ determinant

$$A_n = \det(H_{1-i+j}), \tag{3.19}$$

where we have shown the (ij)th element of the $n \times n$ matrix whose determinant is calculated. Recalling that H_n is the character of the representation with a single row supertableau and that the character of any representation is given by

$$\mathscr{K}_{(n_1,n_2,\cdots)} = \det(H_{n_i - i + j}), \tag{3.20}$$

as in Eq. (2.37), we note that A_n must be identified with the character corresponding to the single column supertableau $A_n = \mathscr{K}_{(1^n)}$. Similarly H_n can be written as a $n \times n$ determinant in terms of the A_k's

$$H_n = \det(A_{1-i+j}). \tag{3.21}$$

A second relation can be established between $H_n(\epsilon,\lambda)$ and $A_n(\epsilon,\lambda)$ by observing in Eqs. (3.17), (3.18) that the generating functions $G(z;\epsilon,\lambda)$ and $g(z;\epsilon,\lambda)$ transform into each other by interchanging (λ_j)'s with (ϵ_i)'s. However, this is just the tilde operation discussed in the last section which relates the superdeterminants in class I and class II representations as inverses of each other. Therefore, $(-1)^n A_n(\epsilon,\lambda)$ is simply $\mathscr{K}_{(n,0,0,\cdots)}$ for class II while $H_n(\epsilon,\lambda)$ is $\mathscr{K}_{(n,0,0,\cdots)}$ for class I representations. We have now found the following relations among them:

$$(-1)^n A_n(\epsilon,\lambda) = H_n(\lambda,\epsilon), \tag{3.22}$$

which follows from the interchange of λ's with ϵ's.

Just as in the ordinary Lie algebra case, we see from the general character formula and Eq. (3.19) that $A_n(\epsilon,\lambda)$ is just the class I character of the completely "antisymmetric" representation with n indices corresponding to a *single column of white* boxes. However, we have also just realized that $(-1)^n A_n(\epsilon,\lambda)$ is the class II character of the completely symmetric representation with n indices corresponding to a *single row of black* boxes. These two representations are related to each other by the tilde operation *plus* interchanging "symmetrization" with "antisymmetrization". From the general character formulas we now obtain the following result: Representations which are related to each other by the tilde operation (conversion of bosons$\longleftrightarrow$fermions) in the graded Hibert space plus the interchange of "symmetrization" and "antisymmetrization," have identical characters which differ at most by a $(-)$ sign.

Finally we note the nontrival relation which follows via Eqs. (3.20), (3.22):

$$(-1)^n H_n(\lambda,\epsilon) = \det[H_{1-i+j}(\epsilon,\lambda)], \tag{3.23}$$

where the λ's and ϵ's are interchanged in the arguments of the H's on opposite sides of the equations. A similar relation holds for the A_n's.

IV. EXTENSION TO ORTHOSYMPLECTIC SUPERGROUPS

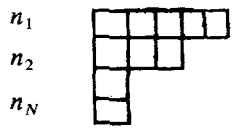
In the first part of this section we will briefly review the character and dimension formulas[10] for the representations of O($2N$)-, O($2N+1$)-, and Sp($2N$)-type Lie groups. The representations of these groups are labeled by a partition into N parts: $\{n_1,n_2,...n_N\}$, where $n_1 \geqslant n_2 > ... > n_N \geqslant 0$. One can rewrite this partition defining $l_i = n_i + N - i$ so that $l_1 > l_2 > ... l_N \geqslant 0$.

For the O($2N$) type groups the character of the irreducible representation corresponding to the partition $\{n_1,n_2,...n_N\}$ is given by[10,15]

$$\chi_{\{n_1,n_2,...n_N\}} = \tfrac{1}{2}\det(h'_{n_j+i-j} + h'_{n_j-j-i+2}) \tag{4.1}$$

$$= \tfrac{1}{2}\begin{vmatrix} h'_{n_1} + h'_{n_1} & h'_{n_2-1} + h'_{n_2-1} & \cdots \\ h'_{n_1+1} + h'_{n_1-1} & h'_{n_2} + h'_{n_2-2} & \cdots \\ \vdots & \vdots & \end{vmatrix},$$

where $h'_m = h_m - h_{m-2}$. Just as in the U(N) case we can associate a tableau with at most N rows (not $2N$ rows) with this representation of O($2N$):



Note that the dimension of the determinant reduces to the number of nontrivial rows in the Young tableau if we take into account that $h_0 = 1$ and $h_n = 0$ for $n =$ negative integer. The complete homogeneous symmetric function h_n can again be expressed as

$$h_n(S) = \oint_c \frac{dz}{2\pi i} \frac{z^{-n-1}}{\det(1 - zS)}, \tag{4.2}$$

where the matrix S is the fundamental representation of $O(2N)$ and c is a contour around the origin. The dimension of the representation $\{n_1,n_2,...,n_N = 0\}$ is

$$d_{\{n_1,n_2,...,n_{N-1},0\}} = \frac{2^{N-1}\Delta(l^2)}{(2N-2)!\,(2N-4)!\cdots 2!}, \tag{4.3}$$

where $\Delta(l^2)$ is the Vandermonde determinant in the arguments $l_1^2, l_2^2, ..., l_N^2$. The dimension of the representation $\{n_1,n_2,...,n_N \neq 0\}$ is

$$d_{\{n_1,n_2,...,n_N\neq 0\}} = \frac{2^N \Delta(l^2)}{(2N-2)!\,(2N-4)!\cdots 2!}. \tag{4.4}$$

Equations (4.3) and (4.4) are obtained by calculating the character of the matrix I:

$$d_{\{n_1,n_2,...,n_N\}} = \chi_{\{n_1,n_2,...n_N\}}(I).$$

For $n_N = 0$, the irreducible representation of $O(2N)$ whose character is given in Eq. (4.1) is also an irreducible representation of $SO(2N)$. But for the case $n_N \neq 0$ this representation is reducible. It splits into two irreducible representations of $SO(2N)$ with the characters

$$\chi^{(1)}_{\{n_1,n_2,...,n_N\neq 0\}} = \tfrac{1}{4}[\det(h'_{n_j - i - j + 2} + h'_{n_j + i - j} + \alpha i^N \det(h_{n_i - i + j - 1} + h_{n_i - i - j + 1})], \tag{4.5a}$$

$$\chi^{(2)}_{\{n_1,n_2,...,n_N\neq 0\}} = \tfrac{1}{4}[\det(h'_{n_j - i - j + 2} + h'_{n_j + i - j}) - \alpha i^N \det(h_{n_i - i + j - 1} + h_{n_i - i - j + 1})], \tag{4.5b}$$

where α can be expressed as

$$\alpha = [\det(S^T - S)]^{1/2}$$

and S is the fundamental representation of $SO(2N)$. The dimensions of these two representations are the same and given by Eq. (4.3).

For the $O(2N+1)$-type groups one also associates irreducible representations with the partitions $\{n_1,n_2,...,n_N\}$. The character of $\{n_1,n_2,...n_N\}$ is given by

$$\chi_{\{n_1,n_2,...,n_N\}} = \tfrac{1}{2}\det(h'_{n_j - i - j + 2} + h'_{n_j + i - j}). \tag{4.6}$$

The dimension of this representation is again found by calculating the character of the unit matrix. One obtains

$$d_{\{n_1,n_2,...,n_N\}} = \frac{\Delta(l)\Pi_{i<j}(l_i + l_j + 1)}{(2N-1)!\,(2N-3)!\cdots 3!\;1!}, \tag{4.7}$$

where $\Delta(l)$ is the Vandermonde determinant in the arguments $l_1,...,l_N$.

Now let us make contact with the above well-known results by employing the symmetrization–antisymmetrization technique. This procedure will teach us how to generalize the character and dimension formulas to the supergroups $OSP(N/2M)$. The symmetrized tensor product of two fundamental (vector) representations of $O(2N)$ or $O(2N+1)$ may be written as

$$\phi_{(ab)} = \phi^{(1)}_a \phi^{(2)}_b + \phi^{(2)}_a \phi^{(1)}_b. \tag{4.8}$$

Unlike the $U(N)$ case $\phi_{(ab)}$ does not form an irreducible representation. Since the Kronecker delta function δ_{ab} is an invariant the orthogonal group, the irreducible basis κ_{ab} can be chosen by imposing the invariant condition $\delta_{ab}\kappa_{ab} = 0$. Therefore, κ_{ab} can be expressed as

$$\kappa_{(ab)} = \phi_{(ab)} - (\delta_{ab}/M)\delta_{cd}\phi_{(cd)} \tag{4.9}$$

for $O(M)$ where $M = 2N$ or $2N+1$. In other words the reducible basis $\phi_{(ab)}$ is split into two irreducible bases: $\kappa_{(ab)}$ and the singlet $\delta_{cd}\phi_{(cd)}$. Under the $O(M)$ group, M odd or even, $\kappa_{(ab)}$ transforms into

$$\kappa_{(ab)} \to [U_{(ab),(a'b')} - \delta_{ab}\,\delta_{a'b'}/M\,]\kappa_{(a'b')}, \tag{4.10}$$

where $U_{(ab),(a'b')}$ is as given in Eq. (2.4). As in Sec. II the character of this representation is then $h_2 - 1 = h_2 - h_0$. Extending the above argument, one shows that the symmetrized tensor product of m-basis vectors is split into irreducible representations in a similar way. The characters of these irreducible representations are given by $h'_m = h_m - h_{m-2}$, $h'_{m-2} = h_{m-2} - h_{m-4},...,h_1$ or h_0. From Eqs. (4.1) and (4.2) one observes that these are the characters of the representations $\{m,0,0,\cdots\}$, $\{m-2,0,\cdots\}$, etc. corresponding to single row tableaux for $O(M)$.

The antisymmetrized tensor product $\phi_{(a,b)} = \phi^{(1)}_a \phi^{(2)}_b - \phi^{(2)}_a \phi^{(1)}_b$ form the basis of an irreducible representation of $O(M)$ since $\delta_{ab}\phi_{(a,b)} = 0$. As a matter of fact Eq. (4.1) gives the character of the representation $\{1,1,...,n_p = 1,n_{p+1} = 0,...,0\}$ as a $p \times p$ determinant:

$$\chi_{\{1,...,n_p=1,n_{p+1}=0,...,0\}} = \tfrac{1}{2}\det(h'_{3-i-j} + h'_{1+i-j}) = \det(h_{1+i-j}), \tag{4.11}$$

which is equal to a_p by Eq. (3.5) which is the character of the representation of $Gl(N)$ or $U(N)$ obtained by antisymmetrizing p basis vectors. Hence completely antisymmetrized tensor products of the fundamental representation form irreducible representations of $O(M)$.

For $Sp(2N)$ type groups the character of the irreducible representation corresponding to the partition $\{n_1,n_2,...,n_N\}$ is[10]

$$\chi_{((n_1,n_2,...,n_N))} = \tfrac{1}{2}\det(h_{n_j+i-j} + h_{n_j-i-j+2}). \tag{4.12}$$

The dimension of this representation can again be found by calculating the character of identity matrix. These formulas can again be related to the symmetrization–antisymmetrization procedure. They can be shown to be intimately connected to the $O(2N)$ case by interchanging the roles of symmetrization with antisymmetrization and by taking C_{ab}, the invariant antisymmetric tensor of $Sp(2N)$, instead of the δ_{ab} of $O(2N)$. Note that

$$C = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix},$$

where I_N is the identity matrix in N dimensions.

Now we can generalize the above results to the OSP($N/2M$)-type supergroups. We denote the basis for the fundamental representation by ζ_A which contains N bosons and $2M$ fermions. Under the supergroup ζ_A transforms into $\zeta'_A = \mathscr{M}_{AB}\zeta_B$, where $\mathscr{M}$ is the element of the supergroup OSP($N/2M$) in the $(N+2M)$-dimensional fundamental representation. Since the ordinary matrix transposition $(\mathscr{M}_1\mathscr{M}_2)^{\mathrm{T}}$ is not equal to $\mathscr{M}_2^{\mathrm{T}}\mathscr{M}_1^{\mathrm{T}}$ when one has fermionic matrix elements, we define the *supertransposition* by interchanging the order of fermions according to Eq. (2.32): $\zeta_A = \mathscr{M}_{AB}\zeta_B = \zeta_B(\mathscr{M}^{\mathrm{ST}})_{BA}$. Here $\mathscr{M}^{\mathrm{ST}}$ is given by $(\mathscr{M}^{\mathrm{ST}})_{BA} = (-1)^{g(B)[g(A)-g(B)]}\mathscr{M}_{AB}$ and satisfies the equation

$$(\mathscr{M}_1\mathscr{M}_2)^{\mathrm{ST}} = \mathscr{M}_2^{\mathrm{ST}}\mathscr{M}_1^{\mathrm{ST}}. \tag{4.13}$$

For OSP($N/2M$)-type supergroups the group element $\mathscr{M}$ should obey the relation[6,7]

$$\mathscr{M}^{\mathrm{ST}}H\mathscr{M} = \mathrm{H}, \quad \mathscr{M}H\mathscr{M}^{\mathrm{ST}} = H^{\mathrm{ST}}, \tag{4.14}$$

where

$$H = \begin{pmatrix} I_N & 0 \\ 0 & C \end{pmatrix} \tag{4.15}$$

with

$$C = \begin{pmatrix} 0 & I_M \\ -I_M & 0 \end{pmatrix}. \tag{4.16}$$

We note that

$$H^2 = \begin{pmatrix} I_N & 0 \\ 0 & -I_{2M} \end{pmatrix}, \quad HH^{\mathrm{ST}} = \begin{pmatrix} I_N & 0 \\ 0 & I_{2M} \end{pmatrix}. \tag{4.17}$$

The "symmetrized" tensor product of two basis vectors $\zeta_A^{(1)}$ and $\zeta_B^{(2)}$ is reducible. Since H_{AB} is an invariant of the OSP($N/2M$)-type supergroups, the irreducible basis $\zeta_{(AB)}$ should satisfy the condition $H_{AB}\zeta_{(AB)} = 0$. We then write

$$\zeta_{(AB)} = \overline{\zeta}_{(AB)} - [(H^{\mathrm{ST}})_{\mathrm{AB}}/(\mathrm{N}-2\mathrm{M})]H_{CD}\overline{\zeta}_{(CD)}, \tag{4.18}$$

where

$$\overline{\zeta}_{(AB)} = \zeta_A^{(1)}\zeta_B^{(2)} + \zeta_A^{(2)}\zeta_B^{(1)}. \tag{4.19}$$

Using the relation

$$H_{AB} = (-1)^{g(A)}H_{BA}, \tag{4.20}$$

one easily shows that $\zeta_{(AB)}$ given above satisfies our condition. Under the supergroup $\zeta_{(AB)}$ transforms into

$$\zeta'_{(AB)} = [\mathscr{M}_{(AB),(A'B')} - (H^{\mathrm{ST}})_{AB}H_{A'B'}/(N-2M)]\zeta_{(A'B')}, \tag{4.21}$$

where

$$\mathscr{M}_{(AB),(A'B')} = \tfrac{1}{2}[(-1)^{g(A')\cdot[g(B)-g(B')]}\mathscr{M}_{AA'}\mathscr{M}_{BB'} + (-1)^{g(A)\cdot g(B)}(-1)^{g(A')\cdot[g(A)-g(B')]} \times \mathscr{M}_{BA'}\mathscr{M}_{AB'}], \tag{4.22}$$

as for the U($N/2M$) group. The character of this representation is $H_2 - 1 = H_2 - H_0$, where

$$H_n = \oint_c \frac{dz}{2\pi i}\frac{z^{-n-1}}{\mathrm{Sdet}(1-z\mathscr{M})}, \tag{4.23}$$

as defined by Eq. (3.16). Similarly the "symmetrized" tensor product of m basis vectors is split into irreducible representations whose characters are given by $H_m - H_{m-2} = H'_m$, $H_{m-2} - H_{m-4} = H'_{m-2}, \ldots, H_1$ or H_0. *This is a direct generalization of the orthogonal group characters to the orthosymplectic group. Note that the generalization consists of formally replacing traces or determinants by supertraces or superdeterminants.*

On the other hand the "antisymmetrized" tensor product of two basis vectors

$$\zeta_{(A,B)} = \zeta_A^{(1)}\zeta_B^{(2)} - \zeta_A^{(2)}\zeta_B^{(1)} \tag{4.24}$$

is the basis of an irreducible representation since it automatically satisfies the condition $H_{AB}\zeta_{(A,B)} = 0$. In general the completely antisymmetrized tensor product of n basis vectors form an irreducible representation whose character is the n-dimensional determinant $\det(H_{1-i+j})$.

Having observed these close correspondences (trace→supertrace) between the simplest characters of the orthogonal groups and the orthosymplectic supergroups, we conclude that the character of the irreducible representation of the OSP($N/2M$) type groups corresponding to the partition $\{n_1,n_2,\ldots\}$ must be given by

$$\mathscr{K}_{\{n_1,n_2,\ldots\}} = \tfrac{1}{2}\det(H'_{n_j+i-j} + H'_{n_j-j-i+2}), \tag{4.25}$$

where $H'_m = H_m - H_{m-2}$.

The dimension of this representation, $D'_{\{n_1,n_2,\ldots\}}$, is found by calculating the character of the matrix $\mathscr{J}$, defined in Eq. (2.39). We get

$$D'_{\{n_1,n_2,\ldots\}} = \tfrac{1}{2}\det(D'_{n_j+i-j} + D'_{n_j-j-i+2}),$$

where $D'_n \equiv D_n - D_{n-2}$. D_n is given by Eq. (2.43).

The character formula (4.25) for OSP($N/2M$)-type supergroups should reduce to the character formulas of O(N) and Sp($2M$) type groups in limiting cases. Let us note some of these limits and check the consistency of our equations. The fundamental representation of the O(N) subgroup has a bosonic basis and the Sp($2M$) subgroup has a fermionic basis. The matrix $\mathscr{M}$ can be written as

$$\mathscr{M} = \begin{pmatrix} \mathscr{A} & \mathscr{B} \\ \mathscr{C} & \mathscr{D} \end{pmatrix}, \tag{4.26}$$

where the matrix elements of $\mathscr{A}$ and $\mathscr{D}$ are bosonic and those of $\mathscr{B}$ and $\mathscr{C}$ are fermionic. The diagonalized form of $\mathscr{M}$ is

$$\mathscr{M}' = \begin{pmatrix} \mathscr{A}' & 0 \\ 0 & \mathscr{D}' \end{pmatrix}. \tag{4.27}$$

The "symmetrized" representation $\{m,0,\ldots,0\}$ of OSP($N/2M$) should reduce to the representation $((1,1,\ldots,n_m=1,n_{m+1}=0,\ldots,0))$ of Sp($2M$) when the matrices $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$ are zero and $\mathscr{D}$ is nonzero. This amounts to the eigenvalues ϵ_i, $i=1,\ldots,N$, of $\mathscr{A}'$ all being zero and the eigenvalues λ_j, $j=1,\ldots,2M$, of $\mathscr{D}'$ being nonzero. In this case the character of the representation $\{m,0,\ldots,0\}$ reduces to (in the notation of Sec. II)

$$H'_m(0,\lambda) = H_m(0,\lambda) - H_{m-2}(0,\lambda), \tag{4.28}$$

which is equal to $\mp[a_m(\lambda) - a_{m-2}(\lambda)]$ by Eqs. (3.16) and (3.17). On the other hand, Eq. (4.12) gives the character of the representation $((1,1,\ldots,n_m=1,n_{m+1}=0,\ldots0))$ of Sp($2M$) as

the $m\times m$ determinant

$$\tfrac{1}{2}\det[h_{3-i-j}(\lambda)+h_{1+i-j}(\lambda)].$$

$$=\begin{vmatrix} h_1 & h_2 & h_3 & \cdots \\ h_0 & h_1 & h_2 & \cdots \\ 0 & h_0 & h_1 & \cdots \\ \vdots & \vdots & \vdots & \end{vmatrix} - \begin{vmatrix} h_0 & h_1 & h_3 & \cdots \\ 0 & h_0 & h_2 & \cdots \\ 0 & 0 & h_1 & \cdots \\ \vdots & \vdots & \vdots & \end{vmatrix}, \tag{4.29}$$

which is again equal to $a_m(\lambda)-a_{m-2}(\lambda)$ by Eq. (3.5). Hence the representation $\{m,0,\cdots\}$ of OSP($N/2M$) reduces to the representation $((1,\ldots,n_m=1,\ n_{m+1}=0,\ldots,0))$ of Sp($2M$) in this limit. We also expect the completely "antisymmetrized" representation $\{1,1,\ldots,n_m=1,n_{m+1}=0,\cdots\}$ of OSP($N/2M$) to reduce to the representation $((m,0,\ldots))$ of Sp($2M$) in the same limit. For OSP($N,2M$) we have

$$\mathcal{K}_{\{1,1,\ldots,n_m=1,\ n_{m+1}=0,\ldots\}}$$
$$=\tfrac{1}{2}\det(H'_{3-i-j}+H'_{1+i-j})=A_m \tag{4.30}$$

by Eq. (3.19) and

$$A_m(0,\lambda)=h_m(\lambda)\ (-1)^m \tag{4.31}$$

by Eq. (3.18). For Sp($2M$) one gets $\chi_{\{(m,0,\ldots,0)\}}=h_m(\lambda)$ by Eq. (4.12). Thus, our results are consistent also for this case, as it should have been. The extra minus sign comes from the existence of an odd number of fermions.

The discussion given above for the class I representations can easily be extended to the class II representations by applying a tilde operation.

V. CALCULATION OF CASIMIR INVARIANTS

Using the character formulas given in the previous sections, one can calculate the Casimir invariants for the various representations of supergroups. Before discussing supergroups we will develop some techniques for SU(N) type groups as a warm-up excercise.

For SU(N) groups the Killing metric can be taken proportional to 1. We take it as δ_{ij}. If $R_{ab}(X_i)$, $i=1,2,\ldots,N^2-1$, is the representation of the generator X_i, then the value of the Casimir operator $C_2(R)$ in the representation R is given by

$$R_{ab}(X_i)R_{bc}(X_j)\delta^{ij}=C_2(R)\delta_{ac}. \tag{5.1}$$

Setting $a=c$ and summing, one arrives at

$$d(R)C_2(R)=\mathrm{Tr}[R(X_i)R(X_i)], \tag{5.2}$$

where $d(R)$ is the dimension of the representation R. Let us relate this equation to the character of the representation. Since any group element can be written as $g=\exp(\theta^i X_i)$, we can write

$$\delta^{ij}[R(X_i)R(X_j)]_{ab}=\delta^{ij}\left[\frac{\partial^2}{\partial\theta^i\partial\theta^j}R_{ab}(g)\right]_{\theta=0}, \tag{5.3}$$

where $R(g)$ is the representation of g. Setting $a=b$ and summing yields

$$d(R)C_2(R)=\delta^{ij}\left[\frac{\partial^2}{\partial\theta^i\partial\theta^j}\chi_R(g)\right]_{\theta=0}. \tag{5.4}$$

We apply this result to the character of the representation $(n,0,\ldots,0)$. Using Eq. (2.15) for this character, we parametrize $g=U=\exp(\theta^i\lambda^i/2)$ in the fundamental representation and take the derivatives as indicated in Eq. (5.4). Then we obtain the quadratic Casimir invariant $C_2^N(n)$ for this completely symmetric representation as

$$d_n C_2^N(n)=\oint\frac{dz}{2\pi i}\frac{z^{-n-1}}{(1-z)^N}\times\left[\frac{z}{1-z}+\frac{z^2}{(1-z)^2}\right]\left[\mathrm{Tr}\left(\frac{\lambda_i}{2}\frac{\lambda_j}{2}\right)\right]\delta^{ij}. \tag{5.5}$$

From Eq. (5.4) we see that

$$\mathrm{Tr}\left(\frac{\lambda_i}{2}\frac{\lambda_j}{2}\right)\delta^{ij}=N\,C_2^N(1),$$

where $C_2^N(1)$ is the quadratic Casimir invariant in the fundamental representation. The Killing form can be related to the normalization condition

$$\mathrm{Tr}\lambda_i\lambda_j=2\delta_{ij}.$$

This yields

$$C_2^N(1)=(N^2-1)/2N. \tag{5.6}$$

Substituting Eq. (5.6) into Eq. (5.5), one obtains

$$d_n C_2^N(n)=\frac{N-1}{2N!}\frac{(N+n)!}{(n-1)!}, \tag{5.7}$$

which gives via Eq. (2.16c)

$$C_2^N(n)=n(N-1)(N+n)/2N. \tag{5.8}$$

Similarly from Eqs. (2.11) and (5.4) one finds the quadratic Casimir invariant $C_2^N(n_1,n_2,\cdots)$, for the representation $(n_1,n_2,\ldots,n_{N-1})$ to be

$$d_{(n_1,n_2,\cdots)}C_2^N(n_1,n_2,\cdots)=\begin{vmatrix} d_{n_1}C_2(n_1) & d_{n_2-1} & \cdots \\ d_{n_1+1}C_2(n_1+1) & d_{n_2} & \cdots \\ \vdots & \vdots & \end{vmatrix}$$
$$+\begin{vmatrix} d_{n_1} & d_{n_2-1}C_2(n_2-1) & \cdots \\ d_{n_1+1} & d_{n_2}C_2(n_2) & \cdots \\ \vdots & \vdots & \end{vmatrix}+\cdots, \tag{5.9}$$

where we need to sum over as many terms as the rank of the determinant, which is equal to the number of nontrivial rows in the Young tableau.

We will use the same method to write down the Casimir invariants of the supergroups explicitly. A supergroup element g can be written as

$$g=\exp(\Theta_A X_A), \tag{5.10}$$

where X_A are the elements of the corresponding Lie superalgebra and the parameters Θ_A are bosonic [for $g(A)=0$] or fermionic [for $g(A)=1$]. Let us represent the generators X_A by the matrices $(\lambda_A/2)$ in the fundamental representation. Then the Killing form metric (g_{AB})[16] can again be related to the normalization of these matrices via the supertrace

$$2g_{AB}=\mathrm{Str}\lambda_A\lambda_B. \tag{5.11}$$

Note that $\mathrm{Str}\lambda_A=0$ for all A. The metric g_{AB} is not symmetric:

$$g_{AB}=(-1)^{g(A)\cdot g(B)}g_{BA}. \tag{5.12}$$

One defines the contravariant metric g^{AB} via the relation

$$g_{AB}g^{BC}=\delta^C{}_A. \tag{5.13}$$

The quadratic Casimir operator $C_2(R)$, in the represen-

tation R, is given as

$$g^{AB}[R(X_A)R(X_B)]_{rs} = [C_2(R)]_{rs}. \tag{5.14}$$

According to the generalization of Schur lemma $C_2(R)$ is proportional to the unity only for the representations where the dimension of the bosonic subspace is different than the dimension of the fermionic subspace[6]:

$$[C_2(R)]_{rs} = C_2(R)\delta_{rs}.$$

For such representations we can take the supertrace and write

$$\mathrm{Str}[R(I)]C_2(R) = g^{AB}\mathrm{Str}[R(X_A)R(X_B)], \tag{5.15}$$

where $R(I)$ is the representation and $\mathrm{Str}[R(I)] = \mathscr{K}_R(I)$ is the character of the identity element. Therefore, for $SU(N/M)$ type supergroups with $N \neq M$, in the fundamental representation this equation reads

$$\begin{aligned}(N-M)C_2^{N,M}(1) &= g^{AB}\mathrm{Str}\left(\frac{\lambda_A}{2}\frac{\lambda_B}{2}\right)\\ &= \tfrac{1}{2}g^{AB}g_{AB},\end{aligned} \tag{5.16}$$

where $N-M$ is the supertrace of the identity element in the fundamental representation of class I. Using Eq. (5.12), the above expression takes the form

$$(N-M)C_2^{N,M}(1) = \tfrac{1}{2}\left(\sum_a \delta_a^a - \sum_\alpha \delta_\alpha^\alpha\right). \tag{5.17}$$

where $\Sigma_a \delta_a^a$ and $\Sigma_\alpha \delta_\alpha^\alpha$ are the number of bosonic and fermionic generators, respectively:

$$\sum_a \delta_a^a = N^2 + M^2 - 1, \tag{5.18a}$$

$$\sum_\alpha \delta_\alpha^\alpha = 2MN. \tag{5.18b}$$

Substituting Eq. (5.18) into Eq. (5.17), we get the quadratic Casimir invariant $C_2^{N-M}(1)$ in the fundamental representation as

$$C_2^{N,M}(1) = (N-M-1)(N-M+1)/2(N-M). \tag{5.19}$$

We see, in fact, that for $N = M$ we must take a different approach, in accordance with the generalized Schur's lemma.[6]

From Eqs. (2.46) and (2.47) we observe that $\mathscr{K}_{(n_1,n_2,\cdots)}(I)$ is the difference of the dimensions of the bosonic and fermionic subspaces of the representation $R = (n_1,n_2,\cdots)$. If this difference is nonzero, we can write the quadratic Casimir invariant, $C_2^{N,M}(R)$, of such representations as

$$\begin{aligned}&\mathscr{K}_{(n_1,n_2,\cdots)}(I)C_2^{N,M}(R)\\ &\quad = g^{AB}\mathrm{Str}[R(X_A)R(X_B)],\end{aligned} \tag{5.20}$$

where $R(X_A)$ is the representation of the generator X_A. In analogy to Eq. (5.4), we obtain in the case of supergroups

$$\begin{aligned}&\mathscr{K}_{(n_1,n_2,\cdots)}(I)C_2^{N,M}(R)\\ &\quad = g_{AB}\left[\frac{\partial}{\partial\theta_B}\frac{\partial}{\partial\theta_A}\mathscr{K}_{(n_1,n_2,\cdots)}(g)\right]_{\theta=0}.\end{aligned} \tag{5.21}$$

Let us apply this equation to the calculation of the quadratic Casimir invariant $C_2^{N,M}(n)$ of the representation $(n,0,\ldots,0)$ of $SU(N/M)$. Using Eq. (2.36) and following the same steps leading to Eq. (5.5) we obtain

$$\begin{aligned}\mathscr{K}_n(I)C_2^{N,M}(n) &= (N-M)C_2^{N,M}(1)\\ &\quad\times\oint\frac{dz}{2\pi i}\frac{(1-z)^{M-N}}{z^{n+1}}\left(\frac{z}{1-z}+\frac{z^2}{(1-z)^2}\right).\end{aligned} \tag{5.22}$$

Substituting Eq. (5.19) into Eq. (5.22), one gets

$$C_2^{N,M}(n) = n(N-M-1)(N-M+n)/2(N-M). \tag{5.23}$$

Similarly from Eqs. (2.37) and (5.21) the quadratic Casimir invariant $C_2^{N,M}(n_1,n_2,\cdots)$ for the representation $(n_1,n_2,\cdots)$ with $\mathscr{K}_{(n_1,n_2,\cdots)}(I)\neq 0$ can be found as

$$\begin{aligned}&\mathscr{K}_{(n_1,n_2,\cdots)}(I)C_2^{N,M}(n_1,n_2,\cdots)\\ &= \begin{vmatrix} \mathscr{K}_{n_1}(I)C_2^{N,M}(n_1) & \mathscr{K}_{n_2-1}(I) & \cdots\\ \mathscr{K}_{n_1+1}(I)C_2^{N,M}(n_1+1) & \mathscr{K}_{n_2}(I) & \cdots\\ \vdots & \vdots & \end{vmatrix}\\ &+ \begin{vmatrix} \mathscr{K}_{n_1}(I) & \mathscr{K}_{n_2-1}(I)C_2^{N,M}(n_2-1) & \cdots\\ \mathscr{K}_{n_1+1}(I) & \mathscr{K}_{n_2}(I)C_2^{N,M}(n_2) & \cdots\\ \vdots & \vdots & \end{vmatrix} + \cdots,\end{aligned} \tag{5.24}$$

where again we need to sum over as many terms as there are nontrivial rows in the supertableau.

Higher order Casimir invariants can be clearly constructed by a straightforward extension of the methods presented in this section by taking higher derivatives.

Eigenvalues of Casimir operators have been calculated in Ref. 6c in terms of the highest weights for typical representations.

VI. DECOMPOSITION OF SOME REPRESENTATIONS OF U(*N/M*)

In this section we will give examples of various branchings of $U(N/M)$ type supergroups into some smaller subgroups which are potentially useful for physical applications. Completely "symmetric" class I representations of such supergroups are used in nuclear physics as discussed elsewhere.[5]

Let us define the symbol $(n]$ for the class I representation $(n,0,0,\cdots)$ of SU(N/M), whose basis is a graded "symmetric" tensor with n indices. We are interested in decomposing this representation into tensor product representations of the subgroup $SU(N)\times SU(M)$:

$$SU(N/M)\supset SU(N)\times SU(M).$$

For notational purposes we define (n) as the representation $(n,0,0,\ldots,0)$ of $SU(N)$ whose basis is a symmetric tensor with n indices and $[m]$ as the representation $(1,1,\ldots,1,0,0\cdots0)$ of $SU(M)$ whose basis is an antisymmetric tensor with m indices. Then, from Eq. (2.43) it follows that $(n]$ decomposes into the following representations of $SU(N)\times SU(M)$:

$$(n] = \sum_m \oplus((n-m),[m]).$$

For SU(6/4) which is a supergroup of interest this takes the

form

$$(n] = ((n),[0]) \oplus ((n-1),[1]) \oplus ((n-2),[2]) \oplus ((n-3),[3]) \oplus ((n-4),[4]).$$

For this group we wish to further decompose the representation according to the following chain of subgroups.

$$SU(6/4) \supset SU(6) \times SU(4) \supset SO(6) \times SU(4) \supset Spin6.$$

For this purpose we define $\{n\}$ as the representation $\{n,0,0,...,0\}$ of $SO(N)$ whose basis is a symmetric traceless tensor with n indices. Then we can write

$$\begin{aligned}((n-m),[m]) &= \sum_l \oplus (\{n-m-2l\},[m]) \\ &= (\{n-m\},[m]) + (\{n-m-2\},[m]) \\ &\quad + \cdots + (\{0 \text{ or } 1\},[m]).\end{aligned}$$

To proceed further, we use the isomorphism of $SO(6) \cong SU(4)$ to write each symmetric SO(6) representation $\{n\}$ in terms of SU(4) notation by replacing an SO(6) index by an antisymmetric pair of SU(4) indices. Then the SO(6) representation $\{n\}$ transforms under SU(4) as $(n,n,0)$. The decomposition to the diagonal SU(4) = Spin6 contained in $SO(6) \times SU(4)$ can now be given as follows:

$$\begin{aligned}(\{n-0-2l\},[0]) &= (n-2l, n-2l, 0), \\ (\{n-1-2l\},[1]) &= (n-2l, n-2l-1, 0) \\ &\quad + (n-2l-1, n-2l-1, 1), \\ (\{n-2-2l\},[2]) &= (n-2l-1, n-2l-1, 0) \\ &\quad + (n-2l-1, n-2l-2, 1) \\ &\quad + (n-2l-3, n-2l-3, 0), \\ (\{n-3-2l\},[3]) &= (n-2l-2, n-2l-2, 1) \\ &\quad + (n-2l-3, n-2l-4, 0), \\ (\{n-4-2l\},[4]) &= (n-2l-4, n-2l-4, 0).\end{aligned}$$

Another potentially useful supergroup chain is

$$SU(7/6) \supset SU(3/2) \supset SU(3) \times SU(2).$$

Again we are interested in the completely "symmetric" representation $(n,0,\ ,0\cdots)$ of SU(7/6). For this purpose it is useful to note that the class I fundamental representation $(1,0,0,\cdots)$ of SU(7/6) transforms as the $(2,0,0,\cdots)$ "symmetric" representation of SU(3/2). This observation leads to the following formula:

$$(n,0,0,\cdots)_{SU(7/6)} = \sum \oplus (2n_1, 2n_2, ..., 2n_i, \cdots)_{SU(3/2)},$$

where the sum is over all partitions which satisfy

$$(n_1 + n_2 + \cdots + n_i + \cdots) = n.$$

and $n_1 \geqslant n_2 \geqslant \cdots \geqslant n_i \geqslant \cdots \geqslant 0$.

Similar decompositions can be found in Ref. 7 using the method of highest weights.

VII. DISCUSSION

We have studied some aspects of the representation theory of supergroups in a form which is suitable for physical applications. Our work is closely related to the fact that as we generalize from the Lie groups to the supergroups, traces and determinants appearing in the invariants of the theory are changed into supertraces and superdeterminants. In this way we have obtained characters, dimensions, and Casimir invariants of some representations. The same method is possibly useful for studying other properties of supergroups starting from the known results of the Lie group theory.

We have investigated only certain finite-dimensional representations of U(N/M)- and OSP($N/2M$)-type supergroups, namely those which can be obtained by taking the Kronecker products of *either* class I *or* class II representations. The tensor products of class I with class II basis vectors also form the basis of new representations which are, in general, reducible. In this paper we have not studied such representations. We have deferred these and direct products with complex conjugate representations to a forthcoming paper now in preparation.

We note that class I and class II representations are not completely independent. They are related to each other by a tilde operation (which interchanges bosons and fermions) or equivalently by the conjugation of the supertableaux. This fact enables us to derive some nontrivial relations among the invariants of the supergroups such as Eq. (3.23). We emphasize that while the representation of the group element g is identical on certain class I and class II representations, the basis vectors (states) are quite different in the boson-fermion content. This can already be seen for the fundamental representations ξ_A and $\tilde{\xi}_A$ in Eqs. (2.17) and (2.18).

We have constructed expressions for the eigenvalues of the Casimir operators of U(N/M), $N \neq M$, type supergroups only for the representations where the generalized Schur's lemma holds, namely whenever the dimension of the bosonic subspace is different from the dimension of the fermionic subspace. Our method is easily generalizable to the OSP($N/2M$) supergroups as well. An extension of this work to the cases where the generalized Schur's lemma fails remains to be done.

It is appropriate to comment on the irreducibility of our representations: for SU(N/M) with any N, M, all representations we have presented in this paper are irreducible. For OSP($N/2M$) all representations appearing here are irreducible provided $N \neq 2M$. Our method yields representations which are not completely reducible for both OSP(2M/2M) and SU(N/N), although those belonging to SU(N/N) have not yet come up in this paper. This point will be discussed in more detail in a forthcoming paper where many more representations are constructed by extending our method to mixed covariant–contravariant and class I–class II representations. In our formalism it is easy to see the irreducibility of our representations as well as the troublesome cases, as described below. We will argue that *for all cases our character formulas correspond to irreducible representations*, even though the corresponding representation presents some difficulty with respect to irreducibility when the number of bosons and fermions are the same in the fundamental representation.

First consider SU(N/N). The basis vector for an arbitrary class I supertableau has the form

$$\begin{aligned}&\xi_{(A_1 B_1 \cdots, A_2 B_2 \cdots, A_3 B_3 \cdots)} \\ &= \xi^{(1)}_{A_1} \xi^{(2)}_{B_1} \cdots \times \xi^{(n_1+1)}_{A_2} \xi^{(n_1+2)}_{B_2} \cdots + \cdots, \qquad (7.1)\end{aligned}$$

where $(A_1B_1\cdots)$ denote the indices corresponding to first row, $(A_2B_2\cdots)$ corresponding to the second row, etc. In this expression if we set all the fermionic variables equal to zero, we obtain the basis of an *irreducible* representation of SU(N) corresponding to the Young tableau of the same shape. Similarly, if all the bosonic variables are set equal to zero, keeping only the fermions we obtain the basis of an *irreducible* representation of SU(M) corresponding to the Young tableau reflected from the diagonal (conjugate Young tableau). The reason for the reflected Young tableau is that symmetrization in superspace implies antisymmetrization of fermionic subspace. *Thus the pure SU(N) and pure SU(M) subspaces of our representations are irreducible.* Now, if any of these superrepresentations were not irreducible, then the pure SU(N) or SU(M) subspace would have to be reducible. Since this is not the case, our SU(N/M) representations are irreducible for all N, M.

Consider the representations of OSP($N/2M$). To illustrate the difference with SU(N/M), it is sufficient to consider the completely symmetric supertraceless representation

$$\xi_{(A_1A_2,\ldots,A_N)} = (\xi^{(1)}_{A_1}\xi^{(2)}_{A_2}\cdots + \xi^{(2)}_{A_1}\xi^{(1)}_{A_2}\cdots + \cdots) - \frac{1}{N-2M}(H^{\mathrm{ST}}_{A_1A_2}\xi_{(A_3A_4\cdots)}\cdots) + \cdots. \tag{7.2}$$

The point is that we have to subtract the invariant subspace $H^{\mathrm{ST}}_{A_1A_2}\xi_{(A_3A_4\cdots)}$, etc. As shown in Eqs. (4.18), (7.2), this involves dividing by the number $(N-2M)$. Such a procedure is necessary also in the construction of the representations of the supergroup element on this basis as shown in Eq. (4.21). When $N \neq 2M$, this operation can be done and we obtain an *irreducible* tensor. The irreducibility of the representation can be shown as in the previous paragraph. When $N = 2M$, we see that the invariant subspace cannot be subtracted even though we have clearly identified it. Therefore, this basis is not completely reducible when $N = 2M$.

For OSP($2M/2M$) the representation matrix in our basis can be reduced to the form

$$\begin{pmatrix} \alpha & \beta \\ 0 & \gamma \end{pmatrix}, \tag{7.3}$$

where γ is the representation of the group applied to the invariant subspace identified above. The character in this representation is $\mathrm{Str}\alpha + \mathrm{Str}\gamma$. Both of these pieces can be recovered *separately* from our character formula by considering the $N = 2M$ case as the limit of $N \to 2M$. In our method, when the character is calculated the $(N-2M)$ in the denominator is canceled by a similar factor in the numerator so that the $N \to 2M$ limit can be taken smoothly. Thus our expressions for the characters of OSP($N/2M$) will yield the invariant pieces $\mathrm{Str}\alpha$ and $\mathrm{Str}\gamma$ separately for the case of OSP($2M/2M$). Therefore our OSP($N/2M$) character formulas correspond to irreducible representations for all N, M, including $N = 2M$.

In a forthcoming paper[17] we consider covariant and contravariant representations of SU(N/M) by distinguishing lower and upper indices. Then we can construct new representations, which do not appear in this paper, in the form $\xi^{(B_1B_2B_3\cdots)}_{(A_1A_2A_3\cdots)}$. Such bases have to be supertracelss:

$$\sum_{A_1}(-1)^{g(A_1)}\xi^{(A_1B_2B_3\cdots)}_{(A_1A_2A_3\cdots)} = 0.$$

Thus, as in the OSP($N/2M$) case, we have to subtract certain invariant subspaces and this involves terms in which $(N-M)$ appear in the denominator. This procedure can be carried out when $N \neq M$, and we obtain irreducible representations. But for SU(N/N) one identifies, in the same way, certain bases which are not completely reducible. However, the character formulas will again correctly spearate out the irreducible parts. These will be discussed in our next paper, now in preparation.[17]

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APPENDIX

The following is a list of characters and dimensions of some low-dimensional representations of U(N) calculated by first symmetrizing with respect to the rows and then antisymmetrizing with respect to the columns of the Young tableaux associated with these representations:

$\chi_{(1,0,\cdots)} = \mathrm{Tr}U,$

$d_{(1,0,\cdots)} = N$ $\square$,

$\chi_{(2,0,\cdots)} = (1/2!)[(\mathrm{Tr}U)^2 + \mathrm{Tr}U^2],$

$d_{(2,0,\cdots)} = \frac{1}{2}N(N+1)$ $\square\square$,

$\chi_{(1,1,0,\cdots)} = (1/2!)[(\mathrm{Tr}U)^2 - \mathrm{Tr}U^2],$

$d_{(1,1,0,\cdots)} = \frac{1}{2}N(N-1)$ $\begin{smallmatrix}\square\\\square\end{smallmatrix}$,

$\chi_{(3,0,0,\cdots)} = (1/3!)[(\mathrm{Tr}U)^3 + 3\mathrm{Tr}U\,\mathrm{Tr}U^2 + 2\mathrm{Tr}U^3],$

$d_{(3,0,0,\cdots)} = (1/3!)N(N+1)(N+2)$ $\square\square\square$,

$\chi_{(2,1,0,\cdots)} = \frac{1}{3}[(\mathrm{Tr}U)^3 - \mathrm{Tr}U^3],$

$d_{(2,1,0,\cdots)} = \frac{1}{3}(N-1)N(N+1)$ $\begin{smallmatrix}\square\square\\\square\end{smallmatrix}$,

$\chi_{(1,1,1,0,\cdots)} = (1/3!)[\mathrm{Tr}U)^3 - 3\mathrm{Tr}U\,\mathrm{Tr}U^2 + 2\mathrm{Tr}U^3],$

$d_{(1,1,1,0,\cdots)} = (1/3!)(N-2)(N-1)N$ $\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}$,

$\chi_{(4,0,0,0,\cdots)} = (1/4!)[\mathrm{Tr}U)^4 + 6(\mathrm{Tr}U)^2\mathrm{Tr}U^2 + 8\mathrm{Tr}U\,\mathrm{Tr}U^3 + 3(\mathrm{Tr}U^2)^2 + 6\mathrm{Tr}U^4],$

$d_{(4,0,0,0,\cdots)} = (1/4!)N(N+1)(N+2)(N+3)$ $\square\square\square\square$,

$\chi_{(3,1,0,0,\cdots)} = \frac{1}{8}[(\mathrm{Tr}U)^4 + 2(\mathrm{Tr}U)^2\mathrm{Tr}U^2 - (\mathrm{Tr}U^2)^2 - 2\mathrm{Tr}U^4],$

$d_{(3,1,0,0,\cdots)} = \frac{1}{8}(N-1)N(N+1)(N+2)$ $\begin{smallmatrix}\square\square\square\\\square\end{smallmatrix}$,

$\chi_{(2,2,0,0,\cdots)} = \frac{1}{12}[(\mathrm{Tr}U)^4 - 4\mathrm{Tr}U\,\mathrm{Tr}U^3 + 3(\mathrm{Tr}U^2)^2],$

$d_{(2,2,0,0,\cdots)} = \frac{1}{12}(N-1)N^2(N+1)$ $\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}$,

$\chi_{(2,1,1,0,\cdots)} = \frac{1}{8}[(\mathrm{Tr}U)^4 - 2(\mathrm{Tr}U)^2\mathrm{Tr}U^2 - (\mathrm{Tr}U^2)^2 + 2\mathrm{Tr}U^4],$

$d_{(2,1,1,0,\cdots)} = \frac{1}{8}(N-2)(N-1)N(N+1)$ $\begin{smallmatrix}\square\square\\\square\\\square\end{smallmatrix}$,

$\chi_{(1,1,1,1,0,\cdots)} = (1/4!)[(\mathrm{Tr}U)^4 - 6(\mathrm{Tr}U)^2\mathrm{Tr}U^2 + 8\mathrm{Tr}U\,\mathrm{Tr}U^3 + 3(\mathrm{Tr}U^2)^2 - 6\mathrm{Tr}U^4],$

$d_{(1,1,1,1,0,\cdots)} = (1/4!)(N-3)(N-2)(N-1)N$ $\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}$

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Infeld–Hull factorization, Galois–Picard–Vessiot theory for differential operators [a)]

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The Infeld–Hull theory of factorization of second order differential operators is related, on the one hand, to the classical Picard–Vessiot theory and, on the other hand, to work by the author, Gel'fand, and Kirillov on Lie algebras contained in the field of fractions or algebraic extensions of the enveloping associative algebra of a Lie algebra.

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I. INTRODUCTION

The paper by Infeld and Hull[1] on the factorization of the linear ordinary differential operators that occur in quantum mechanics is a famous one that has long tantalized those of us who work on the group-theoretic foundations of physics. It seems to suggest that there is a general algebraic framework for certain quantum mechanical problems generalizing the "annihilation–creation operator" theory of the harmonic oscillator. Further, it is known[2] that the martix elements of certain Lie group representations satisfy differential equations which admit Infeld–Hull type factorizations. Thus, via the Infeld–Hull theory there should be a link between quantum mechanical dynamics and the theory of harmonic analysis on Lie groups.

Another circle of ideas that is clearly related comes from the late 19th century when Lie theory was developed. The possibility of factorization of linear ordinary differential operators was very well known in the 19th century, being tied in with the "symbolic" methods of analysis and algebra. Schlesinger's *Handbuch*,[3] for example, discusses it in great detail. It is also linked with Galois theory, tied to the "reducibility" of the Galois groups.

Another feature of the Infeld–Hull theory is the role played by "parameters." (One is the eigenvalue parameter; another provides the "ladder" structure of the solutions.) In terms of contemporary mathematics, this indicates the Infeld–Hull theory is a "deformation" theory.[4–6] Now, similar deformation theories for linear ordinary differential operators play a role in the modern theory of nonlinear waves—the deformations are "isospectral" and "isomonodromic." Both of these sorts of deformations are clearly related to connections in vector bundles, which is related to gauge theories, and so on. There are many possibilities for interconnection between different fields of contemporary mathematics and physics.

Actually, the immediate motivation for this work came from system theory. In working on the algebro–geometric properties of linear, time-invariant finite and infinite-dimensional systems,[7–9] I stumbled onto material that was very reminiscent of the Infeld–Hull ideas.

Another motivation was work that I did almost 15 years ago on what I called the "Gell-Mann formula."[4–6,10,11] This represents one Lie algebra in terms of the skew field of fractions or quadratic extensions of the universal enveloping algebra of another. This is also related to work by Gel'fand and Kirillov.[12] In this way, we could define Lie algebra representations of one Lie algebra in terms of representations of another.

Now, for many of the "special functions" arising from Lie group representations, one can accomplish the needed factorization of the second order operator in terms of the universal enveloping algebra of another, infinite-dimensional Lie algebra. Since the original differential operators (Bessel, Whittaker, Legendre, etc.) arose from the enveloping algebra of finite-dimensional algebras in a well-known way, one sees that the underlying explanation for this phenomena might well lie in the algebraic properties of the quotient fields of the universal enveloping algebras.

Another noteworthy feature of these factorizations is that they suggest relations with algebraic geometry. Namely, the infinite-dimensional Lie algebras that appear in the Infeld–Hull factorization are realized as *differential operators on algebraic fields*. Geometrically, these are then *first order differential operators on compact Riemann surfaces with meromorphic coefficients*. Now, in the examples treated so far, these Riemann surfaces are the simplest, the genus zero. However, there are indications in the 19th century literature that the genus-one Riemann surfaces, i.e., the Abelian varieties, also appear in this way. (Of course, that is the end if one sticks to vector fields—the higher-genus compact Riemann surfaces admit no nonzero mermorphic vector fields.)

Another relation, which will not be pursued here, is with the Muira transformation[13] for the Korteweg–de Vries equations.

II. THE ABSTRACT ALGEBRA OF THE INFELD–HULL PAPER

We now formulate the basic idea of the Infeld–Hull paper in an algebraic way. Let Γ be a vector space with a given field of scalars. (Typically, this is the real or complex numbers.) Let $D,D',D'':\Gamma\to\Gamma$ be linear maps. Consider the following set of linear equations:

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$$D''\gamma' = \lambda'\gamma'', \tag{2.1}$$
$$D'\gamma'' = \lambda''\gamma'.$$

Suppose that

$$D = D'D''. \tag{2.2}$$

Theorem 2.1: If (γ',γ'') is a solution of (2.1) with scalars λ',λ'', then

$$\gamma = \gamma''$$

is an eigenvector of D with eigenvalue $\lambda = \lambda'\lambda''$, i.e.,

$$D\gamma = \lambda\gamma.$$

Proof:

$$D\gamma = D\gamma'' = D'D''\gamma'' = D'\lambda''\gamma' = \lambda''\lambda'\gamma = \lambda\gamma.$$

Thus, by means of the factorization (2.2) of the operator D, the eigenvector equation (2.3) is replaced by a pair (2.1) of equations.

Now, in general, this is of no particular help. However, if D is a second order linear ordinary differential operator, the system (2.1) will be a first order system, which might be easier to solve. Certainly, the solutions of many of the equations that define the "special equations of mathematical physics" are of this form—typically, they involve the recursion relations satisfied by these functions.

Another useful point is that the solution of the system (2.1) often involves nontrivial Lie group theory. To this end, we are particularly interested in the *Lie algebra of linear operators generated by the D',D''*.

III. AN ABSTRACT FORM OF PICARD–VESSIOT THEORY

Let Γ be a vector space over a scalar field. (The scalar field should have zero characteristic. In the applications it will be the real or complex numbers.) Let $L(\Gamma)$ denote the algebra of linear maps: $\Gamma\to\Gamma$. Let $\mathrm{GL}(\Gamma)$ denote the group of automorphisms of Γ.

An *algebraic model of a differential structure* on Γ will be defined by a linear map

$$\delta = \Gamma\to\Gamma,$$

and an *algebra* (under composition) $\mathscr{A}$ of linear operators on Γ such that the following condition is satisfied:

$$[a,\delta] \equiv a\delta - \delta a \in \mathscr{A} \quad \text{for all } a\in\mathscr{A}. \tag{3.1}$$

An *automorphism of the differential structure* will be an element of $g\in\mathrm{GL}(V)$ such that

$$g\delta = \delta g, \tag{3.2}$$
$$gag^{-1}\in\mathscr{A}, \quad \text{for all } a\in\mathscr{A}.$$

A *differential operator associated with the differential structure* will be an element

$$D\in L(\Gamma),$$

which can be written in the form

$$D = a_n\delta^n + \cdots + a_0, \tag{3.3}$$

where $a_0,\ldots,a_n\in\mathscr{A}$.

The smallest integer n such that $a_n \neq 0$ is called the *order* of the differential operator. Let $\mathscr{S}(D)$ be the space of solutions γ of the equation

$$D\gamma = 0,$$

i.e., algebraically, $\mathscr{S}(D)$ is the kernel of D. An automorphism g of the differential structure is said to be a *symmetry* of the differential operator if it satisfies the following condition:

$$g\mathscr{S}(D)\subset\mathscr{S}(D). \tag{3.4}$$

The set of such symmetries forms a group called the *Galois group* of D, denoted by $G(D)$.

In Galois theory, one is interested in two "functors." The assignment

$$D\to\mathscr{S}(D)$$

and

$$D\to G(D).$$

Notice that $G(D)$ by its very nature admits a representation by linear maps in $\mathscr{S}(D)$, called the *Picard–Vessiot representation*.

This is, of course, just a collection of definitions. What is needed to give it more kick is some hypothesis about Γ and δ, and the class of D's which assume that $G(D)$ is a Lie group, and that relates the structure of $G(D)$ to the algebraic structure of the D's.

The traditional example where these conditions are satisfied is that where Γ is the space of functions of a complex variable z, which are analytic in some region of the complex z plane $\delta = d/dz$, and the algebra $\mathscr{A}$ consists of operators of multiplication by analytic functions. The operators of form (3.3) are then the ordinary linear differential operators in the usual sense. One of the main theorems proved by Picard and Vessiot[14,15] is that the reducibility of the Galois group D, as a group of linear transformations on $\mathscr{S}(D)$, is *equivalent* to reducibility of D, in the sense that it can be factored to the product of lower order operators. I will not attempt to prove this result here. Instead, let us examine it for the special case of second order ordinary linear differential operators with rational coefficients.

IV. FACTORING SECOND ORDER DIFFERENTIAL OPERATORS WITH RATIONAL COEFFICIENTS

Let Γ be a vector space of analytic functions in some region of the complex plane, with coordinate z. Suppose Γ is preserved under multiplication by rational functions and differentiation. Let $\mathscr{A}$ be the algebra of linear operators on Γ resulting from multiplication by rational functions. Set

$$\delta = \frac{d}{dz}.$$

Let

$$D = \delta^2 + a_1\delta + a_0 \tag{4.1}$$

be a second order linear differential operator with rational coefficients a_0,a_1.

Let us now try to factor D:

$$\begin{aligned} D &= (\delta + b_0)(\delta + c_0) \\ &= \delta^2 + b_0\delta + \delta c_0 + b_0c_0 \\ &= \delta^2 + (b_0 + c_0)\delta + \delta(c_0) + b_0c_0. \end{aligned} \tag{4.2}$$

Comparing (4.1) and (4.2), we have

$$b_0c_0 = a_1,$$
$$\delta(c_0) + b_0c_0 = a_0. \tag{4.3}$$

This leads to a differential equation for c_0:

$$\delta(c_0) = \frac{dc_0}{dz}$$
$$= a_0 - (a_1 - c_0)c_0. \tag{4.4}$$

This is a Riccati equation for c_0, which is well known to be as difficult to solve as Eq. (4.1)

To deal with this in the fashion of contemporary differential algebra,[16,17] let $\mathcal{F}$ be the smallest field of functions containing the rational functions and the two linearly independent solutions of $Dy = 0$. The Galois group of D is then defined as the subgroup of the automorphisms of $(\mathcal{F},\delta)$ which leave invariant the rational functions.

Now, a solution of the Riccati equation can be obtained from a particular solution y of $Dy = 0$. Set

$$c = -\delta(y)y^{-1}. \tag{4.5}$$

Then,

$$\delta(c) = -\delta^2(y)y^{-1} + \delta(y)^2y^{-2}$$
$$= [\delta(y)a_1 + a_0y]\,y^{-1} + c^2$$
$$= -ca_1 + a_0 + c^2. \tag{4.6}$$

Thus, c and c_0 satisfy the same Riccati differential equation. The steps are reversible; if c_0 is a solution of (4.4), then y_0 such that

$$-\delta(y_0)\cdot y_0^{-1} = c_0 \tag{4.7}$$

is a solution of $Dy_0 = 0$.

Let y_1,y_2 be any two linearly independent solutions of $Dy = 0$, and let y_0 be defined by (4.7). Then, y_0 is a solution of $Dy = 0$. Hence:

There are constants λ_1,λ_2 such that

$$y_0 = \lambda_1y_1 + \lambda_2y_2. \tag{4.8}$$

Now, if D factors in the form (4.2) *with rational coefficients*, then there is a c_0, a rational function, and λ_1,λ_2 complex numbers, such that (4.7) and (4.8) hold.

Now, suppose g is an element of the Galois group of D's, i.e., g is an automorphism of the differential field $\mathcal{F}$ which leaves invariant the rational functions. Then, g maps solutions of $Dy = 0$ into solutions

$$g(y_1) = \sigma_{11}y_1 + \sigma_{12}y_2,$$
$$g(y_2) = \sigma_{21}y_1 + \sigma_{22}y_2,$$

where $\sigma_{11},\ldots,\sigma_{22}$ are scalars. Also,

$$g(c_0) = c_0,$$

since c_0 is rational. Since g commutes with $\delta = d/dz$, we see that

g leaves invariant the linear subspace of $\mathcal{S}(D)$ spanned by y_0.

Thus, in this case, we see quite explicitly how reducibility of the Galois group of D is equivalent to factorizability of D in terms of differential operators *with rational coefficients*.

V. THE INFELD–HULL FACTORIZATION OF THE BESSEL EQUATION

To see a nontrivial example of factorization in the Infeld–Hull sense, take Γ to be a space of an analytic function of the complex variable z, in a region Z of the complex plane. Let $\delta = d/dz$. Set

$$D = \delta^2 + z^{-1}\delta - n^2z^{-2}. \tag{5.1}$$

Then, the eigenvectors of D with eigenvalue $\lambda = 1$ are the solutions of the Bessel equation. Set

$$A_j = \delta + jz^{-1}. \tag{5.2}$$

Let us try to write D as a product:

$$D = A_jA_k$$
$$= (\delta + jz^{-1})(\delta + kz^{-1})$$
$$= \delta^2 + (j + k)z^{-1}\delta - kz^{-2} + jkz^{-2}. \tag{5.3}$$

Compare (5.3) to (5.1):

$$j + k = 1$$
$$-n^2 = jk - n$$
$$= j(1 - j) - n,$$
$$-n^2 + n = j - j^2$$

or

$$j = n, \quad k = 1 - n,$$
$$D = (\delta + nz^{-1})(\delta - (n - 1)z^{-1}) \tag{5.4}$$
$$= A_nA_{-n+1}. \tag{5.5}$$

The Lie algebra generated by the differential operators A is an interesting one:

$$[A_n,A_n] = [\delta + nz^{-1},\delta + mz^{-1}]$$
$$= (n - m)B_2, \tag{5.6}$$

with

$$B_2 = z^{-2}.$$

Set

$$B_n = z^{-n}.$$

Then,

$$[A_n,B_m] = B_{m+1}, \tag{5.7}$$
$$[B_n,B_m] = 0. \tag{5.8}$$

Let $\mathcal{L}$ be the Lie algebra generated by the vector fields A_n. It has an interesting graded structure:

$\mathcal{L}$ = subspace spanned by the A_n,

$\mathcal{L}^{1+j}$ = one-dimensional subspace spanned by B_{1+j}, $j = 1,2\cdots$.

Then,

$$[\mathcal{L}^j,\mathcal{L}^k] \subset \mathcal{L}^{j+k}.$$

Set

$$\mathcal{L}_j = \mathcal{L}^j + \mathcal{L}^{j+1} + \cdots.$$

The $\mathcal{L}_j$ determine a filtered Lie algebra. Then, $\mathcal{L}_2$, $\mathcal{L}_3$,... form abelian ideals. This exhibits a sort of "generalized nilpotent" structure of $\mathcal{L}$.

What we have done is to find a one-parameter family of

differential operators

$$\lambda \to D_\lambda$$

such that:

For $\lambda = 1$, D is the Bessel operator itself.

For $\lambda = 0$, D factors over the rationals.

Thus, the Galois group

$$\lambda \to G_\lambda(D_\lambda)$$

is a one-parameter family of groups—a "deformation"—which becomes reducible for $\lambda = 0$.

VI. THE INFELD–HULL FACTORIZATION FOR THE WHITTAKER EQUATION

The Whittaker functions are generalization of the Bessel functions. (From the Lie group point of view, both sorts of functions are matrix elements of representations of solvable Lie groups.[2])

Consider the following Lie algebra of first order differential operators generated by the vector field

$$V = z^{1/2}\frac{d}{dz}$$

and the functions

$$f_1 = z^{1/2}, \quad f_2 = z^{-1/2}.$$

According to Ref. 2, p. 415, we have

$$(V - \mu f_2 + \tfrac{1}{2}f_1)[V + \tfrac{1}{2}(2\mu - 1)f_2 - \tfrac{1}{2}f_1] - (\mu - \lambda - \tfrac{1}{2}) = z^{-1}\left(\frac{d^2}{dz^2} - \tfrac{1}{4} + \lambda z^{-1} + (\tfrac{1}{4} - \mu^2)z^{-2}\right). \tag{6.1}$$

This is, of course, an Infeld–Hull type of factorization.

It is interesting to calculate the Lie algebra $\mathscr{L}$ generated by the V, f_1, f_2 [the expression on the left-hand side of (6.1) is then on the universal enveloping algebra of $\mathscr{L}$]:

$$V(f_1) = \tfrac{1}{2}$$
$$V(f_2) = -\tfrac{1}{2}z^{-1}$$
$$V(z^{-1}) = -z^{1/2}z^{-2} = -z^{-3/2}$$

and so on.

Notice that the functions obtained in this way are always rational functions in $z^{1/2}$. Thus, $\mathscr{L}$ can be described very elegantly in terms of Riemann surface theory.

Theorem 6.1. The Lie algebra $\mathscr{L}$ involved in the recursion relations and the Infeld–Hull structure of the Whittaker functions can be realized as meromorphic, first order differential operators on the Riemann surface of the algebraic curve

$$w^2 = z.$$

VII. THE LIE ALGEBRA AND INFELD–HULL STRUCTURE FOR THE LEGENDRE FUNCTION

The process we have gone through for Bessel's equation and the Whittaker functions can be repeated for virtually every "special function" given in the treatise by Vilenkin.[2] For example, on p. 137, he proves the following formula:

$$(V - f_{n+1,m})(V + f_{n,m}) - (l - n)(l + n + 1) = (1 - z^2)\frac{d^2}{dz^2} - 2z\frac{d}{dz} + \frac{m^2 + n^2 - 2mnz}{1 - z^2} + l(l + 1), \tag{7.1}$$

where

$$V = (1 - z^2)^{1/2}\frac{d}{dz}, \tag{7.2}$$

$$f_{n,m} = (nz - m)/(1 - z^2)^{1/2}. \tag{7.3}$$

Let $\mathscr{R}$ be the field of rotational functions on the Riemann surface of the algebraic curve

$$w^2 + z^2 = 1. \tag{7.4}$$

V is a derivation of this field, and each $f_{n,m}$ is an element of $\mathscr{R}$. Thus, the Lie algebra $\mathscr{L}$ generated by the operators appearing in the Infeld–Hull factorization of the operator on the right-hand side of (8.4) is a Lie algebra of first order rational differential operators on the Riemann surface.

VIII. THE LIE ALGEBRA OF THE INFELD–HULL RELATIONS IN TERMS OF THE RATIONAL ENVELOPING ALGEBRAS OF FINITE-DIMENSIONAL LIE ALGEBRAS

In previous sections we have presented some calculations which seem to indicate that the Lie algebra $\mathscr{L}$ which generates certain of the Infeld–Hull factorizations are naturally interpreted in terms of compact Riemann surfaces. However, the functions we have been dealing with appear as matrix elements of representations of Lie groups. Thus, we might also look for some more direct relation to Lie groups. We will restrict attention here to the Bessel equation.

Let M be the unit circle in R^2, parameterized by real θ, $0 \leqslant \theta < 2\pi$. Let $F(M)$ be the C^∞, complex-valued functions on M. Let Z denote the complex numbers, with complex coordinate z. Let $\mathscr{A}(Z)$ be the space of analytic functions on z. Let

$$B: F(M) \to \mathscr{A}(Z)$$

be the following mapping:

$$B(f)(z) = \int_0^{2\pi} e^{iz\sin\theta} f(\theta)\, d\theta. \tag{8.1}$$

Let $\mathscr{G}$ be the Lie algebra of operations on $F(M)$ spanned by the following three:

$$C_1 = \frac{\partial}{\partial\theta},$$
$$C_2 = \sin\theta,$$
$$C_3 = \cos\theta.$$

We see that $\mathscr{G}$ is a solvable Lie algebra, isomorphic to the group of rigid motions in R^2. $\mathscr{L}$, the Lie algebra which is generated by the operators

$$\frac{d}{dz}, \qquad z^{-1}.$$

Now,

$$\frac{d}{dz}(B(f)) = iB(C_2(f)).$$

Set

$$C_4 = -i(\cos\theta)^{-1}\frac{d}{d\theta}$$
$$= -iC_3^{-1}C_1.$$

Then,

$$z(B(f)) = B(C_4(f)).$$

Thus, at least formally,

$$z^{-1}B(f) = B(C_4^{-1}(f))$$
$$= B(iC_1^{-1}C_3).$$

Thus, the Lie algebra $\mathscr{L}$ is essentially generated by

$$A_1C_2 \quad iC_1^{-1}C_3.$$

Let us check this out with the commutation relations

$$[C_1,C_2] = C_3,$$
$$[C_1,C_3] = -C_2,$$
$$[C_2,C_3] = 0.$$

Thus,

$$[C_2,C_1^{-1}C_3] = [C_2,C_1^{-1}]C_3$$
$$= -C_1^{-1}[C_2,C_1]C_1^{-1}C_3$$
$$= (C_1^{-1}C_3)^2. \tag{8.2}$$

Again, we see that C_2 and $C_1^{-1}C_3$ generate a graded Lie algebra of a generalized nilpotent type.

Now, algebraically, objects like $C_1^{-1}C_3$ are elements of the "field of fractions of the universal enveloping algebra of $\mathscr{L}$,"[2] denoted as $\mathscr{F}(\mathscr{L})$. Analytically, they are "pseudodifferential operators on the manifold M." Let us formulate this in general terms as follows:

Consider a Lie algebra $\mathscr{G}$. Construct the associative universal algebra $U(\mathscr{G})$. $U(\mathscr{G})$ consists of the polynomials

$$A_1\cdots A_n$$

in the elements of $\mathscr{G}$ subject only to the associative law and to the relations:

$$[A_{12},A_2] = A_1A_2 - A_2A_1.$$

Gel'fand and Kirillov then construct the "quotient field" of rational functions,

$$A_1^{-1}A_2\cdots A_n^{-1}\cdots$$

denote this as $\mathrm{QU}(\mathscr{G})$. It too is a Lie algebra.

Suppose that we have another representation

$$\rho':\mathscr{L}\to\mathrm{QU}(\mathscr{G})$$

for some Lie algebra $\mathscr{G}$. We might be able to construct a representation

$$\alpha:\mathscr{G}\to\mathscr{G}$$

then extends to $U(\mathscr{G})$.

Let us suppose that the algebra $\mathscr{D}$ of differential operators on $\mathscr{A}$ can be enlarged to another Lie algebra $\mathscr{P}\mathscr{D}$ of operators called *pseudodifferential operators*. Let us also say that α can be extended to a representation

$$\alpha:\mathrm{QU}(\mathscr{G})\to\mathscr{P}\mathscr{D}.$$

Suppose finally that there is given another Lie algebra representation

$$\rho':\mathscr{L}\to\mathrm{QU}(\mathscr{G}).$$

Compose this with α_1 to obtain a Lie algebra homorphism

$$\alpha\rho':\mathscr{L}\to\mathscr{P}\mathscr{D}.$$

Thus, we have two representations of $\mathscr{L}$ into the "pseudodifferential operators": the original representation ρ into the *differential* operators and the $\alpha\rho'$ we have just constructed. *It then may be possible to construct a linear map*

$$\beta:\mathscr{A}\to\mathscr{A}$$

which intertwines these two representations of $\mathscr{G}$.

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Isomonodromy as a curvature-zero condition [a)]

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The "isomonodromy deformation" condition is expressed as a curvature-zero condition, thus bringing to the foreground the relations to other approaches in the theory of nonlinear waves.

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I. INTRODUCTION

The theory of nonlinear waves and solitons has focussed attention on a mathematical structure called "isospectral deformation of differential operators."[1,2] It has been discovered that there is a close link between this condition and the theory of connections in fiber bundles.[3–5] Indeed, finding "isospectral deformations" is equivalent to finding certain two-dimensional submanifolds of the base of a fiber bundle with connection such that the curvature differential forms are zero when restricted to this submanifold. This has the added virtue of relating the theory of isospectral deformation with two topics—Cartan's theory of exterior differential systems and connections and the theory of Yang–Mills fields, which also involve connections in fiber bundles and physical equations defined by conditions on the *curvature* of these connections.

There has recently been some attention by mathematicians and physicists to a notion which is related to isospectral deformation, namely, "isomonodromy deformation."[6–9] Here, one tries to define deformations of linear ordinary differential operators so that the monodromy group is preserved. The notion goes back to the classic work of the 19th and early 20th centuries, particularly by Fuchs and Schlesinger. My aim here is to show how "isomonodromy" can be defined as a curvature-zero condition. I show that the partial differential equations which are obtained can be reduced to a system of *ordinary* nonlinear equations.

In Ref. 10, Morris and Dodd have discussed another method of introducing fiber bundles and connections.

II. ISOMONODROMY IN THE SENSE OF FUCHS AND SCHLESINGER AS A CONNECTION

Let Z be a connected open subset of the Riemann sphere, i.e., the complex plane with the point at infinity added on. Let z be the complex coordinate of Z. Let $d = d/dz$, acting on complex-valued functions which are analytic in z. Let

$$D = d^n + a_{n-1}(z)d^{n-1} + \cdots + a_0 \tag{2.1}$$

be a linear differential operator with coefficients which are analytic functions in z. (Of course, they may have singularities at the points of the Riemann sphere which lie outside of Z.) To solve $Dy = 0$ for an analytic function $z \to y(z)$ is the same as finding a flat cross section for an analytic fiber bundle E over Z. Namely, let E locally have coordinates

$$(z, y_0, \ldots, y_{n-1}),$$

with $(y_0, \ldots, y_{n-1})$ the coordinates of the fiber, z the coordinate of the base. Let

$$\begin{aligned} \omega_{n-1} &= dy_{n-1} + (a_{n-1}y_{n-1} + \cdots + a_0 y_0)\,dz, \\ \omega_{n-2} &= dy_{n-2} - y_{n-1}\,dz, \\ &\vdots \\ \omega_0 &= dy_0 - y_1\,dz. \end{aligned} \tag{2.2}$$

The forms $(\omega_0, \ldots, \omega_{n-1})$ then define the connection on the bundle. The structure group in the bundle is a subgroup of $GL(n, \mathbb{C})$, the group of $n \times n$ complex matrices.

Now the curvature of this connection is *zero*. The monodromy group appears as the *holonomy group* of the connection;[11] it is a discrete group, a homomorphic image of the fundamental group of Z.

Now, introduce a new fiber space E', with base $Z \times T$, where T is an interval of real numbers, parametrized by t, and whose fiber is also $\mathbb{C}^n$. Set up a connection in this bundle by introducing the following connection form:

$$\omega_i' = \omega_i + \sum_j b_i^j y_j\,dt. \tag{2.3}$$

The coefficients a and b are continuous functions on $Z \times T$, which are analytic in Z. The b's are independent of t and satisfy

$$\frac{\partial b_0}{\partial t} = 0 = \cdots = \frac{\partial b_{n-1}}{\partial t}. \tag{2.4}$$

Theorem 2.1: Suppose that the curvature of the connection defined by the forms (2.3) is zero, with (2.4) satisfied. Let $G(t)$ be the monodromy group of the differential operator, with the parameter value t considered as a group of $n \times n$ complex matrices, i.e., as a subgroup of the Lie group $GL(n, \mathbb{C})$. Then, there is a continuous map $t \to g(t)$ in $GL(n, \mathbb{C})$ such that

$$G(t) = g(t)G(0)g(t)^{-1} \qquad \text{for all } t.$$

(In the language of deformation theory, the deformation of subgroups $t \to G(t)$ is "trivial.")

Proof: Let us write (2.3) and (2.4) in a matrix notation:

$$\omega = dy - A(z,t)y\,dz - B(z)y\,dt, \tag{2.5}$$

where ω is a $n \times 1$ matrix of 1-forms, A and B are $n \times n$ matrices of functions [analytic on z, jointly continuous in (z,t)]. Let $s \to z(s)$, $-\infty < s < \infty$, be a closed curve in Z with

$$z(s+1) = z(s). \tag{2.6}$$

Construct a connection in the product bundle

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$$R^2 \times \mathbb{C}^n$$

over R^2, with connection form

$$\omega' = dy - A(z(s),t)y(s)\frac{dz}{ds}\,ds - B(z)y\,dt. \tag{2.7}$$

[Geometrically, this is the pull-back of the connection under the map $R \times T \to Z \times T$, $(s,t) \to (z(s),t)$.] The curvature of this connection is also zero. Since the base is simply connected, there are cross sections

$$(s,t) \to y(s,t)$$

which are *flat*, i.e., satisfy the following differential equations:

$$\frac{\partial y}{\partial s} = A(z(s),t)y(s)\frac{dz}{ds}, \tag{2.8}$$

$$\frac{\partial y}{\partial t} = B(z(s))y.$$

(2.8) can be readily solved:

$$y(s,t) = \exp[tB(z(s))]y(s,0)]. \tag{2.9}$$

Then, $s \to y(s,0)$ is the solution of the linear differential equation (2.8) with periodic coefficients.

Hence,

$$y(s+1,0) = My(s,0), \tag{2.10}$$

where M is a *constant* $n \times n$ matrix.

Insert (2.11) into (2.9):

$$y(s+1,t) = \exp[tB(z(s+1))]My(s,0)$$
$$= \exp[tB(z(s+1))]M\exp[-tB(z(s+1))]y(s,t).$$

We see from this that

$$\exp[tB(z(s+1)]]M\exp[-tB(z(s+1))]$$

is the element of the monodromy group of the differential equation (2.1) at the value t of the parameter corresponding to the closed curve $s \to z(s)$. Thus, as the curve varies, we see that the monodromy group of the Eq. (2.1) is conjugate, as a subgroup of $GL(n,\mathbb{C})$, to a fixed group, which is the meaning of "isomonodromy."

III. PARTIAL SOLUTION OF THE ISOMONODROMY DIFFERENTIAL EQUATION

The conditions for zero curvature of a *linear* connection (2.5) are well known. In nonlinear wave theory they are often called the *Zakharov–Shabat equations*:

$$\frac{\partial A}{\partial t} - \frac{\partial B}{\partial z} = [A,B]. \tag{3.1}$$

To this must be added the following isomonodromy condition:

$$\frac{\partial B}{\partial t} = 0. \tag{3.2}$$

Differentiate both sides of (3.1) with respect to t:

$$\frac{\partial^2 A}{\partial t} = \left[\frac{\partial A}{\partial t}, B\right]. \tag{3.3}$$

Hence,

$$\frac{\partial A}{\partial t}(z,t) = \exp[-tB(z)]\frac{\partial A}{\partial t}(z,0)\exp[tB(z)] \tag{3.4}$$

equals, using (3.1)

$$\exp[-tB(z)]\left(\frac{\partial B}{\partial z} + [A(z,0),B(z)]\right)\exp[tB(z)]$$
$$= \mathrm{Ad}\exp[-tB(z)]\left(\frac{\partial B}{\partial z} + [A(z,0),B(z)]\right). \tag{3.5}$$

Hence,

$$A(z,t) = \{\mathrm{Ad}[-B(z)]\}^{-1}\mathrm{Ad}\exp[-tB(z)]$$
$$\times\left(\frac{\partial B}{\partial z} + [A(z,0),B(z)]\right)$$
$$+ A(z,0) - \{\mathrm{Ad}[-B(z)]\}^{-1}\left(\frac{\partial B}{\partial z} + [A(z,0),B(z)]\right). \tag{3.6}$$

Now, if (3.6) is substituted into (3.1), there results a nonlinear differential equation for $B(z)$.

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Factorization of operators . II

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We extend the methods of a previous paper [J. Math. Phys. **21**, 2508 (1980)], factorizing the general, scalar, third-order differential operator, and obtain a Miura transformation for the Boussinesq equation. We give a general factorized eigenvalue problem. We also give a Hamiltonian structure associated with the factorized eigenvalue problem. We derive several isospectral flows, some of Klein–Gordon type.

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1. INTRODUCTION

In a recent paper[1] (referred to below as I), we discussed the factorization of some particular third order Lax operators, with emphasis on "Miura transformations" and their associated modified equation. In this paper we consider the general third order scattering operator

$$L = \partial^3 + v\partial + \tfrac{1}{2}v_x + w, \tag{1.1}$$

(where $\partial \equiv \partial_x \equiv \partial/\partial x$) of which the two operators discussed in I are special cases. This is the scattering operator for the well known Boussinesq equation.[2,3]

In Sec. 2 we factorize this operator, deriving an associated 3×3 matrix scattering problem. The matrices involved all belong to the Lie algebra $sl(3,\mathbb{R})$, a point which we develop in later sections. We derive the first two polynomial isopectral flows, the first of which is trivial, being just the translation equation, and the second of which is related to the Boussinesq equation by a Miura transformations.[4] We shall refer to this system as the "modified Boussinesq equation".

Polynomial flows of higher order may be constructed recursively; in Secs. 3 and 4 we consider a systematic method of constructing the recursion operator. In Sec. 3 we consider the matrix scattering problem in the adjoint and coadjoint representations of $sl(3,\mathbb{R})$. The coadjoint equations are satisfied by analogues of the usual "squared eigenfunctions".[5] By eliminating variables we derive an integro-differential operator, whose adjoint is shown to be a recursion operator[6] relating isospectral flows. In Sec. 4 we give a different derivation of the recursion operator and exploit the relationship between the two expressions to derive a Hamiltonian structure. We indicate how the recursion operator generates the isospectral flows discussed in Sec. 2. We then calculate, as a special case of the fifth order system, the "modified Kupershmidt equation" discussed in I.

In Sec. 5 we consider isospectral flows of Klein–Gordon type. These systems, generalizations of the sinh–Gordon equations, are related to the 3-particle, periodic Toda lattice. We generalize this further to the n-particle lattice in another paper.[7]

2. FACTORIZATION OF THE SCATTERING OPERATOR

The Boussinesq equation

$$v_{tt} = -\tfrac{1}{3}(v_{4x} + 2(v^2)_x), \tag{2.1}$$

written as the system

$$v_t = 2w_x,$$

$$w_t = -\tfrac{1}{6}(v_{3x} + 4vv_x), \tag{2.2}$$

may be represented as a Lax pair[2,3]

$$L_t = [P,L], \tag{2.3}$$

where

$$L = \partial^3 + v\partial + \tfrac{1}{2}v_x + w,$$
$$p = \partial^2 + \tfrac{2}{3}v. \tag{2.4}$$

The scattering operator L may be decomposed into the product

$$L' = (\partial + y - z)(\partial + 2z)(\partial - y - z), \tag{2.5}$$

provided we can find y and z such that

$$v = -(2y_x + 3z^2 + y^2),$$
$$w = -[z_{xx} + 3yz_x + zy_x + 2z(y^2 - z^2)]. \tag{2.6}$$

The eigenvalue problem of L

$$L\psi_1 = \zeta^3\psi_1 \tag{2.7}$$

may then be written as

$$\frac{\partial}{\partial x}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix} = \begin{pmatrix} y+z & \zeta & 0\\ 0 & -2z & \zeta\\ \zeta & 0 & -y+z\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}. \tag{2.8}$$

The matrix on the right of (2.8) is an element of the Lie algebra $sl(3,\mathbb{R})$ (traceless, 3×3 matrices); it can be expanded in terms of any convenient basis of that algebra. Such a basis, together with its commutation relations, is given in the Appendix.

With respect to this basis, Eq. (2.8) is written

$$\partial\psi = (\zeta R_1 + yR_2 + zR_5)\psi, \tag{2.9}$$

where $\psi = (\psi_1,\psi_2,\psi_3)^T$.

The general eigenvalue problem associated with $sl(3,\mathbb{R})$ (keeping ζ in the same position) is

$$\partial\psi = u\psi, \tag{2.10}$$

where $u = \sum_{i=1}^{8} u^i R_i$, $u^1 \equiv \zeta$, and the remaining u^i are arbitrary functions.

Consider a time evolution of ψ of the form

$$\partial_t\psi = A\psi, \tag{2.11}$$

where $A = \sum_{i=1}^{8} A^i R_i \in sl(3,\mathbb{R})$ and the A^i are functions of u^k, their x-derivatives, and ζ.

If (2.11) is to be consistent with (2.10), then

$$\partial_t u - \partial A + [u,A] = 0. \tag{2.12}$$

In terms of the basis $\{R_i\}$ Eq. (2.12) becomes

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$$\partial_t u^k - \partial A^k + u^i A^j C^k_{ij} = 0, \tag{2.13}$$

where C^k_{ij} are the structure constants of $sl(3,\mathbb{R})$ with the given basis.

When the eigenvalue problem is associated with the factorization of a scalar operator, taking the form of (2.9), Eq. (2.13) becomes (with $u^2 = y$ and $u^5 = z$),

$$\begin{aligned}
&\partial A^1 = 2(u^5 A^6 - u^2 A^3),\\
&\partial A^2 = \partial_t u^2 - 3\zeta A^7,\\
&\partial A^3 = \zeta A^2 - u^2(A^1 + A^3) - u^5 A^6,\\
&\partial A^4 = 3\zeta A^3 + 3u^5(A^7 - A^8) - u^2 A^4,\\
&\partial A^5 = \partial_t u^5 + \zeta A^4,\\
&\partial A^6 = 3u^5(A^1 - A^3) - 3\zeta A^5 + u^2 A^6,\\
&\partial A^7 = -\zeta A^6 + u^2(A^7 + A^8) + u^5 A^4,\\
&\partial A^8 = 2(u^2 A^7 - u^5 A^4).
\end{aligned} \tag{2.14}$$

A trivial solution of (2.14) is

$$A = u, \tag{2.15}$$

corresponding to the translation flow

$$u_t = u_x, \tag{2.16}$$

where $u = (u^1, u^5)^T$.

A more interesting solution is given by

$$\begin{aligned}
&A^1 = A^4 = A^7 = 0,\\
&A^2 = 2u^2 u^5 + u^5_x,\\
&A^3 = \zeta u^5,\\
&A^5 = \tfrac{1}{3}[(u^2)^2 - 3(u^5)^2] - \tfrac{1}{2}u^2_x,\\
&A^6 = \zeta u^2,\\
&A^8 = \zeta^2,
\end{aligned} \tag{2.17}$$

which generates the flow:

$$\begin{aligned}
&u^2{}_t = u^5{}_{xx} + 2(u^2 u^5)_x,\\
&u^5{}_t = -\tfrac{1}{3}u^2{}_{xx} - \tfrac{1}{3}[3(u^5)^2 - (u^2)^2]_x,
\end{aligned} \tag{2.18}$$

which we refer to as the modified Boussinesq equation, it being related to (2.2) by the "Miura transformation" (2.6).

These flows and a sequence of higher-order polynomial flows may be generated recursively, as will be discussed in the following sections.

3. COADJOINT STRUCTURE AND SQUARED EIGENFUNCTIONS

The inegrability condition (2.12)

$$A_x - [u,A] = u_t \tag{3.1}$$

is considered as a linear, inhomogeneous equation for A. The corresponding homogeneous equation,

$$\Psi_x = [u,\Psi], \tag{3.2}$$

is the adjoint representation of (2.10), Ψ being an element of $sl(3,\mathbb{R})$. Equation (3.2) may be derived from the requirement that the integral

$$\int \langle \Phi, \Psi_x - [u,\Psi] \rangle \, dx \tag{3.3}$$

be stationary with respect to variation in Φ, where Φ is an element of the vector space dual to $sl(3,\mathbb{R})$ and $\langle\ ,\ \rangle$ denotes the inner product between elements of these spaces.

Requiring this same integral to be stationary with respect to variations in Ψ we obtain the adjoint (it is unfortunate that the word "adjoint" has several distinct meanings) of (3.2):

$$\Phi_x = -\{u,\Phi\}, \tag{3.4}$$

where $\{u,\Phi\} = \mathrm{ad}^*_u \Phi$ is defined by

$$\langle \{u,\Phi\}, \Psi \rangle = \langle \Phi, [u,\Psi] \rangle. \tag{3.5}$$

The linear transformation ad^*_u on the dual of the Lie algebra is a representation, called the coadjoint,[8] of the element $(-u)$ of the algebra.

If Ψ is expanded in terms of the basis $\{R_i\}$ and Φ in terms of its dual basis, then

$$\langle \Phi, \Psi \rangle = \sum_{i=1}^{8} \Phi_i \Psi^i \tag{3.6}$$

so that (3.4) becomes

$$\Phi_{k,x} = -u^j C^i_{jk} \Phi_i. \tag{3.7}$$

Equations (3.1) and (3.4) imply

$$\int \langle \Phi, u_t \rangle \, dx = 0, \tag{3.8}$$

which should be compared with (3.13) below. This equation relates the time evolutions of the eigenvalues and the field variables. In the case developed below these are respectively u^1 and the pair $\{u^2, u^5\}$.

Squared Eigenfunctions: Consider the integral

$$\int \phi(\psi_x - u\psi)\, dx, \tag{3.9}$$

where ϕ and ψ are row and column three-vectors and $u \in sl(3,\mathbb{R})$, and require that it be stationary with respect to variations of ϕ and ψ, obtaining

$$\psi_x = u\psi, \tag{3.10}$$

which is just (2.10); and its adjoint,

$$\phi_x = -\phi u. \tag{3.11}$$

The matrix

$$\Psi = \psi\phi \tag{3.12}$$

is then easily seen to satisfy Eq. (3.2). If we now look for those deformations of u which leave the integral (3.9) stationary under the above mentioned variations, we obtain the condition

$$\sum_{i=1}^{8} \int \dot{u}^i \phi R_i \psi \, dx = 0, \tag{3.13}$$

where $u = \Sigma_{i=1}^8 u^i R_i$ and $\dot{u}$ is the deformation of u.

It is easily seen that the functions

$$\begin{aligned}
\Phi_i &= \phi R_i \psi\\
&= \mathrm{Tr}(R_i \Psi) = \mathrm{Tr}(R_i R_j)\Psi^j
\end{aligned} \tag{3.14}$$

satisfy Eq. (3.7). The matrix $\mathrm{Tr}(R_i R_j)$, known as the trace form, is important in the study of the Hamiltonian structure

associated with the eigenvalue problem (2.10), as will be discussed in the next section.

These Φ_i and Ψ^i are the sets of squared eigenfunctions used for the theory of perturbed solitons.[9] They are also of importance in the theory of periodic solutions.[10,11] The system (3.7) then represents the squared eigenfunction equation, and gives us a way of constructing this explicitly, as will be seen below.

The Recursion Operator: We want to find an operator $M^\dagger$ which maps one isospectral flow into another of higher order. To do this we consider the condition (3.13) and required that the eigenvalue $\zeta \equiv u^1$ be constant [for the eigenvalue problem (2.8)]

$$\int (\dot{u}^2\Phi_2 + \dot{u}^5\Phi_5)\,dx = 0. \tag{3.15}$$

We are thus interested in a linear operator whose eigenfunction is the column vector $(\Phi_2,\Phi_5)^T$. We achieve this by eliminating the remaining components Φ_k from the system of Eqs. (3.7):

$$\begin{aligned}
\Phi_{1,x} &= u^2\Phi_3 - 3u^5\Phi_6,\\
\Phi_{2,x} &= -\zeta\Phi_3,\\
\Phi_{3,x} &= 2u^2\Phi_1 + u^2\Phi_3 - 3\zeta\Phi_4 + 3u^5\Phi_6,\\
\Phi_{4,x} &= u^2\Phi_4 - \zeta\Phi_5 - u^5\Phi_7 + 2u^5\Phi_8,\\
\Phi_{5,x} &= 3\zeta\Phi_6,\\
\Phi_{6,x} &= -2u^5\Phi_1 + u^5\Phi_5 - u^2\Phi_6 + \zeta\Phi_7,\\
\Phi_{7,x} &= 3\zeta\Phi_2 - 3u^5\Phi_4 - u^2\Phi_7 - 2u^2\Phi_8,\\
\Phi_{8,x} &= 3u^5\Phi_4 - u^2\Phi_7.
\end{aligned} \tag{3.16}$$

From this system of equations we derive:

$$\begin{pmatrix}\Phi_6\\ \Phi_3\\ \Phi_1\end{pmatrix} = \frac{1}{\zeta} M_1 \begin{pmatrix}\Phi_2\\ \Phi_5\end{pmatrix},$$

$$\begin{pmatrix}\Phi_4\\ \Phi_7\\ \Phi_8\end{pmatrix} = \frac{1}{\zeta} M_2 \begin{pmatrix}\Phi_6\\ \Phi_3\\ \Phi_1\end{pmatrix}, \tag{3.17}$$

and

$$\begin{pmatrix}\Phi_2\\ \Phi_5\end{pmatrix} = \frac{1}{\zeta} M_3 \begin{pmatrix}\Phi_4\\ \Phi_7\\ \Phi_8\end{pmatrix},$$

where

$$M_1 = \begin{pmatrix} 0 & \tfrac{1}{3}\partial \\ -\partial & 0 \\ -\partial^{-1}u^2\partial & -\partial^{-1}u^5\partial \end{pmatrix},$$

$$M_2 = \begin{pmatrix} u^5 & \tfrac{1}{3}(u^2-\partial) & \tfrac{2}{3}u^2 \\ \partial + u^2 & -u^5 & 2u^5 \\ \partial^{-1}[3(u^5)^2 - (u^2)^2 - u^2\partial] & \partial^{-1}(-u^5\partial + 2u^2u^5) & 0 \end{pmatrix},$$

and

$$M_3 = \begin{pmatrix} u^5 & \tfrac{1}{3}(\partial + u^2) & \tfrac{2}{3}u^2 \\ -\partial + u^2 & -u^5 & 2u^5 \end{pmatrix}. \tag{3.18}$$

Thus, $(\Phi_2,\Phi_5)^T$ satisfies the equation:

$$M\begin{pmatrix}\Phi_2\\ \Phi_5\end{pmatrix} = \zeta^3\begin{pmatrix}\Phi_2\\ \Phi_5\end{pmatrix}, \tag{3.19}$$

where $M = M_3M_2M_1$.

Multiplying the integral (3.13) by ζ^3 and using (3.19) we get

$$\begin{aligned}
0 &= \sum_{i=2,5} \dot{u}^i(M\Phi_i)\,dx\\
&= \sum_{i=2,5} \int (M^\dagger\dot{u}^i)\Phi_i\,dx,
\end{aligned} \tag{3.20}$$

so that $M^\dagger\dot{u}$ is also an isospectral flow; hence $M^\dagger$ is a recursion operator for the eigenvalue problem (2.8).

4. HAMILTONIAN STRUCTURE

In this section we find a relationship between the operator M and its adjoint, and exploit this to construct a Poisson bracket for the systems under discussion.

Since for simple Lie algebras, the trace form

$$g_{ij} = \mathrm{Tr}(R_iR_j) \tag{4.1}$$

is nonsingular, Eq. (3.14) implies

$$\Psi = g^{-1}\Phi. \tag{4.2}$$

In particular,

$$\begin{pmatrix}\Psi^2\\ \Psi^5\end{pmatrix} = \begin{pmatrix}\frac{1}{2} & 0\\ 0 & \frac{1}{6}\end{pmatrix}\begin{pmatrix}\Phi_2\\ \Phi_5\end{pmatrix} = \hat{g}^{-1}\begin{pmatrix}\Phi_2\\ \Phi_5\end{pmatrix}, \tag{4.3}$$

wherer $\hat{g}$ is the appropriate projection of g.

Hence, from Eq. (3.19) we get

$$\tilde{M}\begin{pmatrix}\Psi^2\\ \Psi^5\end{pmatrix} = \zeta^3\begin{pmatrix}\Psi^2\\ \Psi^5\end{pmatrix}, \tag{4.4}$$

where $\tilde{M} = \hat{g}^{-1}M\hat{g}$.

We now look for A^k, polynomials in ζ, satisfying Eq. (3.1). Since u_t^k must be independent of ζ, it is clear from comparison of (3.1) and (3.2) that A^2 and A^5 are polynomials in ζ^3 and their coefficients satisfy

$$\begin{pmatrix}A^2\\ A^5\end{pmatrix}^{(n)} = \tilde{M}\begin{pmatrix}A^2\\ A^5\end{pmatrix}^{(n+3)}. \tag{4.5}$$

Since

$$\begin{pmatrix}u^2\\ u^5\end{pmatrix}_t = \partial\begin{pmatrix}A^2\\ A^5\end{pmatrix}^{(0)}, \tag{4.6}$$

we find that

$$\partial\tilde{M}\partial^{-1} = \partial\hat{g}^{-1}M\hat{g}\partial^{-1} \tag{4.7}$$

is a recursion operator, relating isospectral flows of (2.9). It may be verified that this operator is equal to $M^\dagger$.

Now we consider the adjoint of Eq. (3.19):

$$M^\dagger \begin{pmatrix} \bar{\Phi}^2 \\ \bar{\Phi}^5 \end{pmatrix} = \zeta^3 \begin{pmatrix} \bar{\Phi}^2 \\ \bar{\Phi}^5 \end{pmatrix}, \tag{4.8}$$

where $\bar{\Phi}^2$ and $\bar{\Phi}^5$ are the "adjoint wavefunctions". However, since

$$M^\dagger = \partial \hat{g}^{-1} M \hat{g} \partial^{-1}, \tag{4.9}$$

by taking

$$\begin{pmatrix} \bar{\Phi}^2 \\ \bar{\Phi}^5 \end{pmatrix} = \partial \hat{g}^{-1} \begin{pmatrix} \Phi_2 \\ \Phi_5 \end{pmatrix} \tag{4.10}$$

we may solve Eq. (4.8). Thus, using the fact that eigenfunctions $\Phi(\zeta)$ at one eigenvalue are orthogonal to the adjoint eigenfunctions $\bar{\Phi}(\zeta')$ at a different eigenvalue, we derive

$$\int (\Phi_2, \Phi_5)(\zeta) \partial \hat{g}^{-1} \begin{pmatrix} \Phi_2 \\ \Phi_5 \end{pmatrix} (\zeta')\, dx = 0, \tag{4.11}$$

when $\zeta \neq \zeta'$. Because of Eq. (3.13) we may consider Φ_2 and Φ_5 as the functional derivatives of ζ with respect to u^2 and u^5 respectively. Therefore, Eq. (3.3) may be considered as expressing the involution of distinct eigenvalues with respect to the Poisson bracket

$$\{H,K\} = \int \left(\frac{\delta H}{\delta u^2}, \frac{\delta H}{\delta u^5} \right) \partial \hat{g}^{-1} \begin{pmatrix} \dfrac{\delta K}{\delta u^2} \\ \dfrac{\delta K}{\delta u^5} \end{pmatrix} dx. \tag{4.12}$$

Hence

$$\partial_t \begin{pmatrix} u^2 \\ u^5 \end{pmatrix} = -\partial \hat{g}^{-1} \begin{pmatrix} \dfrac{\delta H}{\delta u^2} \\ \dfrac{\delta H}{\delta u^5} \end{pmatrix} \tag{4.13}$$

are the Hamiltonian equations. It may be checked that the Hamiltonians of distinct flows, generated by the recursion operator $M^\dagger$, are in involution with respected to this Poisson bracket.

Some Polynomial Flows: The first two nontrivial flows (2.16) and (2.18) may both be written as

$$\partial_t \begin{pmatrix} u^2 \\ u^5 \end{pmatrix} = M^\dagger \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{4.14}$$

where the coefficients of each are determined by the constants of integration in $M^\dagger$. Higher flows may be generated by successive application of $M^\dagger$; the subsequent constants of integration may then be set equal to zero as they contribute nothing new. However, the calculations involved are rather tedious, so will be omitted here. Nevertheless, it should be pointed out that the integration invovled in these calculations can always be performed, the integrands being derivatives of the momentum density

$$H_1 = \tfrac{1}{3}(u^2)^2 + (u^5)^2 \tag{4.15}$$

or the modified Boussinesq Hamiltonian density

$$H_2 = u^5 u^2{}_x - u^2 u^5{}_x + 2u^5 [(u^5)^2 - (u^2)^2] \tag{4.16}$$

"along" an isospectral flow, and are hence exact space derivatives, since these densities are conserved.

A special case of some interest is the restriction

$$u^5 \equiv 0. \tag{4.17}$$

This corresponds to choosing the scalar operator L of (2.4) to be skew–Hermitian (the choices $u^2 \pm u^5 = 0$ are easily seen to be equivalent). With this restriction the recursion operator $M^\dagger$ becomes

$$M^\dagger|_{u^5 \equiv 0} = \tfrac{1}{3}\partial \begin{pmatrix} 0 & (u^2+\partial)^2 - 2u^2\partial^{-1}u^2(\partial + u^2) \\ -\tfrac{1}{3}(u^2-\partial)^2 + 2[(u^2)^2 - \partial u^2]\partial^{-1}u^2 & 0 \end{pmatrix}. \tag{4.18}$$

It is now apparent that $M^\dagger|_{u^5 \equiv 0}$ must be applied twice in order that the condition (3.37) be retained. The simplest nontrivial flow which may be generated in this way is thus given by

$$\begin{aligned} \partial_t u^2 &= \tfrac{1}{3}\partial[(u^2+\partial)^2 - 2u^2\partial^{-1}u^2(\partial+u^2)]\tfrac{1}{3}\partial \\ &\quad \times[-\tfrac{1}{3}(u^2-\partial)^2 + 2((u^2)^2 - \partial u^2)\partial^{-1}u^2] \times 0 \\ &= \tfrac{1}{9}\partial[(u^2+\partial)^2 - 2u^2\partial^{-1}u^2(\partial+u^2)] \\ &\quad \times \partial[2(u^2)^2 - \partial u^2)]K_1 \\ &= [u^2{}_{4x} - 5u^2{}_x u^2{}_{xx} - 5u^2(u^2_x)^2 \\ &\quad - 5(u^2)^2 u^2{}_{xx} + (u^2)^5]_x \end{aligned} \tag{4.19}$$

on giving the constant of integration, K_1, the value $-\frac{2}{9}$. This is the system referred to in I as the modified Kupershmidt equation.

5. NONLINEAR KLEIN–GORDON EQUATIONS

In order to generate isospectral flows of nonlinear Klein–Gordon type we require solutions of (2.14) for which A is inversely proportional to ζ

$$A^k = a^k/\zeta. \tag{5.1}$$

We write u^k in potential form

$$u^k = \theta^k{}_x. \tag{5.2}$$

Equations (2.14) may be simplified considerably; to see this, we consider the third member of this set

$$\partial a^3 = \zeta a^2 - \theta^2{}_x(a^1 + a^3) - \theta^5{}_x a^6. \tag{5.3}$$

Since the a's are independent of ζ, a^2 must vanish. By similar arguments we get

$$a^1 = a^2 = a^3 = a^5 = a^6 = 0. \tag{5.4}$$

Equations (2.14) then reduce to

$$\begin{aligned} a^4_x &= 3\theta^5{}_x(a^7 - a^8) - \theta^2{}_x a^4, \\ a^7_x &= \theta^2{}_x(a^7 + a^8) + \theta^5{}_x a^4, \\ a^8_x &= 2(\theta^2{}_x a^7 - \theta^5{}_x a^4), \end{aligned} \tag{5.5}$$

and

$$\begin{aligned} \theta^2{}_{xt} &= 3a^7, \\ \theta^5{}_{xt} &= -a^4. \end{aligned} \tag{5.6}$$

To solve (5.5) we require that the a^k should be functions of θ^2 and θ^5 alone.

We thus obtain

$$a^4 = -\tfrac{3}{2}\beta\exp(3\theta^5 - \theta^2) + \tfrac{3}{2}\gamma\exp(-\theta^2 - 3\theta^5),$$
$$a^7 = \alpha\exp(2\theta^2) - \tfrac{1}{2}\beta\exp(3\theta^5 - \theta^2) - \tfrac{1}{2}\gamma\exp(-\theta^2 - 3\theta^5),$$
$$a^8 = \alpha\exp(2\theta^2) + \beta\exp(3\theta^5 - \theta^2) + \gamma\exp(-\theta^2 - 3\theta^5). \tag{5.7}$$

The equations of motion (5.6) then become

$$\theta^2{}_{xt} = 3\alpha\exp(2\theta^2) - \tfrac{3}{2}\beta\exp(3\theta^5 - \theta^2) - \tfrac{3}{2}\gamma\exp(-\theta^2 - 3\theta^5),$$
$$\theta^5{}_{xt} = \tfrac{3}{2}\beta\exp(3\theta^5 - \theta^2) - \tfrac{3}{2}\gamma\exp(-\theta^2 - 3\theta^5). \tag{5.8}$$

If α, β and γ are all strictly positive, then without loss of generality they may all be taken to be $\frac{1}{3}$. Hence

$$\theta^2{}_{xt} = \exp(2\theta^2) - \exp(-\theta^2)\cosh(3\theta^5),$$
$$\theta^5{}_{xt} = \exp(-\theta^2)\sinh(3\theta^5). \tag{5.9}$$

If θ^5 is allowed to take imaginary values then the system (5.9) possesses multisoliton solutions.

These systems and some generalization of them related to the Toda lattice have been discussed in more detail elsewhere,[7] in which we show they possess a Bäcklund transformation. These general systems have also been considered by Mikhailov[12] and Kupershmidt.[13]

An interesting special case of (5.9) is when

$$\theta^5 \equiv 0, \tag{5.10}$$

which corresponds to the restriction (4.17). Then

$$\theta^2{}_{xt} = \exp(2\theta^2) - \exp(-\theta^2). \tag{5.11}$$

This equation has been discussed by Dodd and Bullough[14] and Ibragimov.[15]

6. CONCLUSIONS

This paper has had two main objects. The first of these was to extend the results of I to the general operator (1.1). The second was to develop a general scheme for constructing appropriate sets of squared eigenfunctions together with a recursion operator for an arbitrary scattering problem. We also constructed, for the eigenvalue problem (2.8), a Hamiltonian structure, as well as several isospectral flows.

The Miura transformation (2.6) which relates the Boussinesq system (2.2) to the modified system (2.3) may also be used to relate their Hamiltonian structures, in the manner described in I. However, starting from (4.12) we do not generate the usual Poisson bracket for the Boussinesq equation, but the "second" Hamiltonian structure discussed by Kupershmidt and Wilson.[16]

The methods of Secs. 3 and 4 are applicable to any simple Lie algebra; for $sl(2,\mathbb{R})$ the usual recursion operator and squared eigenfunction equations discussed by Ablowitz et al.[5] are generated. In the case of the Boussinesq equation this relationship between the adjoint representation and the squared eigenfunctions has been noted by Flaschka.[17]

The results of Sec. 5 can be generalized, not only to $sl(n,\mathbb{R})$, giving Klein–Gordon equations related to the Toda lattice, but also to any simple Lie algebra, giving systems related to Bogoyavlensky's[18] generalized exponential lattices.[19]

APPENDIX

Throughout this paper the following basis is used for $sl(3,\mathbb{R})$:

$$R_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad R_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$R_3 = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 2 & 0 & 0 \end{pmatrix} \quad R_4 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$
$$R_5 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R_6 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$
$$R_7 = \begin{pmatrix} 0 & 0 & 2 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \quad R_8 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

The commutation relations for these are given by:

	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8
R_1	0	R_3	$3R_4$	R_5	$-3R_6$	$-R_7$	$-3R_2$	0
R_2		0	$-2R_1 - R_3$	$-R_4$	0	R_6	$R_7 + 2R_8$	R_7
R_3			0	$-R_5$	$3R_6$	$2R_8$	$-3R_2$	$-3R_2$
R_4				0	$2R_8 - R_7$	$-R_2$	$2R_1$	$-R_3$
R_5					0	$2R_1 - R_3$	$3R_4$	$-3R_4$
R_6						0	$-R_5$	R_5
R_7							0	$3R_6$
R_8								0

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The lump solutions and the Bäcklund transformation for the three-dimensional three-wave resonant interaction

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A Bäcklund transformation is found for the three-dimensional three-wave resonant interaction, and from it, N-lump exact solutions may be constructed. The one-lump solution is analyzed in detail, and it is shown that it describes such effects as pulse decay, upconversion, and explosive instabilities, all in three dimensions.

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I. INTRODUCTION

Since the general initial value problem of the three-dimensional three-wave resonant interaction (3D3WRI) has recently been completed,[1] one may now turn his attention to see how one may make use of this method of solution. Obviously, one would seek first to exploit the simplest classes of solutions. These are called "lump" solutions, the first ones of which were found by Zakharov[2] and later by Craik.[3] They were then rediscovered by Cornille[4] from his integral equations, and were also noted to arise from the many and varied inverse scattering transforms associated with the 3D3WRI.[1,5] Following a suggestion by Professor Corones,[6] it was soon discovered that the complicated machinery required for the general solution of this problem was not needed if one was willing to only generate new solutions. Of course, to solve an initial value problem you still needed this machinery. But if one would only seek to investigate special solutions, then an old observation made by Professor Corones,[6] would allow one to almost immediately construct the Bäcklund transformation for these equations, from which these special lump solutions could be quickly generated.

These lump solutions in three dimensions are *not* analogous to the soliton solutions from one-dimensional inverse scattering theories, although they are similar in some respects. First of all, when the envelope profiles are required to be integrable, and square integrable in three dimensions, the scattering data for the 3D3WRI has been shown to consist of only a continous spectrum, with no bound states allowed.[1,5,7] On the other hand, soliton solutions in one-dimensional inverse scattering theories always correspond to a pure bound state spectrum, with the continous spectrum being distinctly absent. Furthermore, solitons always have a relation between amplitude and width, so that only one is independent, and with a distinct shape or profile. But lump solutions have no such relation between amplitude and widths, and the profile shape can be quite arbitrary. Thus in three dimensions, we have much more freedom in shaping and forming lump solutions than was possible with one-dimensional soliton solutions.

However, there are also similarities. The one-dimensional soliton solutions always have a closed form solution, since the kernels in the one-dimensional inverse scattering equations were separable. The same is true for these lump solutions in three dimensions, in that the kernels are also separable, again allowing closed form solutions. In fact, this is how one can define a lump solution. And as one could construct N-soliton solutions, so can one also construct N-lump solutions. Furthermore, N-soliton solutions can be constructed from a Bäcklund transformation, and as we shall show here, the same can be done for N-lump solutions.

These N-lump solutions are important for another reason too. Nižnik has shown that any set of potentials (envelope profiles) can be approximated to any given accuracy by a suitably chosen N-lump solution.[8] Thus, many physical situations can therefore be reasonably well approximated by these N-lump solutions, at least for a finite time. The latter condition is necessary, because Nižnik's proof is only valid for a given instant of time, and in general one would not expect such an approximation to remain valid for all time.

What we shall do in this paper is to derive the Bäcklund transformation for the 3D3WRI, showing how one may construct an N-lump solution, and shall briefly discuss these solutions. Then we shall use the one-lump solution to analyze the collision of envelopes in the positive and negative energy cases. What we shall find here are solutions illustrating pulse decay, upconversion, and explosive singularities. These effects in three dimensions are shown to be both analogous and different from the corresponding effects in one-dimensional solutions.[9]

II. THE BÄCKLUND TRANSFORMATION

As discussed by Corones,[6] one way to find a Bäcklund transformation is to simply assume that one exists of the form

$$q' = f(q, Q, \lambda), \tag{2.1}$$

where q is a known solution of the nonlinear system, q' is to be a new solution, Q is the pseudopotential (s), and λ is the eigenvalue (if one is present). One now simply requires q' to be a solution of the nonlinear system, which then can determine what the functional form for f must be.

Well, the same basic idea also works for the 3D3WRI, as we shall now illustrate. The nonlinear equations are

$$\frac{\partial q_i}{\partial \chi_i} = \gamma_i q_j^* q_k^*, \tag{2.2}$$

where i, j, k are cyclic and equal to (1,2,3), q_i is the i^{th} envelope, χ_i is the i^{th} characteristic coordinate, defined by

$$\frac{\partial}{\partial \chi_i} = -\partial_t - \mathbf{v}_i \cdot \nabla, \tag{2.3a}$$

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where $\mathbf{v}_i$ is the group velocity for the i^{th} envelope. The γ_i in (2.2) carries the sign of the coupling constants, and we assume the γ's to be real and scaled to unity in magnitude.

We use the characteristic coordinates because of the resulting simplifications in the analysis. From (2.3) one can obtain the transformation from characteristic coordinates to space–time coordinates. Of course, by (2.3a), we only have three characteristic coordinates, and to complete the transformation, we must supplement (2.3a) with

$$(\partial_t + \mathbf{v}_i\cdot\nabla)\chi_4 = 0, \tag{2.3b}$$

which defines a fourth coordinate. A solution of (2.3) for $\mathbf{x}$ and t as functions of χ_i and χ_4 is

$$x = -\sum_{i=1}^{3}\mathbf{v}_i\chi_i + \mathbf{n}\chi_4, \tag{2.4a}$$

$$t = -\sum_{i=1}^{3}\chi_i, \tag{2.4b}$$

where $\mathbf{n}$ is a unit vector parallel to $(\mathbf{v}_1 - \mathbf{v}_2)\times(\mathbf{v}_2 - \mathbf{v}_3)$, and as such, makes an equal angle with all three group velocities (i.e., $-\mathbf{v}_1\cdot\mathbf{n} = \mathbf{v}_2\cdot\mathbf{n} = \mathbf{v}_3\cdot\mathbf{n}$). Note that when we keep any two characteristic coordinates fixed, and let $t\to\pm\infty$, then the free characteristic coordinate approaches $\mp\infty$.

As far as (2.2) is concerned χ_4 is like a dummy coordinate, since no differentials with respect to it occur. Thus, in solving (2.2), we may keep χ_4 fixed, then let χ_4 take on another value, solve (2.2) again, etc. Thus, since χ_4 is a dummy coordinate, we shall ignore it from now on.

The scattering problem for (2.2) is

$$\partial_k\psi_i = \gamma_k q_j^*\psi_k, \tag{2.5a}$$

$$\partial_i\psi_k = \gamma_i q_j\psi_i, \tag{2.5b}$$

where in (2.5), i,j,k are still cyclic, giving six equations altogether. Equation (2.5) has three conservation laws, which are

$$\partial_i(\gamma_k\psi_k^*\psi_k) = \partial_k(\gamma_i\psi_i^*\psi_i), \tag{2.6}$$

and a consequence of these, is that a function D exists such that

$$\partial_i D = -\gamma_i\psi_i^*\psi_i. \tag{2.7}$$

To find a Bäcklund transformation, we now assume that we can find three functions, $\tilde{q}_1,\tilde{q}_2$, and $\tilde{q}_3$, where

$$\tilde{q}_i = \tilde{q}_i(\psi^*,\psi,q,D), \tag{2.8}$$

and such that these functions will then satisfy (2.2). Using (2.2), (2.5), and (2.7), it is rather simple to show that such can be done, and that

$$\tilde{q}_j = q_j + \psi_i^*\psi_k/D \tag{2.9}$$

is one such transformation, provided D is real. With (2.9), one may now generate new solutions of (2.2) from old solutions. Given any solution of (2.2), one constructs ψ_i from (2.5) and D from (2.7). Then these functions inserted into (2.9) will give a new solution.

In particular, we may start with $q_i = 0$, in which case we obtain a one-lump solution. The solution of (2.5) and (2.7) is then

$$\psi_i = g_i(\chi_i), \tag{2.10a}$$

$$D = \delta + \sum_{i=1}^{3}\gamma_i G_i(\chi_i), \tag{2.10b}$$

where δ is some real constant, and

$$G_i(u) = \int_u^\infty g_i^* g_i(u)\,du. \tag{2.11}$$

In (2.10), we may, without loss of generality, assume $\delta = \pm 1$, since (2.5) is linear in ψ, and only the ratio of $\psi_i^*\psi_k/D$ is significant. Furthermore, if we note that (2.2) and (2.5) are invariant under the change of the signs of all the q's and γ's, we may also choose $\delta = +1$, which we shall do.

Then from (2.9) and (2.10), we have the one-lump solution as being

$$q_j = g_i^* g_k/D, \tag{2.12a}$$

where

$$D = 1 + \sum_{i=1}^{3}\gamma_i G_i. \tag{2.12b}$$

Note that in (2.12), g_i is only a function of χ_i, and similarly for G_i.

Given the above solution, one may proceed to obtain a two-lump solution. Denoting the one-lump D in (2.12) by D_g, then the general solution of (2.5) is now

$$\psi_i = h_i(\chi_i) + g_i F/D_g, \tag{2.13}$$

where

$$F = \eta - \sum_{i=1}^{3}\gamma_i\int_{\chi_i}^\infty g_i^* H_i(u)\,du, \tag{2.14}$$

with η being some constant. The solution of (2.7) is then

$$D = D_h - F - F/D_g, \tag{2.15}$$

where

$$D_h = 1 + \sum_{i=1}^{3}\gamma_i H_i(\chi_i), \tag{2.16a}$$

$$H_i(u) = \int_u^\infty h_i^* h_i\,du. \tag{2.16b}$$

This gives the two-lump solution as being

$$q_j = \bar{q}_j/(D_g D_h - F^*F), \tag{2.17a}$$

where

$$\bar{q}_j = D_h g_i^* g_k + h_i^* g_k F + h_k g_i^* F^* + D_h h_i^* h_k. \tag{2.17b}$$

Although we do not now have a general proof, it seems fairly obvious that by this procedure one may generate an arbitrary N-lump solution.

Let us now consider the simple one-lump solution given by (2.11). The simplest form is when one of the q's is zero. If we choose $g_1 = 0$, then

$$q_1 = g_2^*(\chi_2)g_3(\chi_3)/D(\chi_2,\chi_3), \tag{2.18a}$$

$$q_2 = q_3 = 0, \tag{2.18b}$$

which is a trivial solution of (2.2). It has only one nonzero envelope, and thus corresponds to a freely propagating envelope without any interactions. And in the absence of any interactions, it travels along its characteristic, χ_1 without any change (i.e., it is independent of χ_1). It's profile and shape is determined by two independent functions g_2 and g_3, one for each free dimension. (Actually, g_2 and g_3 will also depend on χ_4, but as stated before, we shall ignore this dependence since it can be understood that all functions and parameters

can always depend on χ_4.) Note that these functions are completely arbitrary; thus there is a large amount of freedom in shaping this pulse. However, the shape is not totally arbitrary, because the functional dependence of q_1 on χ_2 and χ_3 is required to be of the form of a simple product, except for the terms in the denominator.

When all the g's are nonzero in general, we have nontrivial interactions and solutions with the general solution being given by (2.12). To obtain the asymptotic initial profiles (the profiles as $t\to-\infty$) according to (2.4b), we take the limit of the corresponding characteristic coordinate going to $+\infty$. Thus, to get the initial profile for g_1, which we shall designate by Q_1, we let $\chi_1\to+\infty$ in (2.12) for $(i,j,k)=(3,1,2)$ giving,

$$Q_1=g_3^*(\chi_3)g_2(\chi_2)/[1+\gamma_2G_2(\chi_2)+\gamma_3G_3(\chi_3)]. \quad (2.19a)$$

Similarly, the other initial profiles are

$$Q_2=g_1^*(\chi_1)g_3(\chi_3)/[1+\gamma_1G_1(\chi_1)+\gamma_3G_3(\chi_3)], \quad (2.19b)$$

$$Q_3=g_2^*(\chi_2)g_1(\chi_1)/[1+\gamma_1G_1(\chi_1)+\gamma_2G_2(\chi_2)]. \quad (2.19c)$$

Again, one should note that we have a large degree of flexibility in shaping any *one* profile in (2.19). However, after the first one is shaped, say Q_3, then g_1 and g_2 have been specified, and only g_3 is left arbitrary. Now, we are only free to specify "one-half," of another profile. So for the general one-lump solution, we may only shape "one and one-half" profiles arbitrarily, subject to the product form in (2.19). Even with this restriction, one can still obtain useful information concerning the nature of the interactions in the 3D3WRI, as we shall illustrate later.

One can similarly obtain the final profiles, designated by $\tilde{Q}_i$, by taking the limit of $t\to+\infty$ in (2.12). This gives

$$\tilde{Q}_j=g_i^*g_k/(1+\gamma_j\Gamma_j+\gamma_iG_i+\gamma_kG_k), \quad (2.20)$$

where

$$\Gamma_j=G_j(-\infty)=\int_{-\infty}^{\infty}g_j^*g_j(u)\,du. \quad (2.21)$$

Lastly, we should comment that the two-lump solution given by (2.17) has six arbitrary functions, whereas the one-lump solution has only three. Thus, with a two-lump solution one may be able to shape the asymptotic initial profiles independently, instead of only "one and one-half", as is the case for the one-lump solution. However, for now we shall only concentrate on the one-lump solution in spite of the restrictions, due to the simplicity.

III. ONE-LUMP INTERACTIONS

In this section, we shall investigate the range of interactions available in the one-lump solutions. What we shall do, in as far as is possible, is to specify the initial actions in the asymptotic envelopes, and determine via the one-lump solution what the final actions must be. In general we will not be concerned with what the exact initial shape or form is. We will only be interested in how much action is in the envelope. As we shall see, although the shapes are cross-correlated as in (2.19), the actions are not, and can be specified independently. Thus due to this simplification, it is well worthwhile to study this case.

We define the action in the j^{th} envelope A_j by

$$A_j(t)=\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{-\infty}^{\infty}dz\,q_j^*q_j. \quad (3.1)$$

In order to evaluate the above integral, we transform to characteristic coordinates. Directly from (2.4) for t constant, one can show that

$$\begin{aligned}dx\,dy\,dz&=J\,d\chi_1\,d\chi_2\,d\chi_4\\&=J\,d\chi_2\,d\chi_3\,d\chi_4\\&=J\,d\chi_3\,d\chi_1\,d\chi_4\end{aligned} \quad (3.2)$$

where

$$J=|(\mathbf{v}_1-\mathbf{v}_2)\times(\mathbf{v}_2-\mathbf{v}_3)|. \quad (3.3)$$

Thus (3.1) becomes

$$A_j(t)=J\int_{-\infty}^{\infty}d\chi_4a_j(\chi_4,t), \quad (3.4)$$

where the "reduced action" a_j is defined by

$$a_j(\chi_4,t)=\int_{-\infty}^{\infty}d\chi_i\int_{-\infty}^{\infty}d\chi_kq_j^*q_j|_{\chi_j=-t-\chi_i-\chi_k}. \quad (3.5)$$

In practice, it is impossible to evaluate (3.5) when $\chi_j=-t-\chi_i-\chi_k$. However, if instead we define

$$\alpha_j(\chi_4,\chi_j)=\int_{-\infty}^{\infty}d\chi_i\int_{-\infty}^{\infty}d\chi_k\,q_j^*q_j, \quad (3.6)$$

and since as $t\to\pm\infty$, q_j becomes independent of χ_j and we have

$$a_j(\chi_4,t\to\pm\infty)=\alpha_j(\chi_4,\chi_j\to\mp\infty), \quad (3.7)$$

thus allowing us to evaluate the initial and final reduced actions from α_j. In fact, from (2.11) and (2.12), we have the closed form solution

$$\alpha_j=\gamma_k\gamma_k\ln\rho_j, \quad (3.8)$$

where

$$\rho_j=\frac{(1+\gamma_i\Gamma_i+\gamma_jG_j)(1+\gamma_k\Gamma_k+\gamma_jG_j)}{(1+\gamma_jG_j)(1+\gamma_i\Gamma_i+\gamma_k\Gamma_k+\gamma_jG_j)}.$$

Directly from this, we have that the asymptotic initial reduced action a_{jo} is

$$a_{jo}=\gamma_i\gamma_k\ln[(1+\gamma_i\Gamma_i)(1+\gamma_k\Gamma_k)/(1+\gamma_i+\Gamma_i+\gamma_k\Gamma_k)], \quad (3.9)$$

and the final reduced action a_{jf} is

$$a_{jf}=a_{jo}+\gamma_i\gamma_k\ln\sigma, \quad (3.10)$$

$$\sigma=\frac{(1+\gamma_1\Gamma_1+\gamma_2\Gamma_2)(1+\gamma_1\Gamma_1+\gamma_3\Gamma_3)(1+\gamma_2\Gamma_2+\gamma_3\Gamma_3)}{(1+\gamma_1\Gamma_1)(1+\gamma_2\Gamma_2)(1+\gamma_3\Gamma_3)(1+\gamma_1\Gamma_1+\gamma_2\Gamma_2+\gamma_3\Gamma_3)}. \quad (3.11)$$

Note that up to a sign carried by $\gamma_i\gamma_k$, the change in the action is the same for all three envelopes, in agreement with the three conservation laws of action, which are

$$\frac{d}{dt}\int d^3\chi(\gamma_iq_i^*q_i+\gamma_jq_j^*q_j)=0, \quad (3.12)$$

Now, according to (3.9), the initial reduced actions are a function of the three Γ's, and one can also invert this to

obtain the Γ's in terms of the initial reduced actions. To do this, one first defines

$$m_j = [\gamma_i\gamma_k - \gamma_i\gamma_k \exp(-\gamma_i\gamma_k a_{jo})]^{1/2}, \tag{3.13}$$

which is always real, and for $a_{jo} \ll 1$,

$$m_j \to (a_{jo})^{1/2}. \tag{3.14}$$

From (3.9) and (3.13) one can show

$$\Gamma_j/(1+\gamma_j\Gamma_j) = m_i m_k/m_j. \tag{3.15}$$

One should note that no nontrivial solution exists when any one of the reduced actions is chosen to be zero. This is a consequence of using the one-lump solution. However, we may choose any reduced action to be as small as desired, but not zero, as long as a physical solution will exist for (3.15).

Assuming that a physical solution does exist for (3.15), σ as given by (3.11) becomes

$$\sigma = \frac{(1-\gamma_2\gamma_3 m_1^2)(1-\gamma_1\gamma_3 m_2^2)(1-\gamma_1\gamma_2 m_3^2)}{1-\gamma_2\gamma_3 m_1^2 - \gamma_1\gamma_3 m_2^2 - \gamma_1\gamma_2 m_3^2 + 2\gamma_1\gamma_2\gamma_3 m_1 m_2 m_3}. \tag{3.16}$$

Then from (3.10), (3.13), and (3.16), one finally obtains

$$m_{jf}^2 = (m_j - \gamma_j m_i m_k)^2/(1-\gamma_j\gamma_k m_i^2)(1-\gamma_i\gamma_j m_k^2), \tag{3.17}$$

where m_f is that value of m corresponding to the final value of the reduced action, as given in (3.13). We shall now consider the two possible physical cases.

A. The positive energy case

When all envelopes have a positive energy one of the γ's must differ in sign from the other two,[9] and that corresponding wave then has the largest central frequency. Without loss of generality we shall choose this wave to be wave number 1, and thus we have

$$\gamma_1 = -\gamma_2 = -\gamma_3. \tag{3.18}$$

We still have a freedom in choosing the sign of γ_1, since we set the value of δ in (2.10b) equal to $+1$, and as we shall see, changing the sign of γ_1 will give a different solution.

In order to orientate ourselves, we first list out the values for m_j^2 and Γ_j. From (3.13)

$$m_1^2 = 1 - e^{-a_{10}}, \quad \text{thus } 0 < m_1 < 1, \tag{3.19a}$$

$$m_2^2 = e^{a_{20}} - 1, \quad \text{thus } 0 < m_2 < \infty, \tag{3.19b}$$

$$m_3^2 = e^{a_{30}} - 1, \quad \text{thus } 0 < m_3 < \infty, \tag{3.19c}$$

and from (3.15),

$$\Gamma_1 = m_2 m_3/(m_1 - \gamma_1 m_2 m_3), \tag{3.20a}$$

$$\Gamma_2 = m_1 m_3/(m_2 + \gamma_1 m_1 m_3), \tag{3.20b}$$

$$\Gamma_3 = m_1 m_2/(m_3 + \gamma_1 m_1 m_2). \tag{3.20c}$$

Note that by (3.19), as the initial reduced actions are increased, the values of m increase also, and that m_1 must be bounded from above by unity, while m_2 and m_3 are unbounded. From (3.20) we shall obtain the allowed range of the initial reduced actions if the collision is to be represented by one-lump solutions.

First we shall consider the $\gamma_1 = +1$ case. Then for Γ_1 to remain positive and finite we must require

$$m_1 > m_2 m_3, \tag{3.21}$$

and then (3.17) becomes

$$m_{1f}^2 = (m_1 - m_2 m_3)^2/(1+m_2^2)(1+m_3^2), \tag{3.22a}$$

$$m_{2f}^2 = (m_2 + m_1 m_3)^2/(1-m_1^2)(1+m_3^2), \tag{3.22b}$$

$$m_{3f}^2 = (m_3 + m_1 m_2)^2/(1-m_1^2)(1+m_2^2), \tag{3.22c}$$

When $m_1 \gg m_2 m_3$ this solution corresponds to a decay of the high frequency pulse q_1 into the two daughter waves q_2 and q_3. To illustrate this, we shall assume $m_2 = m_3$, and then from (3.19) and (3.22) we find that

$$e^{a_{1f}} = e^{a_{20}} e^{a_{10}}/(1 + 2m_1 m_2^2 e^{a_{10}}), \tag{3.23}$$

which for $a_{10} \to \infty$ and $a_{20} \ll 1$ gives

$$a_{1f} \to -\ln(2a_{20}), \tag{3.24}$$

so that the final action in a very intense high frequency pump, will be determined solely by the initial actions in the daughter waves. This is illustrated in Fig. 1, where we have plotted $\log a_{1f}$ vs $\log a_{1o}$ for various values of $a_{20} = a_{30}$. The main feature to note is that as a_{10} increases (for a given value of $a_{20} = a_{30}$), a_{1f} remains equal to a_{10} (i.e., no depletion occurs) until a critical value of about $-\ln(2a_{20})$ is reached, at which point, all additional action in the pump beyond this critical value is dumped into the daughter waves. Note that this is analogous to the soliton decay case in the one-dimensional 3WRI.[9] However, there the critical value depended essentially only on the absolute *area* under the profile of the pump itself, whereas here, it depends on the amount of action in the perturbing *daughter* waves.

This phenomena of pump decay would be expected to hold true even if the three pulse profiles were not one-lump solutions because all that is basically happening is that the daughter waves are traveling through the pump, and at the

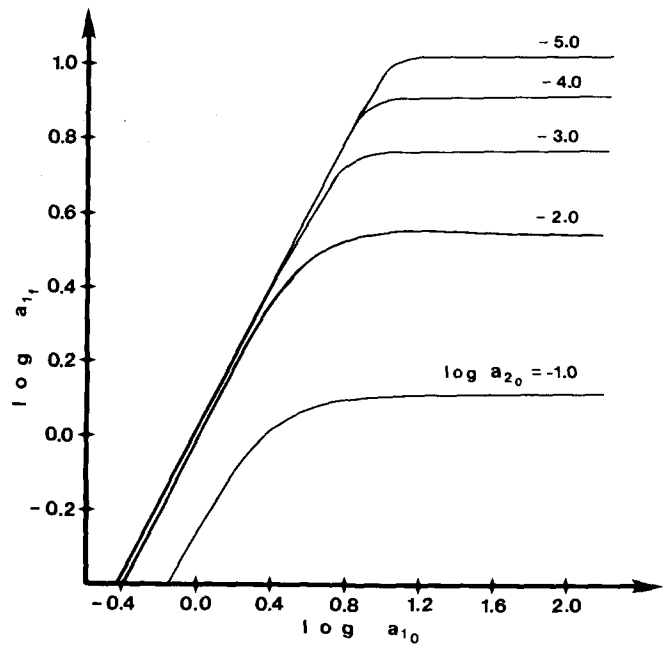

FIG. 1. The decay case. An initially intense high frequency pump of reduced action a_{1o} will decay to a final reduced action of a_{1f}, depending on the initial reduced actions ($a_{20} = a_{30}$) in the daughter waves.

critical value, the growth rate has become equal to the relative pulse width allowing depletion to occur. Beyond this simple picture our result confirms what one would expect. Namely, the relative depletion becomes more and more as the initial action in the pump is increased.

There is another region of this solution where m_1 approaches $m_2 m_3$ from above, and from (3.22a), one can see that for this, virtually total depletion of the pump can occur. But we do not believe this feature to be a general feature. Rather, we consider it to be a special property of 1-lump solutions, and in general it should not occur for general pulses.

When $\gamma_1 = -1$ we have the opposite of decay, which is upconversion. Without loss of generality, we may assume

$$m_3 \geqslant m_2, \tag{3.25a}$$

in which case the allowed physical parameter space, from (3.20), is

$$m_1 < m_2/m_3, \tag{3.25b}$$

and (3.17) becomes

$$m_{f_1}^2 = (m_1 + m_2 m_3)^2/(1 + m_2^2)(1 + m_3^2), \tag{3.26a}$$

$$m_{f_2}^2 = (m_2 - m_1 m_3)^2/(1 - m_1^2)(1 + m_3^2), \tag{3.26b}$$

$$m_{f_3}^2 = (m_3 - m_2 m_1)^2/(1 - m_1^2)(1 + m_2^2). \tag{3.26c}$$

If we again consider the case where $m_2 = m_3$, then (3.25) becomes trivial and no restrictions are placed on our parameter space. Then

$$e^{a_{1f}} = e^{2a_{20}}/[(1 - m_1)(2e^{a_{20}} - 1 + m_1)], \tag{3.27}$$

and for $a_{20} \to \infty$ with $a_{10} \ll 1$, we find

$$a_{1f} \to a_{20} - \ln 2, \tag{3.28a}$$

while in the limit of $a_{10} \to 0$ and $a_{20} \to 0$ we find

$$a_{1f} \to [a_{20} + (a_{10})^{1/2}]^2. \tag{3.28b}$$

Equation (3.28) gives two important limits for the final action in the pump. In Fig. 2, we have plotted $\log a_{1f}$ vs $\log a_{20}$ for various values of $\log a_{10}$. The main features are that as $a_{20} \to 0$, $a_{1f} \simeq a_{10}$, so that no conversion has occured. Then as a_{20} increases, when it reaches the critical value of $a_{20} \simeq (a_{10})^{1/2}$, upconversion starts to occur with a_{1f} rapidly approaching the critical value given by (3.28a). Again, this feature is similar to that which occurs in the one-dimensional 3WRI,[9] except that there the critical value depended only on the absolute areas under the daughter profiles, whereas here it depends only on the amount of action in the high frequency pump. Still, for large amounts of action in the daughter waves, an almost total upconversion can occur.

B. The negative energy case

The only other case which differs from the above is when the high frequency wave is a negative energy wave, in which case

$$\gamma_1 = \gamma_2 = \gamma_3. \tag{3.29}$$

Now, the corresponding expressions for the m's and the Γ's are

$$m_j^2 = 1 - e^{-a_{20}}, \qquad \text{thus } 0 < m_j < 1, \tag{3.30}$$

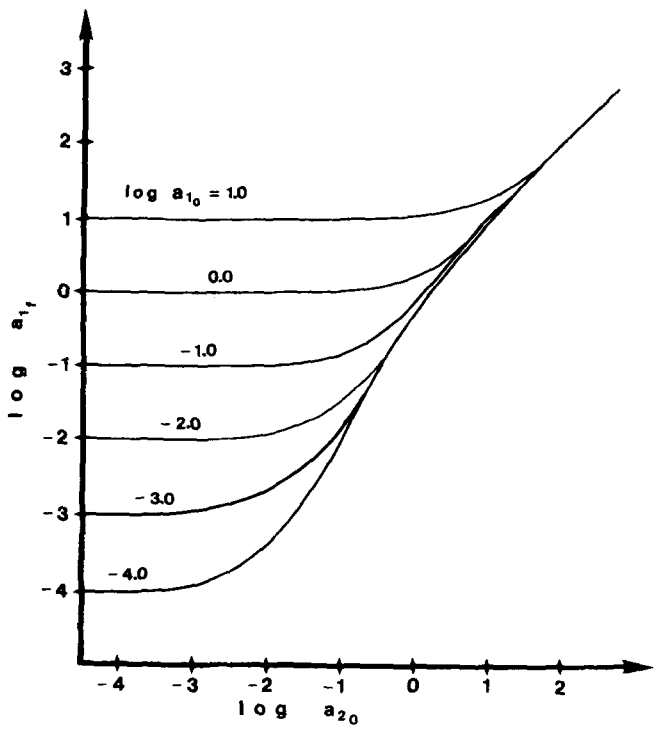

FIG. 2. The upconversion case. Two interacting daughter waves of reduced action $a_{20} = a_{30}$ interact and pump energy into the high frequency wave, creating a pump wave of final reduced action a_{1f} from a_{10}.

$$\Gamma_j = m_i m_k/(m_j - \gamma_1 m_i m_k), \tag{3.31}$$

while (3.17) becomes

$$m_{jf}^2 = (m_j - \gamma_1 m_i m_k)^2/(1 - m_i^2)(1 - m_k^2). \tag{3.32}$$

When $\gamma_1 = -1$ (3.31) gives no restrictions on the parameter space, so we shall handle this solution first. By (3.30), if the final reduced actions are to be real then $m_{jf}^2 < 1$, which by (3.32) requires

$$m_1^2 + m_2^2 + m_3^2 + 2m_1 m_2 m_3 < 1. \tag{3.33}$$

If this requirement is not satisfied by the initial reduced actions, then a singular solution will develop with all three a_j's becoming infinite at some finite time. This can be verified from (2.12). A similar result was obtained in the one-dimensional case.[9] However, here the system seems to be *linearly stable*, since if m_2 and m_3 become infinitesimal, then q_1 is only unstable for m_1 infinitesimally close to unity (i.e., $a_{10} \to \infty$).

In Fig. 3 we show this stability region for the case where $a_{20} = a_{30}$. In this case, the stability line from (3.33) is determined by

$$e^{a_{20}} = 2/[1 + (1 - e^{-a_{10}})^{1/2}]. \tag{3.34}$$

As $a_{10} \to 0$, (3.34) gives that

$$a_{20} \to \ln 2 - (a_{10})^{1/2}, \tag{3.35a}$$

while as $a_{20} \to 0$ we have

$$a_{10} \to -\ln(4a_{20}). \tag{3.35b}$$

If we consider q_1 to be the pump and q_2 and q_3 to be the daughter waves, then (3.35) and Fig. 3 show that once the action in each of the two daughter waves has exceeded ln2, the solution will be unstable for any value of the action in the

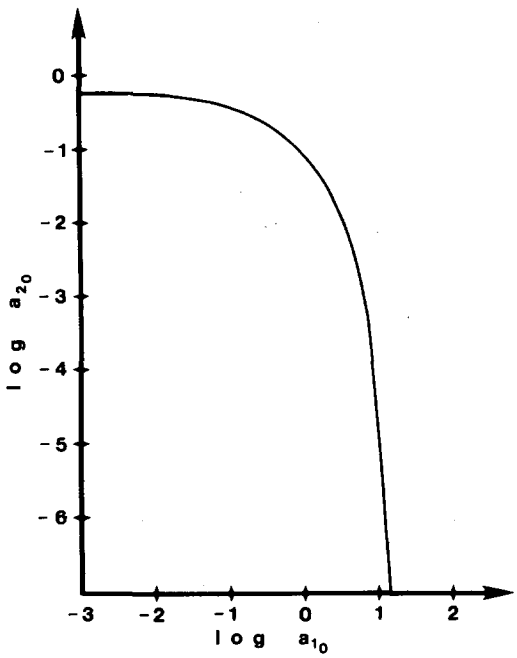

FIG. 3. The negative energy case for $a_{20} = a_{30}$. When the initial reduced actions lie outside and above the curve, the solution will always become singular in a finite time. All solutions under the curve are stable.

pump. On the other hand, as the daughter waves become infinitesimal, a large pump is stable until its action exceeds the value in (3.35b). Thus in theory, a large negative energy pump can be stable, but due to the critical value in (3.35b) being logarithmic, even the smallest finite noise level will place a practical upper limit on this stability.

The $\gamma_1 = +1$ solution is stable, although the parameter space is restricted. Without loss of generality, we can take

$$m_3 \geqslant m_2 \geqslant m_1, \tag{3.36a}$$

in which case (3.31) gives

$$m_1 > m_2 m_3. \tag{3.36b}$$

Now, we use (3.32) to demand that $m_{jf}^2 < 1$ gives

$$m_1^2 + m_2^2 + m_3^2 - 2m_1 m_2 m_3 < 1, \tag{3.37}$$

which due to (3.36) is always satisfied.

IV. CONCLUSIONS

With somewhat remarkable simplicity, we have found a quite interesting set of exact solutions for the 3D3WRI which very nicely illustrate such effects as pulse decay, up-conversion, and explosive instabilities. This was all accomplished by considering the very simple one-lump solution obtained from the Bäcklund transformation. We would expect that two- and three-lump solutions would provide even more interesting results.

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Power series expansion for a crossing-symmetric vertex function

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Starting from a nonlinear system of coupled integral equations for the vertex parts which are irreducible with respect to the s-, t-, and u-channel, a power series is found for the full vertex function in terms of the vertex part Γ^0 which is irreducible with respect to all channels. The problem of finding an expression in closed form remains unresolved, since higher-order products in Γ^0 are nonassociative. In a simplified model, the mathematical properties of the series seem to allow successive rational approximations.

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1. INTRODUCTION

Up to now, all attempts have failed to find a satisfactory solution to the problem of constructing a fully crossing-symmetric vertex function, which plays a central rôle in the Green's function formulation of the many-body theory.[1-5]

The difficulty lies not only in the complexity of an s-, or t-channel Bethe–Salpeter equation as such[4,5] but rather in the problem of finding a suitable input for these equations. Denoting by Γ^s, Γ^t, and Γ^u the respective inputs of the s-, t-, and u-channel equations, i.e., the irreducible parts with respect to s-, t-, and u-channel of the full vertex function Γ, the respective channel equations read

$$\Gamma = \Gamma^s + \Gamma^s \cdot GG \cdot \Gamma, \tag{1.1a}$$

$$\Gamma = \Gamma^t + \Gamma^t * GG * \Gamma, \tag{1.1b}$$

$$\Gamma = \Gamma^u + \Gamma^u \circ GG \circ \Gamma, \tag{1.1c}$$

where dots, stars, and circles indicate the s-, t-, and u-channel connections, respectively, while G denotes the single-particle Green's function. The explicit form of the connections, i.e., the appropriate summation and integration over the labels and energy variables, is given in the next section. The condition that Γ should obey, say, the two equations (1.1a) and (1.1b), is actually a requirement on the quantities Γ^s and Γ^t. In fact, they have to be *determined* in such a way that there exists a vertex function Γ which satisfies Eqs. (1.1)

The question arises as to what the basic quantity is, in terms of which Γ^s, Γ^t, and Γ^u can be evaluated. Migdal[6] suggested introducing a quantity ω which is s- and t-channel irreducible, and deriving a nonlinear integral equation for Γ with ω as input. However, we are not convinced that the equation referred to is correct. Furthermore, ω certainly contains u-reproducible contributions, and is therefore not a suitable candidate for being a basic quantity. Intuitively, one would expect the specific part of Γ, which is irreducible with respect to all three channels, to be a proper basic input quantity from which all three quantities Γ^s, Γ^t, and Γ^u could be constructed.

In this paper we in fact derive a power expansion for Γ^i, $i = s,t,u$, in terms of Γ^0, the vertex part irreducible with respect to all three channels. This expansion can be easily rewritten as an expansion for the full vertex function Γ. We start from a set of coupled nonlinear integral equations for the three quantities Γ^i. In constructing the power series the problem is encountered of nonassociative products, which originates from the different channel connections. This pattern gives rise to certain bracket combinations of an nth order term. They can be obtained in a recursive way from the bracket combinations which originate from the lower-order terms.

Our approach differs from the more traditional ones in that the vertex function is expressed by the basic quantity Γ^0 and not by quantities derived from it, as is the case in Eqs. (1.1). Since we construct the quantities Γ^s, Γ^t, and Γ^u in such a way that Γ obeys Eqs. (1.1), crossing symmetry is guaranteed. Traditional approximations start from *ad hoc* expression for either Γ^s or Γ^t, and then necessarily lead to a noncrossing symmetric vertex function. In our approach, even if Γ^0 is chosen energy independent, the resulting Γ will still be crossing symmetric.

In the following section we set up the nonlinear integral equations. The solution, i.e., the power expansion, is constructed in Sec. 3, while the properties of the series are discussed from various points of view in Sec. 4.

2. THE INTEGRAL EQUATIONS

For reasons of symmetry it is obvious that there is no fermion vertex with an odd number of external lines. As a consequence any diagram can be reducible with respect to at most one channel, since reducibility with respect to two channels would require a 3-fermion vertex. Hence Γ^i, which is defined to consist of all i-channel irreducible parts ($i = s,t,u$), must contain all globally irreducible parts, i.e., Γ^0, and in addition all k-channel reducible parts for $k \neq i$. Since Γ contains all contributions, the expression

$$\gamma^s = \Gamma^s \cdot GG \cdot \Gamma = \Gamma \cdot GG \cdot \Gamma^s$$

yields all s-channel reducible parts. Similarly, the expressions

$$\gamma^t = \Gamma^t * GG * \Gamma = \Gamma * GG * \Gamma^t,$$

$$\gamma^u = \Gamma^u \circ GG \circ \Gamma = \Gamma \circ GG \circ \Gamma^u,$$

yield all the t-channel and u-channel reducible parts, respectively. From the above reasoning we conclude that the three relations

$$\Gamma^s = \Gamma^0 + \Gamma * GG * \Gamma^t + \Gamma \circ GG \circ \Gamma^u,$$

$$\Gamma^t = \Gamma^0 + \Gamma \cdot GG \cdot \Gamma^s + \Gamma \circ GG \circ \Gamma^u, \tag{2.1}$$

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$$\Gamma^u = \Gamma^0 + \Gamma\cdot GG\cdot\Gamma^s + \Gamma * GG * \Gamma^t,$$

must hold. By definition

$$\Gamma = \Gamma^0 + \gamma^s + \gamma^t + \gamma^u,$$

which, using Eqs. (1.1), can be rewritten to yield

$$\Gamma = \tfrac{1}{2}(\Gamma^s + \Gamma^t + \Gamma^u - \Gamma^0). \tag{2.2}$$

Inserting this result into Eqs. (2.1) we obtain a coupled nonlinear system for the quantities Γ^i.

To write down this system in a compact form we introduce the 3-component quantities

$$X = \begin{pmatrix} \Gamma^s \\ \Gamma^t \\ \Gamma^u \end{pmatrix}, \quad A = \begin{pmatrix} \Gamma^0 \\ \Gamma^0 \\ \Gamma^0 \end{pmatrix},$$

as well as a two-face operator $\mathscr{B}$ whose action on vector quantities of the same type as X is defined by

$$Y\mathscr{B}Z = \tfrac{1}{2}\Big(\sum_{i=1}^{3} Y^i\Big)\begin{pmatrix} 0 & *GG* & \circ GG\circ \\ \cdot GG\cdot & 0 & \circ GG\circ \\ \cdot GG\cdot & *GG* & 0 \end{pmatrix}\begin{pmatrix} Z^1 \\ Z^2 \\ Z^3 \end{pmatrix}.$$

With this notation Eqs. (2.1) and (2.2) are combined to yield

$$X = A - \tfrac{1}{3}A\mathscr{B}X + X\mathscr{B}X. \tag{2.3}$$

The nonlinear character of this equation, which originates from the implementation of crossing-symmetry, has been pointed out for relativistic field equations some years ago.[7]

For the sake of completeness we give the explicit expressions for the different channel connections occurring in the operator $\mathscr{B}$. To do so, we choose the three independent energy variables on which all vertex parts depend[3] as

$$s = w_i + w_k = w_l + w_m,$$
$$t = w_l - w_i,$$
$$u = w_l - w_k,$$

and list them as $Z_{iklm}(s,t,u)$ where Z stands for any vertex part. The energies $w_i,\ldots,w_m$ are the off-shell energies associated with the labels $i,\ldots,m$ which refer to a given single-particle basis in which the 4-vertex functions are represented. In that same basis we represent the single-particle propagator G. For convenience later, we give the spectral representation

$$G_{ik}(z) = \sum_{n'\in N_{i'}} \frac{a_{ik}^{(n')}}{z-\omega_{n'}} + \sum_{n\in N_k} \frac{a_{ik}^{(n)}}{z-\omega_n}. \tag{2.4}$$

The s-, t-, and u-channel connections of two vertex parts are then given by[3]

$$Y\cdot GG\cdot Z = -\tfrac{1}{2}\int \frac{dz}{2\pi i} Y_{ik\,pq}(s,z-u,z-t)G_{pp'}\Big(z - \frac{t+u-s}{2}\Big)G_{qq'}\Big(\frac{s+t+u}{2} - z\Big) \times Z_{p'q'lm}(s,t+u-z,z),$$

$$Y * GG * Z = \int \frac{dz}{2\pi i} Y_{pkqm}(z-u,t,z-s)G_{pp'}\Big(z - \frac{s+t+u}{2}\Big)G_{qq'}\Big(z - \frac{s-t+u}{2}\Big) \times Z_{iq'lp'}(z,t,s+u-z),$$

$$Y\circ GG\circ Z = -\int \frac{dz}{2\pi i} Y_{ipqm}(z-t,z-s,u)G_{pp'}\Big(z - \frac{s+t+u}{2}\Big)G_{qq'}\Big(z - \frac{s+t-u}{2}\Big) \times Z_{q'klp'}(z,s+t-z,u),$$

where the summation convention is used. Finally, we mention that the symmetry relations to be fulfilled by Γ, viz.,

$$\Gamma_{iklm}(s,t,u) = -\Gamma_{kilm}(s,u,t) = -\Gamma_{ikml}(s,-u,-t),$$

must be fulfilled by Γ^0 as well. As a consequence, the reducible vertex parts obey

$$\gamma^t_{iklm}(s,t,u) = -\gamma^u_{kilm}(s,u,t) = -\gamma^u_{ikml}(s,-u,-t),$$

while γ^s has the same symmetries as Γ and Γ^0.

3. A POWER SERIES SOLUTION

We consider as given in Eq. (2.3) the quantities A, i.e. Γ^0, and $\mathscr{B}$, i.e. G. The question of the actual availability or rather nonavailability of these quantities, and useful approximations of them, is discussed in the next section.

The individual terms of a power series solution of Eq. (2.3) are expected to be of the form $c_n \cdot A\mathscr{B}A\mathscr{B}\cdots A\mathscr{B}A$ with some coefficients c_n. However, this nth order product is not uniquely defined, since a higher-order product in $\mathscr{B}$ is not associative. In fact, looking for instance at the third component of the vector $(A\mathscr{B}(A\mathscr{B}A))$ we obtain six terms, from which we select one that is typical, viz. $(\Gamma^0\cdot GG\cdot(\Gamma^0 * GG * \Gamma^0))$. This term differs from those generated by the expression $((A\mathscr{B}A)\mathscr{B}A)$; of the nine terms which we obtain, a typical term of the third component now reads $((\Gamma^0\cdot GG\cdot\Gamma^0) * GG * \Gamma^0)$. It is precisely the different channel connections, that

$$(A\mathscr{B}(A\mathscr{B}A)) \neq ((A\mathscr{B}A)\mathscr{B}A).$$

The proper power series solution must therefore have the form

$$X = \sum_{n=0}^{\infty}\sum_{m=1}^{N_n} d_{nm}(\{A\mathscr{B}\}_m^n A), \tag{3.1}$$

where the label m lists all the N_n bracket combinations of an nth order product in the operator $\mathscr{B}$.

The pattern of the bracket combinations, their number N_n and the coefficients d_{nm} are determined in an elementary way. From Eq. (2.3) we find for the first few powers

$$X^{(0)} = A,$$
$$X^{(1)} = \tfrac{2}{3}(A\mathscr{B}A),$$
$$X^{(2)} = \tfrac{4}{9}(A\mathscr{B}(A\mathscr{B}A)) + \tfrac{2}{3}((A\mathscr{B}A)\mathscr{B}A),$$
$$\vdots$$

$$X^{(n+1)} = \tfrac{2}{3}(A\mathscr{B}(X^{(n)})) + ((X^{(n)})\mathscr{B}A) + \sum_{r=1}^{n-1}((X^{(r)})\mathscr{B}(X^{(n-r)})). \tag{3.2}$$

The last expression yields all the information we need. To obtain the number N_n we deduce the recursion formula

$$N_{n+1} = 2N_n + \sum_{k=1}^{n-1} N_k N_{n-k},$$

$$N_1 = 1,$$

the solution of which is

$$N_n = \frac{1}{n}\binom{2n}{n-1}.$$

From Eq. (3.2) it is obvious that the coefficients d_{nm} assume the values

$$d_{nm} = (\tfrac{2}{3})^k, \quad 1 \leqslant k \leqslant n.$$

The value of k is determined by the specific structure of a bracket combination. Since a factor $\frac{2}{3}$ is picked up if and only if we operate with $A\mathscr{B}$ from the left, k is the number of open brackets, with the proviso that accumulated brackets count once. Thus, the combination $(((\cdots(A\mathscr{B}A)\mathscr{B}A)\cdots\mathscr{B}A)$ yields $k = 1$, whereas the combination $(A\mathscr{B}(A\mathscr{B}(\cdots\cdots(A\mathscr{B}A)))\cdots)$ yields $k = n$. For intermediate values of k we find more than one bracket combination. It turns out that n_k, the number of bracket combinations belonging to the same k-family, is

$$n_k = \frac{1}{n}\binom{n}{k}\binom{n}{k-1}.$$

Clearly

$$\sum_{k=1}^{n} n_k = N_n.$$

The strong interrelationship between the three components of the vector X, i.e., between the quantities Γ^s, Γ^t, and Γ^u, becomes fairly obvious by this approach. This is of course not surprising, as we so determined these quantities that each of the Eqs. (1.1) furnishes the same vertex function Γ. The solution Γ of any of Eqs. (1.1) can now also be given by a similar power series using Eq. (2.2). We quote the result, which is obtained in a straightforward way:

$$\Gamma = \Gamma^0 + \sum_{n=1}^{\infty}\sum_{m=1}^{N_n}\left(\left\{\Gamma^0 \sum_{i=s,t,u}{}' (GG)_i\right\}_m^n \Gamma^0\right), \tag{3.3}$$

where $(GG)_s$, $(GG)_t$, and $(GG)_u$ stand for $\cdot GG\cdot$, $*GG*$, and $\circ GG\circ$, respectively.

To evaluate the N_n bracket combinations of nth order, the same lines are followed as those developed above, A being replaced by the term Γ^0, and $\mathscr{B}$ by $\Sigma_i'(GG)_i$. The prime on the summation sign indicates an additional rule: Dismantle a specific bracket combination, and proceed step by step from the outside towards the innermost term, in such a way that when advancing from a term $(GG)_i$ to its next coupled term $(GG)_j$, all three j-values have to occur when they appear to the left of $(GG)_i$, while $j = i$ is excluded when these terms are situated on the right-hand side of $(GG)_i$.

Two examples from the 42 combinations for $n = 5$ illustrate this rule:

$$\left\{\left[\Gamma^0 \sum_i \left(\Gamma^0 \sum_{j'\neq i'} \Gamma^0\right)\right] \sum_i \left[\Gamma^0 \sum_{j\neq i}\left(\Gamma^0 \sum_{j''\neq j} \Gamma^0\right)\right]\right\},$$

$$\left[\Gamma^0 \sum_i \left(\left\{\left[\left(\Gamma^0 \sum_{i'} \Gamma^0\right)\sum_{j'} \Gamma^0\right] \sum_{i''} \Gamma^0\right\} \sum_{j\neq i} \Gamma^0\right)\right].$$

As a result, the actual number Z_n of terms which emerges from the N_n bracket combinations for Γ, is given by

$$Z_n = \sum_{k=1}^{n} 3^{n+1-k}\, 2^{k-1} n_k.$$

It should be noted that the left-right asymmetry introduced above is only apparent: it is a consequence of our specific definition of the operator $\mathscr{B}$. If in Eqs. (2.1) we had used the terms $\Gamma^s \cdot GG \cdot \Gamma$ instead of $\Gamma \cdot GG \cdot \Gamma^s$ and proceeded analogously in the case of the other terms, the definition of $\mathscr{B}$ would have differed accordingly, with the effect that left and right would have interchanged their rôles in the above discussion.

4. DISCUSSION

While the expansion given by Eq. (3.3) constitutes a correct solution to the problem formulated by Eqs. (1.1), there are still many unresolved difficulties. These can be separated into two groups of problems.

The first concerns the input quantities Γ^0 and G. To the best of our knowledge, no equation or any other systematic method except the perturbation approach, has been developed making it possible to construct Γ^0. With regard to the single-particle propagator G, we recall that it depends implicitly on Γ itself.[1-3] However, the value of Eq. (3.3) lies in the fact that it can serve as a starting point of a simplifying model, in which Γ^0 and G are assumed to be given. This approach is similar in spirit to the traditional ones, where Γ^s or Γ^t as well as G are modeled in some way, and Eq. (1.1a) or (1.1b) is then solved. Our approach differs in that we calculate Γ^s and Γ^t [Eq. (3.1)] in order to obtain a consistent Γ. There is, however, a price to be paid for this more ambitious aim, and this leads us to the second group of problems.

Even if Γ^0 and G assume their simplest possible form, i.e., Γ^0 is energy-independent and G contains only one left-hand and one right-hand pole with diagonal residues in Eq. (2.4), a closed expression for the series (3.3) is extremely hard to find. It is to be noted that (3.3) differs completely from any series, similar to a geometric series, such as occurs in the Neumann series of a linear integral equation. There, a solution can at least in principle be obtained by calculating the inverse of an operator. Here, as observed by other authors in a similar context,[8] there does not seem to be an inverse operator whose power expansion would produce the series (3.3). However, there is some prospect of finding acceptable successive approximations in simple cases. We briefly outline the underlying idea.

Consider the model in which an energy-independent Γ^0 is also independent of the labels. We denote this quantity by λ. For G we assume the form described in the previous paragraph, where we denote by ϵ and δ the right-hand and left-hand poles, respectively. The power expansion (3.3) can then be written as

$$\Gamma = \sum_{n=1}^{\infty} \lambda^n \sigma_n(s,t,u). \tag{4.1}$$

Except for $\sigma_1 = 1$, the coefficients σ_n have poles at

$$s = 2\epsilon + k(\epsilon - \delta), \quad s = 2\delta + k(\delta - \epsilon),$$

$$t = \pm(\epsilon - \delta + k(\epsilon - \delta)), \quad u = \pm(\epsilon - \delta + k(\epsilon - \delta)),$$

$$\tfrac{1}{2}(s \pm t \pm u) = 2\epsilon - \delta + k(\epsilon - \delta),$$

$$\tfrac{1}{2}(s \pm t \pm u) = 2\delta - \epsilon + k(\delta - \epsilon),$$

with $k = 0,1,2,\ldots,\leqslant[(n-1)/2]$. In the expression $(s \pm t \pm u)/2$, all four combinations of the signs are understood. The poles listed may be multiple up to at most $(n-1)$th order. These are the only possible singularities of σ_n. In the case considered, a finite radius of convergence can be established around $\lambda = 0$ for energy values outside some finite domains which contain as inner points the poles listed.[9]

We now pose the conjecture that the expansion (4.1) gives rise to a meromorphic function in the energy variables s,t,u with poles only in these variables and in the combination $s \pm t \pm u$, where the pole positions are determined only by λ and the parameters ϵ and δ. This conjecture is supported by results obtained from nontrivial models for Γ (Refs. 4, 5, and 10) and from the fact that, in the model considered, the two-particle propagators derived from Γ are known to be meromorphic. The latter statement means that the expression

$$\Gamma(s,t,u)/[(s - t + u - \eta_1)(s + t - u - \eta_2) \times (s + t + u - \eta_3)(s - t - u - \eta_4)],$$

when integrated over any two of the three variables, is meromorphic in the variable left over. The quantities η_i stand for ϵ or δ, depending on the specific matrix entry considered for the two-particle propagator.

Assuming the conjecture to be correct, we can conclude that Γ is meromorphic in the variable λ. Let us keep two energy variables at some fixed (complex) values and vary the third one, say s. The positions of the singularities in λ, which determine the radius of convergence of the Taylor series (4.1), depend in a genuine nonconstant manner on the distance between the actual value of s and the positions of the poles occurring in σ_n, if this distance is chosen close enough to a pole (otherwise the convergence radius might be determined by the specific choice of the fixed values of t and u, in which case we should continue our reasoning by referring to one of those variables).

In the s plane, in turn, we may view the expansion (4.1) as Laurent expansions around the poles of σ_n by rewriting it in the form

$$\Gamma = \sum_{r=1}^{R} \sum_{n=1}^{\infty} \frac{A_n^{(r)}}{(s - s_r)^n} + C,$$

where s_r, $r = 1,\ldots,R$, are the poles of σ_n nearest to the origin, while C contains all other poles as well as s-independent terms. The radii of convergence inside which the Laurent series diverge, depend on λ; in fact, our conjecture states that, for each r, the singularities on the periphery are poles whose positions depend on λ.

Take now a fixed value s_0 of s in the region of convergence. In the λ plane, we then go, by analytic continuation, on a closed loop around a singularity situated on the periphery of the circle of convergence, so that we arrive at the same λ value. In the s plane, this process has the effect that the actual poles of Γ move around the point s_0, i.e., the situation remains unchanged after the loop is closed. Hence the singularity in the λ plane cannot be a branch point.

Note that this reasoning does not imply that the function which describes the dependence on λ (on s) of the position of the singularity in the s plane (λ plane) has no branch point.

The fact that the expansion (4.1) gives rise to a meromorphic function in λ is an important prerequisite for a successful approximation by rational expressions in λ. Our efforts are directed towards this aim.

Finally we mention that all previous attempts to construct an acceptable vertex function are covered by Eq. (3.3). In the linear model of Ref. 10 only the bracket combinations belonging to the $k = n$ family are taken into account, while Γ^0 and G are replaced by a static term and the unperturbed propagator, respectively. From this the RPA or Galitskii ladder[2] is obtained, if only t or s connections, respectively, are maintained. An important result of the nonlinearity of Eq. (2.3) is that it gives rise to multiphonon propagations. This was discussed in Refs. 4 and 5 in an approximate way and its importance was demonstrated in applications.[11] Again, the contributions dealt within the quoted papers consist only of selective parts of Eq. (3.3), in such a way that crossing symmetry is invalidated. We believe that further advances on all the attempts quoted have to start from an expression such as that given in Eq. (3.3).

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Construction of orthonormal vector sets for atoms and molecules by means of recursive variation

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It is shown using a recursive variation method that the Schmidt orthonormalized vectors are optimal in the sense that the least squared distances are minimized, and that the use of maximal squared overlaps yields a Schmidt canonical orthonormalized vector set which corresponds to the Löwdin canonical vector set. By introducing the Krylov sequence, the method is applied to the derivation of a variational expression for the Lanczos vectors which tridiagonalize any self-adjoint operator. The repeated use of two-step variations is shown to derive a pseudopotential which is useful for the calculations of correlated pair functions.

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I. INTRODUCTION

The classical Schmidt orthonormalization algorithm appears in the literature[1] in such a way that it can necessarily construct an orthonormal vector set from a given set of vectors which are linearly independent. Given nonorthogonal vectors $|\theta_1\rangle$, $|\theta_2\rangle$,···, the Schmidt algorithm yields a recursion formula of the following type for the production of the ith orthonormal vector $|\sigma_i\rangle$ (hereafter called the Schmidt vector):

$$|\sigma_i\rangle = (1 - \sum_{k=1}^{i-1} |\sigma_k\rangle\langle\sigma_k|)|\theta_i\rangle N_i^{-1/2}, \tag{1}$$

$$N_i = \langle\theta_i|(1 - \sum_{k=1}^{i-1} |\sigma_k\rangle\langle\sigma_k|)|\theta_i\rangle, \tag{2}$$

with

$$|\sigma_1\rangle = |\theta_1\rangle N_1^{-1/2}, \quad N_1 = \langle\theta_1|\theta_1\rangle.$$

The alternative orthonormalization algorithm is known as Löwdin's symmetric orthonormalization method,[2] which is expressed as $\boldsymbol{\phi}_s \equiv \boldsymbol{\theta}(\boldsymbol{\theta}^\dagger\boldsymbol{\theta})^{-1/2}$, where $\boldsymbol{\theta}$ denotes a row matrix $\boldsymbol{\theta} \equiv (|\theta_1\rangle|\theta_2\rangle\cdots)$ and $\boldsymbol{\theta}^\dagger$ a column matrix with the elements $\langle\theta_i|$. The method, as can be seen from the form of $\boldsymbol{\phi}_s$, has such an advantage that the vector set $\boldsymbol{\phi}_s$ to be obtained belongs to the same symmetry group as the initial vector set $\boldsymbol{\theta}$ does[3]; that is, it conserves the initial symmetry. In the method, however, a disadvantage appears in such a way that every newly made vector becomes an admixture of all the initial vectors. The Schmidt method, on the other hand, produces recursively the ith vector only from the *previous* vectors, $(i-1)$th, $(i-2)$th,···, while it destroys the natural symmetry properties of the original set. In the present paper, we wish to construct an orthonormal vector set in a recursive manner but in terms of the original vector set by making use of the recursive orthonormality-constrained variation (ONCV) method.[4]

First, we pay attention to Löwdin's successive orthonormalization method[5] in which orthonormal vectors are expressed directly in terms of the original vectors $|\theta_i\rangle$'s. Let the starting set $\{|\theta_1\rangle, |\theta_2\rangle,\cdots,|\theta_{i-1}\rangle\}$ be denoted by a row matrix η_{i-1} and add an extra vector $|\theta_i\rangle$ to it. The ith orthonormal vector is then expressed as $(1 - P_{\eta_{i-1}})|\theta_i\rangle N_i^{-1/2}$, where $P_{\eta_{i-1}}$ is the projection operator and N_i the normalization constant. The algorithm appearing in the successive orthonormalization may thus be regarded as the repeated use of the first two steps of the Schmidt algorithm. In order to obtain such successively orthonormalized vectors in a variational manner, we only have to use the first two steps in our recursive ONCV method[4] repeatedly.[1]

Cook[6] divided the given vectors into two sets, a core set $\boldsymbol{\theta}_c$ and a valence set $\boldsymbol{\theta}_v$, as $\boldsymbol{\theta} \equiv (\boldsymbol{\theta}_c|\boldsymbol{\theta}_v)$, and determined the orthogonal sets $\boldsymbol{\psi}_c = \boldsymbol{\theta}_c$ and $\boldsymbol{\psi}_v = (I - P_c)\boldsymbol{\theta}_v$, where P_c is a projection operator which characterizes the manifold $\boldsymbol{\theta}_c$. The orthogonality of this type is often called "strong orthogonality," the orthogonality between two different groups to which electrons of the system are classified.[7] Application of the symmetric orthonormalization to each of them generates an orthonormal set in which the core set $\boldsymbol{\psi}_c(\boldsymbol{\psi}_c{}^\dagger\boldsymbol{\psi}_c)^{-1/2}$ is not contaminated by the valence set $\boldsymbol{\psi}_v$. It is clear that the essence of this procedure is in the application of the Schmidt method not to vectors but to vector sets. If we divide $\boldsymbol{\theta}$ into $(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2|\cdots)$, where $\boldsymbol{\theta}_1$, for example, denotes a row matrix with the elements $|\theta_{1i}\rangle$'s, then the Schmidt procedure is reformulated, by applying the Löwdin orthonormalization method to vector sets, as

$$\boldsymbol{\sigma}_1 = \boldsymbol{\theta}_1(\boldsymbol{\theta}_1{}^\dagger\boldsymbol{\theta}_1)^{-1/2}, \tag{3}$$

$$\boldsymbol{\sigma}_i = (1 - \sum_{k<i} \boldsymbol{\sigma}_k\boldsymbol{\sigma}_k{}^\dagger)\boldsymbol{\theta}_i\mathbf{N}_i^{-1/2} \quad (i = 2, 3,\cdots), \tag{4}$$

where $\boldsymbol{\theta}_i, \boldsymbol{\sigma}_i$, and $\mathbf{N}_i$ are matrices. Equations (3) and (4) can be expressed in a set form by using a recursive ONCV equation formulated in terms of sets, which leads to an important application since it fulfils the condition of strong orthogonality in the processes of variation.

One feature of the Löwdin symmetric of orthonormalization is known as the resemblance theorem saying that symmetrically orthonormalized vectors $|\phi_{si}\rangle$ resemble the

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original vectors in the sense that they have the least squared distances.[5,8] We show first in the following that a similar optimal property exists in the Schmidt vectors.

II. OPTIMAL PROPERTY OF THE SCHMIDT VECTORS

We recall a method previously called the recursive ONCV.[4] Given an orthonormal set $\rho \equiv (|\rho_1\rangle|\rho_2\rangle\cdots)$, $|\rho_1\rangle$ is first varied into $|\rho_1'\rangle \equiv |\rho_1\rangle + |\delta\rho_1\rangle$ which to first order in $|\delta\rho_1\rangle$ leads to

$$|\bar{\rho}_1\rangle \equiv |\rho_1'\rangle\langle\rho_1'|\rho_1'\rangle^{-1/2}$$
$$= |\rho_1\rangle + |\delta\rho_1\rangle - \tfrac{1}{2}|\rho_1\rangle(\langle\delta\rho_1|\rho_1\rangle + \langle\rho_1|\delta\rho_1\rangle). \quad (5)$$

It is obvious that the variation process $|\rho_1\rangle \to |\bar{\rho}_1\rangle$ maintains the normality. Next, if a normal $|\rho_2\rangle$ is given, then the similar procedure $|\rho_2\rangle \to |\bar{\rho}_2'\rangle$ with

$$|\bar{\rho}_2'\rangle \equiv |\rho_2\rangle + |\delta\rho_2\rangle - \tfrac{1}{2}|\rho_2\rangle(\langle\delta\rho_2|\rho_2\rangle + \langle\rho_2|\delta\rho_2\rangle), \quad (6)$$

also maintains the normality, but in general $|\rho_2'\rangle$ is not orthogonal to $|\rho_1\rangle$. This nonorthogonality has its source in the arbitrariness of $|\delta\rho_2\rangle$. If $|\delta\rho_2\rangle$ is replaced by $(1 - |\rho_1\rangle\langle\rho_1|)|\delta\rho_2\rangle$, then the resulting vector denoted by $|\bar{\rho}_2\rangle$ becomes normal and also orthogonal to $|\rho_1\rangle$ under assumption $\langle\rho_1|\rho_2\rangle = 0$.

Alternatively, the vector $|\bar{\rho}_2\rangle$ can be obtained by the following procedure. First, to make $|\rho_2'\rangle \equiv |\rho_2 + |\delta\rho_2\rangle$ orthogonal to $|\rho_1\rangle$ leads to $(1 - |\rho_1\rangle\langle\rho_1|)|\bar{\rho}_2'\rangle$. Then, by normalization, one obtains

$$(1 - |\rho_1\rangle\langle\rho_1|)|\bar{\rho}_2'\rangle N_2^{-1/2}, \quad (7)$$

with

$$N_2 \equiv \langle\bar{\rho}_2'|(1 - |\rho_1\rangle\langle\rho_1|)|\bar{\rho}_2'\rangle.$$

Note that the process resembles the second step of the Schmidt orthonormalization. Expansion of Eq. (7) in first order yields the vector $|\rho_2\rangle$. In this procedure, the order of the two operations, orthonormalization and normalization, is merely inverted in comparison with the former procedure.

Continuing such recursive processes for a series of the ket-vectors, one arrives at the ith variation:

$$|\rho_1\rangle \to |\bar{\rho}_1\rangle \equiv |\rho_1\rangle + (1 - \sum_{k<i}|\rho_k\rangle\langle\rho_k|)|\delta\rho_i\rangle$$
$$- \tfrac{1}{2}|\rho_i\rangle(\langle\delta\rho_i|\rho_i\rangle + \langle\rho_i|\delta\rho_i\rangle). \quad (8)$$

When the recursive ONCV is applied to the partitioned set (row matrix) $\rho_i, \rho_i \equiv (|\rho_{i1}\rangle|\rho_{i2}\rangle\cdots)$, $\rho \equiv (\rho_1|\rho_2|\cdots)$, the following equation is obtained:

$$\rho_i \to \bar{\rho}_i \equiv \rho_i + (1 - \sum_{k<1}\rho_k\rho_k{}^{\dagger})\delta\rho_i - \tfrac{1}{2}\rho_i(\delta\rho_i{}^{\dagger}\rho_i + \rho_i{}^{\dagger}\delta\rho_i). \quad (9)$$

Here, we feel like adding what follows, which has not been mentioned in our previous paper. In the recursive ONCV, we have seen that

$$\rho_j|\bar{\rho}_i\rangle = 0,$$

and

$$\langle\bar{\rho}_j|\bar{\rho}_i\rangle = \langle\delta\rho_j|\rho_i\rangle \neq 0, \quad (10)$$

for $j < i$, retaining up to first order. We still can work out to derive varied vectors $\tilde{\rho}$ normalized and orthogonalized to each other. Substitution of $(1 - \Sigma_{k<i}|\rho_k\rangle\langle\delta\rho_k|)|\rho_i\rangle$ for the first term $|\rho_i\rangle$ of Eq. (8) yields

$$|\tilde{\rho}_i\rangle \equiv \Big(1 - \sum_{k<i}|\rho_k\rangle\langle\delta\rho_k|\Big)|\rho_i\rangle$$
$$+ (1 - \sum_{k<i}|\rho_k\rangle\langle\rho_k|)|\delta\rho_i\rangle$$
$$- \tfrac{1}{2}|\rho_i\rangle(\langle\delta\rho_i|\rho_i\rangle + \langle\rho_i|\delta\rho_i\rangle)$$
$$= |\rho_i\rangle + |\delta\rho_i\rangle - \tfrac{1}{2}|\rho_i\rangle(\langle\delta\rho_i|\rho_i\rangle + \langle\rho_i|\delta\rho_i\rangle)$$
$$- \sum_{k<i}|\rho_k\rangle(\langle\delta\rho_k|\rho_i\rangle + \langle\rho_k|\delta\rho_i\rangle). \quad (11)$$

and direct calculation gives $\langle\tilde{\rho}_j|\tilde{\rho}_i\rangle = 0$ and $\langle\rho_j|\tilde{\rho}_i\rangle = -\langle\delta\rho_j|\rho_i\rangle \neq 0$, for $j < i$. This procedure is identical with the application of the Schmidt algorithm to a set $\{|\rho_i\rangle + |\delta\rho_i\rangle \equiv |\rho_i'\rangle\}$. Since $|\tilde{\rho}_i\rangle$ contains all lower order variation vectors $|\delta\rho_k\rangle$, $k < i$, characterization of eigenvalues by use of $|\tilde{\rho}_i\rangle$ will be less easy than that by use of $|\bar{\rho}_i\rangle$.

We now apply the recursive ONCV method to the measure, squared distances $\omega_{di} \equiv \||\rho_i\rangle - |\theta_i\rangle\|^2$:

$$\delta'\omega_{di} \equiv \||\bar{\rho}_i\rangle - |\theta_i\rangle\|^2 - \||\rho_i\rangle - |\theta_i\rangle\|^2$$
$$= \langle\delta\rho_i|\{-|\theta_i\rangle + \tfrac{1}{2}|\rho_i\rangle(\langle\rho_i|\theta_i\rangle + \langle\theta_i|\rho_i\rangle)$$
$$+ \sum_{k<i}|\rho_k\rangle\langle\rho_k|\theta_i\rangle\} + \text{h.c.} \quad (12)$$

The notation δ' is used to distinguish it from the arbitrary variation δ. It follows from $\delta'\omega_{di} = 0$ that

$$|\theta_i\rangle = \tfrac{1}{2}|\rho_i\rangle(\langle\rho_i|\theta_i\rangle + \langle\theta_i|\rho_i\rangle) + \sum_{k<i}|\rho_k\rangle\langle\rho_k|\theta_i\rangle, \quad (13)$$

since $|\delta\rho_i\rangle$ is an arbitrary vector. It is easily verified that solutions of Eq. (13) on the manifold θ are just the Schmidt vectors $|\sigma_i\rangle$. Note that solutions of Eq. (13) guarantee normality by the first term and orthogonality by the second term of Eq. (13). In a similar manner, we can derive equations for vector sets:

$$\theta_i = \tfrac{1}{2}\rho_i(\rho_i{}^{\dagger}\theta_i + \theta_i{}^{\dagger}\rho_i) + \sum_{k<i}\rho_k\rho_k{}^{\dagger}\theta_i. \quad (14)$$

It is thus safely said that the Schmidt vectors are optimal in the sense that the squared distances are minimized and that the equations $\delta'\omega_{di} \to 0$ are the variation equations needed for the Schmidt vector construction. As mentioned above, the Löwdin vectors ϕ_s are also optimal so as to fit the initial vectors as closely as possible in the sense of squared distances. It is to be noted that the former is constructed recursively and the latter symmetrically.

Heretofore, we have discussed distances between two vectors as a measure. Next, we will investigate properties of the Schmidt vector, taking overlaps as a measure. The Löwdin canonical vectors[9] $\phi_c \equiv \phi_s U = \theta U D^{-1/2}$, where U is a unitary matrix which diagonalized the matrix $\theta^{\dagger}\theta$, that is $(\theta^{\dagger}\theta)U = UD$, are eigenvectors for the operator $\theta\theta^{\dagger} \equiv \Sigma|\theta_i\rangle\langle\theta_i|$.[5] This is understood from a variational point of view that ϕ_c is optimal in the sense that the squared overlaps are miximized. That is, $\delta'\omega_c = 0$ for the measure

$$\omega_l(\text{optimized}) \equiv \sum_{i,j}|\langle\phi_{ci}|\theta_j\rangle|^2 = \text{tr}(\phi_c{}^{\dagger}\theta\theta^{\dagger}\phi_c). \quad (15)$$

More generally speaking, $\phi_s V$ is a solution to the variation equation $\delta'\omega_c = 0$ provided that V is an arbitrary unitary

matrix; ϕ_c is a specific solution which diagonalizes the operator $\theta\theta^\dagger$.

A similar relation can be obtained for the Schmidt vector set $\{|\sigma_i\rangle\}$. Application of the recursive ONCV, $\rho_i \to \bar{\rho}_i$, to the measure of overlapping

$$\omega_{ci} \equiv |\langle\rho_i|\theta_i\rangle|^2 = \langle\rho_i|\theta_i\rangle\langle\theta_i|\rho_i\rangle, \tag{16}$$

yields

$$\delta'\omega_{ci} = \langle\delta\rho_i|\{(1 - \sum_{k<i}|\rho_k\rangle\langle\rho_k|)|\theta_i\rangle\langle\theta_i|\rho_i\rangle - |\rho_i\rangle\langle\rho_i|\theta_i\rangle\langle\theta_i|\rho_i\rangle\}, \tag{17}$$

which gives an equation for the unknown vector $|\rho_i\rangle$:

$$(1 - \sum_{k<i}|\rho_k\rangle\langle\rho_k|)|\theta_i\rangle\langle\theta_i|\rho_i\rangle = |\rho_i\rangle\langle\rho_i|\theta_i\rangle\langle\theta_i|\rho_i\rangle. \tag{18}$$

A solution to this equation is just the Schmidt vector $|\sigma_i\rangle$. Hence, we can say that the Schmidt vectors are optimized in the sense of maximum overlapping. The variation equation $\delta'\omega_{ci} \to 0$ has unitary invariance among $|\rho_k\rangle$'s, so that the matrix representation of the operator $|\theta_i\rangle\langle\theta_i|$ with respect to $|\rho_k\rangle$'s can be diagonalized by using the freedom of unitary transformation. The vector set $\{|\sigma_i\rangle\}$ thus obtained may be called the Schmidt canonical vectors.

III. APPLICATIONS

A. Variational equation for Lanczos vectors

As a simple example of application of the recursive ONCV equation to construction of orthonormal vectors, we consider the Lanczos algorithm.[10] The algorithm produces a vector set, hereafter called the Lanczos vectors, which tridiagonalizes any self-adjoint operator H given. It is then very useful for practical calculations in quantum mechanical problems,[11,12] since one can easily obtain a diagonalized form from the tridiagonal H.

We introduce the Krylov sequence[13] with respect to $|\theta_i\rangle$'s into Eq. (12); that is, the ith vector is constructed from the $(i-1)$th vector by operating H on it. It follows from the recursive structure of the Schmidt orthonormalization that only the two terms of $\langle\rho_k|H|\rho_i\rangle$ $(k = 1, 2, \cdots < i)$ in Eq. (12) remain; $H|\rho_k\rangle$ is expressed as linear combinations of the vectors which are lower in order than the $(k+1)$th vector inclusive.

Then we have

$$\delta'\omega_{di} = \langle\delta\rho_i|\{-H|\rho_{i-1}\rangle + \tfrac{1}{2}|\rho_i\rangle(\langle\rho_i|H|\rho_{i-1}\rangle + \langle\rho_{i-1}|H|\rho_i\rangle) + |\rho_{i-1}\rangle\langle\rho_{i-1}|H|\rho_{i-1}\rangle + |\rho_{i-2}\rangle\langle\rho_{i-2}|H|\rho_{i-1}\rangle\} + \text{h.c.} \tag{19}$$

The solutions $|\lambda_i\rangle$ for the equations $\delta'\omega_{di} \to 0$ are given by the recursion formula

$$H|\lambda_{i-1}\rangle = (|\lambda_{i-2}\rangle\langle\lambda_{i-2}| + |\lambda_{i-1}\rangle\langle\lambda_{i-1}|)H|\lambda_{i-1}\rangle + |\lambda_i\rangle N_i^{-1/2}, \tag{20}$$

N_i being a normalization factor. Equation (20) is a usually used form for the Lanczos algorithm[11-13], and $|\lambda_i\rangle$'s are just the Lanczos vectors. Note that the second term in Eq. (19) represents the normalization. Solving $|\lambda_i\rangle$ from Eq. (20), one has

$$|\lambda_i\rangle = (1 - |\lambda_{i-1}\rangle\langle\lambda_{i-1}| - |\lambda_{i-2}\rangle\langle\lambda_{i-2}|)H|\lambda_{i-1}\rangle N_i^{1/2}, \tag{21}$$

which is a recursion formula for $|\lambda_i\rangle$'s. It is easily understood that the whole procedure gives rise to a tridiagonalized representation for H.

The method described above leads to a procedure to generate orthonormal functions, for example, the Legendre, Laguerre, and Hermite functions which are well-known in classical mechanics (refer to Ref. 13). To give an instance, if e^{-x} be choosen as a weighting function and $\langle\lambda_0|\lambda_0\rangle = \int_0^\infty \lambda_0^2 e^{-x} dx$ as an inner product, then the set $\{|\lambda_i\rangle\}$ becomes a function system of Laguerre type. We can adopt various optimization methods[14] to solve the variational equations $\delta'\omega_{di} \to 0$ and construct the Lanczos vectors, so that the formulations mentioned above are quite useful in actual applications to quantum mechanical problems.

B. Repeated use of two-step variations

One can consider a modified algorithm in which the first two steps of the Lanczos algorithm are used repeatedly.[15] This procedure can be easily rewritten as two-step variation equations for two sets by means of the recursive ONCV in a manner similar to that mentioned above. The resulting variation equations have the same properties as the modified algorithm has; each iteration yields 2×2 matrices so as to save spaces for computer storage andto avoid manipulation for orthogonalization to the vectors derived in the earlier steps, and only one vector corresponding to the lowest eigenvalue is derived. Once a vector having lowest eigenvalue is obtained, setting a new starting vector so as not to involve the first vector as a component, one obtains the second eigenvalue and eigenvector by the repeated use of the same algorithm. In this manner, the third, fourth,···, eigenvalues and eigenvectors can be found.

Next, we consider a case when the orthogonality between the known set ρ_1 and the set to be obtained plays an important part. The problem to be solved is as in the following[16]:

$$\omega_2 \equiv \text{tr}(\zeta^\dagger H \zeta) \to \text{minimum}, \qquad \rho_1{}^\dagger\zeta = 0, \quad \zeta^\dagger\zeta = \mathbf{I}, \text{ as constraints.} \tag{22}$$

Here, the sets (row matrices) ρ_1 and ζ may be replaced by two ket vectors $|\rho_1\rangle$ and $|\zeta\rangle$. The problem mentioned above is reworded in such a way that given ρ_1, optimize ω_2 under the two constraints with ζ as a set of valuable functions (vectors). When ρ_1 is a core orbital set and ζ an assembly of correlated pair functions (two-electron functions) of valence electrons, the orthogonality condition $\rho_1{}^\dagger\zeta = 0$ is just what is called the strong orthogonality.[7] Evidently, therefore, the second step $\rho_2 \to \bar{\rho}_2$ of the recursive ONCV method,

$$\bar{\rho}_2 \equiv \rho_2 + (1 - \rho_1\rho_1{}^\dagger)\delta\rho_2 - \tfrac{1}{2}\rho_2(\delta\rho_2{}^\dagger\rho_2 + \rho_2{}^\dagger\delta\rho_2), \tag{23}$$

can be used as ζ and applied to the above variational problem. A variational process in which ρ_1 is known and ρ_2 is varied to $\bar{\rho}_2$ has been suggested before,[17] and its practical formulation is quite the same as that applied to a many-shell model.[18] The only difference is that the latter is applied to a

specific shell which one must consider, while the present recursive ONCV method is to be applied to each vector and/or set one after another.

In the variational process $\rho_2 \to \bar{\rho}_2$, however, we have assumed that the initial set ρ_2 is orthogonal to ρ_1 in order to obtain the result $\rho_1^\dagger \bar{\rho}_2 = 0$. Starting from nonorthogonal ρ_1 and ρ_2, a similar variational treatment will become troublesome. On the contrary, we improve the process $\rho_2 \to \bar{\rho}_2$ in such a way as in the following, in order to derive a variational equation in which the given ρ_1 and an arbitrary set (or vector) are involved. Let an arbitrary set (or vector) be η, then $(1 - \rho_1\rho_1^\dagger)\eta \equiv \psi$ turns out to be always orthogonal to ρ_1. Adopting the Löwdin symmetric orthonormalization,[12] we orthonormalize ψ and let it be ρ_2: $\psi(\psi^\dagger\psi)^{-1/2} \equiv \rho_2$. Assuming η receives a variation $\delta\eta$, $\eta \to \eta + \delta\eta \equiv \psi'$, we expand $\psi'(\psi'^\dagger\psi')^{-1/2} \equiv \hat{\rho}_2$ to first order:

$$\hat{\rho}_2 \equiv \psi(\psi^\dagger\psi)^{-1/2} + \delta\psi(\psi^\dagger\psi)^{-1/2} - \tfrac{1}{2}\psi(\psi^\dagger\psi)^{-1} \times (\delta\psi^\dagger\psi + \psi^\dagger\delta\psi)(\psi^\dagger\psi)^{-1/2}. \tag{24}$$

Replacing ψ with $(1 - \rho_1\rho_1^\dagger)\eta$ in Eq. (24), we obtain another form of the recursive ONCV for arbitrary η in which only the first two steps are taken into account. Since the relations $\rho_1^\dagger\rho_2 = 0$ and $\rho_2^\dagger\rho_2 = 1$ evidently hold, $\hat{\rho}_2$ as a function of η can be used for the minimization of ω_2 in Eq. (22).

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Comments on "Higher order modified potentials for the effective phase integral approximation"

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It is pointed out that the comparison made in the paper by Floyd, "Higher order modified potentials for the effective phase integral approximation," between the expansions introduced by Floyd and by the present authors, respectively, is inadequate as a test of the relative merits of the two expansions. In his comparison Floyd used our *unmodified* phase-integral approximations, but for the case considered one should instead use our consistently *modified* phase-integral approximations. The numerical results then obtained are in the present note compared with the numerical results obtained from the expansion derived by Floyd.

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In the method developed by the present authors (see Refs. 1–4 and pp. 126–131 in Ref. 5), a kind of arbitrary-order phase-integral approximations are used which were first derived and examined in unmodified form,[2,3] but were later consistently modified in arbitrary order, both by a direct method[4] and by a transformation method (see pp. 126–131 in Ref. 5). The possibility of this consistent modification grants our method an important feature of generality and flexibility. However, Floyd[6] refers only to the early paper where the unmodified approximations were derived,[2] and disregards the consistently modified approximations, the use of which is sometimes essential for the efficiency of the method in question. Thus, Floyd's comparison in Sec. III of Ref. 6 is inadequate as a test, for the model and the parameter values chosen, of the effectiveness of his expansion compared to ours.

Using our phase-integral approximations of the arbitrary order $2N+1$ in the application treated by Floyd,[6] one obtains the equation

$$\int_0^{\pi} \sum_{n=0}^{N} Y_{2n} Q_{\mathrm{mod}}(x)dx = \nu\pi, \quad |\nu| \neq 1,2,3,\cdots, \tag{1}$$

where $Q_{\mathrm{mod}}(x)$, entering also into the expressions for Y_{2n}, is a so far unspecified function, which shall be chosen conveniently. The first few functions Y_{2n} are

$$Y_0 = 1, \tag{2a}$$

$$Y_2 = \tfrac{1}{2}\left\{\frac{Q^2 - Q_{\mathrm{mod}}^2}{Q_{\mathrm{mod}}^2} + \frac{1}{16Q_{\mathrm{mod}}^6} \times\left[5\left(\frac{dQ_{\mathrm{mod}}^2}{dx}\right)^2 - 4Q_{\mathrm{mod}}^2\frac{d^2Q_{\mathrm{mod}}^2}{dx^2}\right]\right\}, \tag{2b}$$

$$Y_4 = -\tfrac{1}{2}Y_2^2 - \frac{1}{4Q_{\mathrm{mod}}}\frac{d}{dx}\left(\frac{1}{Q_{\mathrm{mod}}}\frac{dY_2}{dx}\right). \tag{2c}$$

Floyd's use of our unmodified approximations means that the expressions for Y_0, Y_2, and Y_4 in his Sec. III correspond to the above formulas (2a), (2b) and (2c), respectively, with

$$Q_{\mathrm{mod}}(x) = Q(x) = [\alpha - 2\gamma\cos(2x)]^{1/2}. \tag{3}$$

This is, however, not a reasonable choice, if one wants to compare the relative effectiveness of our phase-integral approximations and of Floyd's truncated expansion for yielding improved results when one proceeds to higher orders of approximation. For the values of γ considered, it is convenient to choose [cf. Floyd's Eq. (5a)]

$$Q_{\mathrm{mod}}(x) = (\alpha - W_0)^{1/2} = \left(\alpha - \frac{2\gamma\cos(2x)}{1 - 1/\alpha}\right)^{1/2}, \tag{4}$$

TABLE I.

γ	ν	N or exact	α Fröman–Fröman (unmodified)	Fröman–Fröman (modified)	Floyd
		0	0.095	0.0900	0.0900
		1	0.13	0.0895 0551	0.0895 0548
		2	0.19	0.0895 4	0.0895 061
		3	0.27	0.091	0.0895 0555 853
0.03	0.3	4	0.35	0.12	
		5	0.45	0.23	
		6	0.56		
		exact	0.0895	0.0895 0556	0.0895 0555 848
		0	12.291	12.298	12.298
		1	12.2943	12.2946 1	12.2947 5
		2	12.2945 9	12.2946 23	12.2948 0
		3	12.2946 23	12.2946 28	12.2946 6
1.0	3.5	4	12.2946 29	12.2946 305	
		5	12.2946 3094	12.2946 317	
		6	12.2946 3196	12.2946 325	
		exact	12.2946 32	12.2946 32	12.2946 32
		0	20.2747	20.2773	20.2773
		1	20.2759 4	20.2760 022	20.2760 14
		2	20.2760 00	20.2760 0312	20.2760 18
		3	20.2760 031	20.2760 0331	20.2760 0363
1.0	4.5	4	20.2760 0333	20.2760 0335 6	
		5	20.2760 0336 1	20.2760 0336 6	
		6	20.2760 0336 7	20.2760 0336 9	
		exact	20.2760 0336	20.2760 0336	20.2760 0336
		0	30.2665	30.2677	30.2677
		1	30.2670 8	30.2671 0142	30.2671 033
		2	30.2671 009	30.2671 0154 0	30.2671 040
		3	30.2671 0153	30.2671 0155 6	30.2671 0157
1.0	5.5	4	30.2671 0155 68	30.2671 0155 80	
		5	30.2671 0155 821	30.2671 0155 832	
		6	30.2671 0155 835	30.2671 0155 836	
		exact	30.2671 0156	30.2671 0156	30.2671 0156

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TABLE II.

γ	ν	N	$\alpha_{\text{exact}} - \alpha_{\text{approx}}$ Fröman–Fröman (unmodified)	Fröman–Fröman (modified)	Floyd
		0	$-6\cdot10^{-3}$	$-5\cdot10^{-4}$	$-5\cdot10^{-4}$
		1	$-4\cdot10^{-2}$	$5\cdot10^{-8}$	$7\cdot10^{-8}$
0.03	0.3	2	$-1\cdot10^{-1}$	$-3\cdot10^{-5}$	$-5\cdot10^{-7}$
		3	$-2\cdot10^{-1}$	$-2\cdot10^{-3}$	$-5\cdot10^{-11}$
		0	$4\cdot10^{-3}$	$-4\cdot10^{-3}$	$-4\cdot10^{-3}$
		1	$3\cdot10^{-4}$	$2\cdot10^{-5}$	-1.10^{-4}
1.0	3.5	2	$4\cdot10^{-5}$	$9\cdot10^{-6}$	$-2\cdot10^{-4}$
		3	$9\cdot10^{-6}$	$4\cdot10^{-6}$	$-3\cdot10^{-5}$
		0	$1\cdot10^{-3}$	$-1\cdot10^{-3}$	$-1\cdot10^{-3}$
		1	$7\cdot10^{-5}$	$1\cdot10^{-6}$	$-1\cdot10^{-5}$
1.0	4.5	2	$4\cdot10^{-6}$	$2\cdot10^{-7}$	$-1\cdot10^{-5}$
		3	$3\cdot10^{-7}$	$5\cdot10^{-8}$	$-3\cdot10^{-7}$
		0	$6\cdot10^{-4}$	$-6\cdot10^{-4}$	$-6\cdot10^{-4}$
		1	$2\cdot10^{-5}$	$1\cdot10^{-7}$	$-2\cdot10^{-6}$
1.0	5.5	2	$7\cdot10^{-7}$	$2\cdot10^{-8}$	$-2\cdot10^{-6}$
		3	$3\cdot10^{-8}$	$\lesssim 1\cdot10^{-8}$	$-1\cdot10^{-8}$

so that the two kinds of approximations agree in the lowest order ($N = 0$). When our arbitrary-order phase-integral approximations are used in this way, they do not have the same restriction to short wavelengths as the JWKB approximation.

In our Table I, the numerical results displayed in the columns headed *Fröman–Fröman (unmodified)* and *Fröman–Fröman (modified)* have been obtained from (1) with $Q_{\text{mod}}(x)$ chosen according to (3) and (4), respectively. In the column headed *Floyd* we quote from Table I in Ref. 6 the results obtained by Floyd by means of his truncated series. In our Table II we compare the errors $\alpha_{\text{exact}} - \alpha_{\text{approx}}$ of the results obtained in the three ways mentioned above.

The parameter λ is introduced in quite different ways in the arbitrary order phase-integral approximations derived by the present authors and in the truncated series derived by Floyd. Our approximations are expected to be more general and more flexible than Floyd's, not only because of the non-perturbative way in which the parameter λ is introduced and the possibility of adapting the choice of the function $Q_{\text{mod}}(x)$ to the particular problem under consideration, but also because the application of our method is not restricted to situations in which there are no generalized classical turning points, i.e., zeros of $Q^2_{\text{mod}}(x)$. See, for instance, a paper by N. Fröman[7] on a periodic potential, with an application to the Mathieu equation. However, in particular cases of a sufficiently weak potential (i.e., when γ is sufficiently small) and when no zeros of $Q^2_{\text{mod}}(x)$ are encountered, Floyd's truncated series should give more accurate results than our phase-integral approximations. See the results for $\gamma = 0.03$ in our Tables I and II.

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Two-sided Padé approximations for the plasma dispersion function

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Two-sided Padé approximations are determined for the plasma dispersion function. An exact closed form solution is given. The convergence problem is considered with regard to the real axis. Some applications from the theory of charged particle beams are also given

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1. INTRODUCTION

Recently, analytic approximations to the plasma dispersion function have received much interest, both for their application in numerical analysis, and for dispersion equations for linear wave motion in a plasma, see Refs. 1–4. The function is defined by the integral

$$\mathscr{Z}(s)=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{e^{-t^2}}{t-s}\,dt,\quad \mathrm{Im}s>0,$$

or equivalently by the formula

$$\mathscr{Z}(s)=(i\sqrt{\pi})e^{-s^2}-2e^{-s^2}\int_0^s e^{u^2}\,du.$$

In this paper we consider the function

$$f(t)=s^{-1}e^{-s^2}\int_0^s e^{u^2}du,\quad t=s^2.$$

We determine two-sided Padé approximations, namely the rationals

$$R_k(t)=\frac{p_0+p_1t+\cdots+p_{k-1}t^{k-1}}{1+q_1t+\cdots+q_kt^k}$$

for which the terms of the series of the function and rationals agree near $t=0$ and $t=\infty$ for as many terms as possible.

The paper is arranged as follows. In Sec. 2 we give explicit representations for $R_k(t)$ and state some precise results on their convergence. We shall show here that the approximations have geometric convergence rates like $1/3^k$. The proofs are in Sec. 3. Some applications of the results are given in Sec. 4.

2. STATEMENTS OF NEW RESULTS

For a function $g(t)$ which has the representations

$$g(t)\sim\sum_{i=0}^{\infty}a_it^i,\quad t\to 0,\tag{1}$$

$$g(t)\sim\sum_{i=0}^{\infty}b_it^{-i-1},\quad t\to\infty,\tag{2}$$

the rationals $R_k(t)$ can be defined as

$$R_k(t)=\frac{P_k(t)}{Q_k(t)}\tag{3}$$

for which the following two equations are valid, viz.

$$g(t)-R_k(t)=O(t^k),\quad t\to 0,\tag{4}$$

and

$$g(t)-R_k(t)=O(t^{-k-1}),\quad t\to\infty.\tag{5}$$

Rationals satisfying both previous conditions are usually called two-sided Padé approximations.

This concept can be generalized by replacing these conditions by the more general ones, viz.,

$$g(t)-R_k^{(m)}(t)=O(t^{k+m}),\quad t\to 0,\tag{6}$$

$$g(t)-R_k^{(m)}(t)=O(t^{-k+m-1}),\quad t\to\infty,\tag{7}$$

where m is an integer. The reason for this is obvious, we take $k+m$ terms from the series near $t=0$ and $k-m$ terms from the series near $t=\infty$, respectively.

We shall see that there exists an optimal choice of the parameter m.

Next, consider the function $f(t)$; it is well known that

$$f(t)\sim\sum_{i=0}^{\infty}\frac{(-t)^i}{(\frac{3}{2})_i},\quad t\to 0,\tag{8}$$

$$f(t)\sim\tfrac{1}{2}\sum_{i=0}^{\infty}(\tfrac{1}{2})_it^{-i-1},\quad t\to\infty.\tag{9}$$

Hear $(a)_i=a(a+1)\cdots(a+i-1)$, $(a)_0=1$ is Pochhammer's symbol. From conditions (4) and (5) we can get two $2k$ linear equations for $2k$ unknowns: $p_0,p_1,\cdots,p_{k-1},q_1,q_2,\cdots,q_k$;

$$\sum_{j=0}^{l}\frac{(-1)^j}{(\frac{3}{2})_j}q_{l-j}=p_l,\quad l=0,1,2,\cdots,k-1,\tag{10}$$

$$\sum_{j=0}^{k}q_j\frac{(-1)^{i-j}}{(\frac{3}{2})_{i-j}}=0,\quad i=k,k+1,\cdots,k+m-1,\tag{11}$$

$$\tfrac{1}{2}\sum_{j=0}^{i}(\tfrac{1}{2})_{i-j}q_{k-j}=p_{k-1-i},\quad i=0,1,2,\cdots,k-m-1.\tag{12}$$

First, taking the usual case of $m=0$, we state the results

$$f(t)-R_k(t)=S_k(t)/Q_k(t),\tag{13}$$

$$Q_k(t)={}_1\mathscr{F}_1(-k;\tfrac{1}{2}-k;t),\tag{14}$$

$$S_k(t)=\frac{k!t^k}{(\frac{1}{2})_k(\frac{3}{2})_k}{}_1\mathscr{F}_1(k+1;k+\tfrac{3}{2};-t),\tag{15}$$

where ${}_1\mathscr{F}_1$ is the symbol of the confluent hypergeometric function. Functions $P_k(t)$ and $Q_k(t)$ both satisfy the recur-

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sion relations

$$(k^2-\tfrac{1}{4})y_{k+1}=(k-\tfrac{1}{2})(k+\tfrac{1}{2}+t)y_k-kty_{k-1},\quad k=1,2,\cdots, \tag{16}$$

with the initial conditions

$$y_0=\begin{cases}0 & P_k\\ \text{for} & ,\\ 1 & Q_k\end{cases},\quad y_1=\begin{cases}1 & P_k\\ \text{for} & ,\\ 1+2t & Q_k\end{cases} \tag{17}$$

Combining these representations we get a more economic formula for numerical computation:

$$f(t)-\frac{P_k(t)}{Q_k(t)}=\sum_{j=k}^{\infty}\frac{j!}{(\frac{1}{2})_j(\frac{3}{2})_j}\frac{t^j}{Q_j(t)Q_{j+1}(t)}, \tag{18}$$

especially for $k=0$

$$f(t)=\sum_{j=0}^{\infty}\frac{j!}{(\frac{1}{2})_j(\frac{3}{2})_j}\frac{t^j}{Q_j(t)Q_{j+1}(t)}. \tag{19}$$

The first few rationals are as follows:

$$R_1(t)=\frac{1}{1+2t},$$
$$R_2(t)=\frac{3+2t}{3+4t+4t^2},$$
$$R_3(t)=\frac{15+8t+4t^2}{15+18t+12t^2+8t^3}. \tag{20}$$

It is interesting to note that many years ago Wynn published the continued fraction representation[5]

$$f(t)=\cfrac{1}{1+2t-\cfrac{4t^2}{3+2t-\cfrac{8t^2}{5+2t-\cdots}}} \tag{21}$$

which has convergents exactly the same as $R_k(t)$.

Next, we state our result on the geometric convergence of the rationals $R_k(t)$.

Theorem 1: For all $t\geqslant 0$ the rationals $R_k(t)$ converge to $f(t)$ in the order

$$f(t)-R_k(t)=O\left(\frac{k^{\frac{1}{2}}}{2^k}\right),\quad k\to\infty. \tag{22}$$

It should be noted that the convergence for small and large (not moderate) arguments is higher than the geometric one.

TABLE I. The maximal errors E_k in the two-sided Padé approximation and $\mu_k=E_k/E_{k+1}$.

k	E_k	μ_k
1	0.2270(−0)	
2	0.8373(−1)	2.712
3	0.3468(−1)	2.413
4	0.1519(−1)	2.283
5	0.6876(−2)	2.209
6	0.3177(−2)	2.164
7	0.1489(−2)	2.134
8	0.7048(−3)	2.112
9	0.3360(−3)	2.098
10	0.1612(−3)	2.084
11	0.7767(−4)	2.075
12	0.3755(−4)	2.068

TABLE II. The maximal errors $E_k^{(m)}$ in the generalized two-sided Padé approximation.

k	m	$E_k^{(m)}$	$\{E_k^{(m)}/E_{k+3}^{(m+1)}\}^{1/3}$
3	1	0.9821(−2)	
6	2	0.2567(−3)	3.37
9	3	0.7713(−5)	3.22
12	4	0.2455(−6)	3.15

Corollary 1: Let us define the maximal error by E_k

$$E_k=\max_{0\leqslant t\leqslant\infty}|f(t)-R_k(t)|, \tag{23}$$

then

$$\lim_{k\to\infty}\{E_k\}^{1/k}=\tfrac{1}{2}. \tag{24}$$

To illustrate the results of Theorem 1 and Corollary 1 with numerical experiments, we give in Table I the computed value of the maximal error E_k and the quantities $\mu_k=E_k/E_{k+1}$.

Returning to the general case $m\neq 0$ we obtained the following results:

$$f(t)-R_k^{(m)}(t)=S_k^{(m)}(t)/Q_k^{(m)}(t), \tag{25}$$

$$Q_k^{(m)}(t)={}_1\mathcal{F}_1(-k;\tfrac{1}{2}-k-m;t), \tag{26}$$

$$S_k^{(m)}(t)=(-1)^m\frac{\Gamma(\frac{3}{2})\Gamma(m+\frac{1}{2})k!\,t^{k+m}}{\Gamma(k+m+\frac{1}{2})\Gamma(k+m+\frac{3}{2})}\,{}_1\mathcal{F}_1(k+1;k+m+\tfrac{3}{2};-t), \tag{27}$$

$$f(t)-R_k^{(m)}(t)=(-1)^m\Gamma(\tfrac{3}{2})\Gamma(m+\tfrac{1}{2})\times\sum_{j=k}^{\infty}\frac{j!t^{j+m}}{\Gamma(j+m+\frac{1}{2})\Gamma(j+m+\frac{3}{2})}\frac{1}{Q_j^{(m)}(t)Q_{j+1}^{(m)}(t)}. \tag{28}$$

Next, we define the quantities

$$E_k^{(m)}=\max_{0\leqslant t\leqslant\infty}\left|f(t)-\frac{P_k^{(m)}(t)}{Q_k^{(m)}(t)}\right|, \tag{29}$$

$$\varphi(\beta)=\beta^{\beta}(1-\beta)^{1-\beta}2^{\beta-1},\quad 0\leqslant\beta\leqslant 1. \tag{30}$$

Our main result is

Theorem 2: If $\lim_{k\to\infty} m/k=\beta$, $0\leqslant\beta\leqslant 1$, then

$$\lim_{k\to\infty}\{E_k^{(m)}\}^{1/k}=\varphi(\beta). \tag{31}$$

Investigating the function $\varphi(\beta)$, we get

Corollary 2:

$$\lim_{k\to\infty}\{E_k^{(m)}\}^{1/k}\geqslant\tfrac{1}{3}.$$

It means that if $m=[k/3]$, we get the best convergence rate of the two-sided Padé approximations to the function $f(t)$ for $k\to\infty$.

Some numerical experiments are made to show the power of Theorem 2. We give in Table II the values $E_k^{(m)}$.

3. PROOF OF NEW RESULTS

We shall consider the general case only. In proving Theorem 2 we must first establish (26) and (27). From Eqs.

(10)–(12) we select a system of linear equations for the unknowns $q_1, q_2, \cdots, q_k$

$$\sum_{j=0}^{l} \frac{(-1)^j}{(\frac{3}{2})_j} q_{l-j} = \frac{1}{2} \sum_{j=0}^{k-1-l} (\tfrac{1}{2})_{k-1-l-j} q_{k-j},$$

$l = m, m+1, \cdots, k-1,$

$$\sum_{j=0}^{k} q_j \frac{(-1)^{i-j}}{(\frac{3}{2})_{i-j}} = 0, \quad i = k, k+1, \cdots, k+m-1.$$

This, in a more simple form, is

$$\sum_{j=0}^{k} q_j \frac{(-1)^{l-j}}{(\frac{3}{2})_{l-j}} = 0, \quad l = m, m+1, \cdots, k+m-1.$$

From this, with elementary transformations, we are able to get the system

$$\sum_{j=0}^{k} (j+1)_l \Gamma(j-k-m+\tfrac{1}{2}) q_j = 0, \quad l = 0,1,\cdots,k-1.$$

Next, by the orthogonal polynomial method, we solve this system

$$\int_0^\infty u^l e^{-u} \sum_{j=0}^{k} q_j u^j \frac{\Gamma(j-k-m+\frac{1}{2})}{j!} du = 0,$$

$l = 0,1,\cdots,k-1,$

$$\sum_{j=0}^{k} q_j u^j \frac{\Gamma(j-k-m+\frac{1}{2})}{j!} = C \cdot e^u \frac{d^k}{du^k}(u^k e^{-u}),$$

$$q_j = \frac{(-k)_j}{j!(\frac{1}{2}-k-m)_j}.$$

Equation (26) is now proved. To obtain $S_k^{(m)}(t)$, we must compute

$$S_k^{(m)}(t) = \sum_{j=k+m}^{\infty} t^j \sum_{l=0}^{k} q_l \frac{(-1)^{j-l}}{(\frac{3}{2})_{j-l}}.$$

After some transformations we get

$$S_k^{(m)}(t) = \frac{(-t)^{k+m}}{(\frac{1}{2}-k-m)_k} \sum_{j=0}^{\infty} (-t)^j \frac{\Gamma(\frac{3}{2})}{\Gamma(j+m+\frac{3}{2})} \times \sum_{l=0}^{k} \frac{(-k)_l (m+\frac{1}{2})_l}{l!(j+m+\frac{3}{2})_l}$$

$$= (-1)^m \frac{\Gamma(\frac{3}{2})\Gamma(m+\frac{1}{2}) k!\, t^{k+m}}{\Gamma(k+m+\frac{1}{2})\Gamma(k+m+\frac{3}{2})} \times \sum_{j=0}^{\infty} \frac{(-t)^j}{j!} \frac{(k+1)_j}{(k+m+\frac{3}{2})_j}.$$

This is (27) exactly. Next we prove (28). From the theory of hypergeometric functions it follows that functions $Q_k^{(m)}(t)$ and $S_k^{(m)}(t)$ both satisfy the recursion relations

$$[(k+m)^2 - \tfrac{1}{4}] y_{k+1} = (k+m+\tfrac{1}{2}+t)(k+m-\tfrac{1}{2}) y_k - k t y_{k-1}, \quad k = m, m+1, \cdots.$$

Let us consider the difference

$$S_{k+1}^{(m)}/Q_{k+1}^{(m)} - S_k^{(m)}/Q_k^{(m)} = F_k / Q_k^{(m)} Q_{k+1}^{(m)},$$

$$F_k = \frac{kt}{(k+m+\frac{1}{2})(k+m-\frac{1}{2})} F_{k-1},$$

therefore

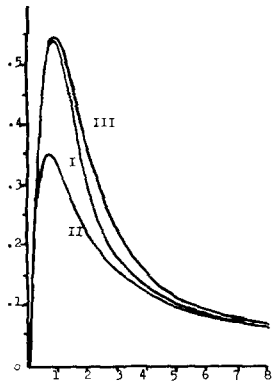

FIG. 1. The function $e^{-x^2} \int_0^x e^{u^2} du$ and its two-sided Padé approximants.

$$F_k = \frac{(-1)^m \Gamma(\frac{3}{2}) \Gamma(m+\frac{1}{2}) k!\, t^{k+m}}{\Gamma(k+m+\frac{1}{2}) \Gamma(k+m+\frac{3}{2})}.$$

Summing the terms from k to ∞ we get

$$f(t) - \frac{P_k^{(m)}(t)}{Q_k^{(m)}(t)} = \sum_{j=k}^{\infty} \frac{F_j}{Q_j^{(m)}(t) Q_{j+1}^{(m)}(t)},$$

which is exactly (28).

In the following we need some asymptotic representation of $Q_j^{(m)}(t)$ for $m = \beta j$, $t = \alpha j$, $j \to \infty$. We investigate the integral representations of $Q_j^{(m)}(t)$

$$Q_j^{(m)}(t) = \frac{j!\Gamma(\frac{1}{2}-j-m)}{\Gamma(\frac{1}{2}-m)} \frac{1}{2\pi i} \oint \frac{e^{-zt}}{(1+z)^{m+\frac{1}{2}} z^{j+1}} dz,$$

If Laplace's method is used it is not difficult to show that the largest contribution of the integrand comes from point z, where z is the root of the equation

$$\alpha + \beta/(1+z) + 1/z = 0.$$

We then get

$$\lim_{j\to\infty} \left| \frac{F_j}{Q_j^{(m)}(t) Q_{j+1}^{(m)}(t)} \right|^{1/j} = \beta^{-\beta} e^{-1-\beta} \alpha^{1+\beta} e^{2\alpha z} z^2 (1+z)^{2\beta}.$$

This term is maximal in α if $\alpha = (1+\beta)^2/[2(1-\beta)]$; thus $z = -(1-\beta)/(1+\beta)$. For this reason

$$\lim_{k\to\infty} \left\{ \max_{0\le t\le\infty} \left| f(t) - \frac{P_k^{(m)}(t)}{Q_k^{(m)}(t)} \right| \right\}^{1/k} = \beta^{\beta} (1-\beta)^{1-\beta} 2^{\beta-1}.$$

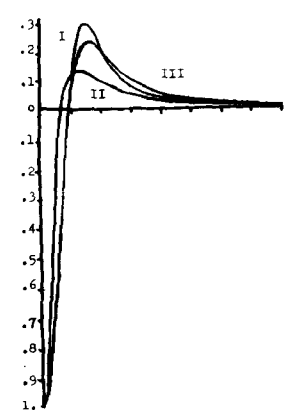

FIG. 2. The function $2xe^{-x^2} \int_0^x e^{u^2} du - 1$ and its two-sided Padé approximants.

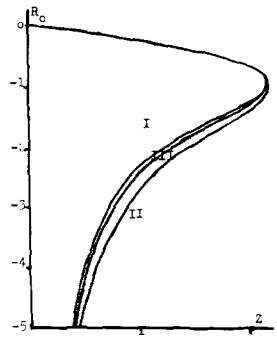

FIG. 3. The angular distribution of the charged beam R_0 versus Z and its two-sided Padé approximants.

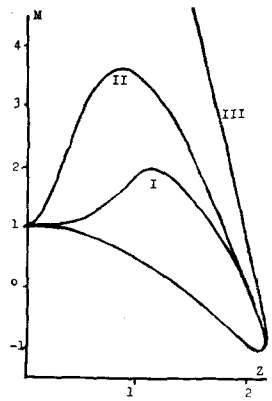

FIG. 4. The increment M versus the reduced axial distance Z and its two-sided Padé approximants.

Theorem 2 is now proved. The proof of Theorem 1 follows from this for $m = 0, \beta = 0$.

4. NUMERICAL APPLICATIONS

The first application is the approximation of the function $e^{-x^2}\int_0^x e^{u^2}\,du$ and its derivative. We compute the Padé approximants with parameters $k = 1$, $m = 0$, and $k = 2$, $m = 1$,

$$\frac{x}{1+2x^2}, \quad \frac{15x+2x^3}{15+12x^2+4x^4},$$

respectively. Figure 1 shows the function with its approximants. The second approximant gives a quite good agreement in a few terms. In Fig. 2 the derivative of the function and the derivatives of the approximants are shown (line I and lines II–III):

$$\frac{2x^2-1}{(1+2x^2)^2}, \quad \frac{8x^6+156x^4+90x^2-225}{(15+12x^2+4x^4)^2}.$$

Line III again gives the better agreement. It is obvious that if higher parameters are taken (i.e. higher approximants) we can get even closer agreement. Another application is the drawing up of constructional curves in engineering.[6] The function appears in the theory of space charge limited beams. Figure 3 shows the angular distribution of the charged beam in a periodically focusing system taken from Ref. 6. Line I is the exact curve, lines II and III are computed by Padé approximants

$$\frac{15x+2x^3}{15+12x^2+4x^4}, \quad \frac{105x+20x^3+4x^5}{105+90x^2+36x^4+8x^6},$$

respectively. It is easy to see that line III fulfills the engineering requirements. The increment M versus the reduced axial distance Z, corresponding to previous approximations is illustrated in Fig. 4. In the stability region $|M| < 1$ line III complies with the requirements of the constructional curve.

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The elastic pendulum: A nonlinear paradigm

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A pendulum with an elastic instead of an inextensible suspension is the simplest realization of an autonomous, conservative, oscillatory system of several degrees of freedom with nonlinear coupling; it can also have an internal 1:2 resonance. A fairly complete study of this system at and near resonance is here undertaken by means of the "slow-fluctuation" approximation which consists in developing the x^2y-type interaction into a trigonometric polynomial and keeping only the term with the slowest frequency. Extensive computations showed that up to moderately large amplitudes the approximate solutions were virtually as accurate as numerical integrations of the exact equations of motion. The slow-fluctuation equations of motion can be completely integrated by quadratures. Explicit solutions for amplitudes and phases are given in terms of elliptic functions, and can be linked to initial conditions. There exist two branches of purely periodic, harmonic, constant-amplitude motions which are orbitally stable but Liapunov unstable. The pure suspension motion is Liapunov unstable and remains orbitally stable only up to and including a critical amplitude; the standard "method of variational equations" leads to a slightly different stability criterion but is shown to be unreliable. In the dynamical neighborhood of the unstable pure suspension mode are motions which convert to it after infinite time. When a motion has an amplitude modulation minimum at or near zero, a phase reversal of the suspension takes place which is shown to be an artefact inherent in the description in terms of amplitudes and phases. In addition there is in the pendulum (but not in the exactly soluble system having the slow–fluctuation Hamiltonian) a fast phase transient which vitiates the slow-fluctuation technique for a few periods around the suspension amplitude minimum; this is the only restriction on the method. An appendix outlines formal isomorphisms between the elastic pendulum and the process of second-harmonic generation in nonlinear optics.

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I. INTRODUCTION

In more than one degree of freedom, a system with Hamiltonian of type

$$\tfrac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \omega_x^2 x^2 + \omega_y^2 y^2) + \gamma x^2 y$$

appears on several counts as the simplest of them all: it is autonomous and conservative, it reduces to a plane, harmonic oscillator for infinitesimal amplitudes and also for vanishing values of γ, it remains bound for moderate amplitudes, and the x^2y-coupling is the simplest which cannot trivially be removed by a coordinate transformation. A perfectly plain realization of such a system (details in Sec. II below) is a pendulum with an elastic instead of an inextensible thread, and constrained to move in a fixed, vertical plane.

This elastic pendulum was introduced by Witt and Gorelik[1] in an important paper which has frequently been misquoted, following Minorski.[2] Their interest centered on a quasiresonant feature of rather simple origins. The centrifugal force accompanying the pendulum swing tugs at the elastic suspension twice in every pendulum period; it will thus excite the suspension mode, or tend to arrest it when the phase relation is the opposite, if the suspension frequency is close to twice the pendulum frequency. The resultant energy exchange is immediately apparent in a rough table-top experiment; it is also familiar as a nuisance[3] in the well-known beginner's experiment to measure a spring constant dynamically by timing vertical oscillations. The pendulum and suspension modes seem to behave just like two coupled, harmonic oscillators, seesawing in amplitude. Some quantitative observation of the turning points quickly shows, however, that the amplitude modulation is not harmonic (see also Figs. 1 and 3 below). Indeed the resonant energy transfer is not harmonic but parametric: the suspension motion periodically alters the pendulum length, and hence the pendulum period. The process is fundamentally nonlinear, and the motion cannot be represented as a superposition of normal modes.

As the paradigm of a conservative, autoparametric system with an internal resonance, the elastic pendulum is mentioned in a number of texts[2,4] at varying levels. Even homework problems have been devised.[5] There is also much analytical work,[1,3,6–10] again of differing sophistication.

We present here a detailed study of the elastic pendulum by means of the slow-fluctuation technique first formulated by one of us[9] which has since been generalized and explored[11,12] in more depth. Given the considerable volume of the existing literature, we feel we should explain why we add to it instead of merely appending our principal results as illustrations to the general exposition[11,12] of the method.

The quoted literature[1–8,10] contains no stringent numerical comparisons between approximations and accurate solutions of the equations of motion. Consequently the authors cannot do full justice either to their own work or to the elastic pendulum. In contrast, we began our studies with extensive numerical integrations and thus possessed a reliable yardstick for checking everything we did later.

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To our surprise we found that our slow-fluctuation solutions approximated the numerical ones with a remarkably, indeed uncannily, small error. We had to conclude that for all intents and purposes, and with only minor limitations, they were comparable in accuracy to the numerical ones. Thus we could confidently use the slow-fluctuation formulae much as if they were exact and discuss the elastic pendulum in considerable depth. This simple system looks like a toy at best, but its behavior is astonishingly complex, with many facets of more than academic luster. What we offer is, therefore, a numerically accurate, analytical study with some aspirations to completeness.

We emphasize that our standards of accuracy are those of the applied mathematician who wishes to compute an oscillation, say, over a hundred periods with an end error of a percent or better in the amplitude and no more than a few degrees of arc in the phase. This is a far cry from the needs of the design engineer who may well be content with 10% and 30°, respectively, after only a half-dozen periods. However, for the sake of the refined study we had in mind, we judged it better to err on the side of pedantry.

We have also been cautious in the matter of notation. It so happens that nearly every feature of the elastic pendulum has a close analog in oscillatory systems of more than two degrees of freedom. We have, therefore, adopted a somewhat elaborate notation in order to facilitate comparisons with the general theory of the slow-fluctuation method.[11,12]

II. BASIC SYSTEM PROPERTIES

Call m the mass of the pendulum bob, k the spring constant of the suspension (assumed massless and elastically linear), l_0 the suspension length in the absence of a load, and l the length under a static load mg. Set

$$g/l = \omega_1^2, \quad k/m = \omega_2^2. \tag{2.1}$$

From the definition of k we have

$$k(l - l_0) = mg, \tag{2.2}$$

and if here we substitute for l and m/k from (2.1) we obtain

$$g/\omega_1^2 - l_0 = g/\omega_2^2,$$

which implies the inequality

$$\omega_1 < \omega_2 \tag{2.3}$$

(overlooked in the literature). If on the other hand we substitute in (2.2) for k/m and g, we obtain

$$\omega_2^2(l - l_0) = l\omega_1^2, \tag{2.4}$$

so that the exact resonance

$$\omega_2 = 2\omega_1 \quad \text{requires } l - l_0 = l/4, \tag{2.5}$$

a convenient rule for experimentation.

The problem suggests polar coordinates, but they lead to very clumsy equations. Oscillatory systems usually are best treated in coordinates which would describe normal modes in the absence of any coupling. We use rectangular q_1, q_2 in a vertical plane with q_1 horizontal and q_2 measured positive upwards; the origin will be placed at the rest position of the bob. Only motions in this plane will be admitted with their amplitudes restricted to small values by

$$q_1^2/(l - q_2)^2 \ll 1 \text{ and } |q_2|/l \ll 1. \tag{2.6}$$

The exact potential energy

$$V = \tfrac{1}{2}k\{[q_1^2 + (l - q_2)^2]^{1/2} - l_0\}^2 + mgq_2$$

can be put into a convenient approximate form by binomial expansion and neglect of higher-order terms in accordance with the conditions (2.6). The result is[6]

$$V = \tfrac{1}{2}m(\omega_1^2 q_1^2 + \omega_2^2 q_2^2) + \gamma q_1^2 q_2, \tag{2.7}$$

except for a constant which we omit, with

$$\gamma = m(\omega_1^2 - \omega_2^2)/2l. \tag{2.8}$$

A Lagrangian for the potential energy (2.7) yields at once the equations of motion

$$\ddot{q}_1 + [\omega_1^2 + (2\gamma/m)q_2]q_1 = 0, \tag{2.9}$$

$$\ddot{q}_2 + \omega_2^2 q_2 = -(\gamma/m)q_1^2. \tag{2.10}$$

As described in the Introduction, the suspension mode behaves as a driven harmonic oscillator (2.10), whereas the pendulum (2.9) is parametric.

The coupling constant (2.8) is always negative,

$$\gamma < 0 \tag{2.11}$$

on account of (2.3). Interestingly enough, it cannot be altered without changing the system itself. If we wish to alter γ while keeping m, ω_1, and ω_2 fixed, we have only l to vary; but because $g/l = \omega_1^2$ we must simultaneously vary g, and then Eq. (2.2) shows that we must vary l_0 too. Thus an essential system parameter has to be changed after all. One must not visualize this pendulum γ as a "small parameter" or an "external perturbation" of the familiar kind which is under control and whose value can be adjusted at will to suit the validity of some approximate technique.

Of course the x^2y- type coupling in the potential energy (2.7) also arises in many analogous series developments. Well known is its occurrence in the vibrational energy of the CO_2-molecule (and of similar ones), where it causes the "Fermi resonance" in the infrared and Raman spectrum.[13] Another important case, with an extensive literature, is the oscillatory and occasionally unstable behavior of a betatron beam.[14] Then there are many occurrences in celestial mechanics.[8,15] And so forth. In all these instances the elastic pendulum can serve as a model or guide, provided only its limitations (2.3) and (2.11) together with the invariability of γ are kept in mind. The dominant feature is always the parametric energy transfer. In fact, if an equation of motion similar to (2.9) is found for some system, the elastic pendulum may have useful analogies to offer even in the absence of other similarities. An example is furnished by the 1:2 resonances between the oscillations of a ship in heave, pitch, and roll which even in a nonconservative approximation[16] bear a strong resemblance to the pendulum swing parametrically excited from the suspension. In a different fashion, by a mathematical analogy arising from the nature of our slow-fluctuation approximation, the elastic pendulum can be related to the process of second-harmonic generation in nonlinear optics, as we show later in the Appendix.

III. NUMERICAL INTEGRATIONS

In all computations we uniformly adopted the value $\omega_2 = 12$ rad/sec, which corresponds to a suspension period close to $\frac{1}{2}$ sec. Near resonance the (full) pendulum period will then be in the neighborhood of 1 sec, and the pendulum length of the order 30 cm, just right for table-top trials. For a fair representation of our graphs and numerical data select a light coil spring, suspend from a standard laboratory tripod, attach a bob of such mass m as to give a vertical period around $\frac{1}{2}$ sec, and lengthen the spring with a piece of twine to satisfy (2.5); to detune at will, lengthen or shorten the twine. For all choices of twine length, the value of γ is automatically determined by (2.8). In the following we quote the chosen ω_1 in terms of the fixed ω_2, or we quote the detuning $2\omega_1 - \omega_2 = \epsilon$.

Using a Runge–Kutta–Simpson technique with variable increment,[17] we integrated the equations of motion (2.9) and (2.10) for various initial conditions and pendulum frequencies ω_1. By never letting the time increment exceed 0.01 sec, we were able to follow the motion satisfactorily over as much as 160 sec (or 300 suspension periods). As a check on accuracy, we calculated the (known, fixed) total energy from the computed solution. We found an energy loss of 0.26% or less for the longest runs. Runs of at most 50 sec (i.e., up to 100 suspension periods) usually sufficed; the energy loss in these amounted to no more than about 0.1% in all cases. We judged this accuracy adequate.

Reference 9 contains an archive of graphs displaying some of our computations. Here we reproduce three typical short runs.

Figure 1 represents a motion at exact resonance, $2\omega_1 = \omega_2$. The bob is released from rest 2 cm below and 0.1 mm to the right of the origin. After about 40 suspension periods an almost complete energy transfer into the pendulum mode has taken place. The transfer then reverses. Figure 2 is an enlarged view of the suspension motion near its amplitude minimum. It is seen that about one half-period is missing, corresponding to an abrupt change of the suspension phase by about 180°. This illustrates the mechanism surmised above: the suspension, driven by the resonant centrifugal tugging, is first arrested and immediately started up again undergoing a 180° phase reversal in the process.

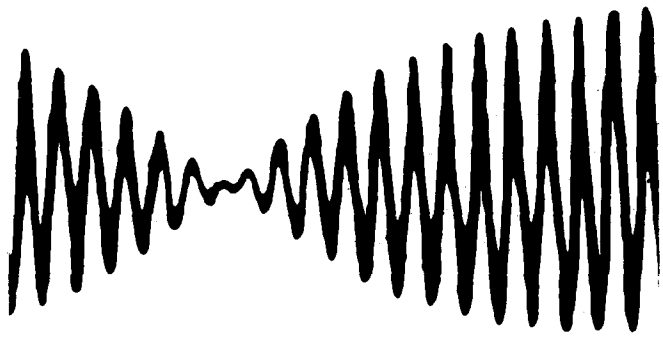

FIG. 2. An enlarged view of the suspension amplitude minimum of Fig. 1. Note the zero crossings; approximately one half-period is missing at the minimum.

Figure 3 shows a case off resonance, with $1.905\omega_1 = \omega_2$ or $\epsilon = 0.095\omega_1$. Bob release is from 1.5 cm below and 2 cm to the right of the origin. No peculiar features are visible. The energy transfer is incomplete but has a regular period. Amplitude modulation and oscillation are not synchronized; from one modulation period into the next the phase is seen to differ slightly, but apparently without sudden shift.

Figure 4 is an example well off resonance, with $\omega_1 = 2\omega_2/3$ instead of the resonant $\omega_2/2$. Bob release is from 1 cm below and 3 cm to the right of the origin. The energy transfer mechanism is here quite ineffective. The amplitude modulation appears as a mere jitter of the turning points. Its period is still quite regular, but it is short and so far out of synchronism with the oscillations that the behavior of the turning points appears at a first glance a little erratic.

In these and many other computed cases we let the amplitudes become fairly large; still consistent with the condi-

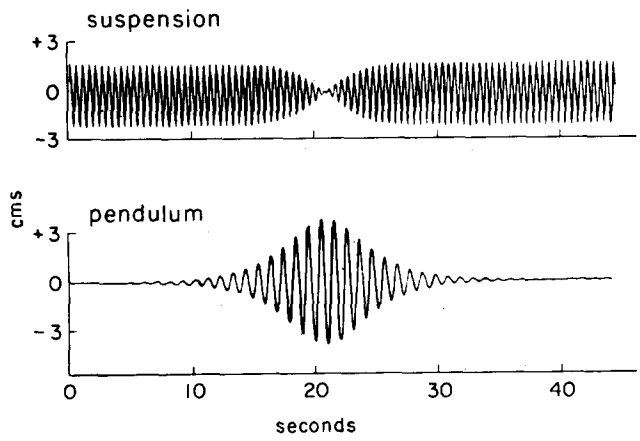

FIG. 1. A numerical integration at exact resonance, $2.000\,\omega_1 = \omega_2$. Initial conditions: release from rest at $t = 0$ with $q_{10} = 0.01$ cm and $q_{20} = -2.00$ cm (notation as in Sec. V).

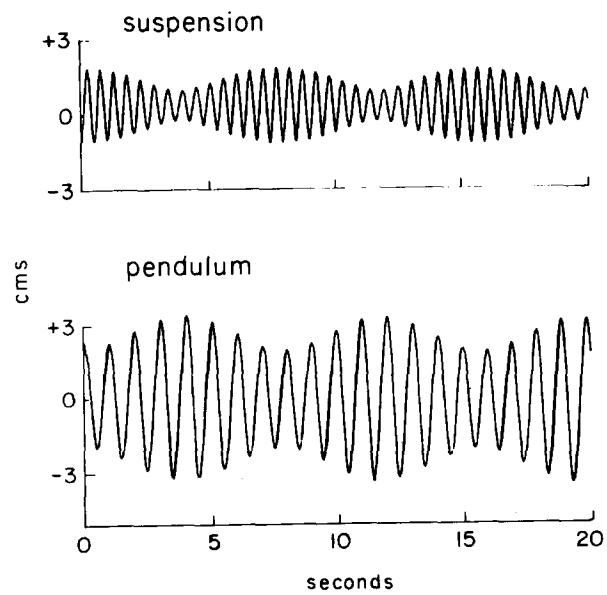

FIG. 3. A numerical integration off resonance, $1.905\,\omega_1 = \omega_2$. Initial conditions: release from rest at $t = 0$ with $q_{10} = 2.00$ cm and $q_{20} = -1.50$ cm.

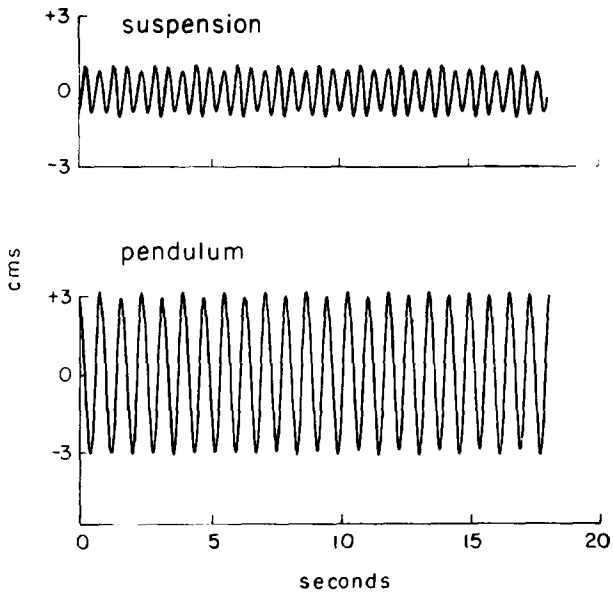

FIG. 4. A numerical integration far from resonance, $1.500\,\omega_1 = \omega_2$. Initial conditions: release from rest at $t = 0$ with $q_{10} = 3.00$ cm and $q_{20} = -1.00$ cm. Note the ineffective energy transfer.

tions (2.6) needed for the validity of the approximation (2.7), but large enough to emphasize nonlinear peculiarities, if any. However, large amplitudes showed nothing else than small ones. We also computed a number of solutions for initial conditions with a nonzero velocity; again, they exhibited nothing new.

IV. THE SLOW-FLUCTUATION METHOD

Energy transfer between the pendulum and suspension modes requires changing phase relations. More formally, we may say that nonlinear oscillators (including parametric ones) generally have their frequencies dependent upon amplitude; evidently, amplitude change implies frequency change. Some substitution such as

$$q_i = A_i \cos(\omega_i t + \beta_i), \tag{4.1}$$

with variable A_i, β_i (always $A_i \geqslant 0$ for uniqueness of β_i) thus becomes unavoidable.

The introduction of amplitudes and phases doubles the number of variables and suggests a Hamiltonian formulation. We shall, instead of the q_i and the pertaining

$$p_i = m\dot{q}_i, \tag{4.2}$$

introduce new coordinates and momenta by the familiar canonical transformation

$$q_i = (2\bar{p}_i/m\omega_i)^{1/2} \cos\bar{q}_i, \tag{4.3}$$

$$p_i = -(2m\omega_i\bar{p}_i)^{1/2} \sin\bar{q}_i, \tag{4.4}$$

which conveniently converts a harmonic oscillator Hamiltonian $\frac{1}{2}(p_i^2/m + m\omega_i^2 q_i^2)$ into $\omega_i\bar{p}_i$. Note that (4.3) is largely (4.1) in disguise with

$$\bar{q}_i = \omega_i t + \beta_i, \tag{4.5}$$

$$\bar{p}_i = \tfrac{1}{2}m\omega_i A_i^2. \tag{4.6}$$

According to (4.6) the new momenta are effectively the squared amplitudes; this suits our purpose well, for it so happens that the method to be developed yields equations, not for the amplitudes themselves, but for their squares.

In terms of the original rectangular coordinates and the momenta (4.2), and with the potential energy (2.7), the Hamiltonian of the elastic pendulum is

$$H(p,q) = (p_1^2 + p_2^2)/2m + \tfrac{1}{2}m(\omega_1^2 q_1^2 + \omega_2^2 q_2^2) + \gamma q_1^2 q_2. \tag{4.7}$$

After the canonical transformation (4.3), (4.4), this becomes

$$\bar{H}(\bar{p},\bar{q}) = \omega_1\bar{p}_1 + \omega_2\bar{p}_2 + \bar{\gamma}(8\bar{p}_1^2\bar{p}_2)^{1/2}\cos^2\bar{q}_1\cos\bar{q}_2, \tag{4.8}$$

where

$$\bar{\gamma} = \gamma(m^3\omega_1^2\omega_2)^{-1/2}.$$

The product of cosines can be resolved into a sum:

$$\cos^2\bar{q}_1\cos\bar{q}_2 = \tfrac{1}{2}\cos\bar{q}_2 + \tfrac{1}{4}\cos(2\bar{q}_1 + \bar{q}_2) + \tfrac{1}{4}\cos(2\bar{q}_1 - \bar{q}_2); \tag{4.9}$$

consequently the exact Hamiltonian equations of motion will also contain sums of terms with trigonometric factors having arguments $\bar{q}_2$, $2\bar{q}_1 + \bar{q}_2$, and $2\bar{q}_1 - \bar{q}_2$. On account of the definition (4.5) these factors can be said to be essentially harmonic with frequencies ω_2, $2\omega_1 + \omega_2$, and $2\omega_1 - \omega_2$, respectively, because the phases β_1 and β_2 vary comparatively much more mildly than $\omega_1 t$ and $\omega_2 t$, respectively, if for the time being we disregard extreme cases like the one depicted in Figs. 1 and 2.

As the system is most interesting near resonance, we assume from now on

$$2\omega_1 - \omega_2 = \epsilon, \quad |\epsilon| \ll \omega_1. \tag{4.10}$$

Then the trigonometric functions with frequencies ω_2 and $2\omega_1 + \omega_2$ fluctuate much faster than those with frequency ϵ. Moreover, they are in the Hamiltonian equations accompanied by factors depending only on the momenta, i.e., on the amplitude modulation functions A_i which vary slowly, as in the typical case of Fig. 3. Hence these rapidly fluctuating terms vary rather symmetrically up-and-down, giving a zero net effect, and can safely be excluded. Note that the distinction of "fast" and "slow" holds good even at rather large detuning ϵ. Suppose $\epsilon = \omega_1/2$, i.e., $1.500\omega_1 = \omega_2$ as for the case depicted in Fig. 4; then $\omega_2 = 3\epsilon$ and $2\omega_1 + \omega_2 = 7\epsilon$, still fairly different from ϵ. Thus the $\ll$ sign in (4.10) may be interpreted liberally.

Deferring quantitative justification until Sec. VII, we henceforth keep only the last term in (4.9) and replace the exact Hamiltonian (4.8) by its "slow-fluctuation" approximation

$$\bar{S}(\bar{p},\bar{q}) = \omega_1\bar{p}_1 + \omega_2\bar{p}_2 + \bar{\gamma}\bar{p}_1(\bar{p}_2/2)^{1/2}\cos(2\bar{q}_1 - \bar{q}_2). \tag{4.11}$$

The first pair of equations of motion $\dot{\bar{p}}_i = -\partial\bar{S}/\partial\bar{q}_i$ is

$$\dot{\bar{p}}_1 = 2\bar{\gamma}\bar{p}_1(\bar{p}_2/2)^{1/2}\sin(2\bar{q}_1 - \bar{q}_2), \tag{4.12}$$

$$\dot{\bar{p}}_2 = -\bar{\gamma}\bar{p}_1(\bar{p}_2/2)^{1/2}\sin(2\bar{q}_1 - \bar{q}_2). \tag{4.13}$$

As they are related by $\dot{\bar{p}}_2 = -\dot{\bar{p}}_1/2$, we have the conservation law

$$\bar{p}_1 + 2\bar{p}_2 = \text{const} = 2\alpha \tag{4.14}$$

($\alpha \geqslant 0$, of course). In terms of the amplitudes, by (4.6),

$$\omega_1 A_1^2 + 2\omega_2 A_2^2 = 4\alpha/m; \tag{4.15}$$

this expresses the conspicuous seesawing between joint extrema.[18] Next, note that (4.14) may be combined with (4.11) into

$$\bar{S} - \omega_2 \alpha = \epsilon \bar{p}_1/2 + \bar{\gamma}\bar{p}_1(\bar{p}_2/2)^{1/2}\cos(2\bar{q}_1 - \bar{q}_2). \tag{4.16}$$

Since the Hamiltonian is conserved,

$$\bar{S}(\bar{p},\bar{q}) = \text{const} = E, \tag{4.17}$$

(4.16) shows that at exact resonance $\epsilon = 0$ the term with $\bar{\gamma}$, i.e., the successor to the nonlinear interaction energy $\gamma q_1^2 q_2$ in (2.7), is separately conserved in our approximation.

In a conservative, autonomous system of two degrees of freedom the existence of a first integral besides the energy permits complete integration by quadratures alone.[19] First eliminate $2\bar{q}_1 - \bar{q}_2$ between (4.11) and (4.12) by squaring and adding,

$$(\bar{S} - \omega_1\bar{p}_1 - \omega_2\bar{p}_2)^2 + \dot{\bar{p}}_1^2/4 = \bar{\gamma}^2\bar{p}_1^2\bar{p}_2/2,$$

and now remove $\bar{p}_2$ and $\bar{S}$ by means of (4.14) and (4.17) with the result[20]

$$\begin{aligned}\dot{\bar{p}}_1^2 &= -\bar{\gamma}^2\bar{p}_1^3 + c_4\,\bar{p}_1^2 + 2\epsilon c_1\bar{p}_1 - c_1^2 \\ &= \bar{f}(\bar{p}_1),\end{aligned} \tag{4.18}$$

where

$$c_1 = 2(E - \omega_2\alpha), \tag{4.19}$$

$$c_4 = 2\bar{\gamma}^2\alpha - \epsilon^2 \tag{4.20}$$

(in a slightly unsystematic numbering which is to facilitate comparisons with the notation in Ref. 9). The solution of this differential equation is the usual

$$t - t_0 = \int d\bar{p}_1/[\bar{f}(\bar{p}_1)]^{1/2}, \tag{4.21}$$

with the sign of the root to be chosen according to the direction of growth of $\bar{p}_1$: + for increase, − for decrease; the resultant $\bar{p}_1(t)$ is an elliptic function of time (including degenerate cases).

It will be convenient to set

$$\begin{aligned}&\bar{f}(\bar{p}_1) = -\bar{\gamma}^2 P(\bar{p}_1), \\ &P(\bar{p}_1) = (\bar{p}_1 - R_1)(\bar{p}_1 - R_2)(\bar{p}_1 - R_3);\end{aligned} \tag{4.22}$$

then comparison of coefficients yields

$$R_1R_2R_3 = -c_1^2/\bar{\gamma}^2, \tag{4.23}$$

$$R_1 + R_2 + R_3 = c_4/\bar{\gamma}^2. \tag{4.24}$$

Let us first assume $c_1 \neq 0$; the degenerate case $c_1 = 0$ will be treated in Secs. IX and XI. From (4.23) we see that one of the three roots of $\bar{f}$ must be negative, say R_3. If the other two were also negative, or if they were complex conjugates, $\bar{f}(\bar{p}_1)$ would be negative for all positive $\bar{p}_1$ which is physically not possible. Hence only R_1, R_2 real and positive needs to be admitted, and then $\bar{f} \geqslant 0$ holds between R_1 and R_2. A general theorem[21] asserts that under these circumstances $\bar{p}_1(t)$ is periodic between turning points R_1 and R_2, and time-reversal symmetric about any of these extrema (with $R_1 = R_2$ a degenerate case yielding constant amplitudes, as discussed in detail in Sec. VIII).

We standardize further developments by putting the zero of the time scale at $\bar{p}_1 = R_1$; thereby (4.21) becomes

$$t = \int_{R_1} d\bar{p}_1/[\bar{f}(\bar{p}_1)]^{1/2}, \tag{4.25}$$

and R_1 assumes the status of an integration constant which eventually needs to be linked to given initial conditions. To be precise, we do not make our calculations in terms of an initial value $\bar{p}_1(t_0)$ prescribed at the specified time t_0, we make them in terms of an initial time $t_0(R_1)$ prescribed at the specified amplitude R_1, only for sheer brevity we also write $t_0 = 0$. Effectively t_0 becomes an independent integration constant; to complete the stratagem we show in the next section how R_1 can be calculated from the special, physical initial conditions which correspond directly to the special formula (4.25). With R_1 thus computable from Eq. (5.3) below, the other roots follow from (4.23) and (4.24) as

$$\begin{aligned}2R_2 &= -c_6 + (c_6^2 + 4c_7)^{1/2}, \\ 2R_3 &= -c_6 - (c_6^2 + 4c_7)^{1/2}, \\ c_6 &= R_1 - c_4/\bar{\gamma}^2, \quad c_7 = c_1^2/\bar{\gamma}^2 R_1,\end{aligned} \tag{4.26}$$

so that the convention $\bar{p}_1(0) = R_1$ neatly skirts the chore of solving the cubic equation $P(\bar{p}_1) = 0$.

The other pair of Hamiltonian equations $\dot{\bar{q}}_i = \partial\bar{S}/\partial\bar{p}_i$ is

$$\dot{\bar{q}}_1 = \omega_1 + \bar{\gamma}(\bar{p}_2/2)^{1/2}\cos(2\bar{q}_1 - \bar{q}_2), \tag{4.27}$$

$$\dot{\bar{q}}_2 = \omega_2 + \tfrac{1}{2}\bar{\gamma}\bar{p}_1(2\bar{p}_2)^{-1/2}\cos(2\bar{q}_1 - \bar{q}_2). \tag{4.28}$$

In passing, note that they may be combined into

$$2\dot{\bar{q}}_1 - \dot{\bar{q}}_2 = \epsilon + \bar{\gamma}(\bar{p}_2/2)^{-1/2}(\bar{p}_2 - \bar{p}_1/4)\cos(2\bar{q}_1 - \bar{q}_2), \tag{4.29}$$

which corresponds to the fact that the Hamiltonian really contains only a generalized coordinate $\bar{q}_1 = 2\bar{q}_1 - \bar{q}_2$. While these observations help to explain[11] the existence of the momentum integral (4.14) as arising from some cyclic coordinate $\bar{q}_2$, (4.29) is less easy to integrate than the equations from which it originates, whence we leave it alone (except for further mention in the Appendix).

Equation (4.28) contains $\bar{p}_2$ in the denominator. If at some time t_1 the suspension amplitude vanishes, or almost vanishes as in Fig. 1, then the necessary Lipschitz condition is not guaranteed near t_1. As Fig. 2 has shown, at t_1 there is also a phase change so rapid that our slow-fluctuation approach can no more be trusted. Thus the extreme cases which we provisionally disregarded above now announce themselves through a singularity in a slow-fluctuation equation. We shall treat these exceptional low-amplitude states in Sec. X; until then we assume that $\bar{p}_2$, i.e., A_2, has a suitably high, positive, uniform lower bound. No such restriction is needed for $\bar{p}_1$; there is no $\bar{p}_1$ in a denominator, and anyway, if $\bar{p}_1$ vanishes at some time then (4.12) shows that it will vanish at all times, so that the pendulum amplitude either never reaches zero, or else we have pure suspension motion.

In (4.27), eliminate the cosine by means of the Hamiltonian (4.11), and then $\bar{p}_2$ by means of (4.14); the result is

$$\dot{\beta}_1 = (E - \omega_1\bar{p}_1 - \omega_2\bar{p}_2)/\bar{p}_1 = (c_1 - \epsilon\bar{p}_1)/2\bar{p}_1. \tag{4.30}$$

Analogous steps throw (4.28) into

$$\dot{\beta}_2 = (c_1 - \epsilon\bar{p}_1)/(4\alpha - 2\bar{p}_1). \tag{4.31}$$

With $\bar{p}_1(t)$ known from (4.21), or from Sec. XI in case $c_1 = 0$, β_1 and β_2 are obtained by time integrations.

The quadrature in (4.30) introduces a further integration constant, say

$$\beta_1(0) = \delta.$$

We now have four free constants: E,α,t_0, and δ. The constant arising in the remaining quadrature (4.31) can, therefore, not be free. Indeed, a glance at Eqs. (4.12) and (4.13) shows that the simultaneous extrema of the amplitudes occur when $\sin(2\bar{q}_1 - \bar{q}_2) = 0$. In particular, at $t = 0$, where we must have such an extremum because of the previous standardization convention (4.25),

$$2\bar{q}_1(0) - \bar{q}_2(0) = 2\beta_1(0) - \beta_2(0) = r\pi, \quad r \text{ integer},$$

is required, or without loss of generality,

$$\beta_2(0) = 2\delta + r\pi, \quad r = 0,1. \tag{4.32}$$

The phase functions $\beta_1(t)$ and $\beta_2(t)$ are necessarily connected[19] by a relation $\Phi(\beta_1,\beta_2) = \text{const}$, but it cannot be obtained explicitly. To see this, introduce $dt = d\bar{p}_1/[\bar{f}(\bar{p}_1)]^{1/2}$ in (4.30) and (4.31). Then β_1 and β_2 emerge as functions of $\bar{p}_1$ after quadratures involving two elliptic integrals of the third kind which have different characteristics n because of the different denominators $2\bar{p}_1$ and $4\alpha - 2\bar{p}_1$. Between the two results $\bar{p}_1$ can be eliminated in principle, but obviously not in closed form.

V. INITIAL CONDITIONS

From the transformation formulae (4.2)–(4.6) we have

$$\dot{q}_i = -\omega_i A_i \sin(\omega_i t + \beta_i) \tag{5.1}$$

and can write out the coordinates and velocity components of the pendulum bob at $t = 0$ as

$$q_1(0) = q_{10} = A_1(0)\cos\delta,$$
$$q_2(0) = q_{20} = A_2(0)\cos(2\delta + r\pi),$$
$$\dot{q}_1(0) = -\omega_1 A_1(0)\sin\delta,$$
$$\dot{q}_2(0) = -\omega_2 A_2(0)\sin(2\delta + r\pi).$$

Evidently the choice $\delta = 0$ singles out a neat subclass of states of motion which have

$$A_1(0) = q_{10} > 0,$$
$$A_2(0) = \pm q_{20} > 0, \quad \text{upper sign } r = 0 \tag{5.2}$$
$$\dot{q}_1(0) = \dot{q}_2(0) = 0.$$

These states are set up by taking the bob to some point to the right of the vertical, and releasing it there from rest. According as we take it up or down from the origin, we must make $r = 0$ or $r = 1$, respectively; if we wanted to take it to the left we should choose $\delta = \pi$, but this need not be mentioned further because it is trivial, the system being symmetrical in q_1. While in a release from rest we necessarily begin the motion at a simultaneous extremum of q_1 and q_2, it is not obvious that this extremum coincides precisely with an extremum of the amplitude modulation.

The four-fold extremum makes it trivially easy to calculate the values of the other integration constants if $\delta = 0$. First from (4.6),

$$R_1 = \bar{p}_1(0) = m\omega_1 q_{10}^2/2. \tag{5.3}$$

Then from (4.15) the amplitude constant

$$\alpha = m(\omega_1 q_{10}^2 + 2\omega_2 q_{20}^2)/4. \tag{5.4}$$

Third, after short reduction, the Hamiltonian (4.11)

$$E = (m/2)(\omega_1^2 q_{10}^2 + \omega_2^2 q_{20}^2) + (\gamma/4)q_{10}^2 q_{20}, \tag{5.5}$$

which differs from the exact total energy (4.7) because keeping only the last term of (4.9) brought a factor 1/4 to the interaction.

Now the constant (4.19) follows readily from (5.4) and (5.5):

$$c_1 = q_{10}^2(m\epsilon\omega_1 + \gamma q_{20})/2. \tag{5.6}$$

If this vanishes we have the special case set aside until Secs. IX and XI. Of course we may have $c_1 = 0$ trivially by $q_{10} = 0$, but since with $\delta = 0$ we also have $\dot{q}_1(0) = 0$, this simply implies pure suspension motion. Nontrivially, $c_1 = 0$ arises from

$$q_{20} = -m\omega_1\epsilon/\gamma. \tag{5.7}$$

Next we obtain the roots of $\bar{f}(\bar{p}_1)$ from (4.26). Straightforward algebra yields with the aid of (4.20), (5.3), and (5.4),

$$c_6 = m\omega_2[(m\epsilon\omega_1)^2 - (\gamma q_{20})^2]/\gamma^2; \tag{5.8}$$

and with (5.3) and (5.6),

$$c_7 = R_1 m\omega_2(m\epsilon\omega_1 + \gamma q_{20})^2/\gamma^2. \tag{5.9}$$

R_2 now follows from the formula in (4.26). Of special interest is the magnitude relation between R_1 and R_2. Using the formula just quoted we may write

$$2(R_2 - R_1) = -(c_6 + 2R_1) + (c_6^2 + 4c_7)^{1/2}.$$

It follows that $R_2 \lessgtr R_1$ as $(c_6^2 + 4c_7)^{1/2} \lessgtr c_6 + 2R_1$. Since in the latter inequality both sides are positive, we may square it; some reduction with the aid of (5.3), (5.8), and (5.9) then leads to the criterion that

$$R_1 \gtrless R_2 \quad \text{as} \quad q_{10}^2 \gtrless 4\omega_2 q_{20}(m\epsilon\omega_1 + \gamma q_{20})/\gamma\omega_1. \tag{5.10}$$

On the whole the $\delta = 0$ states are as tractable as they are easy to set up experimentally. Moreover, from them we can generate other states of motion merely by phase-shifting. Choosing a $\delta \neq 0$ and plotting the $\cos(\omega_i t + \beta_i)$ under the amplitude modulation curves $A_i(t)$ with phase shifts δ and $2\delta + r\pi$, respectively, yields another solution to the equations of motion for the same numerical values of E,α, and R_1. In fact, we exhaust all solutions in this way, for at any physically possible set E,α,R_1 there are no solutions other than those differing by phase constants only, as the quadrature process in the preceding section has shown. Accordingly, the $\delta = 0$ states may serve as representatives of all possible motions.

Emphasizing the $\delta = 0$ states eschews, of course, the awkward problem of determining integration constants for given initial conditions with nonzero velocities. One useful general statement about arbitrary initial conditions may still be made: the three roots of the all-important polynomial $\bar{f}(\bar{p}_1)$ are continuous functions of the initial conditions, whatever these are. Indeed, the roots depend continuously on the coefficients of $\bar{f}$ which are continuous functions of E and α which

in turn are continuous functions of the $\bar{p}$ and $\bar{q}$ and hence, of the initial p and q.

VI. EXPLICIT SOLUTIONS

We proceed to integrate the equations of motion explicitly for $c_1 \neq 0$, referring to the NBS handbook[22] for notation and formulae on elliptic functions. The two cases $R_1 \gtrless R_2$ must be distinguished. The dividing case $R_1 = R_2$ will be discussed separately in Sec. VIII. With initial conditions arbitrary, these three cases can only be recognized after numerical calculation of R_1 and R_2, but for $\delta = 0$ states we can recognize them beforehand by means of (5.10).

If $R_1 < R_2$ (pendulum amplitude modulation a *minimum* at $t = 0$) write Eq. (4.25) as

$$\tfrac{1}{2}[\bar{\gamma}^2(R_2 - R_3)]^{1/2} t = \tfrac{1}{2}(R_2 - R_3)^{1/2} \int_{R_1}^{\bar{p}_1} (-P)^{-1/2}\, d\bar{p}_1, \tag{6.1}$$

using also the abbreviation (4.22). After the substitution NBS (17.4.68),

$$\sin^2\phi = (R_2 - R_3)(\bar{p}_1 - R_1)/(R_2 - R_1)(\bar{p}_1 - R_3), \tag{6.2}$$

(6.1) assumes the canonical form of an elliptic integral of the first kind:

$$\omega_< t = F(\phi \,|\, m_<),$$
$$\omega_< = \tfrac{1}{2}[\bar{\gamma}^2(R_2 - R_3)]^{1/2}, \quad m_< = (R_2 - R_1)/(R_2 - R_3). \tag{6.3}$$

Inversion of (6.3) followed by another use of (6.2) yields[23]

$$\bar{p}_1(t) = \frac{R_1 - R_3 m_< \,\mathrm{sn}^2(\omega_< t \,|\, m_<)}{1 - m_< \,\mathrm{sn}^2(\omega_< t \,|\, m_<)}. \tag{6.4}$$

$A_1(t)$ and $A_2(t)$ now follow from (4.6) and (4.15).

When the integration runs over a half-period of the modulation, $\bar{p}_1$ goes from R_1 to R_2 and ϕ from 0 to 90°. From (6.3) we therefore find the full period $\omega_< T_< /2 = F(\pi/2 \,|\, m_<) = K(m_<)$, or

$$T_< = 4K(m_<)/[\bar{\gamma}^2(R_2 - R_3)]^{1/2} \tag{6.5}$$

The series NBS (17.3.11) shows that

$$T_< = 2\pi/[\bar{\gamma}^2(R_2 - R_3)]^{1/2} + O(m_<), \tag{6.6}$$

with all terms nonnegative since $m_< \geqslant 0$, which implies a lower limit to the period if we let $R_2 \to R_1$ from above.

To integrate (4.30) substitute (6.4) and write first,

$$\beta_1(t) - \beta_1(0) = \int_0^t \frac{c_8 + c_9 \,\mathrm{sn}^2(\omega_< t \,|\, m_<)}{1 - n_{1<} \,\mathrm{sn}^2(\omega_< t \,|\, m_<)} \frac{dt}{2R_1},$$
$$c_8 = c_1 - \epsilon R_1, \quad c_9 = (\epsilon R_3 - c_1) m_<, \quad n_{1<} = m_< R_3/R_1. \tag{6.7}$$

With $\omega_< t = w$ and a decomposition of the integrand into a constant and a partial fraction, the latter yields an elliptic integral of the third kind in its canonical form NBS (17.2.16); finally,

$$\beta_1(t) - \delta = -(c_9/2R_1 n_{1<} \omega_<) \times [\omega_< t - (1 + n_{1<} c_8/c_9) \Pi(n_{1<}; \omega_< t \,|\, m_<)]. \tag{6.8}$$

As Figs. 3 and 4 showed already, the evolution of the pendulum phase $\omega_1 t + \beta_1(t)$ is not synchronized with the amplitude modulation. The system is not strictly periodic, except perhaps under special circumstances. In particular, the four-fold extremum of a $\delta = 0$ state at $t = 0$ does not necessarily recur after one amplitude period.

The integration of (4.31) follows the same pattern except that a different characteristic

$$n_{2<} = m_< (2\alpha - R_3)/(2\alpha - R_1) \tag{6.9}$$

arises from the different denominator. The result, also using (4.32), is

$$\beta_2(t) - (2\delta + r\pi) = -[c_9/(4\alpha - 2R_1) n_{2<} \omega_<] \times [\omega_< t - (1 - n_{2<} c_8/c_9) \Pi(n_{2<}; \omega_< t \,|\, m_<)]. \tag{6.10}$$

If $R_1 > R_2$ (pendulum amplitude *maximum* at $t = 0$), a sign change of the square root in (4.25), the substitution NBS (17.4.69), and minor adaptations of the argument lead to

$$\bar{p}_1(t) = R_1 - (R_1 - R_2)\,\mathrm{sn}^2(\omega_> t \,|\, m_>), \tag{6.11}$$
$$\omega_> = \tfrac{1}{2}[\bar{\gamma}^2(R_1 - R_3)]^{1/2}, \quad m_> = (R_1 - R_2)/(R_1 - R_3),$$
$$T_> = 4K(m_>)/[\bar{\gamma}^2(R_1 - R_3)]^{1/2}, \tag{6.12}$$
$$\beta_1(t) - \delta = -(c_{10}/2R_1 n_{1>} \omega_>) \times [\omega_> t - (1 - n_{1>} c_8/c_{10}) \Pi(n_{1>}; \omega_> t \,|\, m_>)],$$
$$c_{10} = \epsilon(R_1 - R_2), \quad n_{1>} = (R_1 - R_2)/R_1, \tag{6.13}$$
$$\beta_2(t) - (2\delta + r\pi) = -[c_{10}/(4\alpha - 2R_1) n_{2>} \omega_>] \times [\omega_> t - (1 + n_{2>} c_8/c_{10}) \Pi(n_{2>}; \omega_> t \,|\, m_>)], \tag{6.14}$$
$$n_{2>} = (R_2 - R_1)/(2\alpha - R_1).$$

Throughout this section no assumptions about the values of ω_1, ω_2, and γ were made; hence, the formulae remain valid for all systems having a Hamiltonian of the form (4.11), not just the elastic pendulum.

VII. ACCURACY OF THE APPROXIMATION

From the formulae of the preceding section, the final solutions $q_1(t)$ and $q_2(t)$ are obtained by means of Eq. (4.3). We programmed the resultant expressions for computation, using the various procedures given in the NBS handbook,[22] and printed out graphs by an electronic plotter in many cases for which we possessed numerical solutions as described in Sec. III. An archive of such graphs is included in Ref. 9.

When superimposed upon graphs of their numerical counterparts, the slow-fluctuation solutions were nearly always in perfect register over several periods T of the amplitude modulation. Since we graphed on a 1:2 scale, with the bob amplitudes ranging up to some 4 cm and the graph trace no broader than 0.2 mm, we had to conclude that the accuracy of the slow-fluctuation approximation was generally no worse than about 1% in amplitude and at most 10° in phase over time stretches approaching 100 suspension periods.

Discrepancies occurred only under two circumstances. First, the method usually fails in the vicinity of a zero of the suspension amplitude $A_2(t)$. This is the exceptional case set aside until Sec. X.

Second, as the initial amplitudes are increased, errors of a few per cent in the motion peaks begin to appear while the phases still remain accurate. This is to be expected. The slow-fluctuation approximation is exact in the limit of infini-

tesimal amplitudes because in the Hamiltonian (4.11) the coupling term vanishes faster than the other terms. By the same token, the terms *omitted* from that Hamiltonian must soon or late make themselves felt as the amplitudes become larger. We observed that by a pleasant but presumably fortuitous coincidence, the onset of the discrepancies lies in our system at or a little beyond the amplitude levels (2.6) which must not be exceeded anyway in order to guarantee the validity of the basic approximation (2.7). Thus it has no practical importance.

These errors in amplitude develop earlier if the modulation range $|R_2 - R_1|$ is large. Conversely, they remain small at small modulation. In particular, with far off resonance when the modulation is always quite small, we never observed visible error in either amplitude or phase; the comparisons included several rather extreme cases such as the one depicted in Fig. 4, and thereby confirmed our liberal estimate of the $\ll$ sign in the condition (4.10).

In summary, in the elastic pendulum, barring exceptional low-amplitude states (see Sec. X), the slow-fluctuation approximation is virtually as good as an accurate numerical integration in all conditions of practical interest and over a fairly wide range of detuning.

If this exposition sounds long-winded we reiterate that the result came to us as a surprise and prompted us to check it out thoroughly, for we have never seen such accuracy from any of the standard nonlinear approximation methods.

As a first consequence, we may now put the elliptic function developments of Sec. VI aside and proceed to study the elastic pendulum with the aid of the slow-fluctuation formulae in Secs. IV and V virtually as if they were analytically exact.

VIII. PURELY PERIODIC MOTIONS

When a confluence $R_1 = R_2 \neq 0$ occurs the pendulum amplitude $A_1(t)$ remains constant. So does the suspension amplitude $A_2(t)$ on account of the conservation law (4.15); moreover, it cannot vanish, because from the equation of motion (2.10) it follows that $q_2 \equiv 0$ is possible only if also $q_1 \equiv 0$ (no motion at all). If as before, release from rest is adopted as the initial condition, the criterion (5.10) shows that

$$q_{10}^2 = (4\omega_2/\omega_1)\ q_{20}(q_{20} + m\omega_1\epsilon/\gamma) \tag{8.1}$$

is required for the confluence.

At constant, nonvanishing amplitudes the Hamiltonian equations (4.12) and (4.13) can only be satisfied if $\sin(2\bar{q}_1 - \bar{q}_2) \equiv 0$. The two degrees of freedom are therefore strictly synchronized similar to Lissajous figures. Furthermore, the motion is purely harmonic because the phase variations given by Eqs. (4.30) and (4.31) are now constant. With the aid of Eqs. (5.3) and (5.6) the harmonic frequency of the pendulum mode is immediately calculated to be

$$\omega_{1h} = \omega_1 + \dot{\beta}_1 = \omega_1 + (\gamma/2m\omega_1)q_{20} \tag{8.2}$$

in terms of release from rest, while the suspension frequency is $\omega_{2h} = 2\omega_{1h}$.

These constant-amplitude motions were discovered by Witt and Gorelik[1] who called them "purely periodic." The term stuck. Actually, from a more general point of view the periodicity appears subordinate because in more than two degrees of freedom harmonic motions at constant amplitudes still exist but will be strictly synchronized only in exceptional cases.[11]

At exact resonance, $2\omega_1 - \omega_2 = \epsilon = 0$, the condition (8.1) takes the simple form[24]

$$q_{10}^2 = 8q_{20}^2. \tag{8.3}$$

If we release the bob from a point *above* the origin we have $q_{20} > 0$, or $r = 0$ according to Eqs. (5.2). Symmetrically on the other side of the vertical there is another turning point of the motion because of the synchronism. Upon release, the bob will fall, cross the vertical at $q_2 = -q_{20}$ because the suspension motion is simple harmonic, and rise symmetrically on the other side. The orbit is cup-shaped; the frequency from Eq. (8.2) is $\omega_{1h} < \omega_1$ because of the negative γ. If we release from a point with $q_{20} < 0$ or $r = 1$, the bob rises first and goes through a similar but cap-shaped orbit with the increased frequency $\omega_{1h} > \omega_1$ because the second term in Eq. (8.2) is now positive.

Off resonance the two types of motion behave in different ways because the condition (8.1) requires at least that the right-hand side be positive, or

$$q_{20}^2 > -m\omega_1(\epsilon/\gamma)q_{20}. \tag{8.4}$$

For discussion, assume first that $\epsilon/\gamma > 0$. In the elastic pendulum this means that $\epsilon < 0$ (pendulum *longer* than needed for exact resonance), but in a formally similar system with $\gamma > 0$ it would mean $\epsilon > 0$. Now set up a cup motion with $q_{20} > 0$: the requirement (8.4) is fulfilled trivially for any q_{20} however small. The corresponding q_{10} from Eq. (8.1) is also small at first but will always be larger than the value for exact resonance obtained from Eq. (8.3) because of the positive contribution to q_{20} in the parenthesis of Eq. (8.1). Thus the cup motions can be said to develop continuously out of the origin and are flatter than in the resonant case (more saucer than cup). On the other hand, for cap motions with $q_{20} < 0$, the requirement (8.4) implies a minimum amplitude of $|q_{20}| > m\omega_1\epsilon/\gamma$. Let us then start from a pure suspension motion with

$$q_{10} = 0, \quad q_{20} = -m\omega_1\epsilon/\gamma \tag{8.5}$$

[which also has $c_1 = 0$ according to Eq. (5.7), but this is of no concern at the moment]. The cap motions can be developed continuously from this critical suspension motion by releasing the bob from a point still lower than given by Eqs. (8.5), and displaced sideways by a q_{10} satisfying Eq. (8.1) which at first will be quite small. The cap shape is therefore quite peaked at first (like a pierrot hat).

In the opposite case $\epsilon/\gamma < 0$ (pendulum $\epsilon > 0$, length *shorter* than at exact resonance) the system behavior is analogous. The cap motions develop out of the origin and are flatter than at resonance (like a coolie hat); the cup motions develop from a critical suspension motion which is again defined by the release point coordinates (8.5) but with q_{20} now positive, and are deeper than at resonance (like a liqueur glass). In either case the frequency formula (8.2) is not affected by the sign of ϵ.

These various motions are fairly easy to set up in a table-top model. The initial condition (8.1) is not highly critical; evidently the motions neighboring a purely periodic one do not depart far from its cup- or cap-shaped orbit. Thus the purely periodic motions are dynamically stable.

Their stability is *orbital* in the exact sense of Poincaré[25]: for sufficiently small perturbations of the initial condition (8.1) the perturbed orbits in *phase space* will remain within any preassigned, arbitrarily small distance from the unperturbed orbit. For the proof, consider first the polynomial $\bar{f}(\bar{p}_1)$ as defined in Eq. (4.18). Its highest power has a negative coefficient, and in the present case we are given that $R_3 < 0 < R_1 = R_2$; cf. also Eq. (4.23) and the subsequent remarks. It follows that the graph of $\bar{f}$ has the configuration of Fig. 5(a). If then we perturb the initial conditions a little, the roots R_1 and R_2 will in general split with $\bar{f}(\bar{p}_1)$ being *positive between* them, for $\bar{f} < 0$ at all $\bar{p}_1 \geqslant 0$ would leave any physical motion impossible according to Eqs. (4.18) and (4.6). Thus we obtain an amplitude-modulated motion between the new R_1 and R_2,[21] but we can keep R_1 and R_2 as close to their unperturbed location as we please because of the continuous dependence of the roots on the initial conditions. Hence the amplitude $\bar{p}_1(t)$ is stable under the perturbations, and with it $\bar{p}_2(t)$; or equivalently, $A_1(t)$ and $A_2(t)$ are stable.

Now go into the four-dimensional phase space of the p_i and q_i. The phase orbit is given by

$$q_i(t) = A_i \cos(\omega_i t + \beta_i),$$
$$p_i(t) = -m\omega_i A_i \sin(\omega_i t + \beta_i), \quad i = 1,2 \tag{8.6}$$

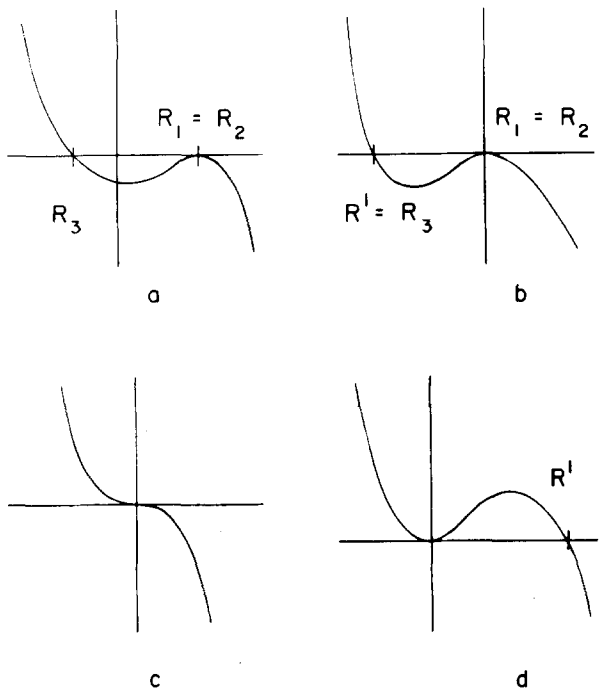

FIG. 5. The four possible configurations of the multiple root of the polynomial (4.18) (schematic). (a) Constant-amplitude motion (orbitally stable). (b) Pure suspension motion in the orbitally stable regime. (c) Critical suspension motion (still orbitally stable). (d) Pure suspension motion in the unstable regime, and "nontrivial $c_1 = 0$" motions which always have the pendulum amplitude finite to start with and zero at the end.

in terms of t as parameter, according to Eqs. (4.3)–(4.6). For a purely periodic motion with constant amplitudes it is a closed curve, and its two projections onto the p_1,q_1 and the p_2,q_2 planes are simply ellipses. After a small perturbation of the initial conditions the projected phase curves must still lie close to these ellipses because of the stability of the A_i. For sufficiently small perturbations the perturbed phase curve will therefore lie as close as we may preassign to the unperturbed one. Q.E.D.

On the other hand, the purely periodic motions are not Liapunov stable, that is, in general the perturbed phase *point* does not remain close to the unperturbed one but will gain distance from it in the course of time. This follows at once from the frequency formula (8.2). Indeed, in the dynamical neighborhood of any one purely periodic motion there are others, but their periods are slightly different. Thus there exist perturbations which will throw a projected phase point from one of the above-mentioned ellipses onto an adjacent ellipse where it now revolves at a *different* rate, and hence must gain a *finite* distance from the unperturbed phase point after a sufficient number of revolutions. Q.E.D.

IX. STABILITY OF THE SUSPENSION MODE

The pure suspension motion $q_1 \equiv 0$ or $\bar{p}_1 \equiv 0$ is a solution to the original equations of motion (2.9) and (2.10) as well as to the slow-fluctuation equations (4.12) and (4.13). Since $\dot{\bar{p}}_1 \equiv 0$ is not possible unless $\bar{f}(\bar{p}_1)$ has a root of (at least) the second order at $\bar{p}_1 = 0$,[21] it is necessary for pure suspension motion that

$$\bar{f}(\bar{p}_1) = \bar{p}_1^2(c_4 - \bar{\gamma}^2 \bar{p}_1) \tag{9.1}$$

[see Eq. (4.18)]. The third root of $\bar{f}$ is then

$$R' = c_4/\bar{\gamma}^2$$

[see also Eq. (4.24)], and is readily expressed with the aid of Eqs. (4.8), (4.20), and (5.4) together with the required $q_{10} = 0$ as

$$R' = m\omega_2(q_{20}^2 - m^2\omega_1^2\epsilon^2/\gamma^2) \tag{9.2}$$

in terms of release from rest. Of course, $|q_{20}| = A_2(t)$ becomes the constant suspension amplitude.

Three regimes with a multiple root at the origin are possible:

$$R' \gtrless 0,$$

as represented in Fig. 5. Under small perturbations they evolve in different ways, but with one important feature in common: Whenever the multiple root at the origin is dissolved there must be one root to the left and two roots to the right of the origin as was proved after Eq. (4.23).

If $R' < 0$, the graph of $\bar{f}$ has the appearance of Fig. 5(b), and R' is seen to be the root previously denoted by R_3. In this regime the motion is orbitally *stable* for the other two roots R_1 and R_2 which after perturbation determine the amplitude modulation will lie as close to the origin as we may want. The pendulum amplitude $A_1(t) = 0$ is therefore stable, and with it the phase orbit, just as in Sec. VIII.

If $R' = 0$, or explicitly,

$$|q_{20}| = m\omega_1|\epsilon/\gamma|, \tag{9.3}$$

the root at $\bar{p}_1 = 0$ is threefold and the graph looks as Fig. 5(c). The motion is still orbitally *stable* because under a small perturbation the roots will split, but again, all remain as close to the origin as we may want.

If $R' > 0$, the graph of $\bar{f}$ has the configuration of Fig. 5(d). In terms of the notation in Sec. IV, $R_3 = R_1 = 0$ and $R' = R_2$. This suspension regime is orbitally *unstable* for the double root at the origin can only split into two with the origin between them; the perturbed pendulum amplitude $\bar{p}_1(t)$ must therefore develop progressively from the new R_1 outwards up to R' and is unstable because an infinitesimal perturbation has resulted in a finite change.

In summary, the pure suspension motion is orbitally unstable iff

$$|q_{20}| > m\omega_1|\epsilon/\gamma|. \tag{9.4}$$

Graphically, the development of instability is heralded by the wandering of a root of $\bar{f}(\bar{p}_1)$ from the left to the right in the sequence of Figs. 5(b)–5(d). Algebraically, we may also go to Eqs. (4.26); noting from Eq. (5.9) that necessarily $c_7 = 0$ if $R_1 = 0$, it is seen that

$$R_1 = 0 \text{ implies } R_2 = (|c_6| - c_6)/2. \tag{9.5}$$

Equation (5.8) shows that c_6 is a holomorphic function of the initial value q_{20}, but evidently R_2 is nonanalytic when $R_1 = 0$: it remains zero up to and including the critical amplitude (9.3) where it makes a kink as c_6 goes through zero, and thereafter continues with the positive value $R_2 = -c_6$.

In the orbitally stable regimes from the critical amplitude (9.3) downwards, the motion is still Liapunov unstable (even though the suspension by itself is an ideal harmonic oscillator!). The phase variation of the suspension motion, $\dot{\beta}_2$, is governed by Eq. (4.31) which contains α, c_1, and $\bar{p}_1$. For a motion in the neighborhood of the pure suspension mode we have $\alpha > 0$ and large, but $c_1 \neq 0$ and small, while $\bar{p}_1$ is small in the orbitally stable case. To the first order in $\bar{p}_1$ we may therefore write

$$\dot{\beta}_2 = [c_1 + (c_1/2\alpha - \epsilon)\bar{p}_1]/4\alpha. \tag{9.6}$$

For the pure suspension mode with $c_1 = 0$ and $\bar{p}_1 \equiv 0$ this vanishes, as it must, because the motion is then harmonic with frequency ω_2. However, it does not in general vanish for neighboring motions which thus take place at somewhat different frequencies.

Assume for definiteness that $R_1 > R_2$; then the exact solution (6.11) applies with $R_1 - R_2$ quite small and therefore $m_>$ small. By a well-known formula, e.g., NBS (16.13.1), $\mathrm{sn}(u|m) \approx \sin u$ holds for small m; also, $\sin^2 u$ can be converted to $(1 - \cos 2u)/2$. The solution (6.11) therefore takes the form

$$\bar{p}_1(t) = \tfrac{1}{2}[(R_1 + R_2) + (R_1 - R_2)\cos 2\omega_> t].$$

Upon insertion of this into Eq. (9.6) it is seen at once that $\dot{\beta}_2$ has a secular term

$$[c_1 + \tfrac{1}{2}(R_1 + R_2)(c_1/2\alpha - \epsilon)]/4\alpha$$

which is a somewhat complicated algebraic function of the initial values q_{10} and q_{20}, cf. Sec. V, but certainly does not vanish identically (in fact, it can be shown to be $\gtrsim 0$ if $\epsilon \lesssim 0$). Hence the frequency ω_2 is augmented by this secular contribution, and the suspension motion cannot be Liapunov stable.

The conspicuous orbital instability of the suspension mode has been a main topic throughout the literature.[1–10] It can be studied by a variety of methods. The above approach through the roots of $\bar{f}(\bar{p}_1)$ seems much the most economical. This use of roots is extensively developed, and reformulated analytically in Ref. 12; the elastic pendulum also appears there again in a broader context. Here we append for contrast a comparison with the "method of the variational equations"[26] which is widely used in nonlinear mechanics.

Regarding $q_2 = q_{20}\cos\omega_2 t$ as a "generating solution," the method represents neighboring motions by

$$q_1 = \xi(t), \quad q_2 = q_{20}\cos\omega_2 t + \eta(t), \tag{9.7}$$

with the deviations ξ and η presumed to be small compared against q_{20}. Insertion of the *ansatz* (9.7) into the exact equation of motion (2.9) yields after omission of a $\xi\eta$ term the "variational equation"

$$\ddot{\xi} + [\omega_1^2 + (2\gamma/m)q_{20}\cos\omega_2 t\,]\xi = 0, \tag{9.8}$$

a Mathieu equation; if we adopt the canonical form

$$\xi'' + (\lambda - 2h^2\cos 2z)\xi = 0,$$

the connection is

$$2z = \omega_2 t, \quad \lambda = (2\omega_1/\omega_2)^2, \quad h^2 = -4\gamma q_{20}/m\omega_2^2. \tag{9.9}$$

Near resonance, $2\omega_1 \approx \omega_2$, the solutions $\xi(t)$ will be unbounded if the (dimensionless) parameter values lie within the $\lambda = 1$ instability region of the Mathieu equation stability chart (e.g., NBS Fig. 20.1) whose stability boundaries are given by $\lambda \approx 1 \pm h^2$. Hence there will be instability if $|h^2| > |\lambda - 1|$, or after insertion of the expressions (9.9) and a little simplification,

$$|q_{20}| > m(\omega_1 - \tfrac{1}{4}\epsilon)|\epsilon/\gamma|. \tag{9.10}$$

This result differs by the $\frac{1}{4}\epsilon$ from the previous criterion (9.4). Given the well-tested accuracy of the slow-fluctuation technique, we submit that its result (9.4) is the correct one of the two. The variational equation technique is, in fact, suspect because it disregards the Liapunov instability of the suspension. Loosely speaking, the cosine in Eq. (9.8) should not have the constant frequency ω_2, but one that depends on ξ and η. More to the point, the deviation $\eta(t)$ of the neighboring motion from the generating one cannot be small because it needs to keep up with a frequency change of q_2 from ω_2 to some slightly different value. Hence the neglect of $\xi\eta$ is not justifiable; there should be an η term accompanying the cosine in Eq. (9.8). It is well known[27] that in equations of the Hill type, $y'' + [\lambda + Q(z)]\,y = 0$, the stability properties are highly sensitive to changes in the periodic function $Q(z)$. See the stability charts for the Whittaker–Hill equation,[28] which is essentially Eq. (9.8) with a second harmonic added to the cosine, or the chart for the Lamé equation,[29] which carries an sn^2 instead of the cosine. In comparison with the Mathieu case the differences border on the drastic. No wonder the disregard of Liapunov instability in the present problem should lead to a spurious $\frac{1}{4}\epsilon$ in formula (9.10), small as this is anyway.[30]

X. EXCEPTIONAL LOW SUSPENSION AMPLITUDES

We now take up the special case excluded since Sec. IV: a suspension amplitude $\bar{p}_2(t)$ or $A_2(t)$ which becomes so small at some time $t = t_1$ that the phase equation (4.28) apparently turns singular. Since the original equations of motion (2.9) and (2.10) are in no way singular, and since the suppression of the "fast fluctuating" terms cannot create a singularity either, we are here faced with an artefact due to the introduction of amplitudes and phases instead of Cartesian coordinates. The specification that an amplitude must not be negative has the consequence that $A_2(t)$ cannot pass through a zero with a smooth tangent at a finite slope; it can only rebound from the zero with the slope reversed in sign. Since the coordinate in the substitution (4.1) must be differentiable, a phase jump by exactly 180° will be needed to compensate exactly for the sign change in the slope of A_2. This is the mathematical origin of the singularity, and of the phase change which was visible already in Fig. 2. A detailed, general discussion[31] of the difficulty is available in Ref. 11. Here we deal with the pendulum is a less formal manner.

Thus, assume that A_2 vanishes at some $t = t_1$. It follows from Eqs. (4.1) and (5.1) that both $q_2(t_1) = 0$ and $\dot{q}_2(t_1) = 0$; to set up such motions we must propel the bob from some position $q_1(t_1)$ on the horizontal through the rest position with any horizontal velocity. This is not easy to do successfully in a table-top experiment except if also $\dot{q}_1(t_1) = 0$ (release from rest) or $q_1(t_1) = 0$ (horizontal hammer blow at the hanging bob). For such initial conditions $A_1(t_1)$ and $\beta_1(t_1)$ can be unambiguously calculated, but $\beta_2(t_1)$ remains indeterminate at first.

Using Eqs. (4.3)–(4.6), the definition of the momentum (4.2) yields at once

$$\dot{A}_2\cos\bar{q}_2 - A_2\ \dot{\beta}_2\sin\bar{q}_2 = 0. \tag{10.1}$$

The same substitutions transform the exact equation of motion (2.10) into

$$\dot{A}_2\sin\bar{q}_2 + A_2\ \dot{\beta}_2\cos\bar{q}_2 = (\gamma/m\omega_2)A_1^2\cos^2\bar{q}_1. \tag{10.2}$$

Now assume for the sake of discussion that $\cos\bar{q}_1(t_1) \neq 0$, i.e., the motion is not being set up by the hammer blow mentioned above. If in Eq. (10.2) we let $t \to t_1$ from the right, A_2 vanishes while $\dot{\beta}_2$ cannot tend to infinity so that $\dot{A}_2\ \sin\bar{q}_2$ must not vanish; in fact, it has the same sign as γ which is negative for the pendulum. Since A_2 can only grow from t_1 onwards, $\dot{A}_2(t_1 +)$ must be positive, and $\sin\bar{q}_2(t_1 +) < 0$ follows. Letting t also approach t_1 in Eq. (10.1), it is seen that $\cos\bar{q}_2(t_1) = 0$, and therefore specifically

$$\sin\bar{q}_2(t_1 +) = -1. \tag{10.3}$$

If on the other hand we make the approach to t_1 from the left, $\dot{A}_2(t_1 -)$ can only be negative and

$$\sin\bar{q}_2(t_1 -) = +1 \tag{10.4}$$

results. Equations (10.3) and (10.4) hold for the pendulum; for a system with positive γ reverse the signs on the right-hand sides. In either case

$$|\beta_2(t_1 +) - \beta_2(t_1 -)| = \pi \tag{10.5}$$

is implied (mod2π of course). This is the mentioned phase jump, demonstrated now in analytic detail rather than colloquially as above. If in the end we were also to let $\cos\bar{q}_1(t_1) \to 0$ the result (10.5) is evidently not affected, but we will have $\dot{A}_2(t_1 \pm) \to 0$; this is the only possibility for the suspension amplitude modulation to reach its zero minimum with a continuous tangent.

Next let us solve Eqs. (10.1) and (10.2) for $\dot{A}_2$ and $A_2\ \dot{\beta}_2$:

$$\dot{A}_2 = (\gamma/m\omega_2)A_1^2\cos^2\bar{q}_1\sin\bar{q}_2,$$

$$A_2\ \dot{\beta}_2 = (\gamma/m\omega_2)A_1^2\cos^2\bar{q}_1\cos\bar{q}_2.$$

Division leads at once to

$$\dot{\beta}_2 = (\dot{A}_2/\sin\bar{q}_2)\times(\cos\bar{q}_2/A_2),$$

and if by l'Hôpital we replace $\cos\bar{q}_2/A_2$ by $-\ddot{\bar{q}}_2\sin\bar{q}_2/\dot{A}_2$, we find

$$\lim\dot{\beta}_2 = -\ddot{\bar{q}}_2(t_1) \quad \text{as } t \to t_1 \pm .$$

Because of $\ddot{\bar{q}}_2 = \omega_2 + \dot{\beta}_2$, this means that

$$\dot{\beta}_2(t) = -\tfrac{1}{2}\omega_2 \quad \text{near } t = t_1. \tag{10.6}$$

Integration in accordance with Eqs. (10.3) and (10.4) yields finally (making also the simplest choice of constants),

$$\beta_2(t) = -\tfrac{1}{2}\omega_2(t + t_1) \mp \tfrac{1}{2}\pi, \quad t \gtrless t_1, \tag{10.7}$$

for t near t_1 (for the pendulum, or $\pm$ for a system with positive γ).

In addition to the phase jump we have here a phase variation so rapid that it entirely vitiates the slow fluctuation approach in the neighborhood of $t = t_1$. Note that the pendulum phase β_1 does not vary fast for the pendulum goes smoothly through a maximum of its energy at $t = t_1$. [In fact, it can easily be shown from the two equations for $\dot{A}_1$ and $\dot{\beta}_1$ analogous to Eqs. (10.1) and (10.2), that $\dot{\beta}_1$ has a double zero at $t = t_1$, but this detail is not needed for our argument.] Hence, in the trigonometric decomposition (4.9) the last term, the one we kept for our approximation, varies near $t = t_1$ as $\cos[\epsilon t + 2\beta_1(t) + \frac{1}{2}\omega_2 t + \text{const}]$, hardly any "more slowly" than the first term which we dropped and which now varies as $\cos(\frac{1}{2}\omega_2 t + \text{const})$.

Of course, one should expect that the rapid variation (10.7) dies out quickly on both sides of the discontinuity as any transient would. This is borne out by comparison of exact numerical integrations with slow-fluctuation solutions computed for the same initial conditions (of release from rest). Again, Ref. 9 contains representative graphs. We first selected some initial conditions involving a fairly large suspension amplitude which we knew from the numerical integrations would be followed by a near-zero of A_2 later on. Figure 1 is a type specimen. The slow-fluctuation solutions in these cases remained in perfect register up to some 2–5 suspension periods from the (exact, numerically found) amplitude minimum; then a phase error develops, the amplitude becomes incorrect, and its minimum is often reached at the wrong time. There are exceptions though. For instance, with $\epsilon = 0$, $q_{10} = 5$ mm, and $q_2 = -16$ mm the amplitude comes down to $A_2 \approx 0.7$ mm after about 11 sec; the slow-fluctuation solution yields a little less, but the minimum lies at the right place and there is no cumulative phase error so that this solution remains in good register throughout the entire next modulation period of $T \approx 22$ sec. On the other hand, when we took the suspension amplitude minimum it-

self as the initial condition, the slow-fluctuation solutions always had a poor start, misrepresented the initial phase transient to a more or less visible degree, developed a visible amplitude error, and often erred seriously in the modulation period T (by 20% in one case).

Evidently the slow-fluctuation solution can always be used safely from the suspension amplitude *maximum* onwards (and backwards) up to 2–5 suspension periods from the minimum, where it must usually be spliced to an accurate numerical solution. On the other side of the minimum another splice can be made, and so forth. The details of the splicing may be delicate, though, if the quoted numerical evidence is an adequate guide. In the light of possible applications (see next section and the Appendix) we believe that this subject deserves a separate, focused study, and we propose to take it up on another occasion.

At all events, note that not the smallness of the amplitude but the sharpness of the phase variation is the important feature. For any state of motion, if the amplitude modulation range $|R_2 - R_1|$ is small compared with $\min(R_1,R_2)$, the phase variations cannot be rapid because little energy is exchanged between the degrees of freedom, and if the suspension amplitude itself is small the validity of the slow-fluctuation method is in no way impaired. In particular, this holds for the constant-amplitude solutions which develop out of the origin with a small suspension amplitude. Thus, the arguments of Sec. VIII stand uncorrected.

The stability arguments of Sec. IX also remain unaffected. If the pure suspension mode is stable, neighboring motions are amplitude modulated with an arbitrarily small range, and there can be no problem even if the suspension amplitude is small to start with. In the unstable case, on the other hand, the unimpaired validity of the slow-fluctuation solutions around a suspension amplitude maximum guarantees that the diagnosis of a *finite* modulation range for neighboring motions will still be correct, even though some of these motions may involve very low suspension amplitude minima.

We must finally ask, what exactly is the phase behavior of the slow-fluctuation solutions at times where $\bar{p}_2(t)$ vanishes? An equivalent question is: suppose we are given a system for which the $\bar{S}$ defined by Eq. (4.11) is the *exact* Hamiltonian,[32] how do the phases behave? The answer is not immediate, for this new system appears exceedingly complex when it is described in terms of the original coordinates q_1 and q_2. Take the trigonometric identity

$$\cos(2\bar{q}_1 - \bar{q}_2) = (\cos^2\bar{q}_1 - \sin^2\bar{q}_1)\cos\bar{q}_2 + 2\sin\bar{q}_1\cos\bar{q}_1\sin\bar{q}_2,$$

and apply the canonical transformation (4.3), (4.4) in reverse to the coupling term in $\bar{S}$; it is found easily that

$$\bar{\gamma}\bar{p}_1(\bar{p}_2/2)^{1/2}\cos(2\bar{q}_1 - \bar{q}_2) = \tfrac{1}{4}\gamma(q_1^2 q_2 - p_1^2 q_2/m^2\omega_1^2 + 2p_1q_1p_2/m^2\omega_1\omega_2). \quad (10.8)$$

Thus the new system comprises most unusual, momentum-dependent couplings which can hardly be understood in straightforward physical terms such as we applied without qualms to the pendulum. New formal arguments are needed.

Assume that $\bar{p}_2$ vanishes at some $t = t_1$. This can only happen for special values of E and α. From the conservation law (4.14) we have first

$$\lim\bar{p}_1 = 2\alpha \quad \text{as } t\to t_1 \pm, \quad (10.9)$$

and from the Hamiltonian (4.11) we have $\bar{S} = E = \omega_1 \lim\bar{p}_1$, whence

$$E = 2\omega_1\alpha. \quad (10.10)$$

The singularity in the phase equation (4.28) is best understood from the equivalent Eq. (4.31). Owing to Eq. (10.9), the denominator $4\alpha - 2\bar{p}_1$ vanishes at $t = t_1$, but use of Eq. (4.19) together with the relation (10.10) shows quickly that the numerator $c_1 - \epsilon\bar{p}_1$ vanishes, too. By l'Hôpital it follows that

$$\dot{\beta}_2(t) = \tfrac{1}{2}\epsilon \quad \text{near } t = t_1; \quad (10.11)$$

compared with the transient (10.6), this one is very mild.

At any rate, the singularity is only apparent, and therefore the original Eq. (4.28) forces us to conclude that $\cos(2\bar{q}_1 - \bar{q}_2) = 0$ at $t = t_1$. In the amplitude equation (4.13) we have then

$$\sin(2\bar{q}_1 - \bar{q}_2) = \pm 1 \quad \text{as } t\to t_1. \quad (10.12)$$

Since $\bar{p}_2$ is essentially A_2^2 and $\dot{\bar{p}}_2$ is $A_2\dot{A}_2$, and since $\dot{A}_2$ again can only be positive/negative to the right/left of t_1, it is seen that in Eq. (10.12) the $\pm$ sign holds as $t\to t_1 \pm$ (for the pendulum analog with a negative γ). Thus there is a certain analogy with Eqs. (10.3) and (10.4). The analogous phase jump occurs in $2\bar{q}_1 - \bar{q}_2$ but is confined to $\bar{q}_2$, of course, because $\dot{\beta}_1$ vanishes at $t = t_1$ according to Eq. (4.27) and is continuous everywhere. This was confirmed by the calculations mentioned above; the suspension phase reversal is quite conspicuous, especially as there is now no notable phase variation right and left of it. Of course, in these numerical studies we did not meet *exact* zeros of $\bar{p}_2$, and so the phase changes did not go abruptly through a full 180°, but smoothly through a little less. The change process is accurately rendered by Eq. (4.31) which in these circumstances has near zeros in its numerator and denominator at slightly different times.

However, at an exact zero of the amplitude, Eq. (4.31) can no longer represent the required phase jump. We must then integrate Eq. (10.11) and choose the constants in accordance with the discontinuity relation (10.12) much as we did above when deriving Eq. (10.7). A complication in the present case is that we must also take account of the phase relation (4.32) which obliges us to provide for two β_2-functions having $r = 0$ and $r = 1$. The result is that

$$\beta_2(t) = \tfrac{1}{2}\epsilon(t + t_1) + 2\beta_1(t_1) + r\pi \mp \tfrac{1}{2}\pi, \quad t \gtrless t_1 \quad (10.13)$$

holds for t near t_1 if $r = 0$, whereas for $r = 1$ the $\mp$ becomes $\pm$ (for γ negative; otherwise reverse both double signs once more). This somewhat opaque formula is best established by direct substitution into Eqs. (10.11) and (10.12).

In summary: (a) the phase reversal through 180° (or nearly) is no more than a transformation artefact; (b) the transient (10.6) in the pendulum is an additional, prominent, physical effect; and (c) the system with coupling (10.8), or Hamiltonian $\bar{S}$, exhibits no such transients over and above the phase reversal.

XI. STATES WITH $c_1 = 0$ (NONTRIVIAL)

If $c_1 = 0$ the polynomial (4.18) always takes the form (9.1) with a double root at $\bar{p}_1 = 0$. We can make $c_1 = 0$ by setting up a pure suspension motion; these are the cases discussed in Sec. IX. However, c_1 can also vanish for initial conditions involving a pendulum amplitude $\bar{p}_1 \neq 0$. The only possible graph for $\bar{f}(\bar{p}_1)$ is then Fig. 5(d). Characteristically, every motion set up with $\bar{p}_1 \neq 0$ and the double zero of $\bar{f}$ at the origin must evolve[21] toward the pure suspension motion $\bar{p}_1 \equiv 0$, either by monotonic pendulum amplitude decrease or by an increase to $\bar{p}_1 = R'$ followed by decrease. The time to reach the pure suspension state is infinite, for the integral (4.21) diverges (logarithmically) if $\bar{f}$ has a double root at the upper limit of integration.

These "nontrivial $c_1 = 0$" motions are impossible to set up in a bench experiment because of the instability of the final suspension motion. The faintest perturbation will split the double root in Fig. 5(d); the pendulum amplitude then goes nearly to zero but eventually returns to $\bar{p}_1 = R'$ with a rather long period. Figure 1 is again typical. We had no passable success either when we experimented with a pendulum of some 7 m length and a heavy bob suspended in a stairwell. Yet the appeal of these motions is not merely esoteric, for they bear the marks of a frequency-doubling device: a more or less mixed pendulum motion is theoretically converted to a pure suspension mode at about twice the frequency.

For explicit treatment we choose $t = 0$ at $\bar{p}_1 = R'$ as before. (In terms of the previous notation, $R_3 = R_2 = 0$ and $R' = R_1$.) If we also assume release from rest, R' is not given by the formula (9.2) which holds only if $q_{10} = 0$. We now have $c_1 = 0$ arising from the condition (5.7), or in full detail

$$q_{10} \text{ arbitrary}, \quad q_{20} = -m\omega_1\epsilon/\gamma \text{ fixed}. \tag{11.1}$$

In the limit as $q_{10} \to 0$ we are again led to the critical suspension motion (8.5), or Fig. 5(c); conversely, the $c_1 = 0$ motions can be said to develop from the latter in branches distinct from the pierrot hat and liqueur glass motions (at $\epsilon/\gamma > 0$ and $\epsilon/\gamma < 0$, resp.) of Sec. VIII. Obviously only one value of r is possible when a $c_1 = 0$ motion is started from rest: $r = 1$ or 0 according as $\epsilon/\gamma > 0$ or < 0; the other value would correspond to a nonzero velocity at $t = 0$. With this in mind, we may now substitute the condition (11.1) into Eq. (5.4) and obtain from Eq. (4.20),

$$R' = c_4/\bar{\gamma}^2 = \tfrac{1}{2}m\omega_1 q_{10}^2, \tag{11.2}$$

for release from rest with $c_1 = 0$.

According to Eqs. (4.25) and (9.1), the pendulum amplitude obeys

$$t = -\int_{R'}^{\bar{p}_1} d\bar{p}_1/\bar{\gamma}\bar{p}_1(R' - \bar{p}_1)^{1/2}.$$

The integral is elementary and yields, after inversion,[33]

$$\bar{p}_1(t) = R'/\cosh^2(\bar{\gamma}R'^{1/2}t/2). \tag{11.3}$$

Remarkably, this does not depend on ϵ. The suspension amplitude is obtained as usual from the conservation law (4.14) or (4.15).

The pendulum phase integration becomes trivial when $c_1 = 0$; from Eq. (4.30),

$$\beta_1(t) = -\tfrac{1}{2}\epsilon t + \delta. \tag{11.4}$$

Thus the pendulum moves at the constant frequency $\omega_1 - \frac{1}{2}\epsilon$; this can be observed in Fig. 1. The suspension phase is different. Using the substitution $dt = -d\bar{p}_1/[\bar{f}(\bar{p}_1)]^{1/2}$, and setting $c_1 = 0$, we find from Eq. (4.31),

$$\beta_2(\bar{p}_1) = \int_{R'}^{\bar{p}_1} \epsilon\, d\bar{p}_1/\bar{\gamma}(4\alpha - 2\bar{p}_1)(R' - \bar{p}_1)^{1/2}. \tag{11.5}$$

The integral is again elementary, but two cases must be distinguished.

Take first $R' < 2\alpha$, or equivalently $\bar{p}_2(0) > 0$ as follows from Eq. (4.14). The integration then yields

$$\beta_2(\bar{p}_1) - (2\delta + r\pi) = -[\epsilon/\bar{\gamma}(2\alpha - R')^{1/2}] \times \arctan[(R' - \bar{p}_1)/(2\alpha - R')]^{1/2}; \tag{11.6}$$

to obtain $\beta_2(t)$, insert the expression (11.3):

$$\beta_2(t) - (2\delta + r\pi) = -[\epsilon/\bar{\gamma}(2\alpha - R')^{1/2}] \times \arctan\{[R'/(2\alpha - R')]^{1/2}\tanh(\bar{\gamma}(R')^{1/2}t/2)\}. \tag{11.7}$$

If in Eq. (4.31) we had integrated from $t = 0$ to $-\infty$ we should have had to change the sign of the $\sqrt{\bar{f}}$ in the substitution, resulting in a sign change of the argument of the arctangent in Eq. (11.6) which in Eq. (11.7) is rendered correctly by writing tanh instead of |tanh|. Thus, Eq. (11.7) is valid as it stands for all t from $-\infty$.

The second case is that $R' = 2\alpha$. According to Eq. (4.20), $R' = c_4/\bar{\gamma}^2 = 2\alpha$ is possible only if $\epsilon = 0$. Equation (4.31) then becomes $\dot{\beta}_2 \equiv 0$ except at $t = 0$, where the denominator also vanishes; the integration has already been done in Eq. (10.13) which applies to just this situation of $\bar{p}_2(0) = 0$, and gives us, using also Eq. (11.4),

$$\beta_2(t) = 2\delta + r\pi \mp \tfrac{1}{2}\pi, \quad t \gtrless 0, \tag{11.8}$$

with r and the double sign as in Eq. (10.13), and t unbounded. So now the suspension phase is constant except for a 180° jump; very nearly this behavior can be observed in Fig. 2. Note how in a $c_1 = 0$ state at exact resonance, both the pendulum and the suspension rigorously move at their normal frequencies ω_1 and ω_2.

The validity of these results requires careful scrutiny. The condition (11.1) shows that for sufficiently large ϵ the suspension amplitude minimum at $t = 0$ will not be so low as to impair the validity of the slow-fluctuation approximation. We can then obtain all solutions by calculating the one for release from rest and providing phase shifts of δ and $2\delta + r\pi$, just as before. At smaller ϵ, the approximation can no more represent the transient (10.6) and fails around $t = 0$. In fact, the various formulae for release from rest, including Eq. (11.2) also must begin to fail. The solutions of the present section still hold *away* from $t = 0$, however. In particular, the universal pendulum amplitude modulation (11.3) can be set up backwards from $t = +\infty$, with the usual phase shifts, to yield all possible solutions down to some moderately small $t > 0$ where a splice to an accurate numerical solution must be made as discussed in the previous section.

For the system having $\bar{S}$ as the *exact* Hamiltonian, all results of this section hold without restriction on ϵ. The totality of solutions is again obtained by applying phase shifts

to the solutions calculated for release from rest. However, the concept of "release from rest" requires a subtle modification. For the actual pendulum, we naturally define "rest" by zero velocity. Velocity is proportional to momentum by the definition (4.2). Thus, the canonical formula (4.4) leads at once to the convenient Eq. (5.1) which was the base for studying the initial conditions. In the system with $\bar{S}$ the momentum is not defined by Eq. (4.2). From the Hamiltonian resolvent equations $\partial S/\partial p_i = \dot{q}_i$ and the interaction (10.8), it is seen that there is a fairly complicated momentum–velocity relation. Consequently we cannot go from Eq. (4.4) to the tractable Eq. (5.1); we must formulate the initial conditions directly in terms of the momentum (4.4), not of the velocity. Correspondingly, "rest" becomes "canonical rest," defined by zero canonical momentum.[34] With this proviso, all our formulae for release from rest remain valid for the $\bar{S}$-system.

Canonical rest is not easy to visualize. Loosely speaking, it is a kind of wobble about a fixed mean position, cf. Ref. 34. Clockwise and anticlockwise types of wobble must be admitted jointly, of course; this explains why in Eq. (11.8) both values of r are possible even for release from rest.

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APPENDIX: SECOND-HARMONIC GENERATION

When the equations of motion (4.12) and (4.13) and the combined-phase equation (4.29) are written in terms of amplitudes with the aid of the relations (4.6), they become

$$\dot{A}_1 = (\gamma/2m\omega_1)A_1A_2\sin\bar{\bar{q}}_1, \tag{A1}$$

$$\dot{A}_2 = -(\gamma/4m\omega_2)A_1^2\sin\bar{\bar{q}}_1, \tag{A2}$$

$$\dot{\bar{\bar{q}}}_1 = \epsilon + (\gamma/m)(A_2/\omega_1 - A_1^2/4\omega_2A_2)\cos\bar{\bar{q}}_1, \tag{A3}$$

where

$$\bar{\bar{q}}_1 = 2\bar{q}_1 - \bar{q}_2.$$

Equations (A1)–(A3) are isomorphic[35] to the equations governing second-harmonic generation in nonlinear optics.[36] The differences are minor. The optical equations describe the *space* variation of a wave propagating along Ox; with kx corresponding to $-\omega t$, replace our $\omega_i t$ by $k_i x$ and reverse the signs of $\bar{\bar{q}}_1$ and of all phase functions and phase constants. Also, dispersion in the medium generally forbids inverse proportionality between ω and k ("phase mismatch"). While $\Delta k = 2k_1 - k_2$ corresponds precisely to $-\epsilon$, the ω_i in the denominators of Eqs. (A1)–(A3) need to be properly related to the k_i. As a result, there are scale factors between our A_i and the optical field amplitudes E_i; they are best found by comparing our conservation law (4.15) with its optical analog (which is called a Manley–Rowe relation[37]).

The theory of second optical harmonics[36] goes back to a pioneering paper by Bloembergen and collaborators.[38] It is strictly analogous to a slow-fluctuation approximation because all combination frequencies except the near-resonant one are neglected. It has not been deliberately formulated and explored in Hamiltonian terms.[39] Thus, the present study has further insights and details to offer. In particular, a complete classification of all solutions now exists: explicit solutions, including phases, are available which can be linked to transparent initial conditions; complete power conversion is seen to be impossible because of the instability of the desired final state; and exact phase coherence obtains (despite "mismatch"!) in the purely periodic solutions, which are orbitally stable and to some extent tunable according to Eq. (8.2).

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[23]A very similar formula was derived by Heinbockel and Struble, Eq. (17) of Ref. 7, from a not very transparent iteration-perturbation approach.

[24]In passing, we quote from Ref. 9 that Eq. (8.3) and the frequency formula (8.2) also result when one seeks (to the first order in γ) purely periodic solutions of the original equations of motion (2.9) and (2.10) (at exact resonance) by means of the standard perturbation method of Poincaré; see, for example, E. Leimanis and N. Minorski, *Dynamics and Nonlinear Mechanics* (Wiley, New York, 1958), Sec. 2.2.

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[30]Munakata, Ref. 29, gives examples of much larger errors. On linear approximations in general, see also Pars, Ref. 4, Chap. 19. Liapunov instability has usually not been considered in such problems; it seems to have rather neat clues to offer.

[31]Such phase jumps have received little attention in the literature although they could be important in some applications. Chapter 8 of Ref. 9 may have been the first serious attempt at a deeper understanding. An interesting case is discussed in some detail by A.H.P. van der Burgh, J. Sound Vib. **49**, 93 (1976).

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[33]This amplitude modulation square has the same waveform as the classical soliton of the Korteweg–deVries equation; see, for example, G. B. Whitham, *Linear and Nonlinear Waves* (Wiley, New York, 1974), Sec. 13.12. The underlying differential equation is formally the same as our Eq. (4.18).

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On the conservation laws in the theory of fields in Finsler spaces

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Some conservation laws are obtained for the fields in some special Finsler spaces such as scalar curvature space, locally Minkowski space, etc.

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I. INTRODUCTION

As is well known,[1,2] Finsler space is a metric space in which the line-element (x, y), instead of the point (x), is chosen as the independent variable, the vector $y(=y^\lambda;\ \lambda=1, 2, 3, 4)$ being regarded, from a physical point of view, as the internal variable associated with each point $x(=x^\kappa;\ \kappa=1, 2, 3, 4)$. From this, it may be said that Riemann space is a point-space, while Finsler space is a line-element-space. In other words, Finsler space is considered the higher order space of order one from the standpoint of the theory of higher order spaces[2] [see Appendix, Subsec. (1)]. Therefore, the y-dependence characterizes essentially the Finslerian field and this y-dependence has been combined with the concept of "anisotropy" or "nonlocality" (cf. Refs. 3 and 4), where the vector y is expected to supply new internal degrees of freedom. In fact, it has been shown that the so-called nonlocal field theory advanced by Yukawa,[5] especially bilocal field theory, can be considered by means of Finsler geometry.[3,4] Along this line, it may be said epistemologically that the Finslerian field corresponds to a nonlocal field obtained by attaching the vector y to each point (x) of a local (i.e., Riemannian) field.

On the other hand, within the theory of gravitational fields in Finsler spaces,[6,7] there arise many interesting and peculiar features caused by the y-dependence and such structurological problems as the field equations, the conservation laws, etc., have been investigated by analogy with Einstein's theory of gravitational field.[8] And on the side of Finsler geometry, the theory of special Finsler spaces has been extensively developed by Matsumoto[1] and his school. Therefore, under these circumstances, it becomes necessary now to consider those problems in more detail by means of the theory of special Finsler spaces. So in this paper, taking account of the y-dependence, we shall focus our attention on the conservation laws for the fields in some special Finsler spaces such as scalar curvature space, locally Minkowski space, etc., and obtain some new conservation laws.

Mathematical preliminaries needed in this paper are summarized in the Appendix.

II. CONSERVATION LAWS—I (SCALAR CURVATURE SPACE)

It goes without saying that in order to obtain conservation laws, it is necessary to take notice of the curvature tensor, as in Einstein's theory,[8] because the field equation is written in terms of the curvature tensor. Among three kinds of curvature tensors of Finsler space [see Appendix, Subsec. (4)], the most Riemann-like one is, of course, the third curvature tensor $R^\kappa_{\nu\lambda\mu}$ (A12). Concerning this, it is easily seen[6] from the Bianchi identity (A23), by contraction of α and κ, that the Ricci tensor $R_{\mu\lambda}(\equiv R^\alpha_{\mu\lambda\alpha})$ becomes, in general, nonsymmetric due to the terms $\{C^\alpha_{\mu\beta}R^\beta_{\lambda\alpha}\}$, where $R^\beta_{\lambda\alpha}$ is the torsion tensor (A13). This is one "non"-Riemannian aspect caused by the y-dependence. Now, in order to proceed to the conservation laws with respect to $R^\kappa_{\nu\lambda\mu}$, it is necessary to find a certain kind of Finslerian tensor constructed by $R^\kappa_{\nu\lambda\mu}$ whose divergence vanishes, as the divergence of the Riemannian Einstein tensor vanishes. For that purpose, we should take account of another Bianchi identity (A24). Then, first, contracting α, λ and then β, κ, we can obtain the following equation[1,6]:

$$(R^\kappa{}_\mu - \tfrac{1}{2}R\delta^\kappa_\mu)_{|\kappa} + \tfrac{1}{2}g^{\beta\kappa}\{P_\beta{}^\lambda{}_{\mu\gamma}R^\gamma_{\lambda\kappa} + P_\beta{}^\lambda{}_{\lambda\gamma}R^\gamma_{\kappa\mu} + P_\beta{}^\lambda{}_{\kappa\gamma}R^\gamma_{\mu\lambda}\} = 0\,, \tag{2.1}$$

where $P_\beta{}^\lambda{}_{\mu\gamma}$ denotes the second curvature tensor (A11), and $R^\kappa{}_\mu \equiv R_{\lambda\mu}g^{\kappa\lambda}$, $R \equiv R^\kappa{}_\mu\delta^\mu_\kappa$. Therefore, it is found from (2.1) that the divergence of the Finslerian Einstein tensor $(R^\kappa{}_\mu - \frac{1}{2}R\delta^\kappa_\mu)$ does not vanish. So, secondly, we must here impose some special conditions on (2.1) in order to obtain the Finslerian conservation laws, which will be actually done in the following. By the way, if there exist some simple relation between $P_\nu{}^\kappa{}_{\lambda\mu}$ and $R^\kappa_{\lambda\mu}$ or $P_\nu{}^\kappa{}_{\lambda\mu}$ and $C^\kappa_{\lambda\mu}$, then (2.1) and the antisymmetric part of $R_{\mu\lambda}$ may be combined with each other, but this is still an open problem.

We shall first consider a Finsler space with scalar curvature in Berwald's sense.[1,9] In this case, Berwald's curvature tensor $H_\nu{}^\kappa{}_{\lambda\mu}$ [(A19) and (A20)] is stipulated as

$$H_{\nu\mu\lambda\kappa}y^\nu X^\mu y^\lambda X^\kappa = K(g_{\nu\lambda}g_{\mu\kappa} - g_{\nu\kappa}g_{\mu\lambda})y^\nu X^\mu y^\lambda X^\kappa\,, \tag{2.2}$$

where the sectional curvature $K(x, y, X)$ is assumed, by definition, not to depend on a tangent vector X^κ at every supporting element (x, y). [The form of $H_{\nu\mu\lambda\kappa}$ itself in this case is given by (A21)]. The following equations are known as the necessary and sufficient conditions for this case (cf. Refs. 1 and 10):

$$R_{\mu\lambda\kappa} = \tfrac{1}{3}\mathfrak{A}_{\lambda\kappa}\{(L^2K|_\lambda + 3Ky_\lambda)h_{\mu\kappa}\}\,,$$

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or

$$R_{\mu 0\kappa}=KL^2h_{\mu\kappa}, \tag{2.3}$$

where $h_{\mu\kappa}$ denotes the angular metric tensor (A3). Then, substituting this torsion $R_{\mu\lambda\kappa}$ into (2.1) and taking account of the relation (A18), we can have (cf. Ref. 10)

$$\{R^{\kappa}{}_{\mu}-\tfrac{1}{2}R\delta^{\kappa}_{\mu}+B_{\nu}(S^{\nu}{}_{\mu}-\tfrac{1}{2}S\delta^{\nu}_{\mu})y^{\kappa}\}_{|\kappa} - B_{\nu|0}(S^{\nu}{}_{\mu}-\tfrac{1}{2}S\delta^{\nu}_{\mu})=0, \tag{2.4}$$

where $B_{\nu}=(1/3L)\partial(KL^3)/\partial y^{\nu}$, and $S_{\nu\mu\lambda\kappa}$ is the first curvature tensor (A10) and $S^{\nu}{}_{\mu}\equiv S_{\alpha}{}^{\beta}{}_{\mu\beta}g^{\alpha\nu}$, $S\equiv S^{\nu}{}_{\mu}\delta^{\mu}_{\nu}$. Therefore, at this stage, we can say the following: If $S^{\nu}{}_{\mu}-\frac{1}{2}S\delta^{\nu}_{\mu}=0$ or $B_{\nu}=0$, then (2.4) reduces to a simple conservation law

$$(R^{\kappa}{}_{\mu}-\tfrac{1}{2}R\delta^{\kappa}_{\mu})_{|\kappa}=0, \tag{2.5}$$

which is quite similar to the Riemannian one. By the way, since the condition $(S^{\nu}{}_{\mu}-\frac{1}{2}S\delta^{\nu}_{\mu}=0)$ is reduced to $S^{\nu}{}_{\mu}=0$ and our case is four-dimensional, $S_{\nu}{}^{\kappa}{}_{\lambda\mu}$ itself vanishes for this case, as has been proved by Matsumoto[11]; if $B_{\nu|0}=0$, then a new conservation law such as

$$\{R^{\kappa}{}_{\mu}-\tfrac{1}{2}R\delta^{\kappa}_{\mu}+B_{\nu}(S^{\nu}{}_{\mu}-\tfrac{1}{2}S\delta^{\nu}_{\mu})y^{\kappa}\}_{|\kappa}=0 \tag{2.6}$$

can be obtained from (2.4). The term $\{B_{\nu}(S^{\nu}_{\mu}-\frac{1}{2}S\delta^{\nu}_{\mu})y^{\kappa}\}$ may play, in a certain sense, a role of sink or source for the (Finslerian) gravitational field.

Next, we shall consider a constant curvature space, where the above-introduced scalar curvature $K(x,y)$ becomes a nonzero constant. In this case, (2.3) is rewritten as, by virtue of (A3) and $\mathfrak{A}_{\lambda\kappa}\{y_{\lambda}l_{\mu}l_{\kappa}\}=0$,

$$R_{\mu\lambda\kappa}=K(y_{\lambda}g_{\mu\kappa}-y_{\kappa}g_{\mu\lambda}), \tag{2.7}$$

and (2.4) is reduced to, because of $B_{\nu}=Ky_{\nu}$, $B_{\nu|0}=0$ and $y_{\nu}S^{\nu}_{\mu}=0$ [cf. (A8) and (A10)],

$$(R^{\kappa}{}_{\mu}-\tfrac{1}{2}R\delta^{\kappa}_{\mu}-\tfrac{1}{2}KSy_{\mu}y^{\kappa})_{|\kappa}=0, \tag{2.8}$$

which has often been cited as a typical example of the Finslerian conservation law (cf. Refs. 1, 6, 7, and 10). Further, it is known[1,6,7] that the Ricci tensor becomes symmetric, because the terms $\{C^{\alpha}_{\mu\beta}R^{\beta}_{\lambda\alpha}\}$ disappear due to (2.7) and (A8), and that Berwald's curvature tensor is given by [see Appendix, Subsec. (5)]

$$H_{\nu\mu\lambda\kappa}=K(g_{\nu\lambda}g_{\mu\kappa}-g_{\nu\kappa}g_{\mu\lambda}). \tag{2.9}$$

Equation (2.9) is often used as another definition of the constant curvature of Finsler space.

Thirdly, if the third curvature tensor $R_{\nu\mu\lambda\kappa}$ itself is given in a form similar to (2.9), i.e.,

$$R_{\nu\mu\lambda\kappa}=A(g_{\nu\lambda}g_{\mu\kappa}-g_{\nu\kappa}g_{\mu\lambda}), \tag{2.10}$$

where A is a nonzero constant, then $S_{\nu\mu\lambda\kappa}=0$ and $P_{\nu\mu\lambda\kappa}=P_{\nu\mu\kappa\lambda}$ hold good [see (A18)], as has been proved by Akbar-Zadeh.[12] In this case, both (2.6) and (2.8) reduce to the same form as (2.5). Equation (2.10) has a form similar to the case of constant curvature of Riemann space, but as mentioned above, the constant curvature of Finsler space is defined by use of Berwald's curvature [see (2.9)].

Now, as mentioned in the Appendix, Subsecs. (3) and (4), the coefficients of connection $F^{\kappa}_{\mu\lambda}$ and $C^{\kappa}_{\mu\lambda}$ are usually assumed to be symmetric with respect to the lower indices. But if the torsion $T^{\kappa}_{\mu\lambda}$ (A14) is assumed to appear, as an example of a more generalized space than Cartan's, then the Bianchi identity (A24) is generalized to (A25). Therefore, starting from (A25), we can repeat the same procedure as the above in order to obtain some new conservation laws for this case. But that is too lengthy to describe here, so that only one new conservation law will be shown in the following. Now, the most interesting and fascinating special form of $T^{\kappa}_{\mu\lambda}$ hitherto known seems to be the following:

$$T^{\kappa}_{\mu\lambda}=\delta^{\kappa}_{\mu}\alpha_{\lambda}-\delta^{\kappa}_{\lambda}\alpha_{\mu}, \tag{2.11}$$

where $\alpha_{\lambda}(x)$ is an arbitrary vector and the coefficient of connection $F^{\kappa}_{\mu\lambda}$ [cf. (A5)] is assumed to depend on x alone. Namely, in this case, the space becomes a Wagner space.[13] Then, under the assumptions of (2.10) and $\alpha_{\lambda}=\partial\alpha/\partial x^{\lambda}$ [$\alpha(x)$ is a scalar], we can obtain from (A25) another new conservation law as follows:

$$(R^{\kappa}{}_{\mu}-\tfrac{1}{2}R\delta^{\kappa}_{\mu}+12A\alpha\delta^{\kappa}_{\mu})_{|\kappa}=0, \tag{2.12}$$

which is a generalization of (2.5).

As for the above-mentioned torsion $T^{\kappa}_{\mu\lambda}$ depending on only x, it has been combined with spin or spin-angular momentum within the Einstein-Cartan theory[14] or the theory of new general relativity,[15] where some "non"-Riemannian features carried by $T^{\kappa}_{\mu\lambda}$ have been noticed. On the other hand, from a more geometrical viewpoint, if the conformal transformation $\overline{L}=L\exp\sigma$ [L is the fundamental function and $\sigma(x)$ is a scalar] is applied to $T^{\kappa}_{\mu\lambda}$ of (2.11), then it is transformed into[13]

$$\overline{T}^{\kappa}_{\mu\lambda}=T^{\kappa}_{\mu\lambda}+\delta^{\kappa}_{\mu}\sigma_{\lambda}-\delta^{\kappa}_{\lambda}\sigma_{\mu}, \tag{2.13}$$

where $\sigma_{\mu}=\partial\sigma/\partial x^{\mu}$. Therefore, if $\alpha_{\lambda}=\partial\alpha/\partial x^{\lambda}$ and $\alpha+\sigma=0$ are assumed, the torsion $\overline{T}^{\kappa}_{\mu\lambda}$ of (2.13) vanishes and the torsion $T^{\kappa}_{\mu\lambda}$ of (2.11) itself is written in terms of the conformal scalar $\sigma(x)$ (cf. Ref. 7). Namely, in this case, the non-Riemannian characteristics may be related to the conformal scalar σ. This kind of thing has often been considered in connection with Dirac's conformally invariant theory (cf. Ref. 16).

III. CONSERVATION LAWS—II (LOCALLY MINKOWSKI SPACE)

As mentioned in Sec. I, the y-dependence characterizes essentially the Finslerian field. Emphasizing this, if we assume that the fundamental function L or the metric tensor $g_{\lambda\kappa}$ (A2) does not depend on x, then we can obtain a locally Minkowski space prescribed by such geometrical conditions as $C_{\mu\lambda\kappa|\nu}=0$ and $R_{\nu\mu\lambda\kappa}=0$.[1,7] In this case, since the second curvature tensor $P_{\nu\mu\lambda\kappa}$ (A11) vanishes too, only the first curvature tensor $S_{\nu\mu\lambda\kappa}$ (A10) appears. Therefore, we must consider the conservation laws with respect to $S_{\nu\mu\lambda\kappa}$. Concerning this, in the same manner that Eq. (2.1) was obtained, contracting the Bianchi identity (A22), we can obtain one conservation law as follows (cf. Refs. 1, 6, and 7):

$$(S^{\kappa}{}_{\mu}-\tfrac{1}{2}S\delta^{\kappa}_{\mu})|_{\kappa}=0, \tag{3.1}$$

which corresponds to (2.5). Here, if we write the field equation in the form

$$S_{\mu\lambda} - \tfrac{1}{2}Sg_{\mu\lambda} = \tau_{\mu\lambda} \quad (\tau_\lambda^\kappa|_\kappa = 0), \tag{3.2}$$

we can obtain $-S = \tau_{\mu\lambda} g^{\mu\lambda}$ and $-\frac{1}{2}S = \tau_{\mu\lambda} l^\mu l^\lambda$ by multiplying (3.2) by $g^{\mu\lambda}$ and $l^\mu l^\lambda$ ($l^\lambda = y^\lambda/L$, unit vector), respectively. Therefore, the energy-momentum tensor $\tau_{\mu\lambda}$ must satisfy the relation $\tau_{\mu\lambda}(g^{\mu\lambda} - 2l^\mu l^\lambda) = 0$, from which $\tau_{\mu\lambda}$ may be given by $\tau_{\mu\lambda} = g_{\mu\lambda} + 2l_\mu l_\lambda$ (cf. Ref. 6).

On the other hand, in the locally Minkowski space there exists no condition imposed on the coefficient of connection $F^\kappa_{\mu\lambda}$ except that $F^\kappa_{\mu\lambda}$ becomes a function of x alone owing to the condition $C_{\mu\lambda\kappa|\nu} = 0$ and satisfies another condition $R_{\nu\mu\lambda\kappa} = 0$, so that the torsion $T^\kappa_{\mu\lambda}$ (A14) can be introduced as in Wagner space [cf. (2.11)]. However, we cannot obtain any conservation law with respect to $S_{\nu\mu\lambda\kappa}$ which includes $T^\kappa_{\mu\lambda}$, because there is no Bianchi identity containing both $S_\nu{}^\kappa{}_{\lambda\mu|\iota}$ (or $S_\nu{}^\kappa{}_{\lambda\mu}|_\iota$) and $T^\kappa_{\mu\lambda}$ simultaneously.

These considerations about the y-dependence are analogous to the case of tangent space, because the tangent space is regarded as a Riemann space at a fixed point and its spatial structure is described by $g_{\lambda\kappa}(y)$, $C_{\mu\lambda\kappa}(y)$, and $S_{\nu\mu\lambda\kappa}(y)$, where $C_{\mu\lambda\kappa}(y)$ becomes equal to the Christoffel three-index symbol derived from $g_{\lambda\kappa}(y)$ and $S_{\nu\mu\lambda\kappa}(y)$ to the Riemannian curvature tensor. Therefore the conservation law (3.1) and the field equation (3.2) can be adapted to this case. However, it should be remarked that the vector y obeys only a linear transformation, so that the tangent space is considered a very restricted Riemann space (cf. Ref. 1).

IV. CONCLUSION

In this paper, we have obtained some conservation laws for the fields in some special Finsler spaces such as scalar curvature space, locally Minkowski space, etc. In Sec. II, the third curvature tensor $R_{\nu\mu\lambda\kappa}$ (A12) has been taken into account and in Sec. III, the first curvature tensor $S_{\nu\mu\lambda\kappa}$ (A10) has been taken up. However, any valuable conservation law with respect to the second curvature tensor $P_{\nu\mu\lambda\kappa}$ (A11) cannot be obtained; this is still an open problem. This seems to be very difficult, because in the Bianchi identity containing $P_\nu{}^\kappa{}_{\lambda\mu|\iota}$ or $P_\nu{}^\kappa{}_{\lambda\mu}|_\iota$, there always exists $R_\nu{}^\kappa{}_{\lambda\mu}$ or $S_\nu{}^\kappa{}_{\lambda\mu}$ and it is necessary to specialize both $P_\nu{}^\kappa{}_{\lambda\mu}$ and $R_\nu{}^\kappa{}_{\lambda\mu}$ or $S_\nu{}^\kappa{}_{\lambda\mu}$ simultaneously. Concerning the above-mentioned conservation laws, we should find some considerable effects of them in future.

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APPENDIX

(1) In the higher-order space of order $M(=1, 2, 3, \cdots)$,[2] an arc length (s) along a curve $x^\kappa = x^\kappa(t)$ is given by the integral

$$s = \int L(x, x^{(1)}, x^{(2)}, x^{(3)}, \ldots, x^{(M)})\, dt, \tag{A1}$$

where L denotes the fundamental function and $x^{(\alpha)} = d^\alpha x/dt^\alpha$. Finsler space is, therefore, regarded as the higher-order space of order one, but the vector y is, in general, not necessarily chosen as $x^{(1)}$ [see also Appendix, Subsec. (2)].

(2) The metric tensor $g_{\lambda\kappa}(x, y)$ of Finsler space is defined by

$$g_{\lambda\kappa} = \tfrac{1}{2}\partial^2 L^2/\partial y^\lambda \partial y^\kappa, \text{ or } L^2 = g_{\lambda\kappa} y^\kappa y^\lambda, \tag{A2}$$

where $L(x, y)$ is the fundamental function and is assumed to be positively homogeneous of degree one with respect to y. And the angular metric tensor $h_{\lambda\kappa}(x, y)$ is defined by

$$h_{\lambda\kappa} = g_{\lambda\kappa} - l_\lambda l_\kappa (= L\partial^2 L/\partial y^\lambda \partial y^\kappa), \tag{A3}$$

where $l_\lambda = y_\lambda/L$, $l_\lambda l^\lambda = 1$ (unit vector). It should be remarked that $g_{\lambda\kappa}$ becomes positively homogeneous of degree 0 in y [i.e., $g_{\lambda\kappa}(x, ay) = g_{\lambda\kappa}(x, y)$ for a positive constant a] and is very singular at $y = 0$, so that $g_{\lambda\kappa}$ cannot be expanded in powers of y. From the standpoint of general theory in Matsumoto's sense,[1] the vector y, which satisfies only a linear transformation, is not necessarily chosen as $x^{(1)}$ [cf. (A1)], so that the relative length (of a vector V) $g_{\lambda\kappa}(x, y)V^\kappa V^\lambda$ differs, in general, from the absolute length $g_{\lambda\kappa}(x, x^{(1)})V^\kappa V^\lambda$.[18]

(3) The absolute differential of an arbitrary vector $V^\kappa(x, y)$ is introduced by

$$DV^\kappa = dV^\kappa + \Gamma^\kappa_{\mu\lambda} V^\mu dx^\lambda + C^\kappa_{\mu\lambda} V^\mu dy^\lambda, \tag{A4}$$

where $\Gamma^\kappa_{\mu\lambda}(x, y)$ and $C^\kappa_{\mu\lambda}(x, y)$ mean the Finslerian coefficients of connection serving as two kinds of gauge fields.[19] From (A4), by replacing dy with Dy, the covariant derivatives are defined as follows[1]:

$$\begin{aligned} DV^\kappa &= (V^\kappa|_\lambda)dx^\lambda + (V^\kappa|_\lambda)Dy^\lambda; \\ V^\kappa|_\lambda &= \frac{\delta V^\kappa}{\delta x^\lambda} + F^\kappa_{\mu\lambda} V^\mu, \\ V^\kappa|_\lambda &= \frac{\partial V^\kappa}{\partial y^\lambda} + C^\kappa_{\mu\lambda} V^\mu, \end{aligned} \tag{A5}$$

where $\delta/\delta x^\lambda = \partial/\partial x^\lambda - N^\nu_\lambda \partial/\partial y^\nu$, $F^\kappa_{\mu\lambda} = \Gamma^\kappa_{\mu\lambda} - N^\nu_\lambda C^\kappa_{\mu\nu}$ and $N^\kappa_\lambda = y^\mu F^\kappa_{\mu\lambda} (\equiv F^\kappa_{0\lambda})$; the symbol 0 means the contraction by y. Concerning $C_{\mu\lambda\kappa} (\equiv C^\nu_{\mu\kappa} g_{\nu\lambda})$, it is assumed to be symmetric for all the indices, so that

$$C_{\mu\lambda\kappa} = \tfrac{1}{2}\partial g_{\mu\lambda}/\partial y^\kappa = \tfrac{1}{2}\partial^3 L^2/\partial y^\mu \partial y^\lambda \partial y^\kappa \tag{A6}$$

holds good by virtue of the metric conditions $Dg_{\lambda\kappa} = 0$, i.e.,

$$\begin{aligned} \frac{\partial g_{\lambda\kappa}}{\partial x^\mu} &= \Gamma_{\lambda\kappa\mu} + \Gamma_{\kappa\lambda\mu}, \\ \frac{\partial g_{\lambda\kappa}}{\partial y^\mu} &= C_{\lambda\kappa\mu} + C_{\kappa\lambda\mu}, \end{aligned} \tag{A7}$$

where $\Gamma_{\mu\lambda\kappa} \equiv \Gamma^\nu_{\mu\kappa} g_{\nu\lambda}$. Of course, $g_{\lambda\kappa|\mu} = 0$ and $g_{\lambda\kappa}|_\mu = 0$. Since $C_{\mu\lambda\kappa}$ becomes positively homogeneous of degree -1 in y, the following relations hold good:

$$C_{\mu\lambda\kappa} y^\mu = C_{\mu\lambda\kappa} y^\lambda = C_{\mu\lambda\kappa} y^\kappa = 0. \tag{A8}$$

As for $\Gamma^\kappa_{\mu\lambda}$ and $F^\kappa_{\mu\lambda}$, they are usually assumed to be symmetric in μ and λ, but in Wagner space the torsion $T^\kappa_{\mu\lambda}$ (A14) appears (see also Sec. II).

(4) In Finsler space there appear, in general, three

kinds of curvature tensors ($S_{\nu}{}^{\kappa}{}_{\lambda\mu}, P_{\nu}{}^{\kappa}{}_{\lambda\mu}, R_{\nu}{}^{\kappa}{}_{\lambda\mu}$) and five kinds of torsion tensors ($R^{\kappa}_{\lambda\mu}, T^{\kappa}_{\lambda\mu}, C^{\kappa}_{\lambda\mu}, P^{\kappa}_{\lambda\mu}, S^{\kappa}_{\lambda\mu}$). They are introduced through the following Ricci identities:

$$\begin{aligned} &V^{\kappa}{}_{|\lambda|\mu} - V^{\kappa}{}_{|\mu|\lambda} = V^{\nu}R_{\nu}{}^{\kappa}{}_{\lambda\mu} - V^{\kappa}{}_{|\nu}T^{\nu}_{\lambda\mu} - V^{\kappa}\big|_{\nu}R^{\nu}_{\mu\lambda}\,, \\ &V^{\kappa}{}_{|\lambda}\big|_{\mu} - V^{\kappa}\big|_{\mu|\lambda} = V^{\nu}P_{\nu}{}^{\kappa}{}_{\lambda\mu} - V^{\kappa}{}_{|\nu}C^{\nu}_{\lambda\mu} - V^{\kappa}\big|_{\nu}P^{\nu}_{\mu\lambda}\,, \\ &V^{\kappa}\big|_{\lambda}\big|_{\mu} - V^{\kappa}\big|_{\mu}\big|_{\lambda} = V^{\nu}S_{\nu}{}^{\kappa}{}_{\lambda\mu} - V^{\kappa}\big|_{\nu}S^{\nu}_{\lambda\mu}\,. \end{aligned} \tag{A9}$$

Their definitions are given as follows:
first curvature tensor:

$$S_{\nu}{}^{\kappa}{}_{\lambda\mu} = \mathfrak{A}_{\lambda\mu}\{\partial C^{\kappa}_{\iota\lambda}/\partial y^{\mu} + C^{\iota}_{\nu\lambda}C^{\kappa}_{\iota\mu}\}, \tag{A10}$$

second curvature tensor:

$$\begin{aligned} P_{\nu}{}^{\kappa}{}_{\lambda\mu} = {}&\partial F^{\kappa}_{\iota\lambda}/\partial y^{\mu} - \delta C^{\kappa}_{\nu\mu}/\delta x^{\lambda} + F^{\iota}_{\nu\lambda}C^{\kappa}_{\iota\mu} - C^{\iota}_{\nu\mu}F^{\kappa}_{\iota\lambda} \\ &+ C^{\kappa}_{\nu\iota}\partial N^{\iota}_{\lambda}/\partial y^{\mu}\,, \end{aligned} \tag{A11}$$

third curvature tensor:

$$R_{\nu}{}^{\kappa}{}_{\lambda\mu} = \mathfrak{A}_{\lambda\mu}\{\delta F^{\kappa}_{\iota\lambda}/\delta x^{\mu} + F^{\iota}_{\nu\lambda}F^{\kappa}_{\iota\mu}\} + C^{\kappa}_{\nu\iota}R^{\iota}_{\lambda\mu}\,, \tag{A12}$$

$$R^{\kappa}_{\lambda\mu} = \mathfrak{A}_{\lambda\mu}\{\delta N^{\kappa}_{\lambda}/\delta x^{\mu}\}, \tag{A13}$$

$$T^{\kappa}_{\lambda\mu} = \mathfrak{A}_{\lambda\mu}\{F^{\kappa}_{\lambda\mu}\}, \tag{A14}$$

$$P^{\kappa}_{\lambda\mu} = \partial N^{\kappa}_{\lambda}/\partial y^{\mu} - F^{\kappa}_{\mu\lambda}\,, \tag{A15}$$

$$S^{\kappa}_{\lambda\mu} = \mathfrak{A}_{\lambda\mu}\{C^{\kappa}_{\lambda\mu}\}\,. \tag{A16}$$

The symbol $\mathfrak{A}_{\lambda\mu}$ means interchange of indices λ, μ and subtraction.[1] In the usual Finsler space in Cartan's sense, $T^{\kappa}_{\lambda\mu} = 0$ and $S^{\kappa}_{\lambda\mu} = 0$ are assumed [cf. (A6)], and $R^{\kappa}_{\lambda\mu} = R_0{}^{\kappa}{}_{\lambda\mu}$ and $P^{\kappa}_{\lambda\mu} = P_0{}^{\kappa}{}_{\lambda\mu}$ hold good. From the definition of $P_{\nu}{}^{\kappa}{}_{\lambda\mu}$ (A11), it is rewritten as

$$P_{\nu\mu\lambda\kappa} = \mathfrak{A}_{\nu\mu}\{C_{\mu\lambda\kappa|\nu} + C^{\iota}_{\nu\lambda}C_{\iota\mu\kappa|0}\}, \tag{A17}$$

from which the following relation can be obtained[1]:

$$\mathfrak{A}_{\lambda\kappa}\{P_{\nu\mu\lambda\kappa}\} = -S_{\nu\mu\lambda\kappa|0}\,. \tag{A18}$$

(5) On the other hand, Berwald's curvature tensor $H_{\nu}{}^{\kappa}{}_{\lambda\mu}$ is defined by Berwald's connection coefficient $G^{\kappa}_{\mu\lambda}$ as follows[1]:

$$H_{\nu}{}^{\kappa}{}_{\lambda\mu} = \mathfrak{A}_{\lambda\mu}\{\delta G^{\kappa}_{\iota\lambda}/\delta x^{\mu} + G^{\iota}_{\nu\lambda}G^{\kappa}_{\iota\mu}\}\,. \tag{A19}$$

By use of the relation between $G^{\kappa}_{\mu\lambda}$ and $F^{\kappa}_{\mu\lambda}$ (i.e., $G^{\kappa}_{\mu\lambda} = F^{\kappa}_{\mu\lambda} + C^{\kappa}_{\mu\lambda|0}$), $H_{\nu}{}^{\kappa}{}_{\lambda\mu}$ and $R_{\nu}{}^{\kappa}{}_{\lambda\mu}$ are related to each other as follows:

$$\begin{aligned} H_{\nu}{}^{\kappa}{}_{\lambda\mu} = {}&R_{\nu}{}^{\kappa}{}_{\lambda\mu} - C^{\kappa}_{\nu\iota}R^{\iota}_{\lambda\mu} \\ &+ \mathfrak{A}_{\lambda\mu}\{C^{\kappa}{}_{\nu|0|\mu} + C^{\kappa}_{\mu\iota|0}C^{\iota}_{\lambda\nu|0}\}\,. \end{aligned} \tag{A20}$$

In the scalar curvature space, $H_{\nu\mu\lambda\kappa}$ is given, with the aid of (2.3) and $H_{\nu}{}^{\kappa}{}_{\lambda\mu} = \partial R^{\kappa}_{\lambda\mu}/\partial y^{\nu}$,[1] by

$$\begin{aligned} H_{\nu\mu\lambda\kappa} = {}&K(g_{\iota\lambda}g_{\mu\kappa} - g_{\nu\kappa}g_{\mu\lambda}) + \mathfrak{A}_{\lambda\kappa}\{(\partial K/\partial y^{\nu})y_{\lambda}g_{\mu\kappa} \\ &+ L(\partial K/\partial y^{\lambda})(2l_{\nu}g_{\mu\kappa} - l_{\kappa}g_{\mu\nu} - l_{\mu}g_{\nu\kappa}) \\ &+ L^2(\partial^2 K/\partial y^{\lambda}\partial y^{\nu})h_{\mu\kappa}\}\,. \end{aligned} \tag{A21}$$

Therefore, if $K = \text{const.}$, (A21) reduces to (2.9).

(6) The following Bianchi identities are used in this paper:

$$\mathfrak{S}_{\mu\lambda\kappa}\{S_{\beta}{}^{\alpha}{}_{\mu\lambda}\,|_{\kappa}\} = 0\,, \tag{A22}$$

$$\mathfrak{S}_{\mu\lambda\kappa}\{R_{\mu}{}^{\alpha}{}_{\lambda\kappa} - C_{\mu}{}^{\alpha}{}_{\beta}R^{\beta}_{\lambda\kappa}\} = 0\,, \tag{A23}$$

$$\mathfrak{S}_{\mu\lambda\kappa}\{R_{\beta}{}^{\alpha}{}_{\mu\lambda|\kappa} + P_{\beta}{}^{\alpha}{}_{\mu\gamma}R^{\gamma}_{\lambda\kappa}\} = 0\,. \tag{A24}$$

The symbol $\mathfrak{S}_{\mu\lambda\kappa}$ means cyclic permutation of μ, λ, κ and summation.[1] In Wagner space,[13] (A24) is extended to

$$\mathfrak{S}_{\mu\lambda\kappa}\{R_{\beta}{}^{\alpha}{}_{\mu\lambda|\kappa} + P_{\beta}{}^{\alpha}{}_{\mu\gamma}R^{\gamma}_{\lambda\kappa} + R_{\beta}{}^{\alpha}{}_{\mu\gamma}T^{\gamma}_{\lambda\kappa}\} = 0\,. \tag{A25}$$

[1] Throughout this paper, with respect to the theory of Finsler spaces, we refer mainly to M. Matsumoto, *Foundation of Finsler Geometry and Special Finsler Spaces* (Deutscher Verlag, Berlin, 1977). See, also E. Cartan, *Les espaces de Finsler* (Hermann, Paris, 1934); H. Rund, *The Differential Geometry of Finsler Spaces* (Springer–Verlag, Berlin, 1959).

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On the theory of fields in Finsler spaces

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Finsler space is a metric space in which the line-element (x, y), instead of the point (x), is chosen as the independent variable, where the vector y is regarded as the internal variable assiciated with each point x. Therefore, the y-dependence characterizes essentially the theory of fields in Finsler spaces and the Finsler field shows many peculiar features depending on y. So, in this paper, with the aid of the theory of special Finsler spaces such as tangent Riemannian space, locally Minkowski space, etc., some physical aspects carried by y are considered by taking into account the intrinsic behavior of y.

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I. INTRODUCTION

Since Einstein[1] used Riemann geometry (or the theory of Riemann spaces) in order to develop his theory of gravitational field, the so-called principle of "geometrization" of physical fields has been employed by many authors, and as a result, in the case of differential geometry, Riemann geometry itself has been generalized or modified in various ways. Among them, Finsler geometry or the theory of Finsler spaces may be regarded as a generalized Riemann geometry of the first order within the sphere of metrical differential geometry (cf. Ref. 2), because the line-element (x, y), instead of the point (x), is chosen as the independent variable, where $y(=y^\lambda; \lambda = 1, 2, \ldots, n; n = 4$ in our case) means the (tangent) vector attached to each point x $(=x^\kappa; \kappa = 1, 2, \ldots, n; n = 4$ in our case) and plays physically the role of internal variable. This way of thinking is derived from the theory of higher order spaces of order $M(=1, 2, 3, \ldots)$,[3] in which an arc length along a curve $x^\kappa = x^\kappa(t)$(t is an arbitrary parameter) is given by the integral

$$S = \int L(x, x^{(1)}, x^{(2)}, \ldots, x^{(M)})dt, \tag{1.1}$$

where L denotes the fundamental function and $x^{(\alpha)} = d^\alpha x/dt^\alpha (\alpha = 1, 2, \ldots, M)$. That is to say, Finsler space is considered the higher-order space of order one (i.e., $y = x^{(1)}$). At any rate, the theory of fields in Finsler spaces is essentially characterized by its y-dependence. So, in this paper, some structurological remarks will be made on the physical aspects carried by the internal variable y.

All the mathematical definitions and notations are referred to in Matsumoto's monograph.[2]

II. ON THE y-DEPENDENCE-I

Since the vector y is attached to each point as the internal variable, the y-dependence may be likened to an introduction of new degrees of freedom representing internal symmetry. From this, it may be said that the vector y embodies the concept of "nonlocality" in Yukawa's sense,[4] where the vectorial internal variable is expected to resolve the so-called "divergence difficulty" (cf. Refs. 4 and 5). In this sense, a Finsler field may be regarded as a "nonlocal" field obtained by "nonlocalizing" a Riemann field. Further, since the concept of "nonlocality" is connected with the "extended model" of elementary particle, the y-dependence may also exert some influence on the "microcausality" (cf. Refs. 5 and 6).

On the other hand, since y is a vector, the y-dependence can represent the concept of "anisotropy". Therefore, for example, the Finslerian gravitational field or cosmology would show some anisotropy inevitably and break some kinds of symmetries (cf. Ref. 7). However, these concepts of nonlocality and anisotropy are taken into account at some microscopic stage, so that after a certain kind of averaging process is performed with respect to y, the resulting macroscopic field would become "local" and "isotropic". This problem will be reconsidered in Sec. 4.

Now, the y-dependence is geometrically represented by the coefficient of connection $C^\kappa_{\mu\lambda}$ appearing in the following absolute differential[2]:

$$DV^\mu = dV^\kappa + \Gamma^\kappa_{\mu\lambda}V^\mu dx^\lambda + C^\kappa_{\mu\lambda}V^\mu dy^\lambda, \tag{2.1}$$

where $V^\mu(x, y)$ is an arbitrary vector, and $\Gamma^\kappa_{\mu\lambda}(x, y)$ and $C^\kappa_{\mu\lambda}(x, y)$ denote the Finslerian coefficients of connection which are also regarded as two different kinds of gauge fields in Yang–Mills' style obeying the principle of minimal coupling (cf. Ref. 8). From (2.1), the covariant derivatives are defined as follows[2]:

$$\begin{aligned} &DV^\kappa = (V^\kappa_{|\lambda})dx^\lambda + (V^\kappa|_\lambda)Dy^\lambda; \\ &V^\kappa_{|\lambda} = \delta V^\kappa/\delta x^\lambda + F^\kappa_{\mu\lambda}V^\mu, \\ &V^\kappa|_\lambda = \partial V^\kappa/\partial y^\lambda + C^\kappa_{\mu\lambda}V^\mu, \end{aligned} \tag{2.2}$$

where $\delta/\delta x^\lambda = \partial/\partial x^\lambda - N^\nu_\lambda(\partial/\partial y^\nu)$, $N^\nu_\lambda = y^\mu F^\nu_{\mu\lambda}$ and $F^\kappa_{\mu\lambda} = \Gamma^\kappa_{\mu\lambda} - N^\nu_\lambda C^\kappa_{\mu\nu}$. Let $g_{\lambda\kappa}(x, y)$ be the Finslerian metric tensor. Then, it is assumed from the beginning that the metric conditions $Dg_{\lambda\kappa} = 0$ (i.e., $g_{\lambda\kappa|\mu} = 0$ and $g_{\lambda\kappa}|_\mu = 0$) hold good [see Appendix (1)]. At this stage, one physical aspect should be noticed: As is well known,[8,9] all the gauge fields in Yang–Mills' style are found to be absorbed into the covariant derivative with respect to x for the purpose of accomplishing gauge invariance of the Lagrangian under some kinds of gauge transformations. Along this line, it may be said from (2.2) that for a Finslerian nonlocal field, the "unified" coefficient of connection $F^\kappa_{\mu\lambda}$, which is introduced into the covariant derivative by x, represents the concept of unified gauge field (cf. Refs. 9 and 10). That is to say,

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the coefficient of connection $F^{\kappa}_{\mu\lambda}$ may be regarded as a unified gauge field between two different kinds of gauge fields $\Gamma^{\kappa}_{\mu\lambda}$ and $C^{\kappa}_{\mu\lambda}$ governing the symmetric properties of the external x- and internal y-coordinates, respectively.

III. ON THE y-DEPENDENCE-II

In this section, in order to emphasize the y-dependence and consider it more concretely, some special conditions are imposed on the Finslerian structure from the standpoint of the theory of special Finsler spaces.[2]

First, if a point x is fixed and only the vector y at the point x is taken into account, then the tangent Riemannian space (M_x) at the point x arises, which corresponds to an internal space spanned by y itself around the point x. This tangent Riemannian space is a four-dimensional Riemann space specified by $g_{\lambda\kappa}(y)$, $C_{\mu\lambda\kappa}(y)$, and $S_{\nu\mu\lambda\kappa}(y)$, where $C_{\mu\lambda\kappa}$ reduces to the Christoffel three-index symbol derived from $g_{\lambda\kappa}$, and the first curvature tensor $S_{\nu\mu\lambda\kappa}$ (A5) becomes the Riemannian curvature tensor. However, it should be remarked that the vector y itself obeys only a linear transformation, so that the spatial structure of M_x must be restricted so as to cope with this transformation (see below).

In the tangent Riemannian space, such a field equation as

$$S_{\mu\lambda} - \tfrac{1}{2} S g_{\mu\lambda} = -\tau_{\mu\lambda} \tag{3.1}$$

may be proposed by analogy with Einstein's one, where $S_{\mu\lambda} = S^{\nu}_{\mu\lambda\nu}$, $S = S_{\mu\lambda} g^{\mu\lambda}$ and $\tau_{\mu\lambda}$ means the energy-momentum tensor. By virtue of the Bianchi identity (A6), the conservation law $(S^{\lambda}_{\mu} - \frac{1}{2} S \delta^{\lambda}_{\mu})|_{\lambda} = 0$ holds good (cf. Ref. 11). Further, if the indicatrix I_x, which is a three-dimensional Riemann space defined by $L = 1$ in M_x, is taken into account, then I_x is made flat by use of the Gauss equation (A9) under the assumption that $S_{\nu\mu\lambda\kappa}$ of M_x is S3-like,[2] i.e.,

$$S_{\nu\mu\lambda\kappa} = A(h_{\nu\lambda} h_{\mu\kappa} - h_{\nu\kappa} h_{\mu\lambda}) \tag{3.2}$$

and $A = -1$, where $h_{\mu\lambda}$ denotes the angular metric tensor (A4) [see Appendix (4)]. This flat indicatrix, which is nothing but a three-dimensional Euclidean space, has been compared to the isotopic space by Asanov.[12] On the other hand, if $A = 0$ in (3.2), then M_x becomes flat and I_x has a constant curvature of 1 [see Appendix (4)]. In this case, the above-mentioned linear transformation of y is limited, for example, to the global Lorentz transformation (cf. Refs. 12 and 13).

Next, as another special case, if it is assumed that there exists a coordinate system in which the fundamental function L or the metric tensor $g_{\lambda\kappa}$ (A1) does not depend on x, then the Finsler space reduces to the locally Minkowski space prescribed by such geometrical conditions as $R_{\nu\mu\lambda\kappa} = 0$ and $C_{\mu\lambda\kappa|\nu} = 0$[2,14]: In this case, $P_{\nu\mu\lambda\kappa} = 0$ holds good too, so that we have only one surviving curvature tensor $S_{\nu\mu\lambda\kappa}$ [cf. (A5)]. And due to the condition that $C_{\mu\lambda\kappa|\nu} = 0$, the coefficient of connection $F^{\kappa}_{\mu\lambda}$ of the locally Minkowski space, which represents the x-dependence, becomes a function of x alone.[14] If $F^{\kappa}_{\mu\lambda}$ is further assumed to be nonsymmetric with respect to μ and λ, then one kind of torsion $T^{\kappa}_{\mu\lambda} (= F^{\kappa}_{\mu\lambda} - F^{\kappa}_{\lambda\mu})$ (A5) appears. Concerning this, if $T^{\kappa}_{\mu\lambda}$ is given by

$$T^{\kappa}_{\mu\lambda} = \delta^{\kappa}_{\mu} \alpha_{\lambda} - \delta^{\kappa}_{\lambda} \alpha_{\mu}, \tag{3.3}$$

where $\alpha_{\mu}(x)$ is an arbitrary vector, then the space becomes a special Wagner space.[15] And one interesting fact has been known[2,15]: if the conformal transformation $\bar{L} = L \exp\sigma(x)$ is applied to (3.3), then the resulting torsion $\bar{T}^{\kappa}_{\mu\lambda}$ is given by

$$\bar{T}^{\kappa}_{\mu\lambda} = T^{\kappa}_{\mu\lambda} + \delta^{\kappa}_{\mu} \sigma_{\lambda} - \delta^{\kappa}_{\lambda} \sigma_{\mu}, \tag{3.4}$$

where $\sigma_{\mu} = \partial\sigma / \partial x^{\mu}$. Therefore, if α_{μ} is given by $\alpha_{\mu} = \partial\alpha / \partial x^{\mu}$ [$\alpha(x)$ is a scalar] and $\alpha + \sigma = 0$ holds good, then $\bar{T}^{\kappa}_{\mu\lambda}$ of (3.4) vanishes. This seems to be very significant, because the scalar σ of the conformal transformation is connected with the Brans–Dicke's scalar $\phi(x)$[16] in the form $\phi^{-1} = G \exp 2\sigma$ {G is the gravitational constant}[17] and α can play a role of another "measure" field cooperating with ϕ. In these cases, the third curvature disappears, i.e., $R_{\nu\mu\lambda\kappa} = 0$ (or $\bar{R}_{\nu\mu\lambda\kappa} = 0$), so that vierbein $(e^{\kappa}_{A}, e^{A}_{\lambda})$ (or $(\bar{e}^{\kappa}_{A}, \bar{e}^{A}_{\lambda})$; $\bar{e}^{\kappa}_{A} = e^{\kappa}_{A} \exp(-\sigma)$, $\bar{e}^{A}_{\lambda} = e^{A}_{\lambda} \exp\sigma$; $A = 1, 2, 3, 4$) can be introduced to give $F^{\kappa}_{\mu\lambda}$ (or $\bar{F}^{\kappa}_{\mu\lambda}$) in the form $F^{\kappa}_{\mu\lambda} = e^{\kappa}_{A} (\partial e^{A}_{\mu} / \partial x^{\lambda})$ (or $\bar{F}^{\kappa}_{\mu\lambda} = \bar{e}^{\kappa}_{A} (\partial \bar{e}^{A}_{\mu} / \partial x^{\lambda}) = F^{\kappa}_{\mu\lambda} + \delta^{\kappa}_{\mu} \sigma_{\lambda}$) (cf. Refs. 12, 14, and 15) and the torsion $T^{\kappa}_{\mu\lambda}$ (or $\bar{T}^{\kappa}_{\mu\lambda}$) plays the leading part in the Finsler field, as in the Einstein–Cartan theory[18] or in the theory of new general relativity.[19] Of course, $y^{A} (= e^{A}_{\lambda} y^{\lambda})$ obeys the affine transformation or the global Lorentz group (cf. Refs. 13 and 19).

IV. OTHER COMMENTS

In the above, only the y-dependence has been considered mainly and special Finsler spaces such as tangent Riemannian space and locally Minkowski space have been taken up. In this section, two other topics will be mentioned briefly: One is the x-dependence represented by the third curvature tensor $R_{\nu\mu\lambda\kappa}$ (A5) and the other is the averaging process with respect to y.

First, $R_{\nu\mu\lambda\kappa}$ is the most analogous curvature tensor to the Riemannian one, but it has, of course, some different characteristics. For example, as is easily understood by contracting α and κ of the Bianchi identity (A7), the Ricci tensor $R_{\mu\lambda} (= R^{\kappa}_{\mu\lambda\kappa})$ is not symmetric due to the quantity $C^{\kappa}_{\mu\lambda}$ and any field equation similar to (3.1) cannot be proposed, because, in general, the conservation law $(R^{\lambda}_{\mu} - \frac{1}{2} R \delta^{\lambda}_{\mu})_{|\lambda} = 0$ cannot be obtained from contraction of the Bianchi identity (A8). Therefore, it is necessary to consider some special forms of $R_{\nu\mu\lambda\kappa}$ in order to obtain the Finslerian conservation laws. For example, if $R_{\nu\mu\lambda\kappa}$ is given by, on the analogy of (3.2),

$$R_{\nu\mu\lambda\kappa} = K(g_{\nu\lambda} g_{\mu\kappa} - g_{\nu\kappa} g_{\mu\lambda}), \tag{4.1}$$

where K is a nonzero constant, then the above-mentioned conservation law holds good and also the Ricci tensor becomes symmetric (cf. Refs. 2, 11, and 20). (Some other special cases including the Wagner space have already been described in a previous paper.[21]

Next, it may be said that the Finsler field itself shows more microscopic aspects than Riemannian ones, because the vector y is attached to each point

as the internal variable. From this viewpoint, there occurs a problem of relationship between the micro- and macrofields, so that it is valuable to consider a certain kind of averaging process with respect to y. This process is geometrically likened, to some extent, to the "reduction" from the Finslerian structure to some non-Riemannian structure under such "osculating" conditions as $dy^\lambda = E^\lambda_\mu(x)dx^\mu$ (cf. Ref. 22). In this case, (2.1) is reduced to

$$DV^\kappa = dV^\kappa + \Gamma^{**}_{\mu\lambda} V^\mu dx^\lambda;$$
$$\Gamma^{**}_{\mu\lambda} = \Gamma^\kappa_{\mu\lambda} + E^\nu_\lambda C^\kappa_{\mu\nu}. \tag{4.2}$$

Therefore, the torsion tensor $T^{**}_{\mu\lambda}(=\Gamma^{**}_{\mu\lambda} - \Gamma^{**}_{\lambda\mu})$ corresponding to $T^\kappa_{\mu\lambda}$ of (3.3) appears, in general, due to the "coarse graining" (or the "nonholonomic" property) associated with the averaging process. This torsion may be connected with the concept of irreversibility or entropy production from a thermodynamical point of view (cf. Ref. 23). By the way, if $Dy^\lambda = 0$, that is to say, if the vector y is displaced in parallel to itself, then the conditions $dy^\lambda = -N^\lambda_\mu(x,y)dx^\mu$ are obtained, so that if y is obtainable as a function of x from those conditions, then $\Gamma^{**}_{\mu\lambda}$ is formally equalized to $F^\kappa_{\mu\lambda}$ of (2.2).

V. CONCLUSIONS

Thus, some structurological remarks have been made on the fields in some special Finsler spaces such as tangent Riemannian space, locally Minkowski space, etc. Of course, there exist many other interesting special spaces,[2] but much to the author's regret, the greater part of them have not yet been used for physical problems. Therefore, the author would like to appeal to physicists and geometricians for seeking for many valuable applications.

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APPENDIX

(1) The metric tensor $g_{\lambda\kappa}(x,y)$ is defined by

$$g_{\lambda\kappa} = \tfrac{1}{2}\partial^2 L^2/\partial y^\lambda \partial y^\kappa, \tag{A1}$$

where $L(x,y)$ denotes the fundamental function, which is assumed to be positively homogeneous of degree 1 with respect to y in order that arc length may be invariant under any parameter transformation [cf. (1.1)]. From metric conditions ($Dg_{\lambda\kappa} = 0$), the following relations are obtained:

$$\partial g_{\lambda\kappa}/\partial x^\mu = \Gamma^\nu_{\lambda\mu} g_{\nu\kappa} + \Gamma^\nu_{\kappa\mu} g_{\lambda\nu},$$
$$\partial g_{\lambda\kappa}/\partial y^\mu = C^\nu_{\lambda\mu} g_{\nu\kappa} + C^\nu_{\kappa\mu} g_{\lambda\nu}. \tag{A2}$$

In the usual Finsler space in Cartan's sense,[2] $C_{\mu\lambda\kappa}$ $(=C^\nu_{\mu\kappa} g_{\nu\lambda})$ is assumed to be symmetric for all indices. Therefore, $C_{\mu\lambda\kappa}$ is uniquely determined by $C_{\mu\lambda\kappa} = \frac{1}{2}\partial g_{\mu\lambda}/\partial y^\kappa$ and becomes positively homogeneous of degree -1 in y, so that

$$C_{\mu\lambda\kappa} y^\mu = C_{\mu\lambda\kappa} y^\lambda = C_{\mu\lambda\kappa} y^\kappa = 0 \tag{A3}$$

hold good. By the way, the angular metric tensor $h_{\lambda\kappa}$ is defined by

$$h_{\lambda\kappa} = g_{\lambda\kappa} - l_\lambda l_\kappa (= L\partial^2 L/\partial y^\lambda \partial y^\kappa), \tag{A4}$$

where $l_\lambda = y_\lambda/L$, $y_\lambda = g_{\lambda\kappa} y^\kappa$.

(2) In Finsler space, there exist, in general, three kinds of curvature tensors $(R^\kappa_{\nu\lambda\mu}, P^\kappa_{\nu\lambda\mu}, S^\kappa_{\nu\lambda\mu})$ and five kinds of torsion tensors $(T^\nu_{\lambda\mu}, R^\nu_{\lambda\mu}, C^\nu_{\lambda\mu}, P^\nu_{\mu\lambda}, S^\nu_{\lambda\mu})$, which are introduced by the following Ricci-identities:

$$V^\kappa{}_{|\lambda|\mu} - V^\kappa{}_{|\mu|\lambda} = V^\nu R^\kappa_{\nu\lambda\mu} - V^\kappa{}_{|\nu} T^\nu_{\lambda\mu} - V^\kappa\big|_\nu R^\nu_{\mu\lambda},$$
$$V^\kappa{}_{|\lambda}\big|_\mu - V^\kappa\big|_{\mu|\lambda} = V^\nu P^\kappa_{\nu\lambda\mu} - V^\kappa{}_{|\nu} C^\nu_{\lambda\mu} - V^\kappa\big|_\nu P^\nu_{\mu\lambda}, \tag{A5}$$
$$V^\kappa\big|_\lambda\big|_\mu - V^\kappa\big|_\mu\big|_\lambda = V^\nu S^\kappa_{\nu\lambda\mu} - V^\kappa\big|_\nu S^\nu_{\lambda\mu}.$$

Their definitions are omitted here for simplicity's sake (see Ref. 2 or 21). $R^\kappa_{\nu\lambda\mu}$ is called the third curvature tensor, derived substantially from $F^\kappa_{\mu\lambda}$; $S^\kappa_{\nu\lambda\mu}$ is the first curvature tensor, derived from $C^\kappa_{\mu\lambda}$; and $P^\kappa_{\nu\lambda\mu}$ denotes the second curvature tensor, which is an intermediate quantity between $R^\kappa_{\nu\lambda\mu}$ and $S^\kappa_{\nu\lambda\mu}$. In Cartan's Finsler space, $T^\nu_{\lambda\mu}$ and $S^\nu_{\lambda\mu}$ are also assumed to vanish, but $T^\nu_{\lambda\mu}$ appears in the Wagner space (cf. Sec. 3).

(3) The following Bianchi identities are cited in this paper:

$$\mathfrak{S}_{\mu\lambda\kappa}\{S^\alpha_{\beta\mu\lambda}\big|_\kappa\} = 0, \tag{A6}$$
$$\mathfrak{S}_{\mu\lambda\kappa}\{R^\alpha_{\mu\lambda\kappa} - C^\alpha_{\mu\beta} R^\beta_{\lambda\kappa}\} = 0, \tag{A7}$$
$$\mathfrak{S}_{\mu\lambda\kappa}\{R^\alpha_{\beta\mu\lambda|\kappa} + P^\alpha_{\beta\mu\nu} R^\nu_{\lambda\kappa}\} = 0. \tag{A8}$$

The symbol $\mathfrak{S}_{\mu\lambda\kappa}$ means cyclic permutation of μ, λ, κ and summation.

(4) The Gauss equation gives the relation between curvatures R_{ijkl} of I_x and $S_{\nu\mu\lambda\kappa}$ of M_x as follows:

$$R_{ijkl} = S_{\nu\mu\lambda\kappa} Y^\nu_i Y^\mu_j Y^\lambda_k Y^\kappa_l + g_{ik} g_{jl} - g_{il} g_{jk}, \tag{A9}$$

where $Y^\nu_i (= \partial y^\nu/\partial u^i)$ is the projection operator, u^i is a parameter of the indicatrix I_x (i.e., $y^\nu = y^\nu(u^i)$; $i = 1,2,3$) and $g_{ij} (= g_{\lambda\kappa} Y^\lambda_i Y^\kappa_j)$ is the induced metric tensor of I_x. If $S_{\nu\mu\lambda\kappa}$ is S3-like [i.e., (3.2)], then R_{ijkl} becomes a constant curvature of $(A+1)$, i.e.,

$$R_{ijkl} = (A+1)(g_{ik} g_{jl} - g_{il} g_{jk}). \tag{A10}$$

Therefore, if $A = -1$, then $R_{ijkl} = 0$ and if $A = 0$, then R_{ijkl} becomes a constant curvature of 1. By the way, $S_{\nu\mu\lambda\kappa}$ of the three-dimensional Finsler space is always written as (3.2), so that the formula of (3.2) is called S3-like.

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Schrödinger equation with time-dependent boundary conditions

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A Schrödinger equation for a well potential with varying width is studied. Generalized canonical transformations are shown to transform the problem into a time-dependent harmonic oscillator problem submitted to fixed boundary conditions. This transformed problem is solved by a perturbation technique and gives the evolution of the average energy of the system according to the motion of the well. Motions corresponding to a renormalization or compaction group are shown to be solvable by separation of variables.

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1. PRESENTATION OF THE PROBLEM

We want to examine the solutions of the Schrödinger equation submitted to time-dependent boundary conditions. This situation arises, for example, when describing the oscillations of a particle in a potential well of time-dependent width.

There are two motivations for this study. The first is mathematical; we will see in what follows that the group of transformations admitted by the problem is an interesting example of Generalized Canonical Transformations (GCT) for which the time variable is submitted to a nonlinear transformation.

The second motivation is physical; as far as we know, apart from limited attempts with harmonic oscillator-type problems with time-dependent frequencies (see Leach[1-3]) or perturbation methods (see Durand[4]), complete analytical solutions of a time-dependent Schrödinger equation are very scarce (see also Burgan, *et al.*[5]). This is partly due to the fact that quantum mechanists are still arguing about the interest of a Schrödinger equation with a time-dependent potential, and partly due to the difficulty of obtaining analytical solutions for a partial differential equation of two variables. We believe that theoretical considerations will remain sterile unless supported by simple exact analytical solutions, and in this respect, this moving-boundary Schrödinger problem is an interesting contribution.

We consider the one-dimensional Schrödinger equation in cartesian coordinates, associated with the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V. \tag{1}$$

The solution is limited to the inner part of a potential well, constituted of two infinite walls. The left boundary is chosen as the origin of position while the right boundary is allowed to undergo an arbitrary time-dependent shift. At any instant t, the position of the right boundary is $LX(t/T)$ where L and T are unit length and unit time and X is an arbitrary dimensionless function. Assuming $X(0) = 1$, L represents the position of the moving wall at the origin of time (see Fig. 1). The constant value of the potential inside the well is chosen as the origin of energies. Under these assumptions the wavefunction must satisfy

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2},\quad 0 \leqslant x \leqslant LX(t), \tag{2}$$

$$\psi(t,x) = 0,\quad \forall t,\ x < 0 \text{ or } x > LX. \tag{3}$$

Since we are interested in evolution problems, we must add the initial condition

$$\psi(t = 0,x) = \psi_0(x). \tag{4}$$

This problem looks simple, since the Schrödinger equation (2) for a potential well is the same whether the boundaries are moving or not. However, the moving-boundary condition renders the equation unsolvable by the usual means. Although the equation is still linear, Laplace or Fourier transforms are in this case incompatible with such boundary conditions. The reader can easily be convinced of the difficulty of the problem by trying a method of separation of variables on (2). The moving-boundary conditions *do not* separate.

Moreover, if $\psi^*\psi$ is to represent a probability density, the wave function must be normalized inside the domain and verify

$$\int_{-\infty}^{+\infty} \psi^*\psi dx = 1 \tag{5}$$

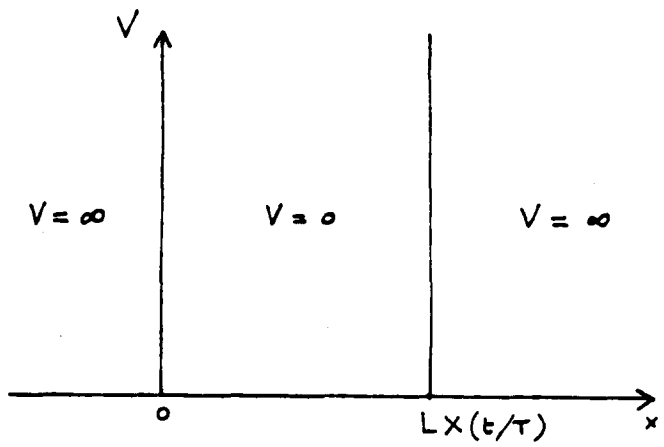

FIG. 1. A moving boundary Schrödinger equation: the time dependent infinite potential well.

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Strangely enough, very little information is available concerning the various properties of the wave function when it comes to dealing with time-dependent conditions. For physical reasons, uniqueness of the solution is required, and we can easily show that this necessitates the continuity of ψ, $\partial\psi/\partial x$, and $\partial^2\psi/\partial x^2$ with respect to x inside the domain. However it is not necessary that $\psi, \partial\psi/\partial x$, and $\partial^2\psi/\partial x^2$ be continuous with respect to t.

The validity of condition (3) is not obvious at all in a time-dependent configuration. All we can say is that is ensures having a unique solution to the problem, and keeps the treatment as simple as possible.

2. FUNDAMENTAL TRANSFORMATION

Our purpose is to change the unsolvable moving-boundary problem into a solvable fixed-boundary problem by means of a group of transformations. We use here a method generalizing a previous work by the authors (see Burgan,[6] Burgan, *et al.*,[5,7,8] Munier[9]) and based on the use of GCT.

Let us define a new rescaled space coordinate

$$\bar{x} = x/X(t/T), \tag{6}$$

a new time variable,

$$\bar{t} = \int_0^t \frac{d\sigma}{X^2(\sigma/T)}, \tag{7}$$

and a new wave function,

$$\bar{\psi}(\bar{t},\bar{x}) = \psi(t,x). \tag{8}$$

Relations (6) and (7) form a particular case of GCT depending solely on the arbitrary function X. For notation convenience we also write $\bar{X}(\bar{t}/T) = X(t/T)$. The generating function of the transformation is

$$\Phi = \bar{p}\bar{x} = \bar{p}x/X, \tag{9}$$

and the momentum is transformed according to

$$\bar{p} = pX. \tag{10}$$

The principle of correspondence of quantum mechanics tells us that the momentum is related to the operator $-i\hbar\partial/\partial x$. Due to the invariance of Hamilton's equations under a GCT, we have

$$\bar{p} \to -i\hbar\partial/\partial\bar{x}. \tag{11}$$

The new Hamiltonian of the problem reads

$$\bar{H} = \bar{X}^2\left(H + \frac{\partial\Phi}{\partial t}\right) = \bar{X}^2\left(\frac{\bar{p}^2}{2m} - \frac{\bar{p}\bar{x}\bar{X}'}{T\bar{X}^3}\right). \tag{12}$$

Using relations (9) and (11), this can be written

$$\bar{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\bar{x}^2} + i\hbar\frac{\bar{x}}{T}\frac{\bar{X}'}{\bar{X}}\frac{\partial}{\partial\bar{x}}, \tag{13}$$

(the prime denotes a derivation with respect to the argument $\bar{t}/T$).

Since the Schrödinger equation has the same structure as the Hamilton–Jacobi equation, it is also invariant under a GCT. One can easily show that

$$i\hbar\frac{\partial\bar{\psi}}{\partial\bar{t}} = \bar{H}\bar{\psi}. \tag{14}$$

Substituting now Hamiltonian (13) into Eq. (14), we see that the moving-boundary problem has been transformed into the following one:

$$i\hbar\frac{\partial\bar{\psi}}{\partial\bar{t}} = -\frac{\hbar^2}{2m}\frac{\partial^2\bar{\psi}}{\partial\bar{x}^2} + i\hbar\frac{\bar{x}}{T}\frac{\bar{X}'}{\bar{X}}\frac{\partial\bar{\psi}}{\partial\bar{x}}, \quad 0 \leqslant \bar{x} \leqslant L, \tag{15}$$

$$\bar{\psi}(\bar{t},\bar{x}) = 0, \quad \forall\bar{t}, \bar{x} < 0 \text{ or } \bar{x} > L, \tag{16}$$

$$\bar{\psi}(\bar{t}=0,\bar{x}) = \bar{\psi}_0(\bar{x}) = \psi_0(\bar{x}). \tag{17}$$

This is a fixed-boundary problem corresponding to the same initial condition. As we can see, the time dependence of the boundary is now entirely conveyed by the gradient term on the right-hand side of Eq. (15).

Although it is possible to use integral transforms (such as Fourier or Laplace transforms) for solving Eq. (15), the procedure is rather cumbersome. Moreover, there are great difficulties (it is probably impossible), in introducing arbitrary initial condition $\psi_0(x)$ *and* arbitrary wall motion $X(t/T)$ when dealing with integrals along complex time-dependent paths obtained by this method.

Equation (15) is not very easy to study as it is, this is why we consider the new wavefunction

$$\hat{\psi}(\bar{t},\bar{x}) = \bar{X}^{1/2}\bar{\psi}(\bar{t},\bar{x})\exp\left(-i\frac{m}{2\hbar}\frac{\bar{X}'}{\bar{X}}\frac{\bar{x}^2}{T}\right). \tag{18}$$

After substitution of this relation into (15), we obtain the new Schrödinger equation

$$i\hbar\frac{\partial\hat{\psi}}{\partial\bar{t}} = -\frac{\hbar^2}{2m}\frac{\partial^2\hat{\psi}}{\partial\bar{x}^2} + \frac{m}{2}\bar{x}^2\Omega^2\hat{\psi}, \tag{19}$$

with

$$\Omega^2(\bar{t}/T) = [\bar{X}''/\bar{X} - 2(\bar{X}'/\bar{X})^2]/T^2 = X^3\ddot{X}/T^2, \tag{20}$$

(the prime and the dot denote differentiation with respect to $\bar{t}/T$ and t/T respectively).

This last quantity can be regarded as a time-dependent pulsation. Equation (19) is consequently equivalent to a harmonic oscillator equation with a time-dependent frequency. The new initial condition associated to the problem is

$$\hat{\psi}_0(\bar{x}) = \hat{\psi}(\bar{t}=0,\bar{x}) = \bar{\psi}_0(\bar{x})\exp\left[-i\frac{m\bar{x}^2}{2\hbar T}\bar{X}'(0)\right], \tag{21}$$

and this relation depends on the time derivative of X at the origin. Invariance of the initial condition is obtained only for $\bar{X}'(0) = 0$, i.e., in the case of a smooth transition of the wall from rest to motion.

3. SOLUTION OF THE PROBLEM

Due to the linearity of the problem, one can express the solution as a series. Hamiltonian (19) can be regarded as the superposition of a time-dependent perturbation with amplitude

$$P(\bar{x},\bar{t}) = (m/2)\bar{x}^2\Omega^2(\bar{t}/T), \tag{22}$$

and of an unperturbed state characterized by $\Omega^2 = 0$.

It must be stressed that, in spite of the appelation "perturbing term" to qualify operator P, the method gives an exact solution (in the form of a series) of the problem, whatever the value of P, which need not be small. Let us write $\varphi_n(\bar{x},\bar{t})$, the eigenfunctions of the unperturbed problem, and $\phi_n(\bar{x})$, the stationary part of these eigenfunctions. The solution of (19) for $\Omega^2 = 0$ is straightforward. We have

$$\phi_n(\bar{x}) = (2/L)^{1/2}\sin(n\pi\bar{x}/L); \tag{23}$$

consequently

$$\varphi_n(\bar{x},\bar{t}) = \phi_n(\bar{x})\exp(-iE_n\bar{t}/\hbar), \tag{24}$$

is the eigenfunction corresponding to the energy level

$$E_n = \frac{\hbar^2}{2m}\left(\frac{\pi n}{L}\right)^2. \tag{25}$$

The theory of time-dependent perturbations tells us that the solution of the perturbed problem can be decomposed over the basis of the eigenfunctions of the unperturbed state (see Durand[4]).

$$\hat{\psi}(\bar{t}/\bar{x}) = \sum_{p=1}^{+\infty} C_p(\bar{t})\varphi_p(\bar{t},\bar{x}), \tag{26}$$

(The $p = 0$ state is excluded since it corresponds to a wavefunction which is strictly zero). Substitution of this series into the Schrödinger equation yields

$$i\hbar\sum_p\left(C_p\frac{\partial\varphi_p}{\partial\bar{t}} + \varphi_p\frac{dC_p}{d\bar{t}}\right) = -\frac{\hbar^2}{2m}\sum_p C_p\frac{\partial^2\varphi_p}{\partial\bar{x}^2} + \sum_p C_p P\varphi_p. \tag{27}$$

We multiply now this relation by ϕ_q^* and integrate with respect to $\bar{x}$ over the interval $[0,L]$, to obtain

$$i\hbar\sum_p\int_0^L \frac{dC_p}{d\bar{t}}\phi_q^*\exp(-iE_p\bar{t}/\hbar)\phi_p d\bar{x} = \sum_p\int_0^L C_p\phi_q^* P\exp(-iE_p\bar{t}/\hbar)\phi_p d\bar{x}. \tag{28}$$

Using now the fact that the functions ϕ_q form a orthornormal basis, we get

$$i\hbar\exp(-iE_q\bar{t}/\hbar)\frac{dC_q}{dt} = \sum_p C_p\exp(-iE_p\bar{t}/\hbar)\int_0^L \phi_q^* P\phi_p d\bar{x}, \tag{29}$$

and we finally obtain a differential equation on C_q:

$$i\hbar\frac{dC_q}{dt} = \sum_p C_p P_{qp}\exp(i\omega_{qp}\bar{t}/\hbar), \tag{30}$$

where P_{qp} represents the components of the operator P in the basis ϕ_q,

$$P_{qp}(\bar{t}) = \int_0^L \phi_q^* P(\bar{x},\bar{t})\phi_p d\bar{x}, \tag{31}$$

and ω_{qp} the energy of transition between the states q and p:

$$\omega_{qp} = E_q - E_p. \tag{32}$$

The Schrödinger problem (19) has consequently been reduced to the solution of an ordinary differential system on $C(t)$, submitted to initial conditions that can easily be obtained from relation (21). If we define

$$\bar{\psi}_0(x) = \psi_0(x) = F(x/L), \tag{33}$$

we have in the transformed space

$$\hat{\psi}_0(\bar{x}) = F(\bar{x}/L)\exp\left[-i\frac{m\bar{x}^2}{2\hbar T}\bar{X}'(0)\right] = \sum_p C_p(0)\phi_p(\bar{x}). \tag{34}$$

After multiplication by ϕ_q^* and integration with respect to $\bar{x}$, this relation gives

$$C_q(0) = (2L)^{1/2}\int_0^1 \exp[(-imL^2u^2\bar{X}'(0)/2\hbar T] \times\sin(q\pi u)F(u)du, \tag{35}$$

with $u = \bar{x}/L$. For a smooth transition at the origin, i.e., for a velocity $\bar{X}'(0) = 0$, the initial condition $C_q(0)$ reduces to the sine-Fourier transform of $F(u)$.

The P_{pq} components of the perturbation matrix are easily obtained after substituting relation (22) into (31) and integrating.

$$P_{qp}(\bar{t}) = (m/2)\Omega^2(\bar{t}/T)\int_0^L \bar{x}^2(2/L)\sin(q\pi\bar{x}/L) \times\sin(p\pi\bar{x}/L)d\bar{x}, \tag{36}$$

or

$$P_{qp}(\bar{t}) = m\Omega^2(\bar{t}/T)L^2\int_0^1 u^2\sin(q\pi u)\sin(p\pi u)du. \tag{37}$$

This gives, according to the values of p and q {with $p,q\in[1,+\infty)$}

$$P_{pq}(\bar{t}) = \frac{mL^2\Omega^2}{\pi^2}\frac{4qp}{(q^2-p^2)^2}, \quad \text{for } p\neq q, \tag{38}$$

$$P_{qq}(\bar{t}) = \frac{mL^2\Omega^2}{\pi^2}\left(\frac{\pi^2}{6} - \frac{1}{4q^2}\right), \quad \text{for } p = q. \tag{39}$$

As one can see, the matrix is symmetrical. The diagonal term which tends to $mL^2\Omega^2/6$ as $q\to\infty$, is seen to be dominant. One easily shows that for $j\geqslant 1$,

$$\frac{P_{q,q+j}}{P_{q,q}} = \frac{(1+j/q)}{j^2(1+j/2q)^2(\pi^2/6 - 1/q^2)}, \tag{40}$$

and this quantity is a decreasing function of j.

4. TRANSITIONS

We want to examine the evolution of a particle, intially described by

$$\psi_0(x) = (2/L)^{1/2}\sin(n\pi x/L) = \phi_n(x) = F(x/L), \tag{41}$$

and corresponding to an eigenstate in a stationary well of width L. The system is then submitted to an arbitrary motion $X(t/T)$ and we calculate the final state at time t_1.

We suppose $\bar{X}'(0) = 0$ in order not to have degenerated levels in the new system, due to a discontinuity of the velocity. We have

$$C_p(0) = 2\int_0^1 \sin(p\pi u)\sin(n\pi u)du = \delta_{pn}. \tag{42}$$

There is only one nonvanishing component of the initial vector $C_p(0)$ and we may apply the preceding theory to solve Eq. (30) and obtain the solution at instant t_1. We are then facing a delicate point. Is the wall stationary at time t_1? In other words is $\bar{X}'(t_1)$ equal to zero followed by $\bar{X}(t) = \text{const}$, or not? If $\bar{X}'(t_1) = 0$, it is possible to expand the solution of the problem in the basis of the eigenfunctions of this new stationary state t_1, and this decomposition may be associated to a measurement. If $\bar{X}'(t_1)\neq 0$, the decomposition process can only represent a "photograph" of a nonstationary phenomenon and it is not obvious whether a measurement can be associat-

ed to this decomposition. To facilitate the interpretation, we choose not only $\bar{X}'(t_1/T)=0$, but we also stop the motion of the boundary from that time on.

At time t_1 the eigenfunctions of the stationary well with width $LX(t_1/T)=LX_1$ are

$$G_s(x)=(2/LX_1)^{1/2}\sin(s\pi x/LX_1); \tag{43}$$

consequently,

$$\psi(t_1,x)=(X_1)^{-1/2}\exp\left(i\frac{mx^2\dot{X}_1}{2\hbar TX_1}\right)\sum_p C_p(\bar{t}_1)\exp(-iE_p\bar{t}_1/\hbar)$$
$$(2/L)^{1/2}\sin\left(p\pi\frac{x}{LX_1}\right), \tag{44}$$

$$\psi(t_1,x)=\sum_s A_s(t_1)(2/LX_1)^{1/2}\sin(s\pi x/LX_1), \tag{45}$$

and we easily deduce

$$A_s(t_1)=2\sum_p C_p(t_1)\exp(-iE_p\bar{t}_1/\hbar)\int_0^1\sin(p\pi u)\sin(s\pi u)du, \tag{46}$$

Therefore,

$$A_s(t_1)=\exp(-iE_s\bar{t}_1/\hbar)C_s(\bar{t}_1), \tag{47}$$

and it is apparent that, save for the phase term, the functions $C_s(\bar{t})$ are the coefficients of probability of transition from one state to the other. Starting from an initial eigenstate n, we end up with a series defined by (45) and (47).

$$\psi(t_1,x)=\sum_s(2/LX_1)^{1/2}\exp(-iE_s\bar{t}_1/\hbar)C_s(\bar{t}_1)\sin(s\pi x/LX_1). \tag{48}$$

Since the initial vector $C_p(0)$ has only one nonvanishing component, and since the smooth transition $\bar{X}'(\bar{t}_1)=0$ implies a one-to-one correspondence between $A_s(t)$ and $C_s(\bar{t})$, it is clear that the degeneration of the initial state comes solely from the nondiagonal terms in the perturbation matrix P_{qp}. *This degeneration of the energy levels is due solely to the variation of the well.*

5. THE MEAN ENERGY

Since the function ψ is not normalized, the mean energy of the system is

$$\langle E(t)\rangle=\int_0^{LX}\psi^*H\psi dx\Big/\int_0^{LX}\psi^*\psi dx. \tag{49}$$

This relation is valid in (x,t) space, with Hamiltonian (2). After substituting the value of ψ and ψ^*, we easily obtain

$$\int_0^{LX}\psi^*\psi dx=\sum_p C_p^*C_p. \tag{50}$$

Hence

$$\sum_p C_p^*C_p\langle E(t)\rangle=-\frac{\hbar^2}{m}\sum_p\sum_q\left[i\frac{m\dot{X}}{\hbar TX}-\left(\frac{q\pi}{LX}\right)^2\right]C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)\int_0^1\sin(p\pi u)\sin(q\pi u)du$$
$$+m(LX)^2\sum_p\sum_q\left(\frac{\dot{X}}{XT}\right)^2C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)\int_0^1u^2\sin(p\pi u)\sin(q\pi u)du$$
$$-\hbar(LX)\sum_p\sum_q\left(\frac{q\pi}{LX}\right)\left(\frac{2i\dot{X}}{XT}\right)C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)\int_0^1u\sin(p\pi u)\cos(q\pi u)du. \tag{51}$$

We can define:

$$Q_{pq}=\int_0^1 u\sin(p\pi u)\cos(q\pi u)du, \tag{52}$$

which gives after integration

$$Q_{pq}=(-1)^{1+p+q}[p/\pi(p^2-q^2)], \quad \text{for } p\neq q, \tag{53}$$

$$Q_{pp}=-1/4\pi p, \quad \text{for } p=q. \tag{54}$$

Consequently, with the help of (36), Eq. (51) yields

$$\sum_p C_p^*C_p\langle E(t)\rangle$$
$$=\frac{1}{X^2}\left[\sum_p E_pC_p^*C_p+\frac{\dot{X}^2}{X\ddot{X}}\sum_p\sum_q C_p^*P_{qp}C_q\exp(i\omega_{pq}\bar{t}/\hbar)\right]$$
$$-i\frac{\dot{X}}{TX}\left[\frac{\hbar}{2}\sum_p C_p^*C_p+2L(2m)^{1/2}\right.$$
$$\left.\times\sum_p\sum_q E_q^{1/2}C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)Q_{pq}\right]. \tag{55}$$

It is possible to determine in the same way, the average of the time derivative of the generating function (9).

$$\left\langle\frac{\partial\Phi}{\partial t}\right\rangle=\left\langle-\tilde{p}x\frac{\dot{X}}{TX^2}\right\rangle. \tag{56}$$

We have

$$\sum_p C_p^*C_p\left\langle\frac{\partial\Phi}{\partial t}\right\rangle=-2\frac{\dot{X}^2}{T^2\Omega^2}\sum_p\sum_q C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)P_{pq}$$
$$+i\frac{\dot{X}}{TX}\sum_p\sum_q C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)E_q^{1/2}2L(2m)^{1/2}Q_{pq}. \tag{57}$$

The average value of operator $\bar{H}$ in space $(\bar{x},\bar{t})$ is

$$\langle\bar{E}(\bar{t})\rangle=\int_0^L\bar{\psi}^*\bar{H}\bar{\psi}d\bar{x}\Big/\int_0^L\bar{\psi}^*\bar{\psi}d\bar{x}, \tag{58}$$

and since

$$\int_0^L\bar{\psi}^*\bar{\psi}d\bar{x}=\frac{1}{\bar{X}}\sum_p C_p^*C_p, \tag{59}$$

this yields

$$\frac{1}{\bar{X}}\sum_p C_p^*C_p\langle\bar{E}(\bar{t})\rangle=\frac{1}{\bar{X}}\sum_p E_pC_p^*C_p-i\frac{\hbar\bar{X}'}{2T\bar{X}^2}\sum_p C_p^*C_p$$
$$-\left(\frac{\bar{X}'}{\bar{X}}\right)^2\frac{1}{\bar{X}T^2\Omega^2}\sum_p\sum_q C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)P_{pq}$$
$$+i\frac{\bar{X}'}{\bar{X}^2}\frac{2L}{T}(2m)^{1/2}\sum_p\sum_q C_p^*C_q\exp(i\omega_{pq}\bar{t}/\hbar)Q_{pq}E_q^{1/2}. \tag{60}$$

Collecting up these different energies, we see that

$$\langle E\rangle = \left\langle \frac{\bar{E}}{\bar{X}^2}\right\rangle - \left\langle \frac{\partial \Phi}{\partial t}\right\rangle. \tag{61}$$

This relation can be compared to the transformation of the Hamiltonian (12). The evaluation of averages is compatible with the Generalized Canonical Transformation.

We notice that, in the case of a linear adiabatic motion (see Burgan[6])

$$X(t/T) = at/T + 1, \tag{62}$$

with $a \ll 1$, then

$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial t}\left(\frac{\bar{p}x}{X}\right) = -\frac{\bar{p}xa}{T(at/T+1)^2} \sim -\frac{a\bar{p}x}{T}. \tag{63}$$

Consequently, relation (61) gives to zero order

$$\langle E\rangle = \langle \bar{E}/\bar{X}^2\rangle. \tag{64}$$

This relation is simply the one we obtain from elementary adiabatic theory, saying that there is to order zero no degeneration of the levels. $\psi(x)$ being the stationary solution, the adiabatic solution reads

$$\psi_{ad}(x) = (X_0/X)^{1/2}\psi(xX_0/X(t)). \tag{65}$$

Finally, we can determine directly the energy in the transformed space:

$$\langle \hat{E}(\bar{t})\rangle = \int_0^L \hat{\psi}^* \hat{H}\hat{\psi} d\bar{x} \Big/ \int_0^L \hat{\psi}^*\hat{\psi} d\bar{x}, \tag{66}$$

with

$$\int_0^L \hat{\psi}^*\hat{\psi} d\bar{x} = \sum_p C_p^* C_p, \tag{67}$$

and we obtain:

$$\sum_p C_p^* C_p \langle \hat{E}(\bar{t})\rangle = \sum_p E_p C_p^* C_p + \sum_p \sum_q C_p^* C_q P_{pq} \times \exp(i\omega_{pq}\bar{t}/\hbar). \tag{68}$$

If the transition between $t = 0$ and t_1 is such that $\dot{X}(0) = \dot{X}(t_1) = 0$ many terms vanish in the various energies and we have

$$\langle E\rangle = \frac{1}{X^2}\left(\sum_p E_p C_p^* C_p\right) \Big/ \left(\sum_p C_p^* C_p\right) = \frac{1}{X^2}\left[\langle \hat{E}\rangle - \left(\sum_p \sum_q C_p^* C_q P_{pq} \exp(i\omega_{pq}\bar{t}/\hbar)\right) \Big/ \left(\sum_p C_p^* C_p\right)\right]. \tag{69}$$

6. CONCLUSION

As a conclusion, we notice that the general problem becomes much simpler for $\Omega^2 = 0$, i.e., when the perturbation in the transformed space becomes zero. Direct integration of Eq. (20) shows that it corresponds to a linear varation of X with respect to time.

$$X = 1 + t/T. \tag{70}$$

After substitution into (7), we obtain the time transformation:

$$\bar{t} = t/(1 + t/T). \tag{71}$$

This particular case was already studied by the authors (see Burgan,[6] Burgan *et al.*[7,8]) and corresponds to what we called "time renormalization." Indeed we see that for $t \in [0, +\infty)$, then $\bar{t} \in [0, T]$. The time variation is therefore bounded in the transformed space.

The second interesting case occurs for $\bar{X}'/\bar{X} = a/2 = \text{const}$ in Eq. (15). We easily see that the corresponding time transformation is logarithmic:

$$a\frac{\bar{t}}{T} = \log\left(1 + a\frac{t}{T}\right). \tag{72}$$

The variation of $\bar{t}$ is not bounded any more as in the renormalization case, but it is drastically reduced, hence the denomination "logarithmic compression."

A solution by separation of variables leads to an ordinary differential equation, the solutions of which can be expressed in terms of parabolic cylinder functions in the integral form (the coefficients of the equation being complex, the solution cannot always lead to Hermite polynomials). The study of integration paths in the complex field are fairly easy, the introduction of boundary conditions however necessitates the search for roots of integral equations and this can be done only numerically.

These two particular cases are the only ones which allow relations (15) and (19) to be solved by separation of variables. If the variation of the well is arbitrary, we use numerical methods for solving the $C_p(\bar{t})$ equation. This numerical and analytical study is done in a space with fixed boundary conditions. The constant potential has become a harmonic oscillator potential with time-dependent frequency.

Other Schrödinger problems with variable potentials can be studied with similar methods. In particular, the Morse potential can be generalized to a law with time-varying coefficients. It must however be stressed that, whenever the spatial domain (possibly time-dependent) is made of several sub-domains with different potentials, great difficulties arise in writing and treating the junction conditions between the different zones.

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Exact propagators for multidimensional quadratic Hamiltonians—Initial-value approach

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A practical method suitable for both analytic and numerical computation of propagators for multidimensional quadratic Hamiltonians in presented. The traditional two-end-point problem is replaced by a manageable initial-value problem. As a by-product, the classical path and action are also obtained as a solution to an initial-value problem. The method is illustrated analytically as well as numerically by solving for the motion of a particle in a constant magnetic field.

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I. INTRODUCTION

There are three reasons for the special role played by quadratic Hamiltonian in both classical and quantal physics: (a) there exist a few important physical systems governed by such Hamiltonians; (b) they can serve as a first approximation (via perturbation or variation techniques) to more complicated Hamiltonians; and (c) they are often analytically solvable. Indeed, the formal solution for the propagator in the quadratic Hamiltonian case has been known for many years.[1] The amplitude to go from the point (q',t') to the point (q'',t'') is given by the semiclassical expression

$$K(q''t'',q't') = \left[\det\left(\frac{1}{-2\pi i\hbar}\frac{\partial^2 S}{\partial q_i' \partial q_j''}\right)\right]^{1/2} \exp\left(\frac{i}{\hbar} S_{\rm cl}\right), \tag{1}$$

where $S_{\rm cl} = \int_{t'}^{t''} L(q,\dot{q},t)\,dt$ is the classical action for the path determined by the two end points.

Equation (1) is exact for quadratic Hamiltonians. Its usefulness depends, however, on the availability of an analytic solution to the classical equations of motion. If such a solution cannot be found, the two-end-point problem can present a formidable numerical task. A partial solution circumventing the classical equations of motion has been recently proposed. Using path-integral technique, Marshall and Pell[2] show that, under certain simplifying assumptions, one can evaluate the determinant in Eq. (1).

The purpose of this paper is to present an initial-value approach to the determination of the multidimensional propagator K, suitable for both numerical and analytic calculation. As a by-product, the classical path and action are obtained as a solution to an initial-value problem. This work is an extention of the work reported earlier[3] on the one-dimensional case.

Section II describes the initial-value formulation for the propagator K. In Sec. III we establish the connection with the semiclassical expression (1). As an example, the motion of a particle in a constant magnetic field is solved in Sec. IV first analytically, and then numerically

II. INITIAL-VALUE FORMULATION

We shall take our Hamiltonian to be of the form

$$H(q,p,t) = \sum a_{ik}\, p_i p_k + \sum b_{ik}(t) q_i q_k + \tfrac{1}{2}\sum c_{ik}(t)[\,p_i q_k + q_k\, p_i\,] + \sum d_i(t)\, p_i + \sum e_i(t)\, q_i + f(t), \tag{2}$$

with a and b symmetric and all coefficient real. Our only assumption is that a is a regular time-independent matrix and that the other coefficients remain finite at $t = 0$. In particular, we do not assume that a is positive definite.[2] An example with nondefinite matrix a, is given in Ref. 3. Our first step will be to diagonalize a. Let Q be a real orthogonal matrix diagonalizing a, that is, $QaQ^{\sim} = \hat{a}$ with $\hat{a}$ diagonal. (Here $\sim$ denotes the transponse.) Defining, similarly, $\hat{b} \equiv QbQ^{\sim}$ etc., we have in terms of the transformed coordinates and momenta, $(\hat{q}) = Q(q)$ and $(\hat{p}) = Q(p)$,

$$H(\hat{q},\hat{p},t) = \sum \hat{a}_{ii}\,\hat{p}_i^2 + \sum \hat{b}_{ik}\hat{q}_i\hat{q}_k + \tfrac{1}{2}\sum \hat{c}_{ik}[\,\hat{p}_i\hat{q}_k + \hat{q}_k\hat{p}_i\,] + \sum \hat{d}_i\,\hat{p}_i + \sum \hat{e}_i\hat{q}_i + f.$$

Since neither the commutation relations nor the properties of H are changed by the above transformation, we shall henceforth assume that a has already been diagonalized and drop the caret from all symbols. (In order to keep $\hat{q}_i$ and $\hat{p}_i$ time-independent, we had to assume a constant matrix a. Had a been diagonal to start with, the assumption could be relaxed.)[3]

Given the Hamiltonian H, we seek a solution to the Schrödinger equation

$$i\hbar\frac{\partial K}{\partial t} = HK \tag{3a}$$

subject to the initial condition

$$K(qt,q't') \underset{t\to t'}{\sim} \prod_{i=1}^{n} \delta(q_i - q_i'). \tag{3b}$$

From the path-integral approach[4] we know that the propagator K is given as a product of a modulating factor $F(t-t')$ (independent of q and q') times $\exp[(i/\hbar)\,S_{\rm cl}(q\,t,q't')]$. We therefore substitute in Eq. (3)

$$K = F(t-t')\exp[(i/\hbar)\,S(qt,q't')], \tag{4}$$

to obtain

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$$i\hbar\left[\frac{\dot F}{F}+\sum\left(a_{ii}\frac{\partial^2 S}{\partial q_i^2}+\tfrac{1}{2}c_{ii}\right)\right]=\frac{\partial S}{\partial t}+H\left(q,\frac{\partial S}{\partial q},t\right). \quad (5)$$

The ansatz

$$\frac{\partial S}{\partial t}+H\left(q,\frac{\partial S}{\partial q},t\right)=0, \quad (6)$$

$$\frac{\dot F}{F}+\sum\left(a_{ii}\frac{\partial^2 S}{\partial q_i^2}+\tfrac{1}{2}c_{ii}\right)=0, \quad (7)$$

with

$$S(q,t)=\alpha(t)+\sum\beta_i(t)q_i+\sum\gamma_{ij}(t)\,q_iq_j\,,\qquad \gamma_{ij}=\gamma_{ji}\,, \quad (8)$$

gives (in matrix notation)

$$\dot\alpha+f+(\tilde\beta)(d)+(\tilde\beta)\,a(\beta)=0, \quad (9a)$$

$$(\dot\beta)+(e)+2\gamma(d)+\tilde c(\beta)+4\gamma a(\beta)=0, \quad (9b)$$

$$\dot\gamma+b+\gamma c+\tilde c\gamma+4\gamma a\gamma=0, \quad (9c)$$

and

$$F(t)=F(t_0)\exp\left[-\int_{t_0}^{t}\mathrm{tr}(2a\gamma+\tfrac{1}{2}c)\,dt'\right]. \quad (10)$$

In the above we have chosen (without loss of generality) $t'=0$ for the initial time. Also, the explicit dependence on the initial position q' has been suppressed. Thus, $S(q,t)\equiv S(qt,q'0)$. In order to obtain the appropriate initial conditions for Eqs. (9) and (10), we shall invoke the representation of the delta function as a limiting form of the free propagator, that is,

$$\frac{1}{(\pi\lambda_i t)^{1/2}}\exp\left[-\frac{(q_i-q_i')^2}{\lambda_i t}\right]\underset{t\to 0^+}{\sim}\delta(q_i-q_i'), \quad (11)$$

where λ_i are constants. Using this representation, namely,

$$K=F(t)\exp\left[\frac{i}{\hbar}S(q,t)\right]\underset{t\to 0^+}{\sim}\prod_{i=1}^{n}\frac{1}{(\pi\lambda_i t)^{1/2}}\times\exp\left[-\frac{(q_i-q_i')^2}{\lambda_i t}\right] \quad (12)$$

with $S(q,t)$ given by Eq. (8), we obtain (up to terms of order t)

$$\alpha(t)\sim i\hbar\sum\frac{q_i'^2}{\lambda_i t}+\alpha^{(0)},$$

$$\beta_i(t)\sim\frac{-2i\hbar q_i'}{\lambda_i t}+\beta_i^{(0)}, \quad (13a)$$

$$\gamma_{ij}(t)\sim\delta_{ij}\frac{i\hbar}{\lambda_i t}+\gamma_{ij}^{(0)}$$

and

$$F(t)\sim\prod_{i=1}^{n}\frac{1}{(\pi\lambda_i t)^{1/2}}. \quad (13b)$$

Substituting these expansions in Eqs. (9b) and (9c) and setting the coefficients of t^{-2} and t^{-1} equal to zero, we secure

$$\lambda_i=4i\hbar a_{ii}\,, \quad (14)$$

and

$$(\beta)\sim-\frac{1}{2t}a^{-1}(q')-\tfrac{1}{2}a^{-1}(d)-\tfrac{1}{4}[a^{-1}c-\tilde c a^{-1}](q') \quad (15a)$$

$$\gamma\sim\frac{1}{4t}a^{-1}-\tfrac{1}{8}[a^{-1}c+\tilde c a^{-1}]. \quad (15b)$$

Here c and (d) are evaluated at $t=0$. Since $\alpha(t)$ does not enter Eq. (9a), the value of $\alpha^{(0)}$ cannot be determined in the same manner. However, by using the explicit expressions (8) and (13) in Eq. (12), we have

$$K=F(t)\exp\left[\frac{i}{\hbar}\left(\alpha+\sum\beta_iq_i+\sum\gamma_{ij}q_iq_j\right)\right]\sim\left[\prod_{i=1}^{n}\delta(q_i-q_i')\right]\times\exp\left[\frac{i}{\hbar}\left(\alpha^{(0)}+\sum\beta_i^{(0)}q_i+\sum\gamma_{ij}^{(0)}q_iq_j\right)\right]. \quad (16)$$

Comparing Eq. (16) with Eq. (3b), we obtain

$$\alpha^{(0)}=-\sum\beta_i^{(0)}q_i'-\sum\gamma_{ij}^{(0)}q_i'q_j', \quad (17)$$

hence [with the aid of (13) and (15)],

$$\alpha\sim\frac{1}{4t}(\tilde q')\,a^{-1}(q')+\tfrac{1}{2}(\tilde q')\,a^{-1}(d)+\tfrac{1}{8}(\tilde q')[3a^{-1}c-\tilde c a^{-1}](q'). \quad (15c)$$

Finally, by Eqs. (13b) and (14)

$$F(t)\sim\prod_{i=1}^{n}\frac{1}{(4\pi i\hbar a_{ii}t)^{1/2}}=\frac{1}{(\det a)^{1/2}}\frac{1}{(4\pi i\hbar t)^{n/2}}. \quad (15d)$$

Using the last result and Eq. (15b), it is not difficult to show that Eq. (10) for the modulating factor $F(t)$ can be rewritten as

$$F(t)=\lim_{t_0\to 0^+}\frac{1}{(\det a)^{1/2}}\frac{1}{(4\pi i\hbar t_0)^{n/2}}\times\exp\left[-\int_{t_0}^{t}\mathrm{tr}(2a\gamma+\tfrac{1}{2}c)\,dt'\right]. \quad (18)$$

Let us review that has been accomplished up to now. In order to evaluate the propagator K, the first-order differential equations (9), subject to the initial conditions (15), must be solved. Starting with Eqs. (9c) and (15b) we solve for γ_{ij}, then [by (9b) and (15a)] for β_i, and finally (by quadratures), for α and F. This can be accomplished analytically in a few cases. In general, we have to resort to numerical integration. Formulated as an initial-value problem, the numerical evaluation of K (as opposed to the two-end-point formulation) is straightforward and fast. In this respect, note that being independent of q_i', $\gamma_{ij}(t)$ can be calculated "once and for all." An example of such a calculation is given in Sec. IV.

III. CONNECTION WITH THE SEMICLASSICAL EXPRESSION

In this section we establish the connection between the semiclassical expression (1) and our initial-value formulation for the propagator K. As a by-product we shall obtain

the classical path and action as a solution to an initial-value problem.

A. The classical path

With the Hamiltonian (2), the classical equations of motion are

$$(\dot{q}) = 2a(p) + c(q) + (d),$$
$$(\dot{p}) = -2b(q) - \tilde{c}(p) - (e). \tag{19}$$

These equations together with the boundary conditions

$$q_i(t') = q_i' \quad \text{and} \quad q_i(t'') = q_i'', \tag{20}$$

determine the path completely. Consider the following change of variables

$$(p) = \left(\frac{\partial S}{\partial q}\right) = (\beta) + 2\gamma(q). \tag{21}$$

Substituting the above expression for (p) into the equations of motion, we obtain

$$[(\dot{\beta}) + (e) + 2\gamma(d) + \tilde{c}(\beta) + 4\gamma a(\beta)] + 2[\dot{\gamma} + b + \gamma c + \tilde{c}\gamma + 4\gamma a\gamma](q) = (0). \tag{22}$$

If this equation is to hold for any (q), (β) and γ must satisfy Eqs. (9b) and (9c). [Conversely, each solution of (9a) and (9b) fulfills (22).] Thus, given (β) and γ, the classical path is determined as the solution to the first-order equation

$$(\dot{q}) = [4a\gamma + c](q) + [2a(\beta) + (d)] \tag{23a}$$

with the initial value

$$(q(t'')) = (q''). \tag{23b}$$

In the Appendix we demonstrate that the above solution, with (β) and γ determined by Eqs. (9) and (15), does indeed pass through the point (q') at the time $t' = 0$.

Can we use the initial condition $(q(t'=0)) = (q')$ instead of (23b)? Inserting the expansions for (β) and γ [Eq. (15)] into Eq. (23a), we end up with an identity

$$(\dot{q}) = \frac{1}{t}[(q(t)) - (q')] + O(t).$$

Thus, the two-end-point classical problem separates neatly into two parts: the point (q') is used to determine (β) and γ and the point (q'') serves to determine the path (q). Equation (23a) must be integrated backwards in time.

B. The classical action

The Lagrangian for the system (2) is

$$L = \sum p_i\dot{q}_i - H = (\tilde{p})(\dot{q}) - [(\tilde{p})a(p) + (\tilde{q})b(q) + (\tilde{p})c(q) + (\tilde{p})(d) + (\tilde{q})(e) + f]. \tag{24}$$

Inserting (p) from Eq. (21) and using Eq. (9) for $\dot{\alpha}$, $(\dot{\beta})$ and γ, we obtain

$$L = \frac{d}{dt}[\alpha + (\tilde{\beta})(q) + (\tilde{q})\gamma(q)] = \frac{d}{dt}S(q(t),t). \tag{25}$$

Hence,

$$S_{\rm cl} = \int_0^{t''} L\,dt = \lim_{t_0\to 0^+}[S(q(t''),t'') - S(q(t_0),t_0)]. \tag{26}$$

Now, by Eq. (15) and the Appendix

$$S(q(t_0),t_0) \sim \sum (q_i(t_0) - q_i')^2/(4a_{ii}t_0) \equiv S_{\rm cl}^{\rm free}(q(t_0)\,t_0,q'0) \underset{t_0\to 0^+}{\to} 0, \tag{27}$$

that is,

$$S_{\rm cl}(q''t'',q'0) = S(q(t''),t'') \equiv S(q''t'',q'0). \tag{28}$$

The classical action is therefore that solution of the Hamilton–Jacobi equation (6), which satisfies the initial condition (27), namely,

$$S_{\rm cl}(q''t'',q'0) \underset{t''\to 0^+}{\sim} S_{\rm cl}^{\rm free}(q''t'',q'0). \tag{29}$$

C. The determinant $|\partial^2 S/\partial q_i'\partial q_j''|$

Having identified $S_{\rm cl}$ with S as given by Eq. (8), we now proceed to calculate the determinant $|\partial^2 S/\partial q_i\partial q_j'|$. According to Eqs. (8), (9b), and (15a), the matrix A where

$$A_{ij} \equiv \partial^2 S/\partial q_i\partial q_j' = \partial\beta_i/\partial q_j', \tag{30}$$

satisfies the differential equation

$$\dot{A} = -[4\gamma a + \tilde{c}]A, \tag{31a}$$

with the initial condition

$$A \underset{t\to 0^+}{\sim} -\frac{1}{2t}a^{-1}. \tag{31b}$$

The determinant of A can now be fixed using a lemma due to Jacobi[5]:

$$\det A(t) = \det A(t_0)\exp\left[-\int_{t_0}^{t}\mathrm{tr}(4\gamma a + \tilde{c})\,dt'\right]. \tag{32}$$

This result is valid as long as the integral in the exponential function exists. Incidently, it serves to show that $A(t)$ is a regular matrix at all times, (when it exists) provided it is regular at $t = t_0$. Letting $t_0 \to 0$ and using the initial condition (31b), we have

$$\det A(t) = \lim_{t_0\to 0^+}\left(-\frac{1}{2t_0}\right)^n \frac{1}{\det a} \times \exp\left[-\int_{t_0}^{t}\mathrm{tr}(4a\gamma + c)\,dt'\right], \tag{33}$$

where $\mathrm{tr}X = \mathrm{tr}\tilde{X}$ has been used. Comparing with Eq. (18), we conclude

$$F(t) = \left[\det\left(\frac{1}{-2\pi i\hbar}\frac{\partial^2 S}{\partial q_i\partial q_j'}\right)\right]^{1/2}. \tag{34}$$

Since $\det X = \det\tilde{X}$, the last result is identical with the semiclassical expression in Eq. (1).

IV. EXAMPLE

As an illustration to the initial-value approach to propagators and classical paths, we shall treat the motion of a particle in a constant magnetic field. Using $\mathbf{B} = \nabla\times\mathbf{A}$ with $\mathbf{A} = (0,Bq_1,0)$, the Hamiltonian for this motion is given by

$$H=\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2$$
$$=(p_1^2+p_2^2+p_3^2)/(2m)+2m\omega^2q_1^2-2\omega p_2q_1,$$
$$\omega\equiv eB/(2mc). \tag{35}$$

Hence,

$$a_{11}=a_{22}=a_{33}=1/(2m),\quad b_{11}=2m\omega^2,\quad c_{21}=-2\omega, \tag{36}$$

and all other coefficients vanish. The equations of motion (9), (7), and (23) take the explicit form

$$\dot\alpha+(\beta_1^2+\beta_2^2+\beta_3^2)/(2m)=0,$$
$$\dot\beta_1-2\omega\beta_2+2(\gamma_{11}\beta_1+\gamma_{12}\beta_2+\gamma_{13}\beta_3)/m=0,$$
$$\dot\beta_2+2(\gamma_{12}\beta_1+\gamma_{22}\beta_2+\gamma_{23}\beta_3)/m=0,$$
$$\dot\beta_3+2(\gamma_{13}\beta_1+\gamma_{23}\beta_2+\gamma_{33}\beta_3)/m=0,$$
$$\dot\gamma_{11}+2m\omega^2-4\omega\gamma_{12}+2(\gamma_{11}^2+\gamma_{12}^2+\gamma_{13}^2)/m=0,$$
$$\dot\gamma_{12}-2\omega\gamma_{22}+2(\gamma_{11}\gamma_{12}+\gamma_{12}\gamma_{22}+\gamma_{13}\gamma_{23})/m=0,$$
$$\dot\gamma_{13}-2\omega\gamma_{23}+2(\gamma_{11}\gamma_{13}+\gamma_{12}\gamma_{23}+\gamma_{13}\gamma_{33})/m=0,$$
$$\dot\gamma_{22}+2(\gamma_{12}^2+\gamma_{22}^2+\gamma_{23}^2)/m=0,$$
$$\dot\gamma_{23}+2(\gamma_{12}\gamma_{13}+\gamma_{22}\gamma_{23}+\gamma_{23}\gamma_{33})/m=0,$$
$$\dot\gamma_{33}+2(\gamma_{13}^2+\gamma_{23}^2+\gamma_{33}^2)/m=0,$$
$$\dot F+F(\gamma_{11}+\gamma_{22}+\gamma_{33})/m=0,$$
$$\dot q_1=2(\gamma_{11}q_1+\gamma_{12}q_2+\gamma_{13}q_3)/m+\beta_1/m,$$
$$\dot q_2=2(\gamma_{12}q_1+\gamma_{22}q_2+\gamma_{23}q_3)/m-2\omega q_1+\beta_2/m,$$
$$\dot q_3=2(\gamma_{13}q_1+\gamma_{23}q_2+\gamma_{33}q_3)/m+\beta_3/m, \tag{37a}$$

with the initial conditions (up to terms of order t_0)

$$\alpha=m(q_1'^2+q_2'^2+q_3'^2)/(2t_0)-m\omega q_1'q_2',$$
$$\beta_1=-mq_1'/t_0-m\omega q_2',\quad \beta_2=-mq_2'/t_0+m\omega q_1',$$
$$\beta_3=-mq_3'/t_0,$$
$$\gamma_{11}=m/(2t_0),\quad \gamma_{12}=m\omega/2,\quad \gamma_{13}=0,$$
$$\gamma_{22}=m/(2t_0),\quad \gamma_{23}=0,\quad \gamma_{23}=m/(2t_0),$$
$$F=(m/2\pi i\hbar t_0)^{3/2}, \tag{37b}$$

and

$$q_1(t'')=q_1'',\quad q_2(t'')=q_2'',\quad q_3(t'')=q_3''. \tag{37c}$$

A. Analytic solution

Inspection of Eq. (37) reveals that

$$\gamma_{13}=\gamma_{23}=0,\quad \gamma_{12}=m\omega/2,\quad \text{and}\quad \gamma_{33}=m/(2t); \tag{38a}$$

hence

$$\gamma_{11}=\gamma_{22}=(m\omega/2)\cot\omega t. \tag{38b}$$

The rest follows straightforwardly:

$$\beta_3=-q_3'/t,\quad \beta_1=-m\omega(q_1'\cot\omega t+q_2'),$$
$$\beta_2=-m\omega(q_2'\cot\omega t-q_1'), \tag{38c}$$
$$\alpha=(m\omega/2)(q_1'^2+q_2'^2)\cot\omega t+mq_3'^2/(2t)-m\omega q_1'q_2', \tag{38d}$$
$$F=[m/(2\pi i\hbar t)]^{1/2}m\omega/(2\pi i\hbar\sin\omega t). \tag{38e}$$

Finally

$$q_3=q_3'+\Delta_3t/t'',$$
$$q_1=q_1'+[(\Delta_1s+\Delta_2c)(1-\cos2\omega t)+(\Delta_1c-\Delta_2s)\sin2\omega t]/(2s), \tag{38f}$$
$$q_2=q_2'+[-(\Delta_1c-\Delta_2s)(1-\cos2\omega t)+(\Delta_1s+\Delta_2c)\sin2\omega t]/(2s),$$

where

$$\Delta_i\equiv(q_i''-q_i'),\quad i=1,2,3,\quad \text{and}\quad s\equiv\sin\omega t'',\quad c\equiv\cos\omega t''. \tag{38g}$$

These results are well known.[6]

B. Numerical solution

In order to check the feasibility of the numerical scheme proposed in Secs. II and III, we solved numerically the differential equations (37a) with the initial conditions (37b) and (37c), using $(q',t')=(1,1,1,0)$ and $(q'',t'')=(2,2,2,1)$ as the two endpoints, and setting $m=\omega=\hbar=1$. Rather than bothering with storage of partial results and numerical quadratures, we simply lumped together all the 14 unknowns of Eq. (37a) into a single vector, and used a Runge–Kutta routine to integrate the system, starting with $t_0=10^{-3}$. The equations were integrated twice. On the forward swipe the coordinated $q_i(t)$ were kept dummy until the end time $t''=1$ has been reached. The backward swipe then generated the path $q_i(t)$ (and regenerated all the other quantities). The results of both swipes were compared with values obtained from the analytic solution (38). All six significant figures printed in the output agreed. At this stage we felt that the feasibility of the method has been demonstrated, and no further checks have been performed.

V. SUMMARY

A practical method suitable for both analytic and numerical computation of the propagators for multidimensional quadratic Hamiltonians has been demonstrated. The traditional two end-point problem has been replaced by a manageable initial-value problem. As a by-product, the classical path and action are also obtained as a solution to an initial-value problem. Work on application of this exact method to the approximate determination of propagators for more a complicated system, is in progress.

APPENDIX

The purpose of this appendix is to show that the path determined by Eq. (23) goes, in fact, through the initial point $(q',t'=0)$, that is, $[q(t'=0)]=(q')$. Let Q be a matrix solution to the equation

$$\dot Q=[4a\gamma+c]\,Q, \tag{A1}$$

with the initial condition

$$Q(t'')=1. \tag{A2}$$

From Jacobi's lemma[5] [see discussion following Eq (32)], we know that $Q^{-1}(t)$ exists. Hence the solution to Eq. (23) can be written as

$$(q) = Q\left\{(q'') - \int_t^{t''} Q^{-1}\,[2a(\beta) + (d)]\,dt'\right\}. \quad \text{(A3)}$$

Let t_0 be a fixed time and let $0 < t \leqslant t_0$. Then, by Eq. (15b), $[4a\gamma + c] = (1/t)[1 + O(t)]$ and

$$Q(t) = Q(t_0)\frac{t}{t_0}\,[1 + O(t)] \equiv Q(t_0)\frac{t}{t_0}B(t) \quad \text{(A4)}$$

is a solution of (A1). Substituting (A4) in (A3) we have

$$\begin{aligned}(q) = Q(t_0)\frac{t}{t_0}B(t)\,\{&(q'') \\ &- \int_t^{t_0} B^{-1}(t')\frac{t_0}{t'}Q^{-1}(t_0)\,[2a(\beta) + (d)]\,dt' \\ &- \int_{t_0}^{t''} Q^{-1}[2a(\beta) + (d)]\,dt'\Big\} \\ = Q(t_0)\frac{t}{t_0}B(t)&\int_t^{t_0} B^{-1}(t')\frac{t_0}{t'^2} \\ &\times Q^{-1}(t_0)(q')\,dt' + O(t), \quad \text{(A5)}\end{aligned}$$

where Eq. (15a) has been used for the last step. Performing the integration [note that $B(t) \equiv 1 + O(t)$], we secure

$$(q) = (q') + O(t). \quad \text{(A6)}$$

Q.E.D.

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High-energy behavior of phase shifts for scattering from singular potentials

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The high-energy behavior of the Jost function in nonrelativistic potential scattering theory is studied for potentials, strongly singular and repulsive at the origin. To be able to give the result in an explicit form, we specialize to the S wave and to pure inverse power potentials. However, the method works for a large class of potentials, and we report briefly on some other cases. We use an asymptotic method, which can be described as a generalization of the JWKB method to arbitrary order, with rigorous error bounds. Some numerical results are given.

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1. INTRODUCTION

Recently, there has been some discussion in the literature[1–4] about the true high-energy behavior of the phase shifts for scattering from singular potentials, in particular from the inverse power potential,

$$V(r) = g^2 r^{-p}, \quad p > 2. \tag{1}$$

As shown by several authors,[1,5–14] most rigorously in Refs. 1 and 14, this high-energy behavior is correctly given by the JWKB approximation. In fact, the present author showed in Ref. 10, and the same result is implicitly contained in Ref. 5, that the JWKB approximation and successive higher-order corrections to it can be arranged to form a whole asymptotic series as the energy goes to infinity.

This short paper is intended to show how this asymptotic series can be constructed with complete mathematical rigor, and with strict error bounds on the rest terms. The method used is the same as in Ref. 10, and rests heavily on the results of Olver (Ref. 15 and original work referred to there).

The paper is organized as follows: in the next section asymptotic methods are used to obtain approximations to the wavefunctions for high energy, valid uniformly in r. Error bounds are provided to any order, explicitly demonstrating the asymptotic character of the approximations. For convenience we restrict ourselves to S waves and to the potential (1), since then most integrals are analytically calculable.

In Sec. 3 we give the asymptotic series for the Jost function and for the phase shift, including error bounds. Section 4 is devoted to the calculation of higher-order terms in the series of Secs. 2 and 3. As can be expected, complexity grows fast with the order, so we stop after a few terms.

In Sec. 5, we discuss what can be said for other potentials and for $l \neq 0$, and in Sec. 6 we give some illustrating numerical results.

2. ASYMPTOTIC APPROXIMATION OF THE WAVEFUNCTION

Consider the S-wave Schrödinger equation with the potential (1). In the scaled variable s,

$$s = r/r_0, \quad r_0 = (k/g)^{-2/p}, \tag{2}$$

this equation reads

$$\left[\frac{d^2}{ds^2} + \nu^2 v(s)\right] u(r_0 s) = 0, \tag{3}$$

where $u = r\Psi$ is the reduced wavefunction and

$$v(s) = 1 - s^{-p}, \quad \nu = kr_0 = g^{2/p} k^{1-2/p}. \tag{4}$$

Here, ν is the large parameter, in which we shall write the asymptotic series. On Eq. (3) we perform the Liouville transformation (Ref. 15, p. 191),

$$\xi = \int_1^s (1 - s^{-p})^{1/2}\, ds, \quad z = -\left(\tfrac{3}{2}\xi\right)^{2/3}, \tag{5}$$

with

$$w(z) = \left(-\frac{dz}{ds}\right)^{1/2} u(r_0 s) = \left(\frac{v(s)}{-z}\right)^{1/4} u(r_0 s). \tag{6}$$

This gives the new differential equation

$$w''(z) = [\nu^2 z + \chi(z)]\, w(z), \tag{7}$$

where the function

$$\chi(z) = \frac{5}{16z^2} + \frac{5[v'(s)]^2 - 4v''(s)v(s)}{16v^3(s)}\, z \tag{8}$$

is regular at $z = 0$, corresponding to the turning pont $s = 1$, $r = r_0$, but has strong singularities at the other zeros of $v(s)$. Equation (7) is completely equivalent to Eq. (3). Equation (5) defines a conformal mapping from the complex s plane to the complex z plane of a region, containing the whole positive real s axis, which is mapped on the real z axis with $s = 0$ corresponding to $z = +\infty$ and $s = \infty$ corresponding to $z = -\infty$.

At this point we take advantage of the specialization to the S wave and to the potential (1) to get the following explicit form of the transformation[16]:

$$\xi = \frac{1}{p} B_v\left(\frac{3}{2}, -\frac{1}{p}\right) = \frac{2}{3p} v^{3/2} F\left(\frac{3}{2}, 1 + \frac{1}{p}; \frac{5}{2}; v\right) \tag{9}$$

and

$$z = -v\left[\frac{1}{p} F\left(\frac{3}{2}, 1 + \frac{1}{p}; \frac{5}{2}; v\right)\right]^{2/3}. \tag{10}$$

Here, B_v is the incomplete beta function[17] and F is the hypergeometric function. Asymptotically, Eq. (9) gives the following relations with the s variable ($|\arg s| < \pi/p$):

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$$\xi = \begin{cases} \left[\frac{2}{p-2}s^{1-p/2} - \frac{1}{p-2}B\left(\frac{1}{2},\frac{1}{2}+\frac{1}{p}\right) \right. \\ \left. + O(s^{1+p/2})\right] \exp\left[\frac{3\pi i}{2}\operatorname{sgn}(\arg s)\right] & \text{for } s\to 0, \\ \frac{2}{3p}(1-s^{-p})^{3/2} + O((1-s^{-p})^{5/2}) & \text{for } s\to 1, \\ s - \frac{1}{2}B\left(\frac{1}{2},1-\frac{1}{p}\right) + O(s^{1-p}) & \text{for } s\to\infty. \end{cases} \tag{11}$$

For z this implies

$$z = \begin{cases} \left(\frac{3}{p-2}\right)^{2/3} s^{-(p-2)/3} + O(s^{(p-2)/6}) & \text{for } s\to 0, \\ -p^{-2/3}(1-s^{-p}) + O((1-s^{-p})^2) & \text{for } s\to 1, \\ -(\frac{3}{2}s)^{2/3} + O(s^{-1/3}) & \text{for } s\to\infty. \end{cases} \tag{12}$$

The points $z_{\pm}$, corresponding to $s = \exp(\pm 2\pi i/p)$, where $\chi(z)$ has singularities can be obtained directly from Eq. (5). The result is that z_+ is in the lower half plane with its argument varying continuously if p is varied, from $-\pi/3$ for $p=2$ through $-\pi/2$ for $p=4$ to approach $-2\pi/3$ for $p\to\infty$. It is never close to the real axis, $|\operatorname{Im} z_{\pm}| \gtrsim 1.8$.

On p. 417 of Ref. 15 we find a very useful theorem about the solutions of Eq. (7). To apply it, we define the following functions:

$$P_j(z) = \operatorname{Ai}(\rho_j z), \quad \rho_0 = 1, \quad \rho_{\pm 1} = \exp(\mp 2\pi i/3), \tag{13}$$

where Ai is the Airy function, and $A_0(z)\equiv 1$,

$$B_n(z) = \tfrac{1}{2}z^{-1/2}\int_0^z dz\, z^{-1/2}[\chi(z)A_n(z) - A_n''(z)],$$

$$A_{n+1}(z) = -\tfrac{1}{2}B_n'(z) + \tfrac{1}{2}\int_{-\infty}^z \chi(z)B_n(z)dz, \quad n = 0,1,2,\cdots. \tag{14}$$

A_n and B_n are real analytic functions in the z-plane cut from $z_{\pm}$ to infinity along the level curves of $\exp(\frac{2}{3}z^{3/2})$. They have strong singularities at $z = z_{\pm}$.

Direct application of Olver's theorem 9.1 (Chap. 11 of Ref. 15) now gives that for each integer N and point α_j in the cut z plane Eq. (7) has a solution $w_{N,j}(\nu,z)$, satisfying

$$w_{N,j}(\nu,z) = P_j(\nu^{2/3}z)\sum_{n=0}^{[(N-1)/2]}\frac{A_n(z)}{\nu^{2n}} + \nu^{-4/3}P_j'(\nu^{2/3}z)\sum_{n=0}^{[N/2-1]}\frac{B_n(z)}{\nu^{2n}} + \epsilon_{N,j}(\nu,z). \tag{15}$$

The error term $\epsilon_{N,j}$ and its derivative are subject to certain bounds given in Ref. 15, (p. 418) for odd N and in Ref. 18 for even N, see Eqs. (21) and (22) below. The solution $w_{N,j}$ is supposed to be fixed by some boundary condition at the point $z = \alpha_j$; therefore $\epsilon_{N,j}$ is zero at this point by definition.

Let now E_j be the functions

$$E_j(z) = |\exp\{\tfrac{2}{3}(\rho_j z)^{3/2}\}|, \quad j = 0, \pm 1, \tag{16}$$

where the principal value is taken for the fractional power and let S_j be the sectors

$$S_j: |\arg(\rho_j z)| < \pi/3, \quad j = 0, \pm 1 \tag{17}$$

of the z plane. Then $E_j > 1$ in S_j, < 1 in the other two sectors.

Define further the auxiliary functions M_j, N_j (see Ref. 15, p. 415 for details) by (cyclic enumeration)

$$M_j(z) = \{E_{j+1}^2(z)|P_{j+1}(z)|^2 + E_{j-1}^2(z)|P_{j-1}(z)|^2\}^{1/2}, \tag{18}$$

$$N_j(z) = \{E_{j+1}^2(z)|P_{j+1}'(z)|^2 + E_{j-1}^2(z)|P_{j-1}'(z)|^2\}^{1/2},$$

the constants μ by

$$\mu_1 = \sup\{\pi|z|^{1/2}M_j^2(z)\}, \quad z\in S_{j-1}\cup S_{j+1},$$

$$\mu_2 = \sup\{\pi E_{j-1}(z)M_j(z)|z^{1/2}P_{j-1}(z)|\}, \quad \cdots, \tag{19}$$

$$\mu_3 = \sup\{\pi E_{j-1}(z)M_j(z)|P_{j-1}'(z)|\}, \quad \cdots$$

and the symbol $\mathscr{V}$ by

$$\mathscr{V}_C(f) = \int_C |f'(z)\,dz|. \tag{20}$$

$\mathscr{V}_C$ denotes the total variation of the function f along the curve C in the complex z plane.

Define finally $\mathscr{L}_j$ to be a piecewise twice differentiable curve without singular points between α_j and the point z, such that $E_j(x)$ is nonincreasing as x moves from α_j to z.

Then the bound for the error term is

$$|\epsilon_{N,j}(\nu,z)| < \frac{M_{j\pm 1}(\nu^{2/3}z)}{E_j(\nu^{2/3}z)}\Delta_{N,j}(\nu,z) \times \exp\left[\frac{4\mu_1}{|\nu|}\mathscr{V}_{\mathscr{L}_j}(z^{1/2}B_0(z))\right], \tag{21}$$

where the suffix on M is $j+1$ when $\nu^{2/3}z\in S_{j-1}\cup S_j$ and $j-1$ when $\nu^{2/3}z\in S_j\cup S_{j+1}$, and further

$$\Delta_{N,j}(\nu,z) = \begin{cases} \frac{4\mu_2}{|\nu|^N}\mathscr{V}_{\mathscr{L}_j}(z^{1/2}B_{(N-1)/2}(z)) & \text{for } N \text{ odd}, \\ \frac{4\mu_3}{|\nu|^N}\mathscr{V}_{\mathscr{L}_j}(A_{N/2}(z)) & \text{for } N \text{ even}. \end{cases} \tag{22}$$

To identify the different solutions $w_{N,j}$ of Eq. (7) with the different physical solutions of Eq. (3) we use the apropriate boundary conditions, that is

$$\varphi(k,r) \underset{r\to 0}{\sim} 2^{-1/2}g^{-1/2}r^{p/4}\exp\left(-\frac{2g}{p-2}r^{-(p-2)/2}\right) \tag{23}$$

for the regular solution φ and

$$f(k,r) \underset{r\to\infty}{\sim} \exp(ikr) \tag{24}$$

for the Jost solution f. The latter function is exponentially small when $\operatorname{Im}(kr)\to+\infty$, that is when $\operatorname{Im}\{\nu(-z)^{3/2}\}\to+\infty$. This is where $P_{-1}(\nu^{2/3}z)$ is exponentially small, and we can identify

$$\varphi(k,r) = C_R(N,\nu)\left(\frac{-z}{v(s)}\right)^{1/4}w_{N,0}(\nu,z),$$

$$f(k,r) = C_J(N,\nu)\left(\frac{-z}{v(s)}\right)^{1/4}w_{N,-1}(\nu,z), \tag{25}$$

where the coefficients $C_{R,J}$ are independent of z, but depend

on the parameter ν and on the number N of terms used in w.

Note that there is no asymptotic approximation involved in Eq. (25)—in each of the two equations the left- and right-hand sides are equal since they are solutions of the same (though transformed) differential equation, satisfying the same boundary condition. Moreover, $C_{R,J}$ can be determined by using the asymptotic formulas for the Airy functions involved in w, putting $\alpha_0 = +\infty$ (corresponding to $r = 0$) and $\alpha_{-1} = \infty \times \exp(-2\pi i/3)$ [corresponding to $\mathrm{Im}(kr) = \infty$] and comparing with Eqs. (23) and (24). This gives

$$C_R^{-1}(N,\nu) = (2\pi)^{-1/2} k^{1/2} \nu^{-1/6} \exp\left[-\frac{\nu}{p-2} B\left(\frac{1}{2}, \frac{1}{2} + \frac{1}{p}\right)\right] \times \left[1 + \sum_{n=1}^{N-1} (-1)^n \frac{\gamma_n}{\nu^n}\right], \tag{26}$$

$$C_J^{-1}(N,\nu) = \tfrac{1}{2}\pi^{-1/2} i^{1/6} \nu^{-1/6} \exp\left[-i\frac{\nu}{2} B\left(\frac{1}{2}, 1 - \frac{1}{p}\right)\right] \times \left[1 - i \sum_{n=0}^{[N/2-1]} \frac{\beta_{2n+1}}{\nu^{2n+1}}\right],$$

where

$$\gamma_{2n} = \lim_{z\to+\infty} A_n(z), \quad \beta_{2n} = \lim_{z\to-\infty} A_n(z) = 0, \tag{27}$$

$$\gamma_{2n+1} = \lim_{z\to+\infty} z^{1/2} B_n(z), \quad \beta_{2n+1} = \lim_{z\to-\infty} (-z)^{1/2} B_n(z),$$

are real constants. Since Eqs. (8) and (12) imply that

$$|\chi(z)| < \mathrm{const}/(1 + |z|^2) \tag{28}$$

outside the neighborhoods of $z_\pm$ it is possible to prove (Ref. 15, p. 419) that $A_n(z)$ and $z^{1/2}B_n(z)$ are uniformly bounded outside some neighborhood of the cuts. It then follows that the limits in Eq. (27) exist and are the same in a large sector around the positive and negative real axis, respectively.

It also follows that the total variations in Eqs. (21) and (22) are finite and therefore that

$$\epsilon_{N,j}(\nu,z) = O(\nu^{-N}) \quad \text{as } \nu\to\infty, \tag{29}$$

uniformly in z outside some neighborhood of the cuts, in particular along the whole real axis.

Note that the fact that $\epsilon_{N,j}$ is zero at the point $z = \alpha_j$ where we compare Eq. (25) with Eqs. (23) and (24) implies that Eq. (26) is an exact relation, without any error term. However, in the wavefunctions of Eq. (25) we still have the error terms implied by Eq. (15).

3. THE PHASE SHIFT

Now that we have good approximations to the wavefunctions, and can control the accuracy of those approximations, we go on to determine the phase shift. The simplest way to determine the Jost function $F(k)$ is to use Corollary 2 of Theorem 2 of Ref. 12, proved in Ref. 14, which says that the Jost function is given by the limit

$$F(k) = \lim_{r\to0}[f(k,r)/\psi(r)], \tag{30}$$

where

$$\psi(r) = 2^{-1/2} g^{-1/2} r^{p/4} \exp\left(\frac{2g}{p-2} r^{-(p-2)/2}\right). \tag{31}$$

Employing Eqs. (15), (25), and (26) this gives the following result for the Jost function

$$F(k) = (2k)^{1/2} \exp\left[-\frac{\nu}{p-2} B\left(\frac{1}{2}, \frac{1}{2} + \frac{1}{p}\right) + \frac{i\nu}{2} \times B\left(\frac{1}{2}, 1 - \frac{1}{p}\right) - \frac{i\pi}{4}\right] \times \left[1 - i \sum_{n=0}^{[N/2-1]} \frac{\beta_{2n+1}}{\nu^{2n+1}}\right]^{-1} \times \left[1 + \sum_{n=1}^{N-1} \frac{\gamma_n}{\nu^n} + \eta_N(\nu)\right], \tag{32}$$

where

$$\eta_N(\nu) = \lim_{z\to+\infty} \frac{\epsilon_{N,-1}(\nu,z)}{P_{-1}(\nu^{2/3}z)}. \tag{33}$$

According to Eq. (21) this error term is bounded by

$$|\eta_N(\nu)| < \Delta_{N,-1}(\nu, +\infty) \exp\left[\frac{4\mu_1}{|\nu|} \mathscr{V}_{(-\infty,\infty)}(z^{1/2}B_0(z))\right], \tag{34}$$

where we can take the variations along the real axis. By using the real form of the Olver theorem this bound can be slightly tightened, the resulting change being

$$4\mu_1 \to 2\lambda, \quad 4\mu_2 \to 2, \quad 4\mu_3 \to 2, \tag{35}$$

where

$$\lambda = \sup_{x\in(-\infty,\infty)} [\pi|x|^{1/2} M^2(x)] \approx 1.04. \tag{36}$$

M is closely related to, but not identical with M_j (Ref. 15, pp. 394–7).

Instead of using Eq. (30), it is also possible to use the standard Wronskian definition of the Jost function, since bounds are available also for the derivative of the error term. After some algebra, the formula obtained that way can be reduced to Eq. (32).

For the phase shift Eq. (32) implies

$$\delta(k) = \delta_{\mathrm{JWKB}}(k) - \arctan\left[\sum_{n=0}^{[N/2-1]} \frac{\beta_{2n+1}}{\nu^{2n+1}}\right] - \theta_N(\nu), \tag{37}$$

where

$$\delta_{\mathrm{JWKB}}(k) = -\frac{\nu}{2} B(\tfrac{1}{2}, 1 - 1/p) + \tfrac{1}{4}\pi \tag{38}$$

is the JWKB phase shift and the error term is given by

$$\theta_N(\nu) = \arctan \frac{\mathrm{Im}\eta_N(\nu)}{1 + \sum_{n=1}^{N-1} \gamma_n/\nu^n + \mathrm{Re}\eta_N(\nu)}. \tag{39}$$

Equations (29) and (34) imply that

$$\theta_N(\nu) = O(\nu^{-N}) \quad \text{as } \nu\to\infty. \tag{40}$$

The main earlier results on the phase shift are the following: Bertocchi, Fubini, and Furlan[5] gave Eqs. (37) and (38) but without proof of the boundedness of the error term. They also determined β_1,

$$\beta_1 = \frac{p+1}{24p} B\left(\frac{1}{2}, \frac{1}{p}\right). \tag{41}$$

Paliov and Rosendorff[6] got the same value for δ_{JWKB}, but a different β_1. Calogero[7] and Jabbur[8] got different values for the coefficient of the leading, linear term. This was, in short, the situation in 1969, described by Frank, Land, and Spector[4] in their review article. There seem to have been no proofs known at that time of the boundedness of the error term. However, studying mainly the large l behavior, Tiktopoulos[9] indeed gave a proof of Eq. (40) for $N = 1$ and the present author[10] a proof of Eq. (29) for general N. Another overlooked result is that of Rofe–Beketov and Hristov, who in Ref. 12 stated that

$$\theta_1(\nu) = o(1) \quad \text{as } \nu \to \infty, \tag{42}$$

giving a rigorous proof in Ref. 14. Finally, Fröman and Thylwe[1] recently gave a rigorous proof of Eq. (40) for $N = 1$.

4. COMPUTATION OF THE HIGHER-ORDER TERMS

In general, it is a difficult task to determine the higher order terms A_n and B_n from Eq. (14), because they are given recursively, and compelxity grows fast with the order. For the first few terms, however, numerical methods should work quite well for a very large class of potentials, because of the regularity of the functions involved. In such a process, special care must be taken of the cancellations between the two terms of Eq. (8) near $s = 1$. We shall not here pursue this line of approach any further.

Let us instead take advantage of the specialization to the potential (1) to determine an analytic expression for B_0,

$$B_0(z) = \tfrac{1}{2} z^{-1/2} \int_0^z dz \left[\frac{5}{16z^{5/2}} + z^{1/2} \frac{5[v'(s)]^2 - 4v''(s)v(s)}{16v^3(s)}\right]. \tag{43}$$

Introduce here a cut along the negative real axis and let C_z denote a curve from a negative real z on the upper rim of the cut, around the origin to the same z on the lower rim of the cut. Then

$$B_0(z) = \frac{i}{4}(-z)^{-1/2} \int_{C_z} dz \left\{\frac{5}{16z^{5/2}} + z^{1/2} \frac{p(1-v)^{1+2/p}[5p - (p-4)v]}{16v^3}\right\}, \tag{44}$$

and the integral can be split into two convergent parts,[5]

$$\frac{5}{16} \int_{C_z} \frac{dz}{z^{5/2}} = \frac{5i}{12}(-z)^{-3/2} \tag{45}$$

and

$$\frac{p}{16} \int_{C_z} \frac{z^{1/2}\, dz}{v^3} [5p - (p-4)v](1-v)^{1+2/p} = \tfrac{1}{16} \int_{C_v} \frac{dv}{(-v)^{5/2}} [5p - (p-4)v](1-v)^{1/p}, \tag{46}$$

respectively, where we used the fact that

$$\frac{dz}{dv} = \frac{dz}{ds}\frac{ds}{dv} = -\left(\frac{v}{-z}\right)^{1/2} \frac{1}{p}(1-v)^{-1-1/p}, \tag{47}$$

and defined C_v to be the image of C_z in the complex v-plane, cut along the positive real axis. C_v goes from a $v \in (0,1)$ on the lower rim of the cut, around the origin to the same v on the upper rim.

Now the incomplete beta function (Ref. 17, p. 263) can be written

$$B_v(a,b) = \int_0^v t^{a-1}(1-t)^{b-1}\, dt = \frac{1}{2i \sin(\pi a)} \int_{C_v} (-v)^{a-1}(1-v)^{b-1}\, dv \tag{48}$$

for noninteger a, and we have thus obtained

$$B_0(z) = -\frac{5}{48z^2} - \frac{(-z)^{-1/2}}{32}\left[5pB_v\left(-\frac{3}{2}, 1 + \frac{1}{p}\right) - (p-4)B_v\left(-\frac{1}{2}, 1 + \frac{1}{p}\right)\right]. \tag{49}$$

Note here that since

$$B_v(a,b) = a^{-1} v^a F(a, 1-b; a+1; v), \tag{50}$$

where the hypergeometric function is regular at $v = 0$, there is no branch point singularity on the right hand side of Eq. (49), just first and second order poles at $z = 0$. Therefore, this expression is valid by analytic continuation in the whole complex v-plane, corresponding to $|\arg s| < \pi/p$. The corresponding region in the z-plane contains, in particular, the whole real axis which is all we need.

Note also that there is a complete cancellation between the poles on the right hand side of Eq. (49), so that B_0 is regular at $z = 0$ as it should be,

$$B_0(z) = \frac{(p+1)(p+11)}{140p^{2/3}} + O(z) \quad \text{as } z \to 0. \tag{51}$$

Calculation of the constants of Eq. (27) is eased by noting that from the properties of the hypergeometric functions (Ref. 17, pp. 556–9) it follows that

$$\lim_{v \to 1} B_v(a,b) = B(a,b) \quad \text{for } b > 0 \tag{52}$$

$$\lim_{v \to -\infty} B_v(a,b) = B(a, 1-a-b) \exp[a\pi i \operatorname{sgn}(\arg v)] \quad \text{for } a + b < 1,$$

also for negative and noninteger z.

Equation (49) then implies Eq. (41) and

$$\gamma_1 = \frac{p+1}{24p} B\left(\frac{1}{2}, \frac{1}{2} - \frac{1}{p}\right). \tag{53}$$

We thus obtain the same β_1 as Bertocchi *et al.*

Next, we determine A_1 by noting that

$$A_1(z) = -\tfrac{1}{2} B_0'(z) + \int_{-\infty}^z z^{1/2} B_0(z) \frac{d}{dz}[z^{1/2} B_0(z)]\, dz, \tag{54}$$

which immediately gives us

$$A_1(z) = -\tfrac{1}{2} B_0'(z) + \tfrac{1}{2} z B_0^2(z) + \tfrac{1}{2}\beta_1^2, \tag{55}$$

implying

$$\gamma_2 = \tfrac{1}{2}\gamma_1^2 + \tfrac{1}{2}\beta_1^2. \tag{56}$$

Determining B_1 is already much harder, but both this coefficient and the higher ones can be expressed in incomplete beta functions. The calculation of the higher order terms can be somewhat simplified with the help of a trick due to Olver (Ref. 17, p. 412, ex. 7.4). Even with this method however, we have not been able to find a general formula for the nth term, due to the growing complexity.

Our result for B_1 is

$$\begin{aligned} B_1(z) = {} & \tfrac{1}{6}zB_0^3(z) + \tfrac{1}{2}\beta_1^2 B_0(z) - \tfrac{1}{2}z^{-1}A_1'(z) \\ & + \tfrac{1}{8}z^{-2}B_0'(z) + \tfrac{1}{32}z^{-3}B_0(z) - \frac{25}{2^{10}\cdot 3^2}z^{-5} \\ & + \frac{(-z)^{-1/2}}{2^{11}}\left[25p^3 B_v\left(-\frac{9}{2},2+\frac{3}{p}\right)\right. \\ & - 10p^2(p-4)B_v\left(-\frac{7}{2},2+\frac{3}{p}\right) \\ & \left. + p(p-4)^2 B_v\left(-\frac{5}{2},2+\frac{3}{p}\right)\right]. \end{aligned} \tag{57}$$

This expression has poles of first to fifth order in the different terms of the right hand side, which cancel completely to give a regular B_1. We have verified this cancellation by explicit calculations, both algebraically for general p and numerically for $p = 4$.

For the corresponding constants Eq. (57) implies

$$\begin{cases} \beta_3 = \tfrac{1}{3}\beta_1^3 + \dfrac{p(p+1)(2p-3)}{2^9\cdot 3}B\left(-\dfrac{5}{2},2+\dfrac{3}{p}\right) \\ \gamma_3 = \tfrac{1}{6}\gamma_1^3 + \tfrac{1}{2}\beta_1^2\gamma_1 - \dfrac{p(p+1)(2p-3)}{2^9\cdot 3} \\ \qquad \times B\left(-\dfrac{5}{2},\dfrac{3}{2}-\dfrac{3}{p}\right). \end{cases} \tag{58}$$

5. OTHER POTENTIALS AND $l \neq 0$

As mentioned above, the restriction to the potential (1) was technical—for this potential we can determine analytically the coefficients of the series in Eqs. (15), (32), and (37). Up to ν^{-3}, inclusive, we have shown this explicitly.

For other potentials, real analytic in a sector around the positive real axis, and having the potential (1) as a repulsive core,

$$V(r) \underset{r\to 0}{\sim} g^2 r^{-p}, \quad p > 2, \tag{59}$$

but otherwise quite arbitrary, the method can be applied as above. Some complications arise, however. The first is with the scaling: the function $v(s)$, and therefore the Liouville transformation (5) and the function $\chi(z)$ in Eqs. (7) and (8) will be ν-dependent. However, this is allowed in the Olver theory. The error term analysis is still applicable, but one has to accept[19] a ν-dependence of A_n, B_n, β_n, and γ_n.

The second complication is, as already implied, that the integrals involved are in general not expressible in known functions. However, as mentioned in Sec. 4, numerical methods could be quite efficient here.

Accepting the above complications, the theory of Secs. 2 and 3 should work for a large class of potentials, but of course a number of points have to be checked in each case, e.g., where the singularities of $\chi(z)$ are. If the potential has the repulsive core (59) the singularities will in the limit $\nu \to \infty$ approach those of the potential (1). For ν large enough, the theory then goes through, and the leading term in the phase shift will be the same as in Eqs. (37) and (38).

To be more precise, assume that

$$V(r) = g^2 r^{-p} + \lambda r^{-q}, \quad 1 < q < p > 2, \tag{60}$$

and put

$$\xi = \int_{s_0}^{s} (1 - s^{-p} - \mu s^{-q})^{1/2}\, ds, \tag{61}$$

where

$$\begin{cases} \mu = \lambda g^{-2(q-2)/(p-2)}\nu^{-2(p-q)/(p-2)} \\ s_0 = 1 + p^{-1}\mu + O(\mu^2), \end{cases} \tag{62}$$

s_0 being defined as the turning point close to 1 for large ν.

A series expansion of the integrand of Eq. (61) gives the small μ (large ν) asymptotic formula

$$\begin{aligned} \xi = {} & \frac{1}{p}B_v\left(\frac{3}{2},-\frac{1}{p}\right) - \frac{\mu}{2p}B_v\left(\frac{1}{2},\frac{q-1}{p}\right) \\ & + O(\mu^{3/2}) + O\left[\mu^2 B_v\left(-\frac{1}{2},\frac{2q-1}{p}\right)\right]. \end{aligned} \tag{63}$$

This implies the following expression for the JWKB phase shift. [Note that Eqs. (37) and (40) are still valid, even though an extra ν-dependence appears in the coefficients of the series]:

$$\begin{aligned} \delta_{\mathrm{JWKB}}(k) = {} & -\frac{\nu}{2}B\left(\frac{1}{2},1-\frac{1}{p}\right) \\ & - \frac{\mu\nu}{2p}B\left(\frac{1}{2},\frac{q-1}{p}\right) + \frac{\pi}{4} + O(\nu\mu^{3/2}). \end{aligned} \tag{64}$$

Thus, adding to the repulsive core a perturbation according to Eq. (60) does not change the leading asymptotic behavior, but can affect the next to leading term. This is so since for

$$q > 1 + \tfrac{1}{2}p, \tag{65}$$

the second term of the right hand side of Eq. (64) dominates the constant term.

Now, if the perturbation of the repulsive core is not as strong as implied by Eq. (65), but only

$$\begin{aligned} \Delta V(r) &= V(r) - g^2 r^{-p} \\ &= \begin{cases} O(r^{-q}) & \text{as } r\to 0,\ q < 1 + \tfrac{1}{2}p \\ O(r^{-1-\epsilon}) & \text{as } r\to\infty,\ \epsilon > 0, \end{cases} \end{aligned} \tag{66}$$

then our method can be applied in another, simpler way. This is because under these conditions, we can keep the transformation (5) and still have everything finite and well defined. The difference is simply that in Eq. (7) and thereafter, χ should be replaced by $\bar{\chi}$, where

$$\Delta\chi(z) = \bar{\chi}(z) - \chi(z) = -[r_0^2 z/v(s)]\Delta V(r_0 s) \tag{67}$$

[compare Eq. (3.06) on page 398 of Ref. 15]. In particular, we obtain

$$\Delta B_0(z) = -\tfrac{1}{2}r_0^2 z^{-1/2}\int_0^z \frac{z^{1/2}dz}{v(s)}\Delta V(r_0 s), \tag{68}$$

which is convergent for all z under the conditions of Eq. (66). Assuming again the potential (60), we get

$$(-z)^{1/2}\Delta B_0(z) = \frac{\sigma}{2p} B_v\left(\frac{1}{2}, \frac{q-1}{p}\right), \tag{69}$$

where

$$\sigma = \lambda\,(\nu/g)^{2(q-2)/(p-2)} \tag{70}$$

is a large or small parameter for large ν, depending on whether q is >2 or <2. The corresponding changes in β_1 and γ_2 are

$$\begin{cases} \Delta\beta_1 = \dfrac{\sigma}{2p} B\left(\dfrac{1}{2}, \dfrac{q-1}{p}\right), \\ \Delta\gamma_1 = \dfrac{\sigma}{2p} B\left(\dfrac{1}{2}, \dfrac{1}{2} - \dfrac{q-1}{p}\right), \end{cases} \tag{71}$$

which for the phase shift implies

$$\delta(k) = -\frac{\nu}{2} B\left(\frac{1}{2}, 1 - \frac{1}{p}\right) + \frac{\pi}{4} - \frac{p+1}{24p\nu} B\left(\frac{1}{2}, \frac{1}{p}\right) - \frac{\sigma}{2p\nu} B\left(\frac{1}{2}, \frac{q-1}{p}\right) + O\left(\frac{1}{\nu^2}\right) + O\left(\frac{\sigma^2}{\nu^2}\right), \tag{72}$$

in accordance with Eqs. (37), (41), and (64).

At this point we are also in a position to test the so-called Langer prescription (see, e.g., Ref. 4) usually described as the replacement $l(l+1) \to (l+\frac{1}{2})^2$. For $l=0$ and the potential (1) this corresponds in our method to using

$$\xi = \int_{s_0}^{s} \left(1 - s^{-p} - \frac{1}{4\nu^2 s^2}\right)^{1/2} ds \tag{73}$$

instead of Eq. (5), where s_0 is the turning point close to 1 for large ν. At the same time we compensate for the extra term by putting

$$\Delta V(r) = -1/4r^2, \tag{74}$$

so that the total differential equation is the same. Now, from Eq. (64) we see that Eq. (73) implies the change

$$\Delta\delta_{\mathrm{JWKB}}(k) = -\frac{1}{8p\nu} B\left(\frac{1}{2}, \frac{1}{p}\right) + O\left(\frac{1}{\nu^2}\right), \tag{75}$$

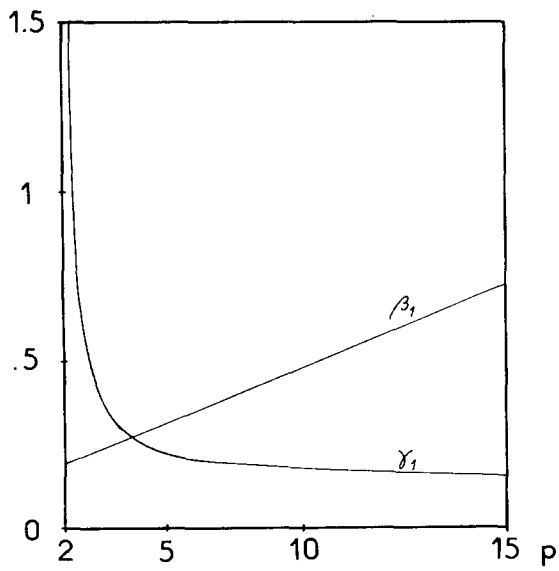

FIG. 1. The variation with p of the coefficients β_1 and γ_1 of the $1/\nu$-terms in Eq. (32), representing the second-order JWKB contribution.

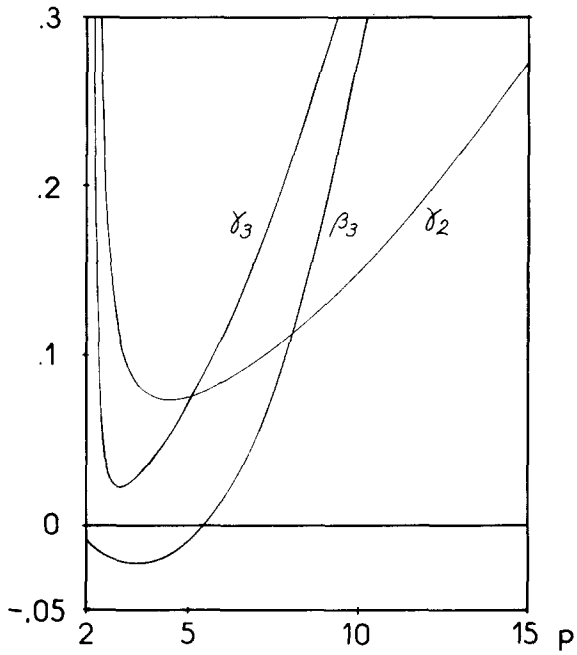

FIG. 2. The variation with p of the coefficients γ_2, β_3 and γ_3 in Eq. (32), representing the third- and fourth-order JWKB contribution.

which in the total phase shift is compensated by the term

$$-\frac{\Delta\beta_1}{\nu} = \frac{1}{8p\nu} B\left(\frac{1}{2}, \frac{1}{p}\right) + O\left(\frac{1}{\nu^3}\right) \tag{76}$$

according to Eqs. (68) and (71). We conclude that the Langer prescription takes care of part of the second order JWKB contribution already in the first order term, so that the remaining second order term is

$$-\frac{\bar{\beta}_1}{\nu} = -\frac{p-2}{24p\nu} B\left(\frac{1}{2}, \frac{1}{p}\right) + O\left(\frac{1}{\nu^3}\right), \tag{77}$$

which is smaller than the old second order term for all p, and zero for $p=2$.

From Eq. (72) we can also get an expression for the $l>0$ phase shift

$$\delta_l(k) = -\frac{\nu}{2} B\left(\frac{1}{2}, 1 - \frac{1}{p}\right) + \frac{\pi}{2}\left(l + \frac{1}{2}\right) - \frac{p-2+3(2l+1)^2}{24p\nu} B\left(\frac{1}{2}, \frac{1}{p}\right) + O\left(\frac{1}{\nu^2}\right). \tag{78}$$

6. SOME NUMERICAL RESULTS

To illustrate the accuracy of the method, we shall finally give some numerical results.

The variation of the first few coefficients of the asymptotic series with the power p of the potential is given in Fig. 1 for β_1 and γ_1 and in Fig. 2 for γ_2, β_3, and γ_3.

Note the nonuniformity in p of the approximations, illustrated by the behavior of γ_N as $p \to 2$ and β_N, γ_N as $p \to \infty$. Note also that $\bar{\beta}_1$ and $\bar{\gamma}_1$, replacing β_1 and γ_1 if we follow the Langer prescription, are obtained from the latter by multiplication with $(p-2)/(p+1)$, among others implying that $\bar{\beta}_1(p=2) = 0$ and $\bar{\gamma}_1(p=2) = 1/12$.

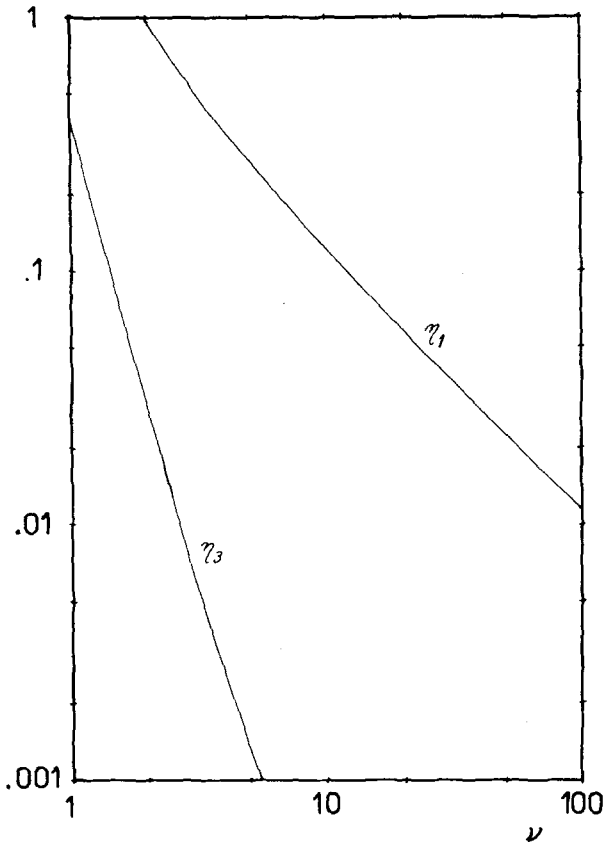

FIG. 3. The variation with ν for fixed $p = 4$ of the error estimate Eq. (34) of the first- and third-order JWKB approximation, respectively.

Even though the size of β_N and γ_N already gives us some hints about the accuracy, we would like to be more precise. The expressions of Eqs. (22) and (34) are here available. They contain the total variations of, in particular, $z^{1/2}B_0(z)$ and $z^{1/2}B_1(z)$. If those functions were monotonic, we would have, e.g.,

$$\begin{cases} \mathscr{V}_{(-\infty,0)}[z^{1/2}B_0(z)] = \beta_1, \\ \mathscr{V}_{(0,\infty)}[z^{1/2}B_0(z)] = \gamma_1. \end{cases} \tag{79}$$

However, we have not been able to prove this for general p—only checked numerically that it is true for $p = 4$.

Also for $p = 4$, we have examined numerically $|z|^{1/2}B_1(z)$ and found that it has a minimum $\simeq -0.02063$ at $z \simeq -3.9$ and a maximum $\simeq 0.00157$ at $z \simeq -1.06$, but is otherwise monotonic and approaches $\beta_3 = -0.02051$ at $z = -\infty$, so that

$$\begin{cases} \mathscr{V}_{(-\infty,0)}[z^{1/2}B_1(z)] = 0.0239 > |\beta_3| \\ \mathscr{V}_{(0,\infty)}[z^{1/2}B_1(z)] = \gamma_3. \end{cases} \tag{80}$$

The resulting bounds for $\mu_1(\nu)$ and $\mu_3(\nu)$ are given in Fig. 3.

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Multipole expansion of stationary asymptotically flat vacuum metrics in general relativity [a)]

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A multipole expansion scheme is introduced for a wide class of stationary, asymptotically flat, vacuum solutions of Einstein's equations using the conformal techniques of Geroch and Hansen. An intrinsic choice of the conformal factor and suitable asymptotic flatness conditions enable one to express the rescaled gravitational mass and angular momentum potentials and the rescaled spatial metric as power series in normal coordinates around a point Λ representing the spatial infinity on the conformal manifold. The coefficients of this expansion are certain nonlinear combinations of the Hansen multipole moments. As an example the Schwarzschild metric is discussed in the present framework.

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I. INTRODUCTION

Although a number of exact solutions of the Einstein equations are now known, their interpretation has almost always been a rather difficult problem. For obtaining a complete intuitive picture of a solution it is important to relate the parameters appearing in the metric written in a certain coordinate system to the physical characteristics of the source. In general relativity quite often a particular coordinate system chosen for the purpose of simplifying the algebraic form of the metric tends to obscure its physical content. Thus, for gaining insight into the physical significance of an exact solution, a manifestly coordinate-free method of treatment is called for. In the context of Newtonian gravitation, the multipole moments provide one such approach. Apart from their usual interpretation as the coefficients of the multipole expansion and the successive moments of the source density, the multipole moments can be identified with a set of trace-free symmetric tensors at spatial infinity which is represented as a single ideal point attached to a three-dimensional manifold with a smooth conformally flat positive definite metric.

From the analogy with the Newtonian case, Hansen,[1] generalizing an earlier work of Geroch,[2] formulated the definition of the multipole moments of a stationary vacuum metric in a generally covariant manner. His method of construction of these moments may be briefly described as follows. The set of all orbits of the timelike Killing vector field constitutes a three-dimensional manifold which is equipped with an induced positive definite "transverse" metric. An additional point Λ is attached to this manifold to represent the spatial infinity. A suitable notion of asymptotic flatness is then introduced in order to represent the gravitational field of an isolated system. This is done by requiring the existence of an appropriate conformal factor such that the rescaled metric is C^∞ everywhere (including at Λ). This allows one to analyze the asymptotic structure of any field on this conformal manifold in terms of its local behavior near Λ. In particular, the norm and the twist of the timelike Killing vector define the two gravitational scalar potentials Φ_M and Φ_J of conformal weight $-1/2$ on this manifold. The vacuum field equations imply that the two rescaled potentials are also C^∞ near Λ. The Hansen multipole moments are then defined recursively as the values at Λ of a sequence of traceless symmetric tensors constructed from the rescaled metric and the rescaled gravitational potentials.

However, an important question remains to be settled. In the case of Newtonian gravity every solution of Laplace's equation vanishing at infinity can be expressed in terms of the multipole moments via the multipole expansion. Thus the Newtonian potential is uniquely specified by its multipole moments about a chosen origin. One might ask whether this is true also in general relativity, that is to say, whether a given set of multipole moments uniquely determines the structure of a stationary asymptotically flat vacuum solution of the Einstein equations at least near spatial infinity. The purpose of this paper is to express the two rescaled gravitational potentials and the rescaled spatial metric tensor as power series around Λ whose coefficients are certain nonlinear combinations of the Hansen multipole moments. This is accomplished by slightly strengthening the usual asymptotic flatness condition. The main idea is to exploit further the analogy with the Newtonian theory and select a conformal factor in an intrinsic way that is applicable to a large class of stationary empty spacetimes. It is hoped that the present work goes a considerable way towards establishing the yet unproven uniqueness theorem and increases our understanding of the asymptotic structure of the gravitational field of a spatially bounded time-independent source.

II. DEFINITION OF THE MULTIPOLE MOMENTS

In this section we give the formal definition of the multipole moments of a stationary, vacuum solution of Einstein's equations asymptotically flat at spatial infinity.

Throughout this paper the greek spacetime indices μ,ν,

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... take the values 0, 1, 2, 3. The components of a spatial tensor are labelled by the indices $i,j,k,\ldots$ in a general coordinate system and by $a,b,\ldots,h$ in a normal coordinate system; they run through 1, 2, 3. The capital latin indices $A, B, \ldots = M, J$. All repeated indices are summed. The (square) round brackets are used for total (anti-) symmetrization of the tensor indices.

Let us consider a spacetime $(\mathscr{M}, g_{\mu\nu})$ with a one-parameter timelike group of motions $\mathscr{G}$ satisfying the vacuum field equations $R_{\mu\nu} = 0$. The norm $\lambda = \xi_\mu \xi^\mu$ and the twist ω (given by $\nabla_\mu \omega = e_{\mu\nu\rho\sigma} \xi^\nu \nabla^\rho \xi^\sigma$) of the associated Killing vector ξ^μ define two scalar fields

$$\Phi_M = \tfrac{1}{4}\lambda^{-1}(\lambda^2 + \omega^2 - 1), \tag{1}$$

$$\Phi_J = \tfrac{1}{2}\lambda^{-1}\omega, \tag{2}$$

on the three-dimensional manifold $\mathscr{V}$ of its trajectories. The canonical projection $\pi: \mathscr{M} \to \mathscr{V} = \mathscr{M}/\mathscr{G}$ induces a positive definite metric h_{ij} on the quotient space $\mathscr{V}$ given by $h_{ij} = -\lambda(\pi_* g)_{ij}$. On the manifold $(\mathscr{V}, h_{ij})$ the equations $R_{\mu\nu} = 0$ reduce to [1,3]

$$(h^{ij}\nabla_i \nabla_j - 2R)\Phi_A = 0, \tag{3}$$

$$R_{ij} = 2[\nabla_i \Phi_A \nabla_j \Phi_A - (1 + 4\Phi^2)^{-1} \nabla_i \Phi^2 \nabla_j \Phi^2], \tag{4}$$

where R_{ij} is the Ricci tensor of $\mathscr{V}$, $R = h^{ij}R_{ij}$ and $\Phi^2 = \Phi_A \Phi_A$.

In order to describe the external field of a spatially bounded source distribution, one usually requires $(\mathscr{V}, h_{ij})$ to be asymptotically flat in the sense of the following definition.

Definition 1: A manifold $(\mathscr{V}, h_{ij})$ is said to be asymptotically flat, if there exists a C^∞ manifold $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$ satisfying the conditions

(i) $\tilde{\mathscr{V}} = \mathscr{V} \cup \Lambda$ where Λ is a single point;

(ii) $\tilde{h}_{ij}$ is a C^∞ positive definite metric on $\tilde{\mathscr{V}}$, such that, (a) $\tilde{h}_{ij} = \Omega^2 h_{ij}$ on $\mathscr{V}$, where Ω is a scalar field (at least C^2) on $\tilde{\mathscr{V}}$ and (b) $[\Omega]_\Lambda = 0, [\Omega_{;i}]_\Lambda = 0, [\Omega_{;ij} - 2\tilde{h}_{ij}]_\Lambda = 0$, where semicolon represents the action of $\tilde{\nabla}_i$, the covariant derivative on $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$. The point Λ thus attached to $\mathscr{V}$ represents the spatial infinity. In terms of the rescaled potentials

$$\tilde{\Phi}_A = \Omega^{-1/2}\Phi_A \tag{5}$$

the field equations on the conformal manifold $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$ are

$$(\tilde{\Delta} - 2\tilde{R})\tilde{\Phi}_A = \tfrac{15}{2}\Omega^{-1}[\tilde{\Delta}\Omega - \tfrac{3}{2}\Omega^{-1}\tilde{h}^{ij}\Omega_{;i}\Omega_{;j}]\tilde{\Phi}_A;$$

$$\tilde{\Delta} = \tilde{h}^{ij}\tilde{\nabla}_i\tilde{\nabla}_j, \tag{6}$$

$$\begin{aligned}\tilde{R}_{ij} = {} & -\Omega^{-1}[\Omega_{;ij} + \tilde{h}_{ij}(\tilde{\Delta}\Omega - 2\Omega^{-1}\tilde{h}^{kl}\Omega_{;k}\Omega_{;l}) \\ & - \tfrac{1}{2}\tilde{\Phi}^2\Omega_{;i}\Omega_{;j}] + 2[\Omega\tilde{\Phi}_{A;i}\tilde{\Phi}_{A;j} + \tfrac{1}{2}\Omega_{;(i}\tilde{\Phi}^2{}_{;j)} \\ & - (1 + 4\Omega\tilde{\Phi}^2)^{-1}(\Omega\tilde{\Phi}^2)_{;i}(\Omega\tilde{\Phi}^2)_{;j}],\end{aligned} \tag{7}$$

where we have set $\tilde{R} = \tilde{h}^{ij}\tilde{R}_{ij}$ and $\tilde{\Phi}^2 = \tilde{\Phi}_A\tilde{\Phi}_A$. Using Eq. (7), Eq. (6) can be rewritten as

$$[\tilde{\Delta}^{(c)} + 15\Omega^{1/2}\tilde{\Delta}^{(c)}(\Omega^{-1/2})]\tilde{\Phi}_A = 0, \tag{8}$$

where $\tilde{\Delta}^{(c)} = \tilde{\Delta} - \frac{1}{8}\tilde{R}$ is the conformally invariant Laplacian on $\tilde{\mathscr{V}}$.

Next we quote two theorems due to Morrey[4,5] on the differentiability properties of the solutions of a system of second order (nonlinear) elliptic differential equations which will be needed in the sequel. Let us consider a system

$$F^\alpha(x,\ u^\beta,\ u^\beta{}_{,i},\ u^\beta{}_{,ij}) = 0,\quad (\alpha, \beta = 1, 2, \ldots, N), \tag{9}$$

on N coupled second order nonlinear differential equations for N functions $u^\beta(x)$ which is elliptic on an open neighborhood $\mathscr{D}_0$, i.e., at every point $x \in \mathscr{D}_0$

$$\det|L^\alpha{}_\beta(x,\xi)| \neq 0 \tag{10}$$

$\forall\ \xi = (\xi_i) \in \mathscr{T}^*_x$, the cotangent space at x $(\xi \neq 0)$, where

$$L^\alpha{}_\beta(x,\xi) = \xi_k \xi_l \left[\frac{\partial F^\alpha}{\partial u^\beta{}_{,kl}}\right](x) \tag{11}$$

and comma denotes ordinary derivative at x.

Theorem 1 (Morrey[4]): If the functions $u^\beta(x)$ are of class C^2 and satisfy Eqs. (9) and (10) on a bounded domain $\mathscr{D}_0 \supset \overline{\mathscr{D}}_1$ (the closure of $\mathscr{D}_1$) and F^α are of class C^1 on the set $\overline{\mathscr{N}}$, the closure of a domain $\mathscr{N}$ which contains the compact set $\{x, u^\beta(x), u^\beta{}_{,k}(x), u^\beta{}_{,kl}(x) | x \in \overline{\mathscr{D}}_1\}$, then $u^\beta(x)$ are of class $C^{2+\mu}$, i.e., $u^\beta{}_{,kl}(x)$ are uniformly Hölder continuous with exponent μ $(0 < \mu < 1)$ on any domain $\mathscr{D}_2$ such that $\overline{\mathscr{D}}_2 \subset \mathscr{D}_1$.

If, moreover, F^α are of class $C^{m+\mu}$, i.e. the mth derivatives of F^α are uniformly Hölder continuous with exponent μ on $\overline{\mathscr{N}}$ $(m = \text{integer} \geqslant 1, 0 < \mu < 1)$, then $u^\beta(x)$ are of class $C^{m+2+\mu}$ on $\mathscr{D}_1$.

Corollary: If the solutions $u^\beta(x)$ of Eqs. (9) and (10) are of class C^2 on $\mathscr{D}_0 \supset \overline{\mathscr{D}}_1$ and F^α are of class C^∞ with respect to all the arguments on $\overline{\mathscr{N}}$, then $u^\beta(x)$ are also C^∞ on $\mathscr{D}_1$.

Theorem 2 (Morrey[5]): If the solutions $u^\beta(x)$ of Eqs. (9) and (10) are of class C^2 on a domain $\mathscr{D}_0 \supset \overline{\mathscr{D}}_1$ and F^α are of class C^ω (i.e., analytic) with respect to all the arguments on $\overline{\mathscr{N}}$, then $u^\beta(x)$ are also of class C^ω on $\mathscr{D}_1$.

Theorem 1 was used by Hansen[1] to infer the smoothness property of the fields $\tilde{\Phi}_A$ in the neighborhood of Λ. A precise statement of his result is contained in the following lemma.

Lemma 1: If

(1) $(\mathscr{V}, h_{ij})$ is asymptotically flat (in the sense of Definition 1),

(2) $\tilde{h}_{ij}$ and $\tilde{\Phi}_A$ satisfy the vacuum Einstein equations, viz. Eqs. (6) and (7) on an open domain $\mathscr{D}_0 \subset \tilde{\mathscr{V}}$ containing Λ,

(3) the quantities $\tilde{\Phi}_A$, $\tilde{\kappa}$ $(\equiv \Omega^{-1/2}\kappa)$ given by

$$\tilde{\kappa}^4 = \tfrac{1}{2}\lambda^{-2}\tilde{h}^{ij}[\lambda_{,i}\lambda_{,j} + \omega_{,i}\omega_{,j}] \tag{12}$$

and

$$\tilde{\Psi} = \Psi = \tfrac{1}{2}\lambda^{-1}(\lambda^2 + \omega^2 + 1) \tag{13}$$

are of class C^2 on an open domain $\mathscr{D}_1$ containing Λ, with $\overline{\mathscr{D}}_1 \subset \mathscr{D}_0$, and

(4) $[\tilde{\Phi}_M]_\Lambda \neq 0$ (i.e. the mass of the system is nonzero), then $\tilde{\Phi}_A$, $\tilde{\kappa}$, $\tilde{\Psi}$ are of class C^∞ on an open domain $\mathscr{D}_2$ containing Λ, such that $\overline{\mathscr{D}}_2 \subset \mathscr{D}_1$.

Proof: The lemma is easily proved using the corollary of Theorem 1, by observing that $\tilde{\Phi}_A$, $\tilde{\kappa}$, and $\tilde{\Psi}$ satisfy a coupled system of (conformally invariant) second order differential equations which is elliptic on an open domain $\mathscr{D}_0 \subset \tilde{\mathscr{V}}$, if $[\tilde{\Phi}_M]_\Lambda \neq 0$:

$$(\tilde{\Delta}^{(c)} - \tfrac{15}{8}\tilde{\kappa}^4)\tilde{\Phi}_A = 0, \tag{14}$$

$$\tilde{\kappa}^7(\tilde{\Delta}^{(c)} - \tfrac{3}{8}\tilde{\kappa}^4)\tilde{\kappa} + \tilde{B}_{ijk}\tilde{B}^{ijk}$$
$$+ \tilde{F}(\tilde{\Phi}_B, \tilde{\Phi}_{B;m}, \tilde{\Phi}_{B;mn}, \tilde{\kappa}, \tilde{\kappa}_{;m}, \tilde{\Psi}, \tilde{\Psi}_{;m}, \tilde{\Psi}_{;mn}) = 0, \quad (15)$$
$$[(\tilde{\Phi}^2)^2(\tilde{\Delta} - 6\tilde{\kappa}^4) - 2\tilde{\Phi}^2\tilde{\Phi}_A\tilde{\Phi}_{A;i}\tilde{\nabla}^i$$
$$+ 2(\tilde{\Psi}^2 - 1)\tilde{h}^{ij}\epsilon_{AB}\tilde{\Phi}_A\tilde{\Phi}_{B;i}\epsilon_{CD}\tilde{\Phi}_C\tilde{\Phi}_{D;j}]\tilde{\Psi} = 0, \quad (16)$$

where $\tilde{B}_{ijk} = L_{i[j;k]}$ is the Bach tensor of $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$, $L_{ij} = \tilde{R}_{ij} - \frac{1}{4}\tilde{h}_{ij}\tilde{R}$ and F is a (rather complicated) conformally invariant function of weight -6, whose explicit form is given in Ref. 1 and will not be needed here. In Eq. (16) ϵ_{AB} denotes the Levi-Civita symbol:

$$\|\epsilon_{AB}\| = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The physical significance of the conditions (3) in Lemma 1 are clarified in the following two lemmas.

Lemma 2: If $\tilde{\Phi}_A$ and Ω are of class C^m in the neighborhood of Λ, then $\tilde{\Psi}$ is also of class C^m there.

Proof: The lemma follows from the obvious relation

$$\tilde{\Psi}^2 = 1 + 4\Omega\tilde{\Phi}^2 \quad (17)$$

by noting that $\tilde{\Psi} \neq 0$ near Λ.

Lemma 3: If $\tilde{\Phi}_A$, Ω and

$$w = \Omega^{-1}\tilde{h}^{ij}\Omega_{;i}\Omega_{;j} \quad (18)$$

are of class C^2 on a domain $\mathscr{D}_0$ containing the point Λ, then $\tilde{\kappa}$ is of class C^2 on an open domain $\mathscr{D}_1$ containing Λ such that $\bar{\mathscr{D}}_1 \subset \mathscr{D}_0$, provided $[\tilde{\Phi}_M]_\Lambda \neq 0$.

Proof: Contracting Eq. (7) and rearranging, we obtain a second order differential equation for the conformal factor Ω:

$$\tilde{\Psi}^2[4(\tilde{\Delta}\Omega - \tfrac{3}{2}w) + \Omega\tilde{R}] - (\tfrac{1}{2}\tilde{\Phi}^2 w + G)\Omega = 0, \quad (19)$$

which is elliptic on $\mathscr{D}_0$, where

$$G = \tilde{h}^{ij}[2\Omega\tilde{\Psi}^2\tilde{\Phi}_{A;i}\tilde{\Phi}_{A;j} + \Omega_{;i}\tilde{\Phi}^2_{;j} - 2\Omega^2\tilde{\Phi}^2_{;i}\tilde{\Phi}^2_{;j}]. \quad (20)$$

From Eqs. (6) and (19) we also obtain a pair of second order elliptic differential equations for $\tilde{\Phi}_A$ on $\mathscr{D}_0$:

$$[\tilde{\Psi}^2\tilde{\Delta}^{(c)} - \tfrac{15}{8}(\tfrac{1}{2}\tilde{\Phi}^2 w + G)]\tilde{\Phi}_A = 0. \quad (21)$$

We now consider open sets $\mathscr{D}_0''$, $\mathscr{D}_0'$, and $\mathscr{D}_1$ containing Λ such that

$$\mathscr{D}_0 \supset \bar{\mathscr{D}}_0'' \supset \mathscr{D}_0'' \supset \bar{\mathscr{D}}_0' \supset \mathscr{D}_0' \supset \bar{\mathscr{D}}_1 \supset \mathscr{D}_1.$$

From the assumptions it follows that $(\frac{1}{2}\tilde{\Phi}^2 w + G)$ is of class C^1 on $\mathscr{D}_0 \supset \bar{\mathscr{D}}_0''$. The first part of Theorem 1 applied to Eqs. (19) and (21) implies that Ω, $\tilde{\Phi}_A$ are $C^{2+\mu}$ on $\mathscr{D}_0'$ $(0 < \mu < 1)$. Consequently $(\frac{1}{2}\tilde{\Phi}^2 w + G)$ is of class $C^{1+\mu}$ on $\mathscr{D}_0'$. A further application of Theorem 1 to Eqs. (19) and (21) then shows that Ω, $\tilde{\Phi}_A$ are $C^{3+\mu}$ on $\mathscr{D}_1$. The relation

$$\tilde{\kappa}^4 = \tilde{\Psi}^{-2}(\tfrac{1}{2}\tilde{\Phi}^2 w + G) \quad (22)$$

then implies that $\tilde{\kappa}^4$ is C^2 on $\mathscr{D}_1$. Since $\tilde{\kappa} \neq 0$ on $\mathscr{D}_1$, the lemma follows. [Note that $[w]_\Lambda = 4$ from Eq. (19).]

Finally, eliminating w in favor of $\tilde{\kappa}$ and $\tilde{\Psi}$ in Eq. (19), we get an elliptic equation for Ω whose coefficients are C^∞ on $\mathscr{D}_2$ by virtue of Lemma 1:

$$(4\tilde{\Delta} + \tilde{R} - \tilde{\kappa}^4)\Omega - 12(\tilde{\Phi}^2)^{-1}(\tilde{\Psi}^2\tilde{\kappa}^4 - G) = 0. \quad (23)$$

Therefore by the corollary to the Theorem 1, it follows that Ω and consequently, on account of (22), w as well are of class C^∞ on an open set $\mathscr{D}$ such that $\mathscr{D}_2 \supset \bar{\mathscr{D}}$. Thus we arrive at

Theorem 3: If

(1) $(\mathscr{V}, h_{ij})$ is asymptotically flat (in the sense of Definition 1),

(2) $\tilde{h}_{ij}$ and $\tilde{\Phi}_A$ satisfy the vacuum Einstein equations, viz. Eqs. (6) and (7) on an open domain $\mathscr{D}_0 \subset \tilde{\mathscr{V}}$ containing Λ,

(3) the quantities $\tilde{\Phi}_A$, Ω and w are of class C^2 on $\mathscr{D}_0$, and

(4) $[\tilde{\Phi}_M]_\Lambda \neq 0$,

then there exists an open set $\mathscr{D}$ containing the point Λ, such that $\bar{\mathscr{D}} \subset \mathscr{D}_0$ and $\tilde{\Phi}_A$, Ω and w are of class C^∞ on $\mathscr{D}$.

The multipole moments $Q_{A_{i_1}\ldots i_s}$ are recursively defined as a set of trace-free symmetric tensors at Λ by the relations

$$Q_{Ai_1\ldots i_s} = [P_{Ai_1\ldots i_s}]_\Lambda,$$
$$P_A = \tilde{\Phi}_A, \; P_{Ai_1} = \tilde{\Phi}_{A;i_1},$$
$$P_{Ai_1\ldots i_{s+1}} = \mathscr{C}[P_{A(i_1\ldots i_s;i_{s+1})} - \tfrac{1}{2}s(2s-1)P_{A(i_1\ldots i_{s-1}}\tilde{R}_{i_s i_{s+1})}], \quad (24)$$

where $\mathscr{C}[\ldots]$ represents the trace-free part of a tensor.

The analogy of the present scheme with the multipole expansion for Newtonian gravity is quite clear. In the latter case the field equations are simply $R_{ij} = 0$ and $\Delta\Phi = 0$ or equivalently $\Delta^{(c)}\Phi = 0$. The rescaled potential $\tilde{\Phi} = \Omega^{-1/2}\Phi$ is a smooth scalar field on $\tilde{\mathscr{V}}$ which satisfies the equation $\tilde{\Delta}^{(c)}\tilde{\Phi} = 0$. The multipole moments $Q_{i_1\ldots i_s}$ are determined from $\tilde{\Phi}$ by relations analogous to (24). In this case we can explicitly construct the conformal manifold $\tilde{\mathscr{V}}$ by transforming the standard Cartesian coordinates x^a to a new set $y^a = r^{-2}x^a$ with $r^2 = \delta_{ab}x^a x^b$, attaching the point $\Lambda = \{y^a = 0\}$ to the original manifold $\mathscr{V}$ and rescaling the original flat metric $dl^2 = \delta_{ab}dx^a dx^b$ to $d\tilde{l}^2 = \Omega_0^2\, dl^2 = \delta_{ab}dy^a dy^b$, $\Omega_0 = r^{-2}$. The conformal factor Ω_0 can also be interpreted as the square of the Euclidean distance from the point Λ: $\Omega_0 = s^2 = \delta_{ab}y^a y^b$ and characterized by the relations

$$\tilde{h}^{ij}\Omega_{0;i}\Omega_{0;j} = 4\Omega_0, \quad (25)$$
$$\Omega_{0;ij} = 2\tilde{h}_{ij}, \quad (26)$$

everywhere on $\tilde{\mathscr{V}}$. Since $\tilde{\mathscr{V}}$ is also flat ($\tilde{R}_{ij} = 0$), $\tilde{\Phi}$ satisfies $\tilde{\Delta}\tilde{\Phi} = 0$. The multipole moments are given by

$$Q_{i_1\ldots i_s} = [\tilde{\Phi}_{;i_1\ldots i_s}]_\Lambda$$

and are automatically totally symmetric and trace-free. The freedom of choice of the conformal factor in fact includes the usual freedom of choice of the origin of expansion in $\mathscr{V}$. It is easily seen that a translation of origin $x^a \to x'^a = x^a + \eta^a$ is equivalent to a rescaling

$$\Omega_0' = \Omega_0(1 + 2\delta_{ab}\, y^a\eta^b + \Omega_0\delta_{ab}\eta^a\eta^b)^{-1},$$

where both Ω_0 and Ω_0' satisfy Eqs. (25) and (26). The general definition of the multipole moments is so chosen that their transformation property under an infinitesimal conformal mapping precisely reproduces their behavior under an infinitesimal shift of origin. The standard Cartesian multipole expansion of Φ is simply the Taylor expansion of the rescaled potential $\tilde{\Phi}$ around Λ:

$$\tilde{\Phi} = Q + Q_a y^a + \tfrac{1}{2}Q_{ab}y^a y^b + \cdots.$$

In the next section we will introduce a similar expansion for the gravitational field of a spatially bounded stationary source in the framework of general relativity.

III. THE MULTIPOLE EXPANSION

We have already seen that for any given stationary vacuum solution of Einstein's equations satisfying the conditions of Theorem 3, there exists a set of well-defined multipole moments. However the asymptotic conditions described in the last section appear to be too weak to allow power series expansion of the quantities $\tilde{\Phi}_A$ and $\tilde{h}_{ij}$ around Λ. In order to have the possibility of such an expansion (at least formally), one is led to impose a somewhat stronger boundary condition at spatial infinity. First we note that in the C^∞ manifold $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$ there exists a unique maximal geodesic $\gamma_X : [0,1] \to \tilde{\mathscr{V}}$ for a nonzero vector X in $\mathscr{T}_\Lambda(\tilde{\mathscr{V}})$ such that [Ref. 6, p. 30]

$$\gamma_X(0) = \Lambda, \quad \frac{d}{dt}\gamma_X(t)|_{t=0} = X.$$

Obviously, $\gamma_{tX}(u) = \gamma_X(tu)$. Analogy with the Newtonian case suggests the quantity σ representing the square of the geodesic distance from Λ in $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$ as an appropriate intrinsic conformal factor. The function σ satisfies the equation

$$\sigma_i \sigma^i = 4\sigma \tag{27}$$

and the boundary conditions

$$[\sigma]_\Lambda = 0, \ [\sigma_i]_\Lambda = 0, \ [\sigma_{;ij}]_\Lambda = 2[\tilde{h}_{ij}]_\Lambda, \tag{28}$$

where we have set $\sigma_i = \sigma_{;i} = \tilde{\nabla}_i \sigma$ and the indices $i, j, k, \ldots$ are raised and lowered by $\tilde{h}_{ij}$. This special conformal factor therefore trivially satisfies the conditions of Theorem 3. We are thus led to replace the usual asymptotic flatness condition by a more restrictive criterion which will be referred to as the "strong asymptotic flatness condition."

Definition 2: The manifold $(\mathscr{V}, h_{ij})$ is said to be strongly asymptotically flat if there exists a C^ω (i.e., analytic) manifold $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$ with the following properties:

(i) $\tilde{\mathscr{V}} = \mathscr{V} \cup \Lambda$ where Λ is a single point, and

(ii) $\tilde{h}_{ij}$ is a C^ω positive definite metric on $\tilde{\mathscr{V}}$ such that, $\tilde{h}_{ij} = \sigma^2 h_{ij}$ on $\mathscr{V}$, where $\sigma = s^2$ is the square of the geodesic distance from Λ in $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$.

This special conformal factor $\Omega = \sigma$ has the remarkable property of preserving (local) geodesic correspondence between the manifolds $(\mathscr{V}, h_{ij})$ and $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$, i.e.

$$\left(\frac{dx^i}{dr}\right)\nabla_i\left(\frac{dx^j}{dr}\right) = 0 \Leftrightarrow \left(\frac{dx^i}{ds}\right)\tilde{\nabla}_i\left(\frac{dx^j}{ds}\right) = 0,$$

with $r = 1/s$.

The field equations on $\tilde{\mathscr{V}}$ are

$$[\tilde{\Delta}^{(c)} - 15(W_i{}^i + \tilde{\Phi}^2)]\tilde{\Phi}_A = 0, \tag{29}$$

$$L_{ij} = -\sigma^{-1}[\sigma_{;ij} - 2\tilde{h}_{ij} - \tfrac{1}{2}\tilde{\Phi}^2\sigma_i\sigma_j] + 2W_{ij}, \tag{30}$$

with

$$\begin{aligned}
W_{ij} &= \sigma A_{ij} + \sigma_{(i}B_{j)} - C\tilde{\Phi}^2\sigma_i\sigma_j - \tfrac{1}{4}\tilde{h}_{ij}(\sigma A_k{}^k + \sigma_k B^k + C), \\
A_{ij} &= \tfrac{1}{2}\tilde{\Phi}_{A;i}\tilde{\Phi}_{A;j} - \sigma(1 + 4\sigma\tilde{\Phi}^2)^{-1}\tilde{\Phi}^2{}_{;i}\tilde{\Phi}^2{}_{;j}, \\
B_i &= \tfrac{1}{2}\tilde{\Phi}^2{}_{;i}(1 + 4\sigma\tilde{\Phi}^2)^{-1}, \\
C &= \tilde{\Phi}^2(1 + 4\sigma\tilde{\Phi}^2)^{-1}.
\end{aligned} \tag{31}$$

Since $(\mathscr{V}, h_{ij})$ is assumed to obey the strong asymptotic flatness condition, Eq. (29) is a pair of elliptic equations for $\tilde{\Phi}_A$ with analytic coefficients. From Theorem 2 it follows that the fields $\tilde{\Phi}_A$ are also analytic in an open neighborhood of Λ in $\tilde{\mathscr{V}}$.

Since the manifold $\tilde{\mathscr{V}}$ is C^∞ and possesses an affine connection, there exist, in accordance with standard theorems of differential geometry [Ref. 6, pp. 32–34], open neighborhoods $\mathscr{N}_0 \subset \mathscr{T}_\Lambda(\tilde{\mathscr{V}})$ and $\mathscr{N}_\Lambda \subset \tilde{\mathscr{V}}$ such that the exponential map $\exp_\Lambda : X \to \gamma_X(1)$ is a C^∞ diffeomorphism of $\mathscr{N}_0$ onto $\mathscr{N}_\Lambda$. If $\mathscr{N}_0$ is chosen to be star-shaped around the origin (i.e. $tX \in \mathscr{N}_0$ for all $X \in \mathscr{N}_0$ and $0 \leqslant t \leqslant 1$), then $\mathscr{N}_\Lambda = \exp_\Lambda \mathscr{N}_0$ is a normal neighborhood of Λ. Moreover $\mathscr{N}_\Lambda$ is also a normal neighborhood of each of its points (Whitehead's theorem). In particular, $\mathscr{N}_\Lambda$ is convex, i.e., two arbitrary points of $\mathscr{N}_\Lambda$ can be joined by exactly one geodesic segment contained in $\mathscr{N}_\Lambda$ (except for a linear change of the affine parameter on the geodesic). Next let $\{\mathbf{e}_a\}$ denote an orthonormal basis in $\mathscr{T}_\Lambda$. The inverse mapping of $\mathscr{N}_\Lambda$ into $\mathbb{R}^3$ given by

$$\exp_\Lambda{}^{-1}(x) = y^a \mathbf{e}_a, \quad x \in \mathscr{N}_\Lambda$$

defines a normal coordinate system around Λ in $\tilde{\mathscr{V}}$. Moreover, in the present case $\exp_\Lambda$ is an analytic diffeomorphism since $\tilde{\mathscr{V}}$ itself is analytic. The pair $(\mathscr{N}_\Lambda, \exp_\Lambda)$ thus represents an analytic chart in $\tilde{\mathscr{V}}$. This enables us to expand $\tilde{\Phi}_A = \sigma^{-1/2}\Phi_A$ and $\tilde{h}_{ab} = \sigma^2 h_{ab}$ as power series in y^a around Λ ($\doteq$ denotes an equality valid only in normal coordinates)[7]:

$$\tilde{\Phi}_A \doteq \sum_{n=0}^{\infty} (n!)^{-1}[\tilde{\Phi}_{A;(a_1 \ldots a_n)}]_\Lambda y^{a_1} \ldots y^{a_n}, \tag{32}$$

$$\begin{aligned}
\tilde{h}_{ab} \doteq{}& \delta_{ab} + \tfrac{1}{3}[\tilde{R}_{aa_1a_2b}]_\Lambda y^{a_1}y^{a_2} + \tfrac{1}{6}[\tilde{R}_{aa_1a_2b;a_3}]_\Lambda y^{a_1}y^{a_2}y^{a_3} \\
&+ \tfrac{1}{20}[\tilde{R}_{aa_1a_2b;a_3a_4} + \tfrac{8}{9}\tilde{R}_{aa_1a_2c}\tilde{R}^c{}_{a_3a_4b}]_\Lambda y^{a_1}y^{a_2}y^{a_3}y^{a_4} + \cdots .
\end{aligned} \tag{33}$$

(These expansions follow from the coordinate condition $\tilde{\Gamma}^a{}_{bc}(y)y^b y^c = 0$.) Furthermore, we note that the Riemann and Ricci tensors of $\tilde{\mathscr{V}}$ are related through the equation

$$\tilde{R}_{ikjl} = 4\tilde{h}_{[i[j}L_{l]k]}. \tag{34}$$

(Since $\tilde{\mathscr{V}}$ is three-dimensional its Weyl tensor is identically zero.)

A straightforward application of the field equations to evaluate the coefficients of these expansions in terms of $Q_{A i_1 \ldots i_n}$ is prevented by the apparent singularity of the right-hand side of Eq. (30) at Λ. This singularity can be removed as follows. By repeated covariant differentiation of Eq. (27) one obtains the coincidence limits[8]

$$[\sigma_{;ijk}]_\Lambda = 0, \ [\sigma_{;ijkl}]_\Lambda = \tfrac{4}{3}[\tilde{R}_{i(jk)l}]_\Lambda \tag{35}$$

and so on. These then yield the following covariant expansion of $\sigma_{;ij}$[9]:

$$\begin{aligned}
\sigma_{;ij} = 2\tilde{h}_{ij} &- \frac{1}{3!}\overset{0}{U}_{ij} + \frac{1}{2\cdot 4!}\overset{1}{U}_{ij} \\
&- \frac{1}{2^2\cdot 5!}\left(\overset{2}{U}_{ij} + \frac{4}{3}\overset{0}{U}_i{}^k\overset{0}{U}_{jk}\right) + \cdots,
\end{aligned} \tag{36}$$

where for brevity we have set

$$\overset{p}{U}_{ij} = \widetilde{R}_{ikjl;m_1\ldots m_p}\sigma^k\sigma^l\sigma^{m_1}\ldots\sigma^{m_p}. \tag{37}$$

Next we introduce the auxiliary quantities

$$\overset{0}{\Lambda}_{ij} = L_{ij}, \overset{p}{\Lambda}_{ij} = L_{ij;m_1\ldots m_p}\sigma^{m_1}\ldots\sigma^{m_p} \quad (p\geqslant 1), \tag{38}$$

$$\overset{p}{V}_i = \overset{p}{\Lambda}_{ij}\sigma^j, \tag{39}$$

and collect a number of useful results in the form of several lemmas.

Lemma 4: For all integers $p\geqslant 0$ the tensors $\overset{p}{U}_{ij}, \overset{p}{\Lambda}_{ij}$ and $\overset{p}{V}_i$ obey the recurrence relations

$$\overset{p+1}{U}_{ij} = \overset{p}{U}_{ij;k}\sigma^k - 2(p+2)\overset{p}{U}_{ij}, \tag{40}$$

$$\overset{p+1}{\Lambda}_{ij} = \overset{p}{\Lambda}_{ij;k}\sigma^k - 2p\overset{p}{\Lambda}_{ij}, \tag{41}$$

$$\overset{p+1}{V}_i = \overset{p}{V}_{i;k}\sigma^k - 2(p+1)\overset{p}{V}_i. \tag{42}$$

Proof: The proof involves a simple direct computation using the relation

$$\sigma_{;ij}\sigma^j = 2\sigma_i. \tag{43}$$

Lemma 5: The vectors $\overset{p}{V}_i$ can be expressed in the form

$$\overset{p}{V}_i = \sigma\overset{p}{G}_i + \sigma_i\overset{p}{H}, \tag{44}$$

where

$$\overset{0}{G}_i = 2[(A_{ik}\sigma^k - \tfrac{1}{4}A_k{}^k\sigma_i) + 2B_i - \sigma_i\widetilde{\Phi}^2(\sigma^k B_k + 3C)], \tag{45}$$

$$\overset{0}{H} = \tfrac{1}{2}(3\widetilde{\Phi}^2 + \tfrac{1}{2}\widetilde{\Phi}^2{}_{;k}\sigma^k), \tag{46}$$

$$\overset{p+1}{G}_i = \overset{p}{G}_{i;k}\sigma^k - 2(p-1)\overset{p}{G}_i \qquad (p\geqslant 0), \tag{47}$$

$$\overset{p+1}{H} = \overset{p}{H}_{;k}\sigma^k - 2p\overset{p}{H} \qquad (p\geqslant 0). \tag{48}$$

In particular the scalars $\overset{p}{H}$ have the form

$$\overset{p}{H} = \tfrac{1}{2}[(p+3)\widetilde{\Phi}^2{}_{;m_1\ldots m_p} + \tfrac{1}{2}\widetilde{\Phi}^2{}_{;im_1\ldots m_p}\sigma^i]\sigma^{m_1}\ldots\sigma^{m_p}. \tag{49}$$

Proof: The case $p = 0$ of Eq. (44) is proved by contracting Eq. (30) with σ^j and using Eqs. (27) and (43). The proof of Eq. (44) for a general value of p can then be carried out by induction from Eq. (42).

Lemma 6: $$\overset{p}{U}_{ij} = 4\sigma\overset{p}{M}_{ij} - 2\sigma_i\sigma_j\overset{p}{H}, \tag{50}$$

where

$$\overset{p}{M}_{ij} = \overset{p}{\Lambda}_{ij} + \widetilde{h}_{ij}(\overset{p}{H} + \tfrac{1}{4}\overset{p}{G}_k\sigma^k) - \tfrac{1}{2}\sigma_{(i}\overset{p}{G}_{j)}. \tag{51}$$

Proof: This lemma is a simple consequence of Eqs. (34) and (44).

From Lemma 6 we can also derive

Lemma 7:

$$\sigma^{-1}\overset{p}{U}_{(i}{}^k\overset{q}{U}_{j)k} = 16\left(\sigma\overset{p}{M}_{(i}{}^k\overset{q}{M}_{j)k} - \sigma_i\sigma_j\overset{p}{H}\overset{q}{H}\right). \tag{52}$$

Armed with these lemmas we now proceed to examine the singularity of the field equation (30) around Λ. With the aid of the expansion (36) and the Lemmas 6 and 7, Eq. (30) can be rewritten as

$$L_{ij} - 2\Big\{W_{ij} + \tfrac{1}{3}\overset{0}{M}_{ij} - \tfrac{1}{24}\overset{1}{M}_{ij} + \Big[\tfrac{1}{240}\overset{2}{M}_{ij} + \tfrac{1}{45}\Big(\sigma\overset{0}{M}_i{}^k\overset{0}{M}_{jk} - \sigma_i\sigma_j\overset{0}{H}{}^2\Big)\Big] - \cdots\Big\}$$
$$= \sigma^{-1}\sigma_i\sigma_j\Big(\tfrac{1}{2}\widetilde{\Phi}^2 - \tfrac{1}{3}\overset{0}{H} + \tfrac{1}{24}\overset{1}{H} - \tfrac{1}{240}\overset{2}{H} + \cdots\Big), \tag{53}$$

where all the singular terms direction dependent at Λ are isolated on the right-hand side. We also note that because of Lemma 7, the terms involving products of the Riemann tensor and its various derivatives do not contribute to the singularity; the only contribution comes from the terms linear in the Riemann tensor and its derivatives. However, in view of Eq. (49) it is obvious that all the singular terms in Eq. (53) proportional to $\sigma^{-1}\sigma_i\sigma_j$ exactly cancel reducing the equation to the form

$$L_{ij} - 2\Big\{W_{ij} + \tfrac{1}{3}\overset{0}{M}_{ij} - \tfrac{1}{24}\overset{1}{M}_{ij} + \Big[\tfrac{1}{240}\overset{2}{M}_{ij} + \tfrac{1}{45}\Big(\sigma\overset{0}{M}_i{}^k\overset{0}{M}_{jk} - \sigma_i\sigma_j\overset{0}{H}{}^2\Big)\Big] - \cdots\Big\} = 0. \tag{54}$$

Equation (54) now involves only quantities manifestly smooth at Λ. However the price we have to pay is that it has now an infinite number of terms.

From now on the calculations proceed in a straightforward iterative manner. From Eq. (54) and its successive covariant derivatives at Λ and the basic coincidence limits [Eqs. (28) and (35)] one obtains

$$[L_{ab}]_\Lambda \overset{*}{=} \frac{3}{2}Q^2\delta_{ab};\ Q^2 = Q_AQ_A, \tag{55a}$$

$$[L_{ab;c}]_\Lambda \overset{*}{=} 6\delta_{(ab}Q_{Ac)}Q_A, \tag{55b}$$

$$[L_{ab;cd}]_\Lambda \overset{*}{=} \tfrac{20}{3}Q_{Aa}Q_{Ab}\delta_{cd} + 8Q_AQ_{A(a|(c}\delta_{d)|b)} + \tfrac{8}{3}Q_{A(a}\delta_{b)(c}Q_{Ad)} + \delta_{ab}\Big[Q_AQ_{Acd} + \tfrac{11}{3}Q_{Ac}Q_{Ad} + \delta_{cd}\Big(2Q^4 - \tfrac{7}{3}Q_{Ae}Q_A{}^e\Big)\Big] + 4\delta_{(a|(c}\delta_{d)|b)} \times\Big(Q^4 + \tfrac{1}{3}Q_{Ae}Q_A{}^e\Big) \tag{55c}$$

and so on. Eq. (29) and its successive covariant derivatives evaluated at Λ together with Eqs. (55a), (55b), (55c) etc. then determine the quantities $[\widetilde{\Phi}_{A;a_1a_2}]_\Lambda$, $[\widetilde{\Phi}_{A;(a_1a_2a_3)}]_\Lambda$, $[\widetilde{\Phi}_{A;(a_1\ldots a_4)}]_\Lambda$, etc. in terms of the multipole moments $Q_{Aa_1\ldots a_s}$ from the definition (24). Moreover, it is apparent that in the present scheme

$$\mathscr{C}[L_{(ij;m_1\ldots m_p)}]_\Lambda = 0. \tag{56}$$

This is most easily seen by dimensional arguments. Assigning the 2^s moment $Q_{Ai_1\ldots i_s}$ a mass dimension $s+1$ we see that the tensor $[L_{(ij;m_1\ldots m_s)}]_\Lambda$ of rank $s+2$ has also mass dimension $s+2$. Since the only tensor available at Λ besides $Q_{Ai_1\ldots i_s}$ is $\widetilde{h}_{ij}$, $[L_{(ij;m_1\ldots m_s)}]_\Lambda$ must be of the form $[\widetilde{h}_{(ij}T_{m_1\ldots m_s)}]_\Lambda$ and must consequently be trace-free. (In fact the same argument applies to the unsymmetrized tensor itself.) Thus the multipole moments are given by the simpler formula

$$Q_{Ai_1\cdots i_s} = \mathscr{C}\,[\tilde{\Phi}_{A;(i_1\cdots i_s)}]_{\Lambda}. \tag{57}$$

Combining these results, one obtains the desired multipole expansion (up to fourth order)[10]:

$$\begin{aligned}\tilde{\Phi}_A \overset{*}{=}\ & Q_A + Q_{Aa_1}y^{a_1} + (\tfrac{1}{2}Q_{Aa_1a_2} + \delta_{a_1a_2}Q^2Q_A)y^{a_1}y^{a_2} + [\tfrac{1}{6}Q_{Aa_1a_2a_3} + \delta_{(a_1a_2}(Q_{Aa_3)}Q^2 \\ & + 2Q_{Ba_3)}Q_BQ_A)]y^{a_1}y^{a_2}y^{a_3} + (\tfrac{1}{24}Q_{Aa_1a_2a_3a_4} + \delta_{(a_1a_2}\{Q_{Ba_3a_4)}Q_BQ_A \\ & + \tfrac{4}{7}Q_{Aa_3a_4)}Q^2 + \tfrac{2}{21}(11Q_{Ba_3}Q_{Ba_4)}Q_A + 20\,Q_{Aa_3}Q_{Ba_4)}Q_B) \\ & + \delta_{a_3a_4)}[\tfrac{2}{21}(Q_{Bb}Q_B{}^bQ_A - 2Q_{Ab}Q_B{}^bQ_B) + Q^4Q_A]\})y^{a_1}\cdots y^{a_4} + O(y^5),\end{aligned} \tag{58}$$

$$\begin{aligned}\tilde{h}_{ab} \overset{*}{=}\ & \delta_{ab} + [Q^2 + \tfrac{4}{3}Q_AQ_{A_1}y^{a_1} + \tfrac{1}{2}(Q_AQ_{Aa_1a_2} \\ & + Q_{Aa_1}Q_{Aa_2})(y^{a_1}y^{a_2} - \tfrac{1}{3}\sigma\delta^{a_1a_2})](y_ay_b - \sigma\delta_{ab}) \\ & - \tfrac{4}{3}\delta_{[a|[b}Q_{Aa_2]|}Q_{Aa_1}y^{a_1}y^{a_2}\sigma + O(y^5), \quad y_a = \tilde{h}_{ab}y^b \overset{*}{=} \delta_{ab}y^b,\end{aligned} \tag{59}$$

together with $\sigma \overset{*}{=} \delta_{ab}y^ay^b$. It is to be emphasized that the expansions (58) and (59) can, in principle, be extended to any desired order. However, the computations become increasingly tedious in higher orders. One may still hope to find a closed form for the general term of these expansions inductively by extending the calculation to several higher orders.

IV. SOME SIMPLE EXAMPLES

In order to express a given stationary vacuum metric in our representation, first one has to solve Eq. (27), which is equivalent to an eikonal equation

$$h^{ij}R_{,i}R_{,j} = 1 \tag{60}$$

on the compactified (but singular) manifold $(\tilde{\mathscr{V}}, h_{ij})$ for the function $R = \sigma^{-1/2}$. This is readily done in the cases (e.g. the Kerr metric) where it is separable in some coordinate system. For the Schwarzschild metric the problem is further simplified by the spherical symmetry. In this case it is natural to choose $(\tilde{\mathscr{V}}, \tilde{h}_{ij})$ also to be spherically symmetric. Spherical symmetry together with static nature implies that all the moments except Q_M are zero. In terms of a new radial variable ρ defined from the standard Schwarzschild radial coordinate r by $r = \rho^{-1}(1 + \frac{1}{2}m\rho)^2$, the spatial metric has the form

$$dl^2 = \rho^{-4}(1 - \tfrac{1}{4}m^2\rho^2)^2 dl_0^2,$$

where dl_0^2 is the flat metric in spherical polar coordinates (ρ, θ, ϕ). In this case an appropriate solution of Eq. (60) is $R = \rho^{-1}(1 + \frac{1}{4}m^2\rho^2) = r - m$. Then the conformal metric and the rescaled gravitational potentials are given by

$$d\tilde{l}^2 = \left[\frac{1 - \frac{1}{4}m^2\rho^2}{(1 + \frac{1}{4}m^2\rho^2)^2}\right]^2 dl_0^2, \tag{61}$$

$$\tilde{\Phi}_M = -m\left[\frac{1 + \frac{1}{4}m^2\rho^2}{1 - \frac{1}{4}m^2\rho^2}\right]^2, \quad \tilde{\Phi}_J = 0, \tag{62}$$

with the point $\{\rho = 0\}$ identified as Λ. In terms of σ, $\tilde{\Phi}_M$ takes the simple form

$$\tilde{\Phi}_M = -m(1 - m^2\sigma)^{-1}. \tag{63}$$

This is seen to agree with the general expression (58) (up to fourth order) with the identification $Q_M = -m$ when all other moments are set equal to zero. It is to be noted that the series expansion of (63) converges in the entire exterior region $r > 2m$ outside the event horizon.

Next let us choose $Q_M = -m, Q_J = -l$. Since the conformal metric $\tilde{h}_{ab}$ (and consequently σ) are functions of Q^2 alone, they can be obtained by the formal substitution $m^2 \to m^2 + l^2$ in the corresponding expressions for the Schwarzschild solution. The rescaled scalar potentials $\tilde{\Phi}'_A$ for this new solution are now given by

$$\tilde{\Phi}'_M + i\tilde{\Phi}'_J = -(m + il)[1 - (m^2 + l^2)\sigma]^{-1}.$$

We note that the potentials $\Phi'_A (= \sigma^{1/2}\tilde{\Phi}'_A)$ are related to those of the Schwarzschild solution by the relation

$$\Phi'_M + i\Phi'_J = e^{i\alpha}(\Phi_M + i\Phi_J), \alpha = \tan^{-1}(l/m).$$

This solution is therefore readily identified as the NUT (Newman–Unti–Tamburino) metric.

V. DISCUSSIONS

Although in Sec. III we have completed the basic formulation of the problem, enormous calculational complexities have prevented us from displaying a closed formula for the general term of the multipole expansion. Beyond the $O(y^4)$ term, the computation involves manipulating increasingly long and unwieldy expressions. However certain general features already begin to emerge in the lowest order terms. They exhibit clearly the effect of mixing of the multipole moments due to curvature and nonlinearity. The coefficient of the $O(y^s)$ term involves, besides the 2^s order moment, "trace parts" depending on all moments up to order 2^{s-2}. Thus the local structure of the external field of a bounded stationary source described by a strongly asymptotically flat vacuum metric, like that of its Newtonian analog, is determined completely by its multipole moments at least near spatial infinity. In spite of the rather complicated form of the general expansions, the simplicity of the Schwarzschild solution is somewhat encouraging. Relatively simple expressions are expected also for the Kerr and the Weyl metrics. It would also be of great interest to know whether there are exact stationary vacuum solutions which are asymptotically flat by the usual criterion but do not obey our stronger condition.

The present expansion scheme is valid only in a neighborhood of Λ where geodesics emerging from Λ do not cross one another. Knowledge of the general structure of the expansion is necessary to put bounds on the rate of growth of

the 2^s- moment with s in order to ensure its convergence in a domain of nonzero radius around Λ. For the Schwarzschild metric the expansion is indeed valid everywhere outside the event horizon.

Finally we remark that all the weaknesses of a power series method are, of course, inherent in the present scheme. The expansion as such does not yield any information about the global properties of the solution, for instance, the location of singularities and other pathologies. It should also be mentioned that the problem of relating the multipole moments to the actual source distribution by integral relations analogous to the Newtonian case remains completely unsolved in this line of approach.

Note added in proof: Recently a full analyticity theorem has been proved for the entire set of rescaled field variables $\tilde{\Phi}_A$ and $\tilde{h}_{ij}$ for a special choice of the conformal factor which makes $\tilde{\Phi}^2 = \text{const.}$[11] However, it seems very difficult to prove a similar strong result for the present choice $\Omega = \sigma$.

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On almost causality

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The almost causal precedence concept proposed by Woodhouse and a causality axiom based on it are analyzed. Properties of the almost future are examined and the above causality axiom is shown to be deducible for a causally continuous space–time. It is shown to be coinciding with known causality conditions for a reflecting space–time. Also the equivalence of various causality conditions for a reflecting space–time and a reduction of the causal continuity axiom are obtained. It is next shown that the above causality axiom is not stable under metric perturbations. Then the Seifert future concept has been analyzed and the Woodhouse causality is proved to be strictly weaker than the stable causality condition. It is concluded that as far as the uncertainties in the form of metric perturbations are concerned, the Seifert future is useful but not the almost future.

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1. INTRODUCTION

In the general theory of relativity, the space–time universe is considered as a collection of all events which admits a 4-dimensional differentiable manifold structure. In the recent developments concerning the theory of occurrence of singularities in a space–time, the causal structure of the space–time has been extensively discussed and various conditions like strong causality, stable causality, causal continuity, etc. have been considered in detail, which would give a physically reasonable space–time so far as the causality is concerned.

However, Woodhouse[1] stressed that the differential and causal structures of space–time could be deduced rigorously from a set of physically well-motivated axioms. He imposed only two global causality restrictions on the space–time of which the second one was more important and it essentially aimed at taking into account the uncertainties involved in the measurements, as implied by the quantum uncertainty principle. A very appealing justification was provided for the introduction of this second axiom, which related the causal and topological structures of space–time also.

Here we aim to consider in detail the second causality principle given by Woodhouse. This causality principle turns out to be related to other global concepts concerning causality, like stable causality, causal continuity, etc. It allows to define a new set in the space–time, called the "almost future" of an event, which is always closed. Having introduced some preliminaries in the next section, Sec. 3 analyzes the properties of the almost future. Section 4 shows that this causality principle by Woodhouse is very closely related to other known causality conditions on a space–time. It can be deduced from the causal continuity of the space–time and for a reflecting space–time it actually coincides with some of the well-known causality conditions. In this section, a reduction of the causal continuity condition of Hawking and Sachs[2] has also been obtained. Section 5 then shows that in fact the Woodhouse causality principle is *not* a stable property of a space–time in the sense that a slightest perturbation in the metric could destroy it. Finally, the almost future definition has been compared with the Seifert future definition which was introduced by Seifert.[3] With the help of the analysis here it is proved that the second causality axiom of Woodhouse is strictly included in the stable causality condition for a space–time. It is concluded that, where as the almost future concept cannot take the metric perturbations into account as shown by us, Seifert's definition is a more useful concept so far as the uncertainties involved in the observations are concerned.

2. PRELIMINARIES

Here M denotes a space–time which is a 4-dimensional differentiable manifold. M is a topological space under the natural manifold topology and is assumed to be connected, Hausdorff, paracompact, and time–orientable. A globally defined metric tensor is defined on M which allows us to speak of nonspacelike curves. The notations and conventions used will be the same as those of Hawking and Ellis.[4]

Following Woodhouse,[1] we now state the concept of "almost causal precedence." He argued that since a real physical experiment can never be made sure to have been performed at a precise event of the space–time, we should think of an event as the limit of a converging sequence of neighborhoods. Hence we shall say that an event x *almost causally precedes* another event y, denoted by $x\mathrm{A}y$, if for all $z\in I^-(x)$, $I^+(z)\supset I^+(y)$; or equivalently, if for all $z\in I^+(y)$, $I^-(z)\supset I^-(x)$. It would be more reasonable physically to say that "x almost causally precedes y," rather than saying that "there is a nonspacelike curve from x to y." This is because if $x\mathrm{A}y$, then every neighborhood of x in the manifold topology would contain events which will precede chronologically some events in any neighborhood of y. Because of this, no physical experiment will be able to tell that x and y are *not* causally related. As the causal precedence definition defines

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the causal future (past) $J^+(x)$ for all $x \in M$, with the help of the above almost causal precedence concept one can define the *almost future* and *almost past* for any $x \in M$:

$$A^+(x) = \{ y | x \text{ almost causally precedes } y \},$$

$$A^-(x) = \{ y | y \text{ almost causally precedes } x \}.$$

This means

$$A^+(x) = \{ y | x A y \},$$

$$A^-(x) = \{ y | y A x \}.$$

Based on this, Woodhouse proposed the following principle of causality for a space–time: If for any $x,y \in M$ we have xAy and yAx, then we must have $x = y$. Note that this formulation includes the nonoccurrence of closed nonspacelike curves, because if such a curve occurred, then for any two different points x and y on it, it is easy to see that we have both xAy and yAx, which contradicts the Woodhouse causality principle. The concept of almost causal precedence is made explicit by Fig. 1.

Before we begin to analyze actually how successful this formulation of almost causal precedence idea is in taking the uncertainties into account, some more definitions are in order: Let $S \subset M$ be an open set. Then the chronological *common future* $\uparrow S$ is the set of all those points such that there is a timelike curve to any of these points from all points in S. Formally,

$$\uparrow S = \text{Int} \left\{ z \in M \left| \begin{array}{l} \text{for all } s \in S, \text{ there is a future} \\ \text{directed timelike curve from } s \text{ to } z \end{array} \right. \right\}.$$

The set $\downarrow S$ can be defined dually. Note that $\downarrow S$ and $\uparrow S$ are always open sets.

A space–time M is said to be *reflecting* if for all $x,y \in M$, $I^+(x) \supseteq I^+(y)$ if and only if $I^-(y) \supseteq I^-(x)$. M is said to be *causal* if it contains no closed nonspacelike curves. For the definitions as well as discussion on various other higher-order causality conditions like future (past) distinguishingness, strong causality, stable causality, etc. we refer to Ref. 4. A space–time M is said to be *causally continuous* if it is both reflecting and distinguishing. Hawking and Sachs[2] introduced this assumption on a space–time, which removes many global pathologies from it and the desirable features like the continuity of global time functions etc. are introduced in M. The following lemma which is proved in Ref. 2. will be useful.

Lemma 1: Let M be a reflecting space–time. Then

$$\uparrow I^-(x) = I^+(x), \quad \downarrow I^+(x) = I^-(x).$$

Since the quantum uncertainty principle implies impreciseness in the measurements, it will not be possible to measure the exact values of the metric at any point and hence the metric perturbations are to be taken into account. To achieve this, Seifert[3] defined the set $J_s^+(x)$ as follows:

$$J_s^+(x) = \bigcap_{\bar{g} > g} J^+(x, \bar{g}).$$

Here $\bar{g} > g$ means that the light cones of $\bar{g}$ are everywhere wider than g, i.e., every nonspacelike vector with respect to g becomes timelike with respect to $\bar{g}$. We shall call the set $J_s^+(x)$ as the *Seifert future* of the event x and shall analyze it later. Hawking and Sachs[2] have proved the following in this connection.

Lemma 2: Let M be a causally continuous space–time. Then

$$J_s^+(x) = \overline{J^+(x)} \quad \text{for all } x \in M.$$

Lemma 3: $J_s^+(x)$ is closed for all $x \in M$.

Also Seifert[3] proved the following:

Lemma 4: Let $\{ p_n \}$ be a sequence in $I^-(p)$ such that $p_n \to p$. Then

$$\bigcap_{n=1}^{\infty} J_s^+(p_n) \subset J_s^+(p).$$

Lemma 5: A space–time M is stably causal if and only if J_s^+ is a partial ordering on M.

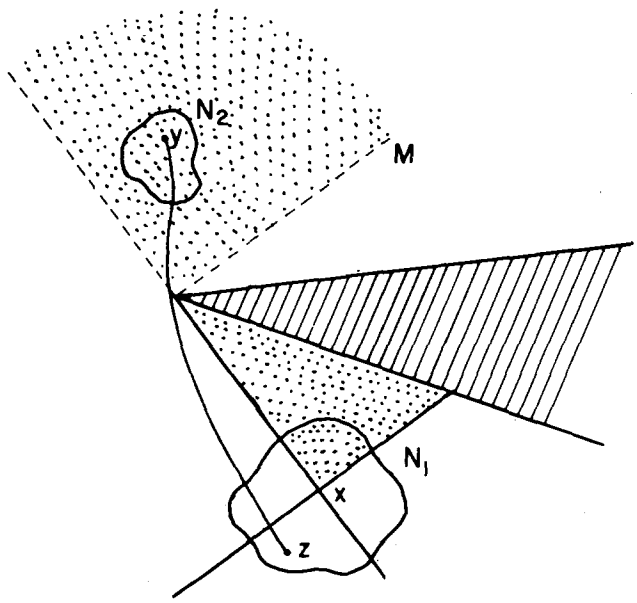

FIG. 1. The shaded region denotes a cut in the space–time. Here $y \in A^+(x)$ but $y \notin I^+(x)$. Note that $A^+(x) \supset I^+(x)$. From every neighborhood N_1 of x, there is a nonspacelike curve to every neighborhood N_2 of y. Since $I^-(y) \supset I^-(x)$, $y \in \uparrow I^-(x)$ also holds. The dotted regions show $A^+(x)$, in which the boundary of the region is also included.

3. SOME PROPERTIES OF ALMOST FUTURE

Here we would like to prove certain results describing some properties of the almost future as defined with the help of the concept of almost causual precedence. These will illustrate the nature of the almost future and also they will be useful for further examination of Woodhouse's formulation of causality principle.

The following proposition follows from the definition of the almost future.

Proposition 1: For all $x,y \in M$, $y \in A^+(x)$ if and only if $x \in A^-(y)$.

It is known that for a general space–time, the causal future $J^+(x)$ of some $x \in M$ need not be closed in the manifold topology. However, one can prove that the almost future of an event is always closed.

Proposition 2: The almost future $A^+(x)$is closed in the manifold topology for all $x \in M$.

Proof: Let p be a limit point of $A^+(x)$ in the manifold

topology on M. Then there is a sequence $\{p_n\}$ in $A^+(x)$ such that $p_n \to p$. Let now $y \in I^+(p)$, then $p \in I^-(y)$, which is open, and hence a neighborhood of p. So there exists a positive integer n_0 such that $p_n \in I^-(y)$ for all $n \geqslant n_0$. So $y \in I^+(p_n)$ for all $n \geqslant n_0$. Since $p_n \in A^+(x)$ for all n, this gives $I^+(p_n) \subset I^+(z)$ for all $z \in I^-(x)$. So $y \in I^+(z)$ for all $z \in I^-(x)$. Thus finally we have $I^+(p) \subset I^+(z)$ for all $z \in I^-(x)$ and so $p \in A^+(x)$.

Thus, whenever a sequence of events is in the future of an event, its limit it also in the future of that event according to the Woodhouse's definition, which is a physically reasonable feature. Also we note that the closeness of $A^+(x)$ in general may help to obtain a topology on the space–time in the same way as the openness of $I^+(x)$ gives a topology on it.

In Fig. 1 the event $y \in A^+(x)$. However clearly $y \in \uparrow I^-(x)$ also. This suggests some relation between the almost future and the common future of the past of the event, which is established in general by the following:

Proposition 3:

$$\mathrm{Int}[A^+(x)] = \uparrow I^-(x).$$

Proof: Let $p \in \mathrm{Int}[A^+(x)]$. Then there is a simple region N containing p and contained within $A^+(x)$. Let $q \in I^-(p) \cap N$. Then $p \in I^+(q)$ and $q \in A^+(x)$. Therefore $I^+(q) \subset I^+(z)$ for all $z \in I^-(x)$. This gives $p \in I^+(z)$ for all $z \in I^-(x)$. In the similar manner one can see that any point of N belongs to $I^+(z)$ for all $z \in I^-(x)$. Hence $p \in \uparrow I^-(x)$.

Conversely, suppose $p \in \uparrow I^-(x)$. Since $\uparrow I^-(x)$ is an open set, there is a simple region N such that $p \in N \subset \uparrow I^-(x)$. So every point of N could be joined by a timelike curve from any point of $I^-(x)$. This gives $p \in N \subset A^+(x)$. Hence $p \in \mathrm{Int} A^+(x)$.

The $A^+(x)$ definition attempts to take into account the imprecision of the measurements and the $\uparrow I^-(x)$ provides information about future as decided by the overall past; both of which have turned out to be almost the same. This suggests the possibility that some information from the past of an event should probably determine its almost future. This is established to be true in general in the following result.

Proposition 4: Let $x \in M$ and $\{x_n\}$ be a sequence in $I^-(x)$ such that $x_n \to x$. Then

$$A^+(x) = \bigcap_{n=1}^{\infty} \overline{I^+(x_n)} = \bigcap_{n=1}^{\infty} \overline{J^+(x_n)}.$$

Proof: Let $p \in A^+(x)$. Then $I^+(p) \subset I^+(x_n)$ for all n. Now let $s \in I^+(p)$. Then $I^+(s) \subseteq I^+(p) \subseteq I^+(x_n)$, so $s \in \overline{I^+(x_n)}$. This gives $p \in \overline{I^+(p)} \subseteq \overline{I^+(x_n)}$ for all n. Hence $p \in \cap_{n=1}^{\infty} \overline{I^+(x_n)}$ and so $A^+(x) \subset \cap_{n=1}^{\infty} \overline{I^+(x_n)}$.

Conversely, let $p \in \cap_{n=1}^{\infty} \overline{I^+(x_n)}$. So $p \in \overline{I^+(x_n)}$ for all n, implying that $I^+(p) \subseteq I^+(x_n)$ for all n. Now let $z \in I^-(x)$. Then $x \in I^+(z)$, and $I^+(z)$ being open, $x_n \in I^+(z)$ after certain stage. Then for such x_n, $I^+(z) \supseteq I^+(x_n) \supseteq I^+(p)$. So $p \in A^+(x)$. Since $\overline{I^+(x)} = \overline{J^+(x)}$ is always true, the equality $A^+(x) = \cap_{n=1}^{\infty} \overline{J^+(x_n)}$ follows.

4. WOODHOUSE CAUSALITY AND OTHER CAUSALITY CONDITIONS

We would like to examine here the relationship between Woodhouse's causality principle and other known causality conditions like strong causality, stable causality, causal continuity etc. We call a space–time to be W-causal whenever $x \mathrm{A} y$ and $y \mathrm{A} x$ implies $x = y$ for all events.

It will be convenient first to consider the relationship between causal continuity and W-causality. We shall prove below that the W-causality of a space–time can be deduced from its causal continuity, i.e., causally continuous space–times will be always W-causal. Thus W-causality turns out to be not an entirely new feature of a space–time but is deducible from its reflectingness and distinguishing nature.

To see the above, we prove two more results. The following proposition shows that for a reflecting space–time, the almost future of a point turns out to be a simple and well-known set.

Proposition 5: Let M be a reflecting space–time. Then,

$$A^+(x) = \{y | x \mathrm{A} y\} = \overline{I^+(x)}.$$

Proof. By Proposition 3, $\mathrm{Int}[A^+(x)] = \uparrow I^-(x)$. Now by Lemma 1, $\uparrow I^-(x) = I^+(x)$. Hence taking closures on both the sides provides the result.

Again a reflecting space–time exhibits a special type of symmetry in the following sense:

Proposition 6: Let M be a reflecting space–time. Then,

$$I^+(x) = I^+(y) \text{ iff } x \mathrm{A} y, y \mathrm{A} x \text{ iff } I^-(x) = I^-(y).$$

Proof: Let $I^+(x) = I^+(y)$. Then by the definition of the almost causal precedence, we have both $x \mathrm{A} y$ and $y \mathrm{A} x$. Again, when $x \mathrm{A} y$ and $y \mathrm{A} x$ are both true, by the Proposition 5, $y \in \overline{I^+(x)}$ and $x \in \overline{I^+(y)}$. This then gives $I^+(y) \subseteq I^+(x)$ and $I^+(x) \subseteq I^+(y)$. This proves $I^+(x) = I^+(y)$. The final part also can be similarly proved.

Thus for a reflecting space–time, the W-causality axiom can be stated as: $x \in \overline{I^+(y)}$, $y \in \overline{I^+(x)} \Rightarrow x = y$. Now when M is causally continuous, let $x \mathrm{A} y$ and $y \mathrm{A} x$ hold. Then by Proposition , $I^+(x) = I^+(y)$. So the distinguishingness implies that $x = y$, which finally shows that M is W-causal. Thus we have proved the following now:

Theorem 7: Let M be a causally continuous space–time. Then M is W-causal.

However, the converse of this theorem is not true. The example in Fig. 2 is a space–time which is W-causal but not causally continuous. Thus causal continuity strictly includes W-causality.

Also with the help of Proposition 6 it is possible to reduce the assumption of causal continuity. Causal continuity requires both reflectingness and distinguishingness as originally defined by Hawking and Sachs. However when M is reflecting, we have $I^+(x) = I^+(y)$ if and only if $I^-(x) = I^-(y)$. Because, suppose M is future distinguishing and reflecting, then $I^-(x) = I^-(y)$ would imply $I^+(x) = I^+(y)$ by Proposition 6, which would give $x = y$ by assumption. This proves that M is past distinguishing also. Hence we proved that the whole assumption of distinguishingness is not required to define causal continuity.

Proposition 8: A space–time M is causally continuous if and only if it is reflecting and future (past) distinguishing.

Such an equivalence between future and past distinguishing conditions does not hold for a general space–time

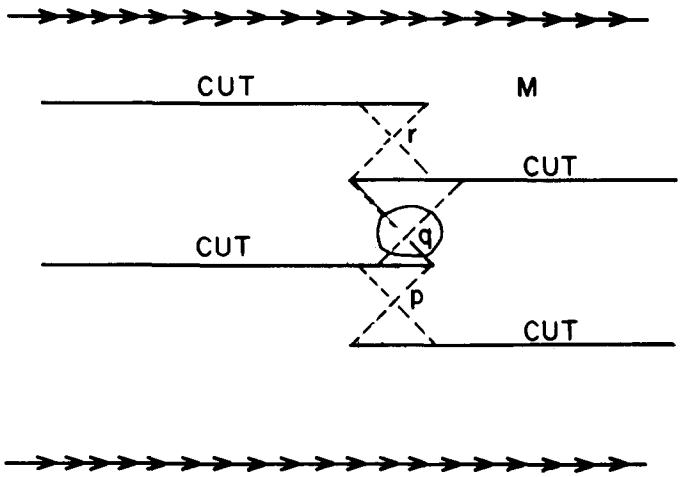

FIG. 2. Arrows denote identificaton. Here M is causal, since there are no closed nonspacelike curves. Also M is W-causal, but a slightest perturbation in the metric opens up the light cones and closed nonspacelike curves are produced; hence causality and W-causality both break down. Also, M is not stably causal or reflecting, but is strongly causal.

which is not reflecting (see, for example, Fig. 37 of Ref. 4). Here M is past distinguishing but not future distinguishing.

Now it is possible to point out the unifying power of the reflecting condition on a space–time in view of various other causality conditions, and also the relation of W-causality with them. Consider a reflecting space–time which is future distinguishing. Then Proposition 8 has shown that it will be past-distinguishing also, and hence M is distinguishing. Then Theorem 7 shows that M must be W-causal. Now Woodhouse[1] has shown that a W-causal space–time is distinguishing in general. Hence for a reflecting space–time, the W-causality and distinguishingness are equivalent. Again Hawking and Sachs[2] have shown that a reflecting space–time which is distinguishing (i.e., a causally continuous space–time) is always stably causal and strongly causal. Now, since it is known that stable causality imply strong causality which in turn implies distinguishingness (e.g., see Hawking and Sachs[2]), we have proved the following:

Theorem 9: Let (M,g) be a reflecting space–time. Then the following are equivalent:

(a) M is future distinguishing,
(b) M is past distinguishing,
(c) M is distinguishing,
(d) M is W-causal,
(e) (M,g) is stably causal,
(f) M is strongly causal.

Thus for a reflecting space–time only future or past distinguishingness or W-causality would become the single reasonable global causality condition, with no need to assume anything more about causality; which is not the case for a general space–time, where there is a separate need for each causality condition.

5. ON THE STABILITY OF W-CAUSALITY

The W-causality formulation that we have been examining here has the merit of having a simple and intuitively clear physical interpretation. However, the previous results concerning the almost future and W-causality principle do not give the feeling that the new formulation could have superior features in comparison to what causality conditions are known. In particular, for a reflecting space–time, it just coincides with distinguishingness or any other condition mentioned in Theorem 9.

Of course, this by itself does not decrease the importance of W-causality formulation. The essential purpose for introducing the concept of almost causal precedence in the place of causal precedence is to take the observational uncertainties into account. Hence the important question which is to be asked is: Suppose (M,g) is a space–time which is W-causal. Shall it remain W-causal even after a small perturbation in the metric? One would require an affirmative reply to this in order to have the stability of the W-causality formulation.

To reply this, we construct here in Fig. 2 an explicit example of a space–time in which W-causality holds, but which will breakdown with a slightest perturbation in the metric. In this space–time, for no two different points x and y, both $x\mathrm{A}y$ and $y\mathrm{A}x$ holds; which implies W-causality. However, as soon as a slightest perturbation is made in the metric to open up the light cones, closed nonspacelike curves arise. For any two different points x and y on any such curve, both $x\mathrm{A}y$ and $y\mathrm{A}x$ would hold as can be easily seen, and hence the new space–time is no longer W-causal. Thus the W-causality formulation may not be considered very useful so far as the metric perturbations are to be taken into account.

Will it be possible to make the W-causality formulation a stable property of a space–time by changing the definition of almost causal precedence somewhat? The following result shows that going to neighborhoods of events rather than considering pasts or futures of the events woud be of no help.

Proposition 10: Let $x,y\in M$. Then x almost causally precedes y if and only if for every neighborhood N_x of x and N_y of y, there is a future directed nonspacelike curve from N_x to N_y.

Proof: Suppose $x\mathrm{A}y$ holds. Then $I^+(y)\subset I^+(z)$ for all $z\in I^-(x)$. Now let $p\in N_x\cap I^-(x)$. Then $p\in I^-(x)$ and so $I^+(y)\subset I^+(p)$. Hence $N_y\cap I^+(y)\subset I^+(p)$. Hence if we choose $q\in N_y\cap I^+(y)$, then there will be a nonspacelike curve from p to q, i.e, from N_x to N_y.

Conversely, suppose p is any point of $I^+(y)$. Then $y\in I^-(p)$ which is a neighborhood of y, since $I^-(p)$ is open. Again let z be any point of $I^-(x)$. Then in the similar manner $I^+(z)$ is a neighborhood of x. Hence by assumption there must be a nonspacelike curve from some $t\in I^+(z)$ to some event $s\in I^-(p)$. So $p\in I^+(s)\subset I^+(t)\subset I^+(z)$. Therefore we have $I^+(y)\subset I^+(z)$ for all $z\in I^-(x)$, that is $x\mathrm{A}y$ holds.

For a reflecting space–time the W-causality fully concurs with other well-known causality axioms. Where does it stand for a general space–time? To have an idea about this, again the example given in Fig. 2 is useful. Here the space–time is strongly causal but not stably causal. This suggests that W-causality should lie between strong causality and stable causality for a general space–time. We shall prove in the next section that the stable causality implies W-causality in general.

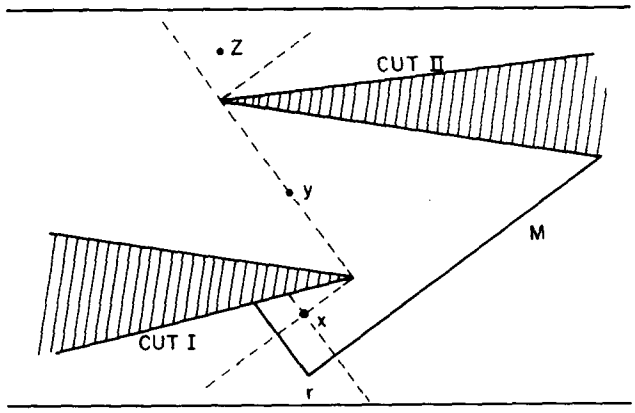

FIG. 3. In the space-time here, $z \notin A^+(x)$ but $z \in J_s^+(x)$, so $A^+(x) \neq J_s^+(x)$. Again xAy and yAz hold but not xAz. On the other hand, $y \in J_s^+(x)$, $z \in J_s^+(y)$ and $z \in J_s^+(x)$ also hold.

6. THE ALMOST FUTURE AND THE SEIFERT FUTURE

As it has been mentioned earlier, Seifert[3] defined the future $J_s^+(x)$ of an event x in the space–time by taking metric perturbations into account. It should be interesting to compare this definition of the future with the almost futurer definitions, since both have a similar type of motivation. Though the almost future concept failed to take the metric perturbations into account, the Seifert future accounts for these properly. The following result shows when these two types of futures are always equal in a space–time.

Proposition 11: Let M be a causally continuous space–time. Then

$$J_s^+(x) = A^+(x) \quad \text{for all } x \in M.$$

Proof: For such a space–time

$$J_s^+(x) = \bigcap_{\bar{g} > g} J^+(x,\bar{g}) = \overline{J^+(x)} \text{ by Lemma 2.}$$

Again, $\overline{J^+(x)} = \overline{I^+(x)} = A^+(x)$ for such a space–time as Proposition 5 shows.

However, for a general space–time they are not equal. Consider the space–time given in Fig. 3. Here the event $z \notin A^+(x)$ because the future of any event $r \in I^-(x)$ is fully obstructued by cuts in M and so it cannot contain the future of the event z. But clearly for all metrics $\bar{g} > g$, $z \in J_{\bar{g}}^+(x)$ because a slightest perturbation in the metric would open up the light cones to give way to a nonspacelike curve to reach from x to z. Hence $z \in J_s^+(x)$ and the two futures are not equal.

There is an essential difference between the almost future and the Seifert future. The relation J_s^+ between events in a space–time is a transitive one, i.e., $y \in J_s^+(x)$ and $z \in J_s^+(y)$ imply $z \in J_s^+(x)$. However, this is not the case for the relation A^+, which is again clear from Fig. 3. There clearly xAy and yAz hold, but as we have seen, xAz is not true; which is the breakdown of the transitivity property.

The relationship between the almost future and the Seifert future of an event in a general space–time is obtained in the following result.

Proposition 12: Let M be a space–time. Then for all $x \in M$, $A^+(x) \subseteq J_s^+(x)$.

Proof: By the definition of $J_s^+(x)$, clearly $\overline{I^+(x)} \subset J_s^+(x)$. Now by Lemma 3, $J_s^+(x)$ is closed, hence $\overline{I^+(x)} \subseteq J_s^+(x)$. Let now $p \in A^+(x)$. Then $I^+(p) \subset I^+(z)$ for all $z \in I^-(x)$. Consider now a sequence $\{p_n\}$ in $I^-(x)$ converging to x. Then by Lemma 4 we have $\cap_{n=1}^{\infty} J_s^+(p_n) \subset \overline{J_s^+(x)}$. Now $I^+(p) \subset I^+(z)$ for all $z \in I^-(x)$ implies that $p \in \overline{I^+(z)}$ for all $z \in I^-(x)$. So $p \in J_s^+(z)$ for all $z \in I^-(x)$ and so $p \in \cap_{n=1}^{\infty} J_s^+(p_n)$, since $p_n \in I^-(x)$ for all n. This gives $p \in J_s^+(x)$.

With the help of the above result now it can be established that the W-causality principle is strictly weaker to the stable causality condition.

Theorem 13: Let M be a space–time which is stably causal. Then M satisfies the W-causality principle.

Proof: Seifert[3] has shown that the stable causality of M implies that the relation J_s^+ is a partial order on M, i.e., $x \in J_s^+(y)$, $y \in J_s^+(x)$ implies $x = y$. Now suppose xAy and yAx hold. Then $y \in A^+(x)$ and $x \in A^+(y)$. Since $A^+(x) \subset J_s^+(x)$ for all $x \in M$, this gives $y \in J_s^+(x)$ and $x \in J_s^+(y)$. This implies $x = y$, that is, M is W-causal.

The W-causality principle is stated as whenever $y \in A^+(x)$ and $x \in A^+(y)$ then we must have $x = y$. This means that the relation A^+ between the events in the space–time must be antisymmetric. We have shown that this is not a stable property of the space–time. On the other hand, Seifert[3] has proved that whenever the relation J_s^+ is a partial order on M, M must be stably causal. Since J_s^+ is reflexive and transitive by definition, this means that the antisymmetry of J_s^+ ensures the stability of a particular causality formulation. Hence the perturbations in the metric, which are important in view of the quantum uncertainty principle, have been suitably taken into account by the Seifert definition but not by the almost causal precedence idea.

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Null Killing vectors

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Space–times admitting a null Killing vector are studied, using the Newman–Penrose spin coefficient formalism. The properties of the eigenrays (principal null curves of the Killing bivector) are shown to be related to the twist of the null Killing vector. Among the electrovacs, the ones containing a null Maxwell field turn out to belong to the twist-free class. An electrovac solution is obtained for which the null Killing vector is twisting and has geodesic and shear-free eigenrays. This solution is parameterless and appears to be the field of a zero-mass, spinning, and charged source.

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1. INTRODUCTION

The earliest known example of space–times admitting a null Killing vector is the class of plane-fronted waves.[1] In contrast to the case with timelike or spacelike Killing symmetries, the existence of a null motion is restrictive enough a condition on a space–time to attempt a full analysis of the governing equations. Indeed, Dautcourt[2] has completely solved the vacuum Einstein equations under the condition. Electrovacua consisting of a source-free Maxwell field and of gravitation have apparently a much richer structure. Kramer[3] has studied electrovacua admitting a hypersurface-orthogonal null Killing field using scalar potentials. As for matter sources, the perfect fluid does not allow physically meaningful metrics with a hypersurface-orthogonal null motion.[4] The twisting perfect fluid problem, restricted to algebraically special metrics, has been taken up by Wainwright[5] (cf. Table I).

In this paper we approach the null Killing vector using the Newman–Penrose spin coefficient formalism.[6] We believe that spin coefficients suit ideally this particular type of study; and further, that a formalism does not grow "old" (unlike people who apply it).

When the tetrad vector l^μ is chosen to be the null Killing vector, the Killing equation can be expressed as a set of algebraic conditions on the spin coefficients (Sec. 2). While experimenting with several conceivable gauge conditions on the rest of the null tetrad, we came across the notion of eigenrays or principal nuli curves of the Killing bivector.[7] This notion, quite unexpectedly, turns out to be useful also with a null Killing vector, thus we present a detailed analysis of it in Sec. 3. We find that there are two eigenray congruences which coincide when the Killing field is hypersurface-orthogonal. The null Killing trajectories themselves are eigenrays. When they are twisting, it is possible to orient the tetrad vector n^μ along the second eigenray congruence. In this gauge, most of the curvature invariants are given algebraically and the number of NP equations to be integrated diminishes substantially.

In Secs. 4–6 we apply our ideas on electrovac fields. In Sec. 4 we show that the second eigenray has a preferred orientation also with respect to the Maxwell field (although this relation is nonlocal). In Sec. 5 we prove that the null Killing vector is hypersurface-orthogonal in the presence of a null Maxwell field. Finally, in Sec. 6 we find a new solution of the Einstein–Maxwell equations characterized by both eigenray congruences geodesic and shearfree. Remarkably, this latter condition characterizes also the Kerr–Newman metric.[8] However, the structure of our parameterless solution is completely fixed. It has a twisting null Killing vector and a non-null Killing vector commuting with the null one. The solution appears to represent the field of a charged, spinning particle moving with the speed of light, the Maxwell field strangely twisting around the world line of the source.

TABLE I. Space–times admitting a null Killing vector.

Source \ l^μ	hypersurface-orthogonal	twisting
Vacuum	Dautcourt[2]	none
Perfect fluid	$\rho + p = 0$ only[4]	Wainwright[5]: alg. special
Electrovac	Kramer[3]	this paper

2. BASIC STRUCTURES

The existence of a null Killing vector l_μ satisfying

$$l_{\mu;\nu} + l_{\nu;\mu} = 0 \tag{2.1}$$

and

$$l_\mu l^\mu = 0 \tag{2.2}$$

entails some basic relations in any space-time. Thus the covariant derivative of Eq. (2.2) with Eq. (2.1) gives

$$l_{\mu;\nu} l^\nu = 0. \tag{2.3}$$

The null Killing vector l^μ is tangent to a null geodesic congruence.

For further discussion, it will be quite advantageous to introduce the complex null vector m^μ and the real null vector n^μ, in addition to l^μ, thereby completing a Newman–Penrose (NP) null tetrad.[6] Recall that the nonvanishing scalar products of these vectors are $l_\mu n^\mu = 1$, $m_\mu \bar{m}^\mu = -1$. We then express the Killing property (2.1) of l^μ in terms of spin coefficients. From Eq. (2.3) we obtain

$$\kappa \equiv l_{\mu;\nu} m^\mu l^\nu = 0. \tag{2.4a}$$

We find from Eq. (2.1) that the shear and the divergence of

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the null Killing congruence vanish:

$$\sigma \equiv l_{\mu;\nu} m^\mu m^\nu = 0, \tag{2.4b}$$

$$\rho + \bar{\rho} \equiv l_{\mu;\nu}(m^\mu \bar{m}^\nu + \bar{m}^\mu m^\nu) = 0. \tag{2.4c}$$

The rest of the tetrad components of Eq. (2.1) read

$$\bar{\alpha} + \beta + \tau \equiv l_{\mu;\nu}(n^\mu m^\nu + m^\mu n^\nu) = 0, \tag{2.4d}$$

$$\gamma + \bar{\gamma} \equiv l_{\mu;\nu} n^\mu n^\nu = 0, \tag{2.4e}$$

$$\epsilon + \bar{\epsilon} \equiv l_{\mu;\nu} n^\mu l^\nu = 0. \tag{2.4f}$$

A null Killing vector l^μ is a principal null vector of the curvature. This follows at once from the Ricci equation (4.2b) of NP,

$$\Psi_0 = 0. \tag{2.5}$$

We can choose any propagation law for the tetrad vectors m^μ and n^μ which preserves scalar products. We find it convenient to require Lie propagation along l^μ. Thus we set

$$\mathcal{L}_l n^\mu \equiv n^\mu{}_{;\nu} l^\nu - l^\mu{}_{;\nu} n^\nu = 0,$$

$$\mathcal{L}_l m^\mu \equiv m^\mu{}_{;\nu} l^\nu - l^\mu{}_{;\nu} m^\nu = 0. \tag{2.6}$$

Taking tetrad components of (2.6) we have

$$\bar{\tau} + \pi = 0, \tag{2.7a}$$

$$\rho - 2\epsilon = 0. \tag{2.7b}$$

With this choice of the tetrad, the action of the absolute derivative operator $D \equiv l^\mu \nabla_\mu$ on any spin coefficient or curvature invariant gives zero.

3. EIGENRAYS

We next consider the algebraic properties of the Killing bivector $l_{\mu;\nu}$. We find that the clarity of the discussion is enhanced in a spinor notation.

The symmetric spinor representing a Killing bivector can be written

$$G_{AB} = \nabla_{(A}{}^{A'} l_{B)A'}, \tag{3.1}$$

where $\nabla_A{}^{A'}$ is the covariant spinor derivative. The principal spinors η_A of G_{AB} are defined by the eigenvalue problem,[7]

$$G_A{}^B \eta_B = \chi \eta_A. \tag{3.2}$$

This equation has two solutions for the eigenspinor η_A. When the two eigenspinors are proportional to each other we say that the Killing bivector is degenerate. The integral curves of the eigenspinors are also termed the *eigenrays* of the gravitational field.[7]

When the Killing vector is null, it can be written in spinor terms as

$$l_{AA'} = o_A \bar{o}_{A'}. \tag{3.3}$$

Equation (3.1) takes the form

$$G_{AB} = o_{(A} \nabla_{B)}{}^{A'} o_{A'} + \bar{o}_{A'} \nabla_{(A}{}^{A'} o_{B)}. \tag{3.4}$$

Transvecting (3.4) with the dyad spinors o_A and ι_A ($o_A \iota^A = 1$), we obtain

$$G_{00} \equiv G_{AB} o^A o^B = 0, \tag{3.5a}$$

$$G_{01} \equiv G_{AB} o^A \iota^B = -\rho, \tag{3.5b}$$

$$G_{11} \equiv G_{AB} \iota^A \iota^B = \bar{\tau} - \bar{\beta} - \alpha. \tag{3.5c}$$

By Eq. (3.5a), the null Killing trajectories themselves are eigenrays, a fact recognized already by Debney.[9] Equation (3.5b) shows the condition of degeneracy to be $\rho = 0$. This is to say that the Killing trajectories are hypersurface-orthogonal. In vacuum, the Ricci equation (4.2a) of NP reads $\rho^2 = 0$. Thus a null Killing field *in vacuo* is always hypersurface-orthogonal. (An exhaustive treatment of the vacuum problem has been presented by Dautcourt[2].) The electrovac fields admitting a hypersurface-orthogonal null Killing vector have been studied by Kramer.[3] In what follows we shall consider algebraically general (or twisting) null Killing fields characterized by

$$\rho = 2\epsilon \neq 0. \tag{3.6}$$

Since the Killing bivector Lie propagates along the Killing vector l^μ, we are free to choose the dyad spinor ι^A, the second principal spinor of G_{AB}. With this choice, the tetrad vector n^μ becomes tangent to the corresponding eigenrays. From Eq. (3.5c) we have $\bar{\tau} - \bar{\beta} - \alpha = 0$. Comparing with (2.4d), we find that our eigenray condition is

$$\tau = 0. \tag{3.7}$$

The remaining indeterminacy in the phase of the basic spinors amounts to a freedom in choosing the phase of the tetrad vector m^μ:

$$m^\mu \to e^{iC} m^\mu, \tag{3.8}$$

where $DC = 0$.

The vector n^μ could, of course, be given any orientation, preferably consistent with Lie propagation. In Sec. 5, for example, it will prove useful to choose n^μ along a principal null direction of the Maxwell field. An interesting consequence of our eigenray condition $\tau = 0$, when imposed upon the null tetrad, is that most components of the Weyl tensor but Ψ_4 are given by algebraic expressions, according to the Ricci equations

NP (4.2):

$$\text{(b)} \quad \Psi_0 = 0, \tag{3.9a}$$

$$\text{(c)} \quad \Psi_1 = -\Phi_{01}, \tag{3.9b}$$

$$\text{(h)} \quad \Psi_2 = 2\epsilon\mu - 2\Lambda, \tag{3.9c}$$

$$\text{(i)} \quad \Psi_3 = 2\epsilon\nu - \Phi_{21}. \tag{3.9d}$$

The remaining Ricci equations are, eliminating ρ by Eq. (2.7b) and setting $\tau = \pi = 0$,

NP (4.2)

$$\text{(a)} \quad 4\epsilon^2 + \Phi_{00} = 0, \tag{3.10a}$$

$$\text{(d)} \quad \bar{\delta}\epsilon = -\Phi_{10}, \tag{3.10b}$$

$$\text{(f, h)} \quad \Delta\epsilon = -\epsilon(\mu + \bar{\mu}), \quad \Phi_{11} = -\epsilon(\mu - \bar{\mu}) + 3\Lambda \tag{3.10c}$$

$$\text{(g)} \quad 2\epsilon\lambda = \Phi_{20}, \tag{3.10d}$$

$$\text{(j)} \quad \Delta\lambda - \bar{\delta}\nu = -(\mu + \bar{\mu} - 4\gamma)\lambda + 2\alpha\nu - \Psi_4, \tag{3.10e}$$

$$\text{(l)} \quad \delta\alpha + \bar{\delta}\bar{\alpha} = 4\alpha\bar{\alpha} + 4\epsilon\gamma + 6\Lambda, \tag{3.10f}$$

$$\text{(m)} \quad \delta\lambda - \bar{\delta}\mu = 2(\epsilon\nu + 2\bar{\alpha}\lambda + \Phi_{21}), \tag{3.10g}$$

$$\text{(n)} \quad \delta\nu - \Delta\mu = \mu^2 + 2\bar{\alpha}\nu + \lambda\bar{\lambda} + \Phi_{22}, \tag{3.10h}$$

$$\text{(r)} \quad \Delta\alpha - \bar{\delta}\gamma = \epsilon\nu + \bar{\alpha}\lambda + \Phi_{21} - (2\gamma + \bar{\mu})\alpha. \tag{3.10i}$$

Operators δ and Δ each commute with D and their nonvanishing commutators are

$$\delta\Delta - \Delta\delta = -\bar{\nu}D + \bar{\lambda}\bar{\delta} + (\mu - 2\gamma)\delta, \tag{3.11a}$$

$$\delta\bar{\delta} - \bar{\delta}\delta = (\mu - \bar{\mu})D + 4\epsilon\Delta - 2\alpha\delta + 2\bar{\alpha}\bar{\delta}. \tag{3.11b}$$

Equations (3.10) and (3.11), together with the appropriate matter equations, govern space–times admitting a twisting null Killing vector.

4. ELECTROVACS

Electrovac fields consisting of a source-free Maxwell field ϕ_m and of gravitation are characterized by the components of energy–momentum,

$$\Phi_{mn} = \phi_m \bar{\phi}_n, \quad \Lambda = 0. \tag{4.1}$$

The algebraic field Eqs. (3.10a), (3.10c), and (3.10d) become

$$\phi_0\bar{\phi}_0 = -4\epsilon^2, \tag{4.2a}$$

$$\phi_1\bar{\phi}_1 = -\epsilon(\mu - \bar{\mu}), \tag{4.2b}$$

$$\phi_2\bar{\phi}_0 = 2\epsilon\lambda. \tag{4.2c}$$

Equations (4.2) are satisfied by setting

$$\phi_0 = -2i\epsilon e^{iH}, \tag{4.3a}$$

$$\phi_1 = \phi e^{iH}, \tag{4.3b}$$

$$\phi_2 = i\lambda e^{iH}, \tag{4.3c}$$

where the real function H is a common phase of the Maxwell field and ϕ is a complex function subject to

$$\phi\bar{\phi} = -\epsilon(\mu - \bar{\mu}). \tag{4.4}$$

In Eqs. (4.3), the spin coefficients ϵ and λ feature as amplitudes of the Maxwell field. Recall, however, that the tetrad has been oriented along the two eigenrays of the non-degenerate Killing bivector (cf. preceding chapter). And we find here as a bonus that the tetrad shows a preferred orientation also with respect to the Maxwell field.

The admissible phase transformations $m^\mu \to m^\mu e^{iC}$ [Eq. (3.8)] affect the electromagnetic field components as follows,

$$\begin{aligned} &\phi_0 \to \phi_0 e^{iC}, \\ &\phi_1 \to \phi_1, \\ &\phi_2 \to \phi_2 e^{-iC}. \end{aligned} \tag{4.5}$$

Comparing with (4.3) we have

$$H \to H + C, \tag{4.6a}$$

$$\phi \to \phi e^{-iC}. \tag{4.6b}$$

Maxwell's equations in terms of spin coefficients [Eqs. (A1) of NP] can now be written

$$i\phi DH + 2\epsilon\bar{\delta}H = 4i\alpha\epsilon + 8\phi\epsilon, \tag{4.7a}$$

$$\lambda DH + \bar{\delta}\phi + i\phi\bar{\delta}H = -2i\epsilon\lambda, \tag{4.7b}$$

$$\delta\phi + i\phi\delta H - 2\epsilon\Delta H = 2i\epsilon(\bar{\mu} + 2\gamma), \tag{4.7c}$$

$$i\delta\lambda - \lambda\delta H - \Delta\phi - i\phi\Delta H = 2i\epsilon\nu + 2\mu\phi + 2i\bar{\alpha}\lambda. \tag{4.7d}$$

We take the D derivative of Eqs. (4.7) and recall that the derivative operators all commute with D. Noting that H is the only quantity here with a possibly nonvanishing D derivative, we obtain

$$\begin{bmatrix} i\phi & -2\epsilon \\ \lambda & i\phi \end{bmatrix} \begin{bmatrix} DDH \\ D\bar{\delta}H \end{bmatrix} = 0, \tag{4.8}$$

$$\begin{bmatrix} i\phi & -2\epsilon \\ \lambda & i\phi \end{bmatrix} \begin{bmatrix} D\delta H \\ D\Delta H \end{bmatrix} = 0.$$

Each of these equations has the determinant,

$$\text{Det} = 2\epsilon\lambda - \phi^2. \tag{4.9}$$

When Det = 0, we have

$$\phi_0\phi_2 - \phi_1^2 = 0, \tag{4.10}$$

characterizing an algebraically special Maxwell field. Then, Eqs. (4.8) do not completely determine the D dependence of the phase H. Such algebraically special Maxwell fields will be the subject of Sec. 5.

When the Maxwell field is algebraically general, Eqs. (4.8) tell us that all derivatives of DH vanish. Thus,

$$DH = 2c, \tag{4.11}$$

where c is a real constant. The condition $DH = 0$ characterizes Maxwell fields sharing the null symmetry of the space–time, i.e., having a vanishing Lie derivative along l^μ. In Sec. 6 we shall investigate algebraically general Maxwell fields for which both eigenray congruences are geodesic and shear-free.

5. NULL MAXWELL FIELDS

In this section we show that at least one of the null Killing fields in an electrovac space–time containing a degenerate Maxwell field,

$$\phi_0\phi_2 - \phi_1^2 = 0, \tag{5.1}$$

[Eq. (4.10)] is hypersurface-orthogonal. We do so by assuming first that l^μ has a curl, $\text{Im}\rho = -2i\epsilon \neq 0$, and finding subsequently that n^μ is a hypersurface-orthogonal null Killing field.

We find it convenient to dispense with the eigenray condition adopted for the spinor dyad in other chapters of this paper. Instead, we choose the dyad spinor ι^A coincident with with the principal null direction of the (degenerate) Maxwell field. This is possible according to the Ricci equation $\phi_0\bar{\phi}_0 + 4\epsilon^2 = 0$ [Eq. (4.2) of NP], from which $\phi_0 \neq 0$, i.e., the principal null direction of the Maxwell field does not coincide with the Killing vector l^μ. We then have

$$\begin{aligned} &\phi_0 = -2i\epsilon e^{iH}, \\ &\phi_1 = 0, \\ &\phi_2 = 0, \end{aligned} \tag{5.2}$$

where H is a real phase function. We use the phase freedom (3.8) to make

$$\tau \equiv l_{\mu;\nu} m^\mu n^\nu = \bar{\tau}.$$

For the reader's convenience we now list some necessary equations from NP. First, Maxwell's equations [(A.1) of NP] become

$$\begin{aligned} &\bar{\delta}\epsilon + i\epsilon\bar{\delta}H = (\tau + 2\alpha)\epsilon, \\ &0 = \lambda\epsilon, \\ &-\Delta\epsilon - i\epsilon\Delta H = (\mu - 2\gamma)\epsilon, \\ &0 = \nu\epsilon. \end{aligned} \tag{5.3}$$

Since $\epsilon \neq 0$ by assumption, in what follows we have

$$\lambda = \nu = 0.$$

From the Ricci identities and commutators we need

NP (4.2d) $\bar{\delta}\tfrac{1}{2}\ln\epsilon = \tau,$ (5.4a)

NP (4.2e) $\delta\tfrac{1}{2}\ln\epsilon = \tau,$ (5.4b)

NP (4.2f) $\Delta\tfrac{1}{2}\ln\epsilon = (1/2\epsilon)(\tau^2 - \Psi_2),$ (5.4c)

NP (4.2g) $\delta\tau = -2\bar{\alpha}\tau,$ (5.4d)

NP (4.2h) $\bar{\delta}\tau = 2\epsilon\bar{\mu} + 2(\alpha + \tau)\tau + \bar{\Psi}_2,$ (5.4e)

NP (4.2i) $\Delta\tau = -2\gamma\tau + \Psi_3,$ (5.4f)

NP (4.2j) $\Psi_4 = 0,$ (5.4g)

NP (4.2l) $\delta\alpha - \bar{\delta}\beta = \alpha\bar{\alpha} + \beta\bar{\beta} - 2\alpha\beta + \epsilon(3\mu - \bar{\mu} + 4\gamma) - \Psi_2,$ (5.4h)

NP (4.2r) $\Delta\alpha - \bar{\delta}\gamma = -(2\gamma + \bar{\mu})\alpha - 2\tau\gamma - \Psi_3,$ (5.4i)

NP (4.4) $\bar{\delta}\delta - \delta\bar{\delta} = (\bar{\mu} - \mu)D - 4\epsilon\Delta - (2\bar{\alpha} + \tau)\bar{\delta} + (2\alpha + \tau)\delta,$ (5.4j)

$\delta\Delta - \Delta\delta = 2\tau\Delta + (\mu - 2\gamma)\delta.$ (5.4k)

Computing $(\bar{\delta}\delta - \delta\bar{\delta})\tfrac{1}{2}\ln\epsilon$ and using (5.4a), (5.4b), and (5.4d) we get

$$\Psi_2 = \tau^2 + \tfrac{1}{2}\epsilon(\mu + \bar{\mu}), \tag{5.5}$$

which, together with (5.4d) and (5.4e), yields

$$8\alpha\tau + 6\tau^2 + \epsilon(3\bar{\mu} - \mu) = 0. \tag{5.6}$$

Using (5.4) in the Maxwell equations (5.3), we obtain

$$\delta H = i(2\bar{\alpha} - \tau),$$

by means of which we have

$$\begin{aligned} &\delta \ln\phi_0 = 3\tau - 2\bar{\alpha}, \qquad D\ln\phi_0 = 10iq \\ &\bar{\delta}\ln\phi_0 = 2\alpha + \tau, \\ &\Delta\ln\phi_0 = 2\gamma - \mu, \end{aligned} \tag{5.7}$$

where $q = \frac{1}{10}DH$, and

$$\delta q = \bar{\delta}q = \Delta q = 0. \tag{5.8}$$

Application of the commutators (5.4j), (5.4k), and the complex conjugate of (5.4k) on $\ln\phi_0$, and use of (5.4b) and (5.4i), gives us

$$\tau^2 + (\epsilon - iq)(\bar{\mu} - \mu) = 0, \tag{5.9a}$$

$$\bar{\delta}\mu = 2\mu\tau - \bar{\mu}\tau + \Psi_3, \tag{5.9b}$$

$$\bar{\delta}\bar{\mu} = -\bar{\mu}\tau - 5\Psi_3, \tag{5.9c}$$

respectively. The action of the complex conjugate of (5.4k) on τ yields

$$\bar{\delta}\Psi_3 = (4\tau - 2\alpha)\Psi_3. \tag{5.10}$$

Assume now $\tau \neq 0$ and take the δ derivative of (5.9a). Using the same Eq. (5.9a) together with (5.6), (5.9b), (5.9c), (5.10), and (5.4a), we get

$$\epsilon(7\bar{\mu} - 5\mu) + (\epsilon - iq)(2\mu - 6\bar{\mu} - 12\xi) = 0, \tag{5.11}$$

where $\xi = \Psi_3/\tau$, and we have $\bar{\delta}\xi = 4\Psi_3$. Applying $\bar{\delta}$ twice on Eq. (5.11) and using Eq. (5.9), (5.6), (5.10), and (5.4a) again, we get two further relations of a similar structure;

$$\epsilon(-4\mu - 16\xi) + (\epsilon - iq)(\mu + \bar{\mu} - 4\xi) = 0, \tag{5.12a}$$

$$\epsilon(-7\mu + 3\bar{\mu} - 54\xi) + (\epsilon - iq)(\mu - \bar{\mu} - 10\xi) = 0. \tag{5.12b}$$

The determinant of the homogeneous system (5.11) and (5.12) for the unknowns μ, $\bar{\mu}$, and ξ is

$$\begin{vmatrix} -3\epsilon - 2iq & \epsilon + 6iq & -12\epsilon + 12iq \\ -3\epsilon - iq & \epsilon - iq & -20\epsilon + 4iq \\ -6\epsilon - iq & 2\epsilon + iq & -64\epsilon + 10iq \end{vmatrix}.$$

It does not vanish unless $q = 0$. In this case, however, we have from Eq. (5.11) and from (5.12a) that $\xi = 0$ and $\mu = 0$. The latter, using (5.9a) gives $\tau = 0$. Whether or not the determinant vanishes we have

$$\mu = 0, \quad \tau = 0, \quad \Psi_3 = 0,$$

contradicting our assumption $\tau \neq 0$.

Now we have arrived back to the eigenray condition $\tau = 0$ and the freedom of the choice of C in (3.8) is again at our disposal. The spin coefficients α and γ transform under (3.8) as

$$\begin{aligned} &\alpha \to \alpha + \tfrac{1}{2}i\bar{\delta}C, \\ &\gamma \to \gamma + \tfrac{1}{2}i\Delta C. \end{aligned} \tag{5.13}$$

The Ricci equations (5.4h) and (5.4i) are just the integrability conditions ensuring the existence of a real function F such that

$$\begin{aligned} &\alpha = -i\bar{\delta}F, \\ &\gamma = i\Delta F, \\ &DF = 0. \end{aligned} \tag{5.14}$$

Choosing $C = F$, we can set $\alpha = \beta = \gamma = 0$.

Summarizing our results on the null Maxwell field, the spin coefficients all vanish except ϵ and ρ (which are constant) and $\Psi_i = 0$ ($i = 0, 1, 2, 3,$ and 4). The space–time is conformally flat, and by replacing $l^\mu \to n^\mu$ in Eqs. (2.4), n^μ is a hypersurface-orthogonal null Killing vector. Thus we have reduced the class containing an algebraically special Maxwell field to one that has been studied by Kramer.[3]

6. THE SOLUTION WITH GEODESIC AND SHEAR-FREE SECOND EIGENRAYS

In this section we present a new class of electrovacs with a twisting null Killing vector. What we require is that the second eigenray congruence be also geodesic and shear-free. We borrow this condition from the timelike Killing problem where solutions with geodesic and shear-free eigenrays are some plane-fronted wave and Kerr–Newman metrics.[1,8]

The eigenrays with tangent vector n^μ are geodesic and shear-free when

$$\tau = 0, \quad \nu = \lambda = 0. \tag{6.1}$$

From Ricci equations (3.9) and from (4.3c),

$$\Psi_0 = \Psi_3 = \Psi_4 = \phi_2 = 0. \tag{6.2}$$

Let us denote real field variables by Roman capitals. Then

$$\epsilon = iE, \tag{6.3}$$

$$\rho = 2iE. \tag{6.4}$$

The nonvanishing components of the Maxwell tensor are [cf. Eqs. (4.3)]

$$\phi_0 = 2Ee^{iH}, \tag{6.5}$$

$$\phi_1 = \phi e^{iH}. \tag{6.6}$$

Using the phase transformation $m^\mu \to e^{iC} m^\mu$ [Eq. (3.8)], it is possible to eliminate the spin coefficients α and γ [cf. Eq. (5.13)],

$$\alpha = \gamma = 0. \tag{6.7}$$

A constant phase shift in m^μ remains still allowable. Ricci equations (3.9) and (3.10) and Maxwell's equations (4.7) become

$$\left.\begin{aligned} \Psi_1 &= -2E\bar{\phi} \\ \Psi_2 &= 2iE\mu \end{aligned}\right\}, \quad E = \tfrac{1}{2}\mathrm{Im}\rho \neq 0, \tag{6.8}$$

$$\delta \ln E = -2i\bar{\phi}, \tag{6.9a}$$

$$\Delta \ln E = -(\mu + \bar{\mu}), \tag{6.9b}$$

$$\bar{\delta}\mu = 0, \tag{6.9c}$$

$$\Delta\mu = -\mu^2, \tag{6.9d}$$

$$\phi\bar{\phi} = -iE(\mu - \bar{\mu}), \tag{6.9e}$$

$$D\phi = 0, \tag{6.10a}$$

$$\delta\phi = 2iE\Delta H - (\tfrac{1}{2}DH - 4E)(\mu - \bar{\mu}) - 2E\bar{\mu}, \tag{6.10b}$$

$$\bar{\delta}\phi = -iE^{-1}(\tfrac{1}{2}DH - 4E)\phi^2, \tag{6.10c}$$

$$\Delta\phi = -i\phi\Delta H - 2\mu\phi. \tag{6.10d}$$

The nonvanishing commutators (3.11) take the form

$$\Delta\delta - \delta\Delta = -\mu\delta, \tag{6.11a}$$

$$\delta\bar{\delta} - \bar{\delta}\delta = (\mu - \bar{\mu})D + 4iE\Delta. \tag{6.11b}$$

We shall assume $\phi \neq 0$ since the Maxwell field would otherwise be degenerate. Then Eq. (4.11) holds:

$$DH = 2c, \quad c = \text{const}. \tag{6.12}$$

Commutator (6.11b), when acting on H, yields

$$\Delta H = -\frac{i}{2}\frac{c^2 - 10cE + 20E^2}{(c - 5E)E}(\mu - \bar{\mu}). \tag{6.13}$$

All the derivatives of the Maxwell field are now given explicitly. Equation (6.9e) provides us $\delta\mu$. We obtain further new equations by application of the commutators (6.11a) and (6.11b) on the spin coefficients and on ϕ. When the commutators are applied to the spin coefficients involving E, only identities result. On the other hand, from the commutators of μ we get

$$c(\mu - \bar{\mu}) = 0. \tag{6.14}$$

Thus when $c \neq 0$, μ must be real. However, Eq. (6.9e) yields $\phi = 0$ when μ is real which has been excluded. Thus we have established the

Theorem: Metrics with a twisting null Killing symmetry and with both eigenrays geodesic and shear-free require, by the Einstein–Maxwell equations, a nonnull electromagnetic field to Lie propagate along the Killing vector.

Assuming now that the Maxwell field Lie-propagates along l^μ, i.e., $c = 0$, the field equations form a closed system under the commutators. Since D and Δ commute we can choose a coordinate system $x^\mu = (u, v, \zeta, \bar{\zeta}), \mu = 0, 1, 2, 3$ in which

$$l^\mu = \delta_0^\mu, \quad n^\mu = \delta_1^\mu \tag{6.15}$$

and

$$m^\mu = \omega\delta_0^\mu + \Omega\delta_1^\mu + \xi^a\delta_a^\mu, \quad a = 2, 3. \tag{6.16}$$

There remains the coordinate freedom

$$\begin{aligned} u' &= u + F(\zeta, \bar{\zeta}), \\ v' &= v + G(\zeta, \bar{\zeta}), \\ \zeta' &= \zeta'(\zeta). \end{aligned} \tag{6.17}$$

Applying the commutators (6.11) on the coordinates, we obtain equations for the quantities

$$(m^i) = (\omega, \Omega, \xi^a), \quad i = 0, 1, 2, 3.$$

These are

$$\begin{aligned} &Dm^i = 0, \\ &\Delta m^i + \mu m^i = 0, \end{aligned} \tag{6.18}$$

and

$$\begin{aligned} &\delta\bar{\omega} - \bar{\delta}\omega = \mu - \bar{\mu}, \\ &\delta\bar{\Omega} - \bar{\delta}\Omega = 4iE, \\ &\delta\bar{\xi}^a - \bar{\delta}\xi^a = 0. \end{aligned} \tag{6.19}$$

The D and Δ equations among (6.9), (6.10) and (6.18) can be immediately integrated with the results

$$\begin{aligned} &\mu = 1/[v + iW^\circ(\zeta, \bar{\zeta})], \\ &E = E^\circ(\zeta, \bar{\zeta})/(v^2 + W^{\circ 2}) \\ &\phi = \phi^\circ(\zeta, \bar{\zeta})/(v - iW^\circ)^2, \\ &H = H^\circ(\zeta, \bar{\zeta}) + 2i\ln((v + iW^\circ)/(v - iW^\circ)), \\ &\phi^\circ\bar{\phi}^\circ + 2E^\circ W^\circ = 0, \\ &m^i = m^{i\circ}(\zeta, \bar{\zeta})/(v + iW^\circ), \end{aligned} \tag{6.20}$$

where, as usual, a degree sign denotes functions independent of u, v. Substituting these expressions into the remaining equations we get, introducing the "edh" operator $\eth = \xi^{0a}\partial_a$,

$$\eth E^\circ = 0, \tag{6.21a}$$

$$\eth H^\circ = 0, \tag{6.21b}$$

$$\eth\bar{\phi}^\circ = 0, \tag{6.21c}$$

$$\eth\phi^\circ = -2E^\circ, \tag{6.21d}$$

$$\phi^\circ = \bar{\eth}W^\circ, \tag{6.21e}$$

$$\Omega = i\bar{\phi}^\circ, \tag{6.21f}$$

$$\phi^\circ\bar{\phi}^\circ + 2E^\circ W^\circ = 0, \tag{6.21g}$$

$$\eth\bar{\omega}^\circ - \bar{\eth}\omega^\circ = -2iW^\circ, \tag{6.21h}$$

$$\eth\bar{\xi}^{a^\circ} - \bar{\eth}\xi^{a^\circ} = 0. \tag{6.21i}$$

The first Eq. (6.21a) means $E^\circ \equiv 2a = \text{const}$. By constant dilation of l^μ, either $a = 1$ or $a = 0$ can be achieved.

Similarly, $H^\circ = \text{const}$ by (6.21), giving a constant duality angle. A constant duality transformation is a trivial symmetry of the Einstein–Maxwell equations. Equation (6.21i) shows that

$$\xi^{a^\circ} = \delta^a_2 + i\delta^a_3 \tag{6.22}$$

can be set by the transformations (6.17).

The rest of Eqs. (6.21) can be integrated easily to obtain

$$\phi_0 = 4a\frac{v - iW^\circ}{(v + iW^\circ)^3}, \quad \phi_1 = \frac{2a\bar{\zeta}}{(v + iW^\circ)^2}, \quad \phi_2 = 0,$$
$$\Psi_0 = 0, \quad \Psi_1 = \frac{-8a^2\zeta}{v^2 + W^{\circ 2}}\frac{1}{(v + iW^\circ)^2},$$
$$\Psi_2 = \frac{4ia}{v^2 + W^{\circ 2}}\frac{1}{v + iW^\circ}, \tag{6.23}$$
$$\Psi_3 = \Psi_4 = 0.$$

We construct the metric by using

$$g^{\mu\nu} = l^\mu n^\nu + n^\mu l^\nu - m^\mu \bar{m}^\nu - \bar{m}^\mu m^\nu. \tag{6.24}$$

Thus we obtain, setting $\zeta = re^{i\varphi}$,

$$ds^2 = 2(du + \tfrac{1}{4}ar^4 d\varphi)(dv + ar^2 d\varphi) - \tfrac{1}{2}(v^2 + a^2r^4)(dr^2 + r^2 d\varphi^2), \tag{6.25}$$

where $a = 0$ or 1 and $W^\circ = ar^2$. When $a = 0$, we have the line element of Minkowski space–time in a strange coordinate system. These coordinates present a special case of what Synge calls Gödel-type metrics.[10] We find that usual Minkowski coordinates are given by the transformation

$$u = (t + z)/\sqrt{2} + r^2 v/4,$$
$$v = (t - z)/\sqrt{2}, \tag{6.26}$$
$$x = vr\cos\varphi,$$
$$y = vr\sin\varphi.$$

Our solution has no free parameter and it has two Killing vectors only:

$$K^\mu_1 = \delta^\mu_0, \tag{6.27}$$
$$K^\mu_2 = \delta^\mu_1.$$

$K^\mu_1 = l^\mu$ is the null vector we started with, and K^μ_2 can be interpreted as a rotational symmetry around the z axis when $v^2 - r^4 > 0$. Otherwise K^μ_2 is not spacelike. The curvature invariants vanish when v or r goes to infinity. The limit $v \to \infty$ with r kept finite leads us into a Minkowskian region.

When $v = \text{const}$ and r goes to infinity, the curvature invariants vanish, but K^μ_2 becomes timelike: this region differs substantially from a Minkowski space–time. There is a singularity at $v = r = 0$. This solution makes it difficult to present a picture of its own source since no continuous flat-space limit of it exists. Nevertheless, we attempt to make a guess based on the related Minkowski metric with coordinates (6.26). Thus the singularity appears as a point source moving along the z axis with the speed of light.

Our solution is not the only one where a source moving with the speed of light creates also an electromagnetic field. Rather, it appears to be the spinning analog of Bonnor's "nullicle" solution.[11] However, unlike in the case of the nullicle, the charge and spin parameters are both fixed now.

Although the metric (6.25) is axially symmetric, a phase factor in the Maxwell field [cf. Eq. (6.23)] depends on φ. Hence this solution may be viewed as an explicit example of a zero-mass geon.

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Exterior spacetimes for rotating stars

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The algorithms are studied which construct stationary axisymmetric asymptotically flat spacetimes. The multipole moment structure of the resulting spacetimes is determined. The static metric and the transformations which generate any stationary metric are obtained.

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1. INTRODUCTION

Stationary axisymmetric solutions of the Einstein equation attracted the interest of early investigators since the asymptotic flat ones are candidates for the description of the exterior gravitational field of a uniformly rotating star. Their interest was further increased when their study revealed the existence of an enormous algebraic structure, namely, the existence of an infinite dimensional symmetry group of transformations which preserve the equations. This symmetry group, discovered first by Geroch,[1] was further enlarged by Kinnersley and Chitre[2–5] by the inclusion of electromagnetism and it was adapted to a form suitable for generating solutions of the Einstein or Einstein–Maxwell equations. Utilizing these developments, a method was developed[6,7] which applied to any known stationary, axisymmetric, asymptotically flat solution produces a new asymptotically flat solution with any (finite) number of additional parameters. It was also conjectured[6,7] that the method applied to the general static (Weyl) solution gives the general stationary, axisymmetric, asymptotically flat solution. But although the required steps for the construction of the new solutions are straightforward and completely algebraic, the required calculations for the introduction of more than a few additional parameters soon become formidable.

In the present paper we study the multipole moment structure of the spacetimes which are obtained by applying the method of (I)[7] to the general Weyl metric. More precisely:

i) We determine the leading multipole moments of the resulting solutions.

ii) We determine the Weyl solution which should be used and the transformations which should be applied for the construction of any given stationary, axisymmetric solution.

iii) We obtain the above i) and ii) for all three different algorithms suggested in (I).

The central idea is to apply the algorithms (which correspond to different sets of transformations) on the axis of the aximuthal symmetry. It was realized that by restricting the consideration to the axis it was possible to perform the otherwise formidable calculations. It turns out that, although insufficient to determine the metric itself, the knowledge of the Ernst[8] potential on the axis (which is what the algorithms compute) is sufficient to determine the mutipole moment behavior of the solution.

Section 2 reviews the method. Section 3 determines the multipole moments of the solution and Sec. 4 determines the transformations which generate any given solution.

2. REVIEW

Let (M, g_{ab}) be a stationary, axisymmetric, vacuum spacetime which satisfies the Einstein equation $Rab = 0$ and which admits two independent Killing fields which commute and for which the two-dimensional submanifolds orthogonal to the Killing fields are integrable and spacelike. Then the spacetime line element can be cast into the form

$$ds^2 = \lambda_0(dt)^2 + 2\lambda_1(dt)(d\phi) + \lambda_2(d\phi)^2 - \Omega^2[(d\rho)^2 + (dz)^2], \tag{1}$$

where the λi's, essentially the (squared) norms of the two Killing fields, satisfy

$$\lambda_1^2 - \lambda_0\lambda_2 = \rho^2, \tag{2}$$

and Ω is a conformal factor on the two-dimensional manifold of orbits. The λi's and Ω are functions only of the cylindrical coordinates ρ and z. Introduce the twist (potential) ω_0 of the timelike Killing field by

$$\left.\begin{aligned} \omega_{0,\rho} &= \frac{\lambda_0^2}{\rho}\left(\frac{\lambda_1}{\lambda_0}\right)_{,z} \\ \omega_{0,z} &= -\frac{\lambda_0^2}{\rho}\left(\frac{\lambda_1}{\lambda_0}\right)_{,\rho} \end{aligned}\right\}. \tag{3}$$

Then, the vacuum Einstein equation is equivalent[1,8] to the following set of equations:

$$\left.\begin{aligned} \nabla^2\lambda_0 &= \frac{(\nabla\lambda_0)^2 - (\nabla\omega_0)^2}{\lambda_0} \\ \nabla^2\omega_0 &= \frac{2(\nabla\lambda_0)\cdot(\nabla\omega_0)}{\lambda_0} \end{aligned}\right\} \tag{4}$$

$$\left.\begin{aligned} \frac{2}{\rho}(\ln\Omega)_{,\rho} &= \frac{\lambda_{0,\rho}^2 - \lambda_{0,z}^2 + \omega_{0,\rho}^2 - \omega_{0,z}^2}{2\lambda_0^2} - \frac{1}{\rho}(\ln\lambda_0)_{,\rho} \\ \frac{2}{\rho}(\ln\Omega)_{,z} &= \frac{\lambda_{0,\rho}\lambda_{0,z} + \omega_{0,\rho}\omega_{0,z}}{\lambda_0^2} - \frac{1}{\rho}(\ln\lambda_0)_{,\rho} \end{aligned}\right\}, \tag{5}$$

where ∇^2 and ∇ are the Laplacian and the gradient operators in three dimensional flat space. In looking for solutions, the difficult step is to obtain solutions of Eqs. (4). Then, Eqs. (3) determine λ_1, Eq. (2) determines λ_2, and Eqs. (5) determine Ω. The gauge freedom associated with this formulation is the

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addition of a constant to λ_1/λ_0, the multiplication of Ω by a constant, the simultaneous multiplication of λ_0 and ω_0, also of ρ and z, by a constant, and the addition of a constant to z.

The method of (I) *constructs, completely algebraically, solutions* (λ_0, ω_0) *of Eqs.* (4).

More precisely, three different algorithms have been proposed in (I) which construct, from any solution (λ_0,ω_0) of Eqs. (4) a more general solution of the same equations with any finite number of additional parameters. All these algorithms are utilizations of the same basic idea for the performance of the exponentiation of the Kinnersley–Chitre[3] transformations and they are expected to be, in principle, equivalent. However, I feel that it is necessary to consider all three algorithms because it is not yet clear which algorithm minimizes the massive amount of computations involved or which one is more convenient for answering specific questions about the solutions.

The common first step in all three algorithms is the evaluation of the generating function $G(s,t,\rho,z)$ of the original solution, where ρ and z are spacetime coordinates and s and t are two auxiliary variables. For most of the known stationary axisymmetric solutions $G(s,t)$ has already been evaluated.[5,7] Here we give $G(s,t)$ for the general asymptotically flat Weyl solution, i.e., the solution of Eqs. (4) with $\omega_0 = 0$ and $\lambda_0 = \exp[2\delta(r,\theta)]$, where

$$\delta(r,\theta) = \sum_{n=0}^{\infty} m_n r^{-n-1} P_n(\cos\theta), \tag{6}$$

with P_n Legendre polynomials and m_n arbitrary constants. It has been obtained[7] that

$$G(s,t) = -\frac{it}{2S(t)}\cdot\left[1+\frac{s+t-4stz}{sS(t)+tS(s)}\right] \times\exp[\beta(s)+\beta(t)], \tag{7}$$

where

$$S(t) = [(1-2tz)^2 + 4t^2\rho^2]^{1/2} \tag{8}$$

and

$$\beta(t) = S(t)\sum_{n=0}^{\infty}\sum_{k=0}^{n} m_n (2t)^{n-k} r^{-k-1} P_k(\cos\theta). \tag{9}$$

For $\beta(t) = \beta(s) = 0$ Eq. (7) gives the generating function for the flat space.

Having obtained $G(s,t)$, the instructions for computing the new solutions are the following:

First Algorithm:

A.1) Evaluate

$$G_{m,n}(s,t) = \frac{s^m t^n}{m!n!}\left(\frac{\partial}{\partial s}\right)^m\left(\frac{\partial}{\partial t}\right)^n G(s,t), \qquad 0\leqslant m,n\leqslant N, \tag{10}$$

essentially the derivatives of $G(s,t)$.

A.2) Consider the matrix

$$\delta_{ij} - \sum_{p=j}^{N} \alpha^{(p)} G_{i,p-j}(u,u) \tag{11}$$

and evaluate its determinant Δ_A and the determinants $\Gamma_{(A)k}$, $0\leqslant k\leqslant N$, of the matrices obtained by substituting the k th column of the matrix (11) by the column

$$\left(\left[\frac{\partial}{\partial t} G_{i0}(u,t)\right]_{t=0}\right).$$

A.3) The Ernst potential of the new solution is given by

$$\tilde{E} = \tilde{\lambda}_0 + i\tilde{\omega}_0 = \lambda_0 + i\omega_0 + \frac{i}{\Delta_A}\sum_{p=0}^{N}\sum_{k=0}^{p} \alpha^{(p)} G_{0,p-k}(0,u)\Gamma_{(A)k}. \tag{12}$$

$\alpha^{(p)}$, $0\leqslant p\leqslant N$, and u are the additional parameters.

Second Algorithm:

B.1) Construct the new generating function

$$\bar{G}(s,t) = G(s^{-1},t^{-1})$$

and evaluate

$$\bar{G}_{mn}(s,t) = \frac{(-1)^{m+n}}{m!n!} s^m t^n \left(\frac{\partial}{\partial s}\right)^m\left(\frac{\partial}{\partial t}\right)^n \bar{G}(s,t). \tag{13}$$

B.2) Consider the matrix

$$\delta_{ij} - \sum_{p=j}^{N} \delta^{(p)} \bar{G}_{i,p-j}(u,u) \tag{14}$$

and evaluate its determinant Δ_B and the determinants $\Gamma_{(B)k}$, $0\leqslant k\leqslant N$ of the matrices obtained by substituting the k th column of the matrix (14) by the column

$$\left(\lim_{t\to-\infty} t\bar{G}_{i0}(u,t)\right).$$

B.3) The new solution is given by

$$\tilde{E} = \tilde{\lambda}_0 + i\tilde{\omega}_0 = \lambda_0 + i\omega_0 + \frac{i}{\Delta_B}\sum_{p=0}^{N}\sum_{k=0}^{p} \delta^{(p)} \bar{G}_{0,p-k}(-\infty,u)\Gamma_{(B)k}. \tag{15}$$

Now, $\delta^{(p)}$, $0\leqslant p\leqslant N$, and u are the additional parameters.

Third Algorithm:

C.1) Consider the matrix

$$\delta_{ij} - \beta^{(j)} G(u_i,u_j) \tag{16}$$

(no summation) and evaluate its determinant Δ_C and the determinants $\Gamma_{(C)k}$, $1\leqslant k\leqslant N$, of the matrices obtained by substituting the k th column of the matrix (16) by the column

$$\left(\left[\frac{\partial}{\partial t} G(u_i,t)\right]_{t=0}\right).$$

C.2) The new solution is given by

$$\tilde{E} = \lambda_0 + i\omega_0 + \frac{i}{\Delta_C}\sum_{p=1}^{N} \beta^{(p)} G(0,u_p)\Gamma_{(C)p}. \tag{17}$$

The additional parameters are $\beta^{(p)}$ and u_p, $1\leqslant p\leqslant N$. Note that the third algorithm does not require the evaluation of the derivatives of the generating function.

In the terminology of (I) all three algorithms express the application of the transformation $T = \Sigma_{k=0}^{\infty} a_k \gamma^{(k)}{}_{22}$ to a known stationary axisymmetric solution. Different transformations correspond to different choices of the parameters a_k. In the first algorithm we apply the combined N th rank transformation $\Sigma_{p=0}^{N} A^{(p)}$, for which

$$a_k = \sum_{p=0}^{N} \alpha^{(p)}\binom{k}{p} u^k \tag{18}$$

and in the second we apply the transformation $\Sigma_{p=0}^{N} D^{(p)}$, for which

$$a_k = \sum_{p=0}^{N} \delta^{(p)} \binom{k+p-1}{p} u^{-k}. \tag{19}$$

In the third algorithm we apply repeated zero rank transformations with different "u" parameters, i.e., we choose

$$a_k = \sum_{p=1}^{N} \beta^{(p)} u_p^k . \tag{20}$$

$G(s,t) = \Sigma_{m,n}^{0,\infty} s^m t^n N^{(mn)}_{11}$ is the generating function for the potentials $N^{(mn)}_{11}$.

3. MULTIPOLE MOMENTS

Our objective is to study the multipole moment structure of the spacetime obtained by applying the algorithms outlined in the previous section to the most general asymptotically flat Weyl metric. More precisely, we will determine the leading, i.e., the first nonvanishing, mass and angular momentum multipole moments of the new spactimes. Note that, aside from being the most interesting, the leading multipole moments are the only ones which are unambiguously defined; higher multipole moments depend on the choice of the origin.

It has already been mentioned that the central idea is to perform the calculations and evaluate the new solution on the axis $\rho = 0$ of the azimuthal symmetry. In this case the computations simplify considerably. In fact, because the algorithms require the evaluation of the derivatives of the generating function only with respect to the auxiliary variables s and t, the initial ingredient for all three algorithms is the generating function $G(s,t,0,z)$ evaluated on the axis. For convenience we will assume that $s<0$ and $t<0$ and we will consider the $r = z > 0$ part of the axis.[9] For pedagogical reasons, we will proceed in two steps: first, we will apply the algorithms to a flat metric and introduce a finite number of additional parameters. And second, by working in a particular gauge, we will easily generalize the results to the case when the original metric is the general Weyl metric.

On the axis, $S(s) = 1 - 2sr$ and the flat space generating function simplifies to

$$G(s,t) = it/(2tr-1). \tag{21}$$

Then from Eq. (10) we obtain

$$G_{0,n}(s,t) = i(-t)^n (2r)^{n-1} (2tr-1)^{-n-1}, \quad n \geqslant 1 \tag{22}$$

and $G_{m,n}(s,t) = 0 \ \forall m \geqslant 1, \forall n$. the application of the first algorithm then gives

$$\Delta_A = 1 - \sum_{p=0}^{N} \alpha^{(p)} G_{0,p}(u,u),$$

$$\Gamma_{(A)k} = -i\delta_{0k}, \quad 0 \leqslant k \leqslant N,$$

and finally the new solution

$$\widetilde{E} = [1 - iA(r)]^{-1},$$

where

$$A(r) = \frac{\alpha^{(0)} u}{2ur-1} + \sum_{n=1}^{N} \alpha^{(n)} (-1)^n u^n \frac{(2r)^{n-1}}{(2ur-1)^{n+1}}. \tag{23}$$

The last expression can be further simplified. By rescaling the coordinates $r \to (2u)^{-1} r$ and redefining the parameters $\alpha^{(p)} \to u^{-1} \alpha^{(p)}$ we obtain

$$\widetilde{E} = [1 - iB_A(r)]^{-1}, \tag{24}$$

where

$$B_A(r) = \frac{\alpha^{(0)}}{r-1} + \sum_{n=1}^{N} (-1)^n \alpha^{(n)} \frac{r^{n-1}}{(r-1)^{n+1}}. \tag{25}$$

For application of the second algorithm we first obtain that on the axis

$$\overline{G}(s,t) = -i(t-2r)^{-1}, \tag{26}$$

and therefore

$$\overline{G}_{0,n}(s,t) = -it^n (t-2z)^{-n-1}, \quad n \geqslant 1, \tag{27}$$

and

$$\overline{G}_{m,n}(s,t) = 0, \quad \forall m \geqslant 1, \ \forall n.$$

We obtain, as before,

$$\Delta_B = 1 - \sum_{p=0}^{N} \delta^{(p)} \overline{G}_{0,p}(u,u),$$

$$\Gamma_{B(k)} = -i\delta_{0k}, \quad 0 \leqslant k \leqslant N,$$

and after the rescalings $r \to 2^{-1} ur$, $\delta^{(p)} \to u\delta^{(p)}$

$$\widetilde{E} = [1 - iB_B(r)]^{-1}, \tag{28}$$

where

$$B_B(r) = \sum_{n=0}^{N} \frac{(-1)^n \delta^{(n)}}{(r-1)^{n+1}}. \tag{29}$$

Finally, for the last algorithm, we have on the axis

$$G(u_i,u_j) = iu_j (2u_j r - 1)^{-1}, \tag{30}$$

from which we obtain

$$\Delta_C = 1 - \sum_{p=1}^{N} \beta^{(p)} G(0,u_p),$$

$$\Gamma_k = -i, \quad 1 \leqslant k \leqslant N,$$

and

$$\widetilde{E} = [1 - iB_C(r)]^{-1} \tag{31}$$

with

$$B_C(r) = \sum_{n=1}^{N} \frac{\beta^{(n)} u_n}{2ru_n - 1}. \tag{32}$$

Next we consider, on the axis, the generating function for the Weyl metric. For $\theta = 0$ Eq. (9) gives

$$\begin{aligned} \beta(t) &= \sum_{n=0}^{\infty} \frac{m_n}{r^{n+1}} - \sum_{n=0}^{\infty} m_n (2t)^{n+1} \\ &= \delta(r,0) - \delta(1/2t,0), \end{aligned} \tag{33}$$

where $\delta(r,\theta)$ has been defined in Eq. (6). Hence we obtain that, on the axis,

$$G_{\text{Weyl}}(s,t) = \frac{e^{2\delta(r,0)}}{e^{\delta(1/2s,0)} e^{\delta(1/2t,0)}} G_{\text{flat}}(s,t). \tag{34}$$

We can further simplify $G_{\text{Weyl}}(s,t)$ by using the "gauge" freedom of the generating functions, which arises from the fact that the potentials $N^{(mn)}_{11}$ are defined via differential equations. It is known[5,10] that the gauge freedom associated with

the generating function $G(s,t)$ of any static, axisymmetric solution is the multiplication of $G(s,t)$ by $c(s)c(t)$, where $c(s)$ is any smooth function of one variable (independent of the coordinates) for which $c(0)=1$. Therefore, since $\delta(1/2s,0)|_{s=0}=0$, the denominator in Eq. (34) can be absorbed by such a gauge transformation. Hence we conclude that there exists a gauge for which, on the $z>0$ part of the axis,

$$G_{\text{Weyl}}(s,t)=f(r)G_{\text{flat}}(s,t), \tag{35}$$

where

$$f(r)=e^{2\delta(r,0)}=\lambda_0(r,0) \tag{36}$$

is the squared norm of the timelike Killing field evaluated on the axis. We adopt this gauge. Note, parenthetically, that this is precisely the gauge which was used in (I), Eq. (2.24) to make $\beta(t)$ well behaved for $t\to\infty$.

Because the generating functions for the Weyl and flat solutions differ only by a factor which is independent of s and t, it is very easy to write on the axis the solution obtained when the original metric is the Weyl instead of the flat metric. Indeed, one can immediately write the new Ernst potentials by changing the parameters $\alpha^{(p)},\delta^{(p)},\beta^{(p)}$ into $f(r)\alpha^{(p)}$, $f(r)\delta^{(p)},f(r)\beta^{(p)}$ respectively— i.e., change $B_X(r)$ to $f(r)B_X(r)$, $X=A,B,C$—and simultaneously change the squared norm of the original solution from 1 to $f(r)$. We obtain

$$\tilde{E}=f+\frac{ifB}{1-ifB}=\frac{f-if(f-1)B}{1-ifB}, \tag{37}$$

where $B(r)$ stands for B_A, B_B, or B_C of Eqs. (25), (29), and (32) respectively, depending on the particular algorithm which has been applied. In the expression (37), $f(r)$ contains all the information about the Weyl solution which was used and $B(r)$ contains the information of the transformations which were applied.

We now study the multipole moments of the solution (37).

Recall[11] that for stationary asymptotically flat spacetimes one defines the mass and the angular momentum multipole moment potentials by

$$\phi_M=\frac{\lambda_0^2+\omega_0^2-1}{4\lambda_0},\qquad \phi_J=\frac{\omega_0}{2\lambda_0}. \tag{38}$$

The multipole moments of the spacetime are obtained in terms of the derivatives of the above potentials. Although higher multipole moments are difficult to calculate, the leading multipole moments are readily obtained as the coefficients of the leading terms of the expansions of ϕ_M and ϕ_J in powers of $1/r$.

For the solution (37) we have (dropping the tildes)

$$\lambda_0=\frac{f[1+f(f-1)B^2]}{1+f^2B^2}, \tag{39}$$

$$\omega_0=\frac{fB}{1+f^2B^2}, \tag{40}$$

$$\phi_M=\frac{(f^2-1)+f^3(f-2)B^2}{4f[1+f(f-1)B^2]}, \tag{41}$$

$$\phi_J=\frac{B}{2[1+f(f-1)B^2]}. \tag{42}$$

f and B admit expansions of the form

$$f=1+\sum_{n=1}^{\infty}\frac{p_n}{r^n},\qquad B=\sum_{n=1}^{\infty}\frac{b_n}{r^n}. \tag{43}$$

Asymptotic flatness requires that

$$\lambda_0=1+\frac{m}{r}+O\left(\frac{1}{r^2}\right),\qquad \omega_0=\frac{a}{r^2}+O\left(\frac{1}{r^3}\right), \tag{44}$$

for constants m and a and it holds for $b_1=0$. (It turns out that even solutions with $b_1\neq 0$ can be transformed into asymptotically flat solutions by the application of a suitable Ehlers transformation,[7] but we will not consider this case here.) Instead we will assume that

$$\left.\begin{aligned} f&=1+\frac{p_n}{r^n}+O\left(\frac{1}{r^{n+1}}\right), && n\geqslant 1\\ B&=\frac{b_s}{r^s}+O\left(\frac{1}{r^{s+1}}\right), && s\geqslant 2\end{aligned}\right\}. \tag{45}$$

Using Eqs. (41), (42), and (45) it is straightforward to obtain that

$$\phi_M=\begin{cases}\dfrac{p_n}{2r^n}+O\left(\dfrac{1}{r^{n+1}}\right) & \text{if } n<2s\\[2ex] \dfrac{-b_s^2}{4r^{2s}}+O\left(\dfrac{1}{r^{2s+1}}\right) & \text{if } n>2s\\[2ex] \dfrac{(2p_n-b_s^2)}{4r^n}+O\left(\dfrac{1}{r^{n+1}}\right) & \text{if } n=2s \text{ and } b_s^2\neq 2m_n\\[2ex] \dfrac{p_{n+1}}{2r^{n+1}}+O\left(\dfrac{1}{r^{n+2}}\right) & \text{if } n=2s \text{ and } b_s^2=2m_n\end{cases} \tag{46}$$

$$\phi_J=\frac{b_s}{2r^s}+O\left(\frac{1}{r^{s+1}}\right). \tag{47}$$

Equations (46) and (47) determine the leading multipole moments of the new solution. Observe that for the original Weyl metric $\phi_M=p_n/2r^n+O(r^{-n-1})$. Therefore, *for $n<2s$ all three algorithms preserve the leading mass multipole moment of the original Weyl metric.* In particular it could be argued that physically realistic solutions should possess a nonzero total mass, i.e., they would have $p_1\neq 0$. Hence, since $s\geqslant 2$, we conclude, as in (I), that the application of the algorithm does not change the mass.

4. CONSTRUCTION OF PRESCRIBED SOLUTIONS

A. Specific leading multipole moments

It might be desirable to construct the metric of a spacetime representing a relativistically rotating star with predetermined leading mass and angular momentum multipole moments. With the analysis of the previous section this can now be readily achieved. Equations (46) and (47) can be used to obtain the required $f(r)$ and $B(r)$, which contain, respectively, all the information about the original Weyl metric and the choice of the parameters in the algorithms which construct such a metric.

To determine the required Weyl metric is trivial; for $f(r)$ to be of the form given by the first of Eqs. (45) one simply has to choose $m_{n-1} = p_n/2$ as the first nonvanishing parameter in the expression (6) for $\delta(r,\theta)$. Hence, we will concentrate on the slightly more complicated issue of determining the required transformations, namely, on how to choose the parameters $\alpha^{(n)}$, $\delta^{(n)}$, $\beta^{(n)}$ in $B_A(r)$, $B_B(r)$, $B_C(r)$ [Eqs. (25), (29), (32) respectively] such that they admit a power series expansion of the form $b_s r^{-s} + O(r^{-s-1})$, for $s \geqslant 2$. For $B_B(r)$ this is immediate by the choice $\delta^{(n)} = 0$, $0 \leqslant n \leqslant s-2$, which actually reflects that the transformations $D^{(p)}$ used in the second algorithm were constructed to generate pure multipole moments. We proceed with the determination of the parameters in B_A and B_C because such an approach can be generally used to find additional transformations which generate pure multipole moments. To avoid massive calculations while presenting the idea we will consider a particular case, namely, the choice of the parameters in Eqs. (25) and (32) for which B_A and B_C are of the form $b_5/r^5 + O(r^{-6})$.

For B_A we have to choose particular $\alpha^{(n)}$, $0 \leqslant n \leqslant 4$, $\alpha^{(n)} = 0$ for $n \geqslant 5$. By changing $r \to r+1$ (to simplify the calculations) and requiring that the coefficients of the first four powers of $1/r$ vanish we obtain $\alpha^{(0)} = 0$, $3\alpha^{(1)} = \alpha^{(2)} = \alpha^{(3)} = 3\alpha^{(4)}$. Therefore, the required transformation, of the form (18), is

$$a_k = \sum_{p=0}^{4} \alpha^{(p)} \binom{k}{p} u^k = \frac{\alpha^{(4)}}{24} u^k k(k+1)(k+2)(k+3) = \alpha^{(4)} \binom{k+3}{4} u^k,$$

i.e., a transformation of the form (19), used in the second algorithm.

For $B_C(r)$ we again choose $\beta^{(p)} = 0, p \geqslant 6$ while specifying $\beta^{(p)}$ for $1 \leqslant p \leqslant 5$. By writing

$$B_C(r) = \sum_{n=0}^{\infty} \left[\sum_{p=1}^{N} \frac{\beta^{(p)}}{2^{n+1} u_p{}^n} \right] r^{-n-1} \tag{48}$$

and requiring that the coefficients of the first four powers of $1/r$ vanish we now obtain the four linear equations

$$\sum_{n=1}^{5} \beta^{(n)} u_n{}^{-p} = 0, \quad 0 \leqslant p \leqslant 3, \tag{49}$$

which constrain the coefficients. A particularly nice expression is obtained by choosing $u_n = nu$, $1 \leqslant n \leqslant p$ and expressing, using Eqs. (49), all $\beta^{(n)}$'s in terms of $\beta^{(1)}$. We obtain

$$a_k = \sum_{p=1}^{5} \beta^{(p)} u_p{}^k = \epsilon^{(5)} [1 - 4(2^{k+3}) + 6(3^{k+3}) - 4(4^{k+3}) + 5^{k+3}] u^k, \tag{50}$$

for some constant $\epsilon^{(5)}$.

In fact, proceeding by induction one can show that the transformations with

$$a_k = \epsilon^{(p+1)} \left[\sum_{n=0}^{p} (-1)^n \binom{p}{n} (1+n)^{k+p-1} \right] u^k \tag{51}$$

generate a solution with $(p+1)$-leading angular momentum multipole moment. Of course, by making the choice (51) one works with repeated zero rank transformations with different u-parameters.

B. The Geroch conjecture

With the discovery of the infinite dimensional group of transformations which preserve the stationary axisymmetric equations, Geroch[1] conjectured that it should be possible to generate their general asymptotically flat solution by applying the transformations to flat space. His evidence was mainly the observation that the available transformations were sufficient to generate a solution with two infinite sets of arbitrary parameters, representing the mass and the angular momentum multipole moments. A stronger conjecture was made in (I). Since the algorithms generate solutions with any finite number of additional parameters, it was conjectured that, applied to the Weyl metric, they will provide the general solution. This conjecture, together with an earlier proof by Kinnersley and Chitre[4] that the Weyl solution can be generated from the flat solution would settle completely Geroch's conjecture.

Our aim here is to present overwhelming evidence that the conjecture in (I) is true; we will display the Weyl solution which should be used as the original solution and the particular choice of the paremeters in the algorithms which generate any given solution. Here are the instructions: For any given stationary, axisymmetric, asymptotically flat solution evaluate its norm and twist potential $\lambda_0(r)$ and $\omega_0(r)$ on the axis. Then evaluate

$$f(r) = [2\lambda_0 + 1 - (1 - 4\omega_0^2)^{1/2}]/2 \tag{52}$$

and

$$B(r) = 2\omega_0 [2\omega_0^2 + \lambda_0 (1 + (1 - 4\omega_0^2)^{1/2})]^{-1}. \tag{53}$$

From $f(r)$ obtain $\delta(r,0)$ and then $\delta(r,\theta)$ by using Eqs. (36) and (6) respectively, to determine the Weyl solution. Finally, equate the above $B(r)$ to B_A, B_B, or B_C of Eqs. (25), (29), or (32) (depending on the algorithm which will be applied) to determine the parameters $\alpha^{(p)}$, $\delta^{(p)}$ or $\beta^{(p)}$.

The above expressions (52) and (53) have been obtained by solving

$$E = \frac{f - if(f-1)B}{1 - ifB} = \lambda_0 + i\omega_0$$

for f and B and choosing the solution which reduces to $(f,B) = (\lambda_0, 0)$ for $\omega_0 = 0$. Note that for an asymptotically flat solution (λ_0, ω_0) the above $f(r)$ and $B(r)$ have the "correct" [cf. Eq. (45)] asymptotic behavior.

We close the section with the remark that the present analysis does not prove the conjecture completely; it only determines the original metric and the required transformations which will construct any solution provided that the conjecture is true. What is further required to complete the proof is a uniqueness proof for the solutions of the elliptic system (4) with initial data given on the axis and with asymptotic behavior as in Eq. (44), i.e., the asymptotic behavior which guarantees asymptotic flatness.

5. DISCUSSION

It would appear from Eq. (20) that the application of the third algorithm to the general Weyl metric would produce a metric with three infinite sets of independent parameters $\{m_i, \beta^{(i)}, u_i\}_{i=1}^{\infty}$ Moreover, one could possibly consider further combinations of the different transformations, e.g., by choosing

$$a_k = \sum_{i=1}^{M} \sum_{p=0}^{N} a_i^{(p)} \binom{k}{p} u_i^k, \tag{54}$$

and introduce, seemingly, even more infinite sets of parameters. But these contradict the expectation (mainly based on physical intuition) that the general stationary axisymmetric asymptotically flat solution depends on precisely two infinite sets of parameters. The present analysis suggests that the apparent abundance of parameters might be superfluous. It turns out that it is possible to write an algorithm for the application of the transformations (54) and to perform the computations on the axis. The resulting solution, on the axis, depends exactly on two infinite sets of parameters.

The determination of the original Weyl, needed to generate a stationary metric, by Eq. (52) has the slightly unfortunate feature that $f(r)$ depends, except on λ_0, on ω_0 as well. As a result, a stationary metric generalizing a given static metric is not obtained by applying the algorithms to this static metric. For instance, to generate the Kerr solution by using the present algorithms, the static solution needed is not the Schwarzschild solution but some other, rather complicated Weyl solution. The situation should be contrasted with the transformations used in Ref. (5) which generate the Kerr solution from the Schwarzschild solution. However, the numerous advantages of the present transformations certainly outweigh this deficiency.

The idea of performing the computations on the axis might be useful in other studies as well, for instance, in the study of solutions of the Einstein–Maxwell equations. Proceeding as in (I), it is possible to write algorithms for the generation of stationary axisymmetric solutions of the Einstein–Maxwell equations, but as far as I am aware nobody has studied them in any detail. An analysis for these algorithms similar to the analysis done here will reveal the required transformations which generate solutions with any desired multipole moment structure.

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$$G(s,t) = -\frac{iS(s)}{2s\lambda_0} F_{11}(s)F_{11}(t)\left[1 + \frac{s+t-4stz}{sS(t)+tS(s)}\right],$$

where $F_{11}(s)$ has been defined in Refs. 5 and 7. Then, the gauge freedom for $G(s,t)$ is immediately obtained from the freedom for $F_{11}(s)$, Eq. (2.35) of Ref. 5. Note the change in notation, $G(s,t) = G_{11}(s,t)$ and $\lambda_0 = f$.
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Exact composite nearest neighbor degeneracies for one-dimensional lattice spaces

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Expressions are developed which describe exactly the composite, nearest neighbor degeneracy specified by the three kinds of nearest neighbor pairs created when simple indistinguishable particles are distributed on a one-dimensional lattice space.

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I. INTRODUCTION

In the present paper we determine the composite, exact nearest neighbor degeneracy for the following situation: a one-dimensional lattice space which consists of N equivalent sites (each of which can accommodate one single simple particle only) arranged in a linear array; q single, indistinguishable particles each of which occupies a single lattice site; three kinds of nearest neighbor pairs, arising when the particles are distributed on the space, (1) occupied nearest neighbor pairs [1–1 type], (2) mixed nearest neighbor pairs [0–1 type] and (3) vacant nearest neighbor pairs [0–0 type].

Previous papers[1–3] have dealt with a determination of the exact degeneracy of arrangements in those situations where one type of nearest neighbor pair is specified. The present paper seeks to extend those results to a determination of the composite degeneracy of arrangements for which the numbers of occupied, mixed, and vacant nearest neighbor pairs are all prescribed.

Within the constraints imposed by the nearest neighbor approximation, the most general expression for E_i, the interaction energy, is

$$E_i = n_{11}V_{11} + n_{01}V_{01} + n_{00}V_{00}, \tag{1}$$

where n_{11} is the number of occupied nearest neighbor pairs on an array, n_{01} is the number of mixed (one site occupied and an adjacent site vacant) nearest neighbor pairs on an array, and n_{00} is the number of vacant nearest neighbor pairs on an array; V_{11}, V_{01}, and V_{00} are associated potential energies of interaction, respectively.

Clearly, the present notation, appropriate to the occupation of lattice sites, can be transformed readily to situations involving the distributions of two kinds of dissimilar particles or any binary distributions of, for example, magnetic spins of sign $+$ and $-$.

The partition function associated with Eq. 1 is written

$$\sum_{n_{11},n_{01},n_{00}} A\,[N, q, n_{11}, n_{01}, n_{00}]\exp[(-E_i/kT)], \tag{2}$$

where $A\,[N, q, n_{11}, n_{01}, n_{00}]$ is the degeneracy or multiplicity of those arrangements having a prescribed number of 1–1 (occupied nearest neighbor) pairs *and* a prescribed number of 0–1 (mixed nearest neighbor) pairs *and* a prescribed number of 0–0 (vacant nearest neighbor) pairs—when q indistinguishable particles are distributed on the lattice space consisting of N equivalent sites. Here the sum is taken over all states specified by permissible values of n_{11}, n_{01}, and n_{00}. The present paper is concerned primarily with determining the exact composite nearest neighbor degeneracies for one-dimensional lattice spaces.

We first note here that the quantities n_{11}, n_{01}, n_{00} are not independent but are related by the fact that their sum is the total number of nearest neighbor pairs which can exist on an array regardless of the number of particles present, i.e.,

$$N - 1 = n_{11} + n_{01} + n_{00} \tag{3}$$

There will be developed in the next section additional relationships between the five variables N, q, n_{11}, n_{01}, and n_{00}.

II. DETERMINATION OF $A[N, q, n_{11}, n_{01}, n_{00}]$

To calculate $A\,[N, q, n_{11}, n_{01}, n_{00}]$, we must consider the situations when n_{01} is even and when it is odd.

A. n_{01} odd

If n_{01} is odd, then one and only one end compartment is occupied (see Fig. 1). Assuming that the occupied end compartment is on the right-hand side of lattice, we construct "units" which consist of one or more contiguous particles and the adjacent vacancy (or vacancies) to the left of the particle(s) which separate the particles of a "unit" from the particle(s) to their left. With each "unit," except for the one at the right hand side of the array, there are two nearest neighbor pairs of the 0–1 type; one at the right-hand end of the "unit" and one on the left. For the "unit" on the right-hand end of the space there is one mixed nearest neighbor pair. Thus, there must always be a total of $[(n_{01} + 1)/2]$ "units," regardless of the number of occupied or vacant sites.

There are n_{11} occupied nearest neighbor pairs which can be distributed among the $[n_{01} + 1)/2]$ "units." If we consider the "units" as identical boxes into which we can distribute the n_{11} identical nearest neighbor pairs with no restric-

FIG. 1. In this figure $n_{01} = 7$ (denoted by x's), $n_{11} = 3$ (denoted by $=$), and $n_{00} = 1$ (denoted by $-$). The compartment on the right-hand end is occupied while the left-hand compartment is vacant. There are four $(n_{01} + 1)/2 = 4$ "units" (denoted by the dashed boxes).

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tion as to the number of occupied nearest neighbor pairs in each box, then there are

$$\binom{[(n_{01}+1)/2]+n_{11}-1}{n_{11}}=\binom{[(n_{01}-1)/2]+n_{11}}{n_{11}} \quad (4)$$

independent arrangements which can be created as the occupied paris are permuted among the boxes.[4]

By permuting the vacant nearest neighbor pairs among the "units," additional independent arrangements can be created without influencing the number of "units" or the distribution of the n_{11} occupied nearest neighbor pairs within the "units." Again we consider $[(n_{01}+1)/2]$ "units" to be indistinguishable boxes into which we may place the n_{00} indistinguishable vacant nearest neighbor pairs with no constraint as to the number of vacant nearest neighbor pairs which can be placed in each box. By so doing

$$\binom{[(n_{01}+1)/2]+n_{00}-1}{n_{00}}=\binom{[(n_{01}-1)/2]+n_{00}}{n_{00}} \quad (5)$$

independent arrangements can be created.

Because the manipulations leading to Eqs. (4) and (5) represent statistically independent events, the total number of arrangements possible, when n_{01} is odd and the right-hand end compartment is occupied, is simply their product

$$\binom{[(n_{01}-1)/2]+n_{11}}{n_{11}}\binom{[(n_{01}-1)/2]+n_{00}}{n_{00}}. \quad (6)$$

A similar expression can be derived when n_{01} is odd and when the end compartment on the left-hand side is occupied. Because the occupation of the left-hand end compartment is statistically equivalent to the situation when the right-hand end compartment is occupied, $A(N, q, n_{11}, n_{01}, n_{00})$, the total number of arrangements possible when n_{01} is odd, is just twice Eq. (6), i.e.,

$$A(N, q, n_{11}, n_{01}, n_{00}) = 2\binom{[(n_{01}-1)/2]+n_{11}}{n_{11}}\binom{[(n_{01}-1)/2]+n_{00}}{n_{00}}, \quad n_{01}\text{ odd}. \quad (7)$$

B. n_{01} even

When n_{01} is even, two situations can arise:

(a) the compartments on both ends of the array are empty (see Fig. 2).

(b) both ends compartments are occupied (see Fig. 3).

For those arrangements described by (a), we create "units" which consist of a particle or group of contiguous particles and the vacancy or group of vacancies which separated the particle(s) of the "unit" from the particle(s) to the left (see Fig. 2). Thus on the array there are always $[n_{01}/2]$ "units" (because each "unit" has two mixed nearest neighbor pairs).

The "units" may be considered to be identical boxes into which we may place the n_{11} identical occupied nearest neighbor pairs to form

$$\binom{[n_{01}/2]+n_{11}-1}{n_{11}}=\binom{[n_{01}/2]+n_{11}-1}{[n_{01}/2]-1}$$

independent arrangements.

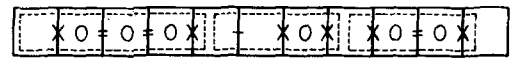

FIG. 2. In this figure $n_{01}=6$ and both end compartments are empty, $n_{11}=3$ (denoted by $=$), and $n_{00}=1$ (denoted by $-$). There are 3 "units" $n_{01}/2=3$ (denoted by dashed lines).

The n_{00} vacant nearest neighbor pairs can be distributed among the $[n_{01}/2]$ "units" and the vacancy or groups of contiguous vacancies at the right-hand end of the aray. Thus there are $[n_{01}/2]+1$ boxes into which the n_{00} vacant nearest neighbor pairs may be placed; this can be done in

$$\binom{[n_{01}/2]+n_{00}}{n_{00}}$$

independent ways.

Thus $A(q, N, n_{11}, n_{01}, n_{00})$, the total number of independent arrangements possible when both end compartments are empty, is given by

$$A(N, q, n_{11}, n_{01}, n_{00}) = \binom{[n_{01}/2]+n_{11}-1}{n_{11}}\binom{[n_{01}/2]+n_{00}}{n_{00}}. \quad (8)$$

For situation (b) (Fig. 3) we form "units" which consist of a particle or group of contiguous particles and the adjacent vacancy (or vacancies) just to the left of the particles; the "unit" on the left-hand end of the array needs no vacancy(ies) to separate it from the rest of the array. Because the particle or group of contiguous particles on each end of the array has only one mixed nearest neighbor pair associated with it, there are $[(n_{01}+2)/2]$ "units."

The n_{11} occupied nearest neighbor pairs may be distributed among the $[(n_{01}+2)/2]$ boxes to form

$$\binom{[(n_{01}+2)/2]+n_{11}-1}{n_{11}}=\binom{[n_{01}/2]+n_{11}}{n_{11}}=\binom{[n_{01}/2]+n_{11}}{\frac{n_{01}}{2}}$$

independent arrangements.

Similarly, the n_{00} vacant nearest neighbor pairs may be distributed among the $[(n_{01}+2)/2]$ boxes in

$$\binom{[n_{01}/2]+n_{00}}{n_{00}}=\binom{[n_{01}/2]+n_{00}}{n_{01}/2}$$

independent ways.

Thus, when the compartments at both ends of the array are occupied, $A(q, N, n_{11}, n_{01}, n_{00})$ is given by

$$A(N, q, n_{11}, n_{01}, n_{00}) = \binom{[n_{01}/2]+n_{11}}{n_{11}}\binom{[n_{01}/2]+n_{00}}{n_{00}}. \quad (9)$$

Equations (7), (8), and (9) are, of course, subject to the

FIG. 3. In this figure $n_{01}=6$ and both end compartments are occupied, $n_{11}=2$ (denoted by $=$), and $n_{00}=3$ (denoted by $-$). The number of "units" is 4, $(n_{01}+2)/2$ (denoted by dashed boxes).

constraints imposed by Eq. (3); however, to express Eqs. (7), (8), and (9) in terms of N and q we note that when n_{01} is odd (i.e., one and only one end compartment is occupied), then the number of mixed nearest neighbor pairs is related to N, q, n_{11}, and n_{00} by the relationships

$$2q - 1 = n_{01} + 2n_{11}, \tag{10}$$

$$2(N - q) - 1 = n_{01} + 2n_{00}. \tag{11}$$

These relationships can be seen from Fig. 4 in which [for Eq. (10)] lines are drawn from both sides of each compartment which is occupied. An accounting of the lines leads to Eq. (10). Equation (11) may be derived in the same manner where the lines are drawn from both sides of each compartment which is vacant.

In light of Eqs. (10) and (11), Eq. (7) becomes

$$A(N, q, n_{11}, n_{00}) = 2\binom{q-1}{n_{11}}\binom{N-q-1}{n_{00}}, \quad n_{01} \text{ odd}. \tag{12}$$

When n_{01} is even and both end compartments are vacant,

$$2q = n_{01} + 2n_{11}, \tag{13}$$

$$2(N - q) - 2 = n_{01} + 2n_{00}, \tag{14}$$

so that Eq. (8) becomes

$$A(N, q, n_{11}, n_{00}) = \binom{q-1}{n_{11}}\binom{N-q-1}{n_{00}}, \quad n_{01} \text{ even}. \tag{15}$$

When n_{01} is even and both end compartments of the array are occupied,

$$2q - 2 = n_{01} + 2n_{11}, \tag{16}$$

$$2(N - q) = n_{01} + 2n_{00}, \tag{17}$$

then Eq. (9) may be written

$$A(q, N, n_{11}, n_{00}) = \binom{q-1}{n_{11}}\binom{N-q-1}{n_{00}}, \quad n_{01} \text{ even} \tag{18}$$

Equations (12), (15), and (18) reflect the permutations of the total number of separations between the particles with those separations which are occupied nearest neighbor pairs and the permutation of the total number of separations between the vacancies with those separations which are vacant nearest neighbor pairs.

To determine, from Eqs. (12), (15), and (18), $A(N, q, n_{11})$, the number of arrangements of q indistinguishable particles on a one-dimensional lattice of N equivalent sites which yield n_{11} occupied nearest neighbor pairs, we sum over all possible values of n_{00}. There are, however, only three possible values of n_{00}. This can be seen from the following considerations:

For a fixed value of n_{11} there are, on any single array, $q - n_{11}$ groups terminated at each end by a mixed nearest neighbor pair unless the group is at the end of the array. Thus

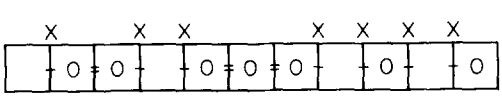

FIG. 4. Accounting for the number nearest neighbor pairs in terms of the number of occupied and vacant sites. There are three occupied nearest neighbor pairs (=); seven mixed nearest neighbor pairs; seven particles.

$$2(q - n_{11} - 1) \leqslant n_{01} \leqslant 2(q - n_{11}). \tag{19}$$

This corresponds to the three cases discussed above: the one case when n_{01} is odd and the two cases when n_{01} is even.

In the light of Eq. (3), Eq. (19) becomes

$$2(q - n_{11} - 1) \leqslant N - 1 - n_{11} - n_{00} \leqslant 2(q - n_{11}) \tag{20}$$

so that the three values of n_{00} are contained in

$$N - 2q + n_{11} - 1 \leqslant n_{00} \leqslant N - 2q + n_{11} + 1. \tag{21}$$

We note by the subtraction of Eq. (13) from Eq. (14) that the lower limit corresponds to the vacancy of the compartments at each end of the array; by the subtraction of Eq. (10) from Eq. (11), that is, $n_{00} = N - 2q + n_{11}$, means that n_{01} is odd and that one and only one end compartment is occupied; and by the subtraction of Eq. (16) from Eq. (17) we note that the upper limit is associated with n_{01} even and that the compartments at both ends are occupied.

Thus

$$\begin{aligned} A(N, q, n_{11}) &= \sum_{n_{00} = N - 2q + n_{11} - 1}^{N - 2q + n_{11} + 1} A(N, q, n_{11}, n_{00}) \\ &= \binom{q-1}{n_{11}}\left[\binom{N-q-1}{q-n_{11}-1} + 2\binom{N-q-1}{q-n_{11}} \right. \\ &\quad \left. + \binom{N-q-1}{q-n_{11}+1}\right] \\ &= \binom{q-1}{n_{11}}\binom{N-q+1}{q-n_{11}}, \end{aligned} \tag{22}$$

a result previously reported.[1] In Eq. (22), we have assumed that $A(N, q, n_{11}, n_{00})$ is given alternately by Eqs. (15), (12), and (18).

Similarly, $A(N, q, n_{00})$ is obtaining by summing $A(N, q, n_{11}, n_{00})$ over all values of n_{11}, $(2q - N + n_{00} - 1 \leqslant n_{11} \leqslant 2q - N + n_{00} + 1)$, i.e.,

$$\begin{aligned} A(N, q, n_{00}) &= \sum_{n_{11} + 2q - N + n_{00} - 1}^{2q - N + n_{00} + 1} A(N, q, n_{11}, n_{00}) \\ &= \binom{N-q-1}{n_{00}}\binom{q+1}{N-q-n_{00}}. \end{aligned} \tag{23}$$

Again in Eq. (23), $A(N, q, n_{11}, n_{00})$ is given alternately by Eqs. (12), (15), and (18). The result contained in Eq. (23) has been reported previously.[1]

To determine the degeneracy of those arrangements containing a prescribed number of mixed nearest neighbor pairs we note from Eq. (12) that when n_{01} is odd,

$$\begin{aligned} A(N, q, n_{01}) &= 2\sum_{n_{11}}\binom{q-1}{n_{11}}\binom{N-q-1}{N-1-n_{11}-n_{01}} \\ &= 2\binom{q-1}{(n_{01}-1)/2}\binom{N-q-1}{(n_{01}-1)/2} \end{aligned} \tag{24}$$

because, from Eq. (10), n_{11} takes on only one value:

$$n_{11} = q - [(n_{01} + 1)/2]. \tag{25}$$

When n_{01} is even n_{11} can take on two values $q - n_{01}/2 - 1$ and $q - n_{01}/2$ so that

$$A(N,q,n_{01}) = \binom{N-q-1}{n_{01}/2-1}\binom{q-1}{n_{01}/2} + \binom{N-q-1}{n_{01}/2}\binom{q-1}{n_{01}/2-1} = 2\left[\frac{N-n_{01}}{n_{01}}\right]\binom{N-q-1}{n_{01}/2-1}\binom{q-1}{n_{01}/2-1}. \tag{26}$$

Equations (24) and (26) represent the exact degeneracy of those arrangements containing a prescribed number of mixed nearest neighbor pairs[3] and as such it is to be compared with an approximate solution developed by Ising (1925) in his treatment of one-dimensional ferromagnetic phase transitions.[5]

III. NORMALIZATION

The zeroth moment of the statistics characterized by $A[N,q,n_{11},n_{01},n_{00}]$ is determined by summing the composite degeneracy over all values of n_{11}, n_{01}, and n_{00}, i.e.,

$$\sum_{n_{11}}\sum_{n_{00}}\sum_{n_{01}} A[N,q,n_{11},n_{01},n_{00}]. \tag{27}$$

From Eqs. (3), (12), (15), (18), (22), and (23) and the Vandermonde theorem[6] we see that Eq. (27) reduces to

$$\sum_{n_{11}=0}^{q-1}\binom{q-1}{n_{11}}\binom{N-q+1}{q-n_{11}} = \binom{N}{q} \tag{28}$$

or

$$\sum_{n_{00}=0}^{N-q-1}\binom{q+1}{N-q-n_{00}}\binom{N-q-1}{n_{00}} = \binom{N}{q}. \tag{29}$$

Similarly, from Eqs. (24) and (26) we see that

$$\begin{aligned}\sum_{n_{01}} A[N,q,n_{01}] &= \left\{2+2\left[\frac{N-2}{2}\right]+2\binom{q-1}{1}\binom{N-q-1}{1}+2\left[\frac{N-4}{4}\right]\times\binom{q-1}{1}\binom{N-q-1}{1}+2\binom{q-1}{2}\binom{N-q-1}{2}\right.\\ &\left.+2\left[\frac{N-6}{6}\right]\binom{q-1}{2}\binom{N-q-1}{2}+\cdots\right\}\\ &= \sum_j\left[\frac{N}{j+1}\right]\binom{q-1}{j}\binom{N-q-1}{j}\\ &= \left[\frac{N}{q}\right]\sum_j\binom{q}{j}\binom{N-q-1}{j}\\ &= \left[\frac{N}{q}\right]\binom{N-1}{q-1} = \binom{N}{q}.\end{aligned} \tag{30}$$

IV. FIRST MOMENT

In this section we consider the mean values of the number of nearest neighbor pairs, for random distributions.

The mean value of n_{11} and n_{00} can be calculated using the results of Eqs. (22) and (23), respectively, and have been reported previously.[1] The mean value of n_{01} can be determined to be

$$\langle n_{01}\rangle = \binom{N}{q}^{-1}\sum_{n_{01}} n_{01}A(N,q,n_{01}), \tag{31}$$

where for odd and even values of n_{01} Eqs. (24) and (26) are utilized to express $A(N,q,n_{01})$ as n_{01} varies over its permissible values. Thus

$$\begin{aligned}\langle n_{01}\rangle = 2\binom{N}{q}^{-1}&\left\{1+(2)\left[\frac{N-2}{2}\right]+(3)\binom{q-1}{1}\times\binom{N-q-1}{1}+4\left[\frac{N-4}{4}\right]\binom{N-q-1}{1}\binom{q-1}{1}\right.\\ &+5\binom{q-1}{2}\binom{N-q-1}{2}+6\left[\frac{N-6}{6}\right]\left.\times\binom{N-q-1}{2}\binom{q-1}{2}+\cdots\right\}.\end{aligned} \tag{32}$$

By grouping the first and second terms, the third and fourth terms, etc., we obtain

$$\begin{aligned}\langle n_{01}\rangle &= 2\binom{N}{q}^{-1}\left\{(N-1)+(N-1)\binom{q-1}{1}\binom{N-q-1}{1}+(N-1)\binom{q-1}{2}\binom{N-q-1}{2}+\cdots\right\}\\ &= 2(N-1)\binom{N}{q}^{-1}\sum_j\binom{q-1}{j}\binom{N-q-1}{j}\\ &= 2(N-1)\binom{N}{q}^{-1}\binom{N-2}{N-q-1} = \frac{2q(N-q)}{N}.\end{aligned} \tag{33}$$

Thus, the maximum value of $\langle n_{01}\rangle/N$ is $\frac{1}{2}$ and occurs at a lattice coverage of $\frac{1}{2}$.

V. SUMMARY

The exact degeneracy of those arrangements exhibiting prescribed numbers of occupied, mixed, and vacant nearest neighbor pairs has been determined. By the reduction of this degeneracy, the degeneracies of arrangements arising when only one kind of nearest neighbor is specified are also determined exactly.

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Asymptotic decay of correlations in the spin-$\frac{1}{2}$ Ising model [a)]

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We show that in the high-temperature region the spin–spin correlation function decays asymptotically like $e^{-\kappa r}/r^b$, $0 \leqslant b \leqslant \frac{1}{2}(d-1)$.

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Perhaps the simplest tenable, quantitative approximation one can make to the two-point, spin–spin, correlation function is that of Ornstein and Zernike.[1] Their approximation results, in general dimension,[2] in the decay of the spin–spin correlation function like

$$\langle \sigma_0 \sigma_{\mathbf{r}} \rangle \propto e^{-\kappa r}/r^{\frac{1}{2}(d-1)}. \tag{1}$$

We have been able to show that their simple approximation represents, at least for the spin-$\frac{1}{2}$ Ising model, above the critical temperature, the limit of what is possible. This behavior is known to be correct for the two-dimensional, nearest-neighbor Ising model from the exact solution.[3] Also it is already known[4] that the decay must be approximately exponential in this region

We set

$$\langle \sigma_0 \sigma_{\mathbf{R}} \rangle = G(\mathbf{R}). \tag{2}$$

It has been proved, for sufficiently high temperatures[5] and for $R = ||\mathbf{R}||_2$, large enough, that:

$$G(\mathbf{R}) \propto e^{-R\kappa(\hat{R})}/R^{\frac{1}{2}(d-1)}, \tag{3}$$

where $\hat{R}$ is the unit vector in the $\mathbf{R}$ direction. The mass gap $\kappa(\hat{R})$ has a nontrivial but explicit dependence on the direction.

It is therefore natural to postulate for the ferromagnetic spin-$\frac{1}{2}$, nearest neighbor, Ising model, that for $\mathbf{R} \in \mathbb{Z}^d$ and $||\mathbf{R}||_2 > R_1$, there exists $0 < A_- \leqslant A_+$, $\kappa(\hat{R}) > 0$ and $b(\hat{R})$ such that:

$$A_- \frac{e^{-R\kappa(\hat{R})}}{R^{b(\hat{R})}} \leqslant \langle \sigma_0 \sigma_{\mathbf{R}} \rangle \leqslant A_+ \frac{e^{-R\kappa(\hat{R})}}{R^{b(\hat{R})}}. \tag{4}$$

Let us call $\hat{O}$ the direction along a given axis of the lattice. Under this hypothesis and either hypothesis:

$$(\mathrm{H}_1) \quad \begin{cases} \kappa(\hat{O}) \leqslant \kappa(\hat{R}) \\ b(\hat{O}) \leqslant b(\hat{R}) \end{cases} \tag{5}$$

or

$$(\mathrm{H}_2) \quad G(\mathbf{R}) \leqslant G(||\mathbf{R}||_2,\ 0,\ 0,\ldots 0). \tag{6}$$

We shall prove that

$$0 \leqslant b(\hat{O}) \leqslant (d-1)/2. \tag{7}$$

Hypothesis (H_2) seems to be likely and expresses the fact that spin–spin correlation function has to have its maximum along the axis of the lattice when considered on a large sphere. An inequality of the same type but in the reverse direction has been obtained by Hegerfeldt[6]

$$G(||\mathbf{R}||_1,\ 0,\ 0,\ldots 0) \leqslant G(\mathbf{R}). \tag{8}$$

We first prove that $b(\hat{R}) \geqslant 0$. Since $\sigma^2 = 1$ we may write

$$\langle \sigma_\alpha \sigma_\beta \rangle = \langle \sigma_\alpha \sigma_\gamma^2 \sigma_\beta \rangle \geqslant \langle \sigma_\alpha \sigma_\gamma \rangle \langle \sigma_\gamma \sigma_\beta \rangle \tag{9}$$

by Griffith's second inequality.[7] Thus by the hypotheses of the theorem, and by taking the points α, β, γ in the same direction, $\hat{R}$, and by choosing,

$$R = |\alpha - \beta| = 2|\alpha - \gamma| = 2|\gamma - \beta|, \tag{10}$$

we get

$$A_+ \frac{e^{-R\kappa(\hat{R})}}{R^{b(\hat{R})}} \geqslant A_-^2 \frac{e^{-R\kappa(\hat{R})}}{R^{2b(\hat{R})}}. \tag{11}$$

We have at once, when $R \to \infty$ that $b(\hat{R}) \geqslant 0$. To prove that $b(\hat{O}) \leqslant (d-1)/2$, choose $\alpha = (0,0,\cdots 0)$ and $\beta = (2R,0,0,\cdots 0)$, $R > R_1$.

Then, setting for convenience $\kappa(\hat{O}) = \kappa$ and $b(\hat{O}) = b$, we have

$$A_- \frac{e^{-2\kappa R}}{2^b R^b} \leqslant \langle \sigma_0 \sigma_{2R} \rangle \leqslant \sum_{\gamma \in \mathscr{B}} \langle \sigma_0 \sigma_\gamma \rangle \langle \sigma_\gamma \sigma_{2R} \rangle \tag{12}$$

by Simon's inequality[8] where the ball $\mathscr{B}$ must surround the origin. We choose for it the $(d-1)$ hyperplane $\mathscr{H}_{d-1}$, which bisects the line (α,β). Using the hypothesis (H_1), we get

$$\begin{aligned} A_- \frac{e^{-2\kappa R}}{2^b R^b} &\leqslant \langle \sigma_0 \sigma_{2R} \rangle \\ &\leqslant A_+^2 \sum_{\gamma \in \mathscr{H}_{d-1}} \frac{\exp[-2||\gamma||_2 \kappa(\hat{\gamma})]}{||\gamma||_2^{2b(\hat{\gamma})}} \\ &\leqslant A_+^2 \sum_{\gamma \in \mathscr{H}_{d-1}} \frac{\exp(-2\kappa||\gamma||_2)}{||\gamma||_2^{2b}} \end{aligned} \tag{13}$$

and for hypothesis (H_2)

$$\begin{aligned} A_- \frac{e^{-2kR}}{2^b R^b} &\leqslant \langle \sigma_0 \sigma_{2R} \rangle \\ &\leqslant \sum_{\gamma \in \mathscr{H}_{d-1}} \langle \sigma_0 \sigma_{||\gamma||_2} \rangle \langle \sigma_{||\gamma||_2} \sigma_{2R} \rangle \\ &\leqslant A_+^2 \sum_{\gamma \in \mathscr{H}_{d-1}} \frac{\exp(-2\kappa||\gamma||_2)}{||\gamma||_2^{2b}} \end{aligned} \tag{14}$$

which leads in both cases to the same result:

$$A_- \frac{e^{-2\kappa R}}{2^b R^b} \leqslant \langle \sigma_0 \sigma_{2R} \rangle \leqslant A_+^2 \sum_{\gamma \in \mathscr{H}_{d-1}} \frac{\exp(-2\kappa||\gamma||_2)}{||\gamma||_2^{2b}}. \tag{15}$$

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Introducing a suitable system of coordinates in $\mathbb{Z}^{d-1} \approx \mathscr{H}_{d-1}$ we get from (15)

$$A_- \frac{e^{-2\kappa R}}{2^b R^b} \leqslant A_+^2 \sum_{(p_1,p_2,\cdots,p_{d-1})}^{+\infty} \frac{\exp[-2\kappa(R^2+p_1^2+\cdots+p_{d-1}^2)^{1/2}]}{[R^2+p_1^2+\cdots+p_{d-1}^2]^b}. \tag{16}$$

Lemma: Consider a function $f(p_1^2+p_2^2+\cdots+p_{d-1}^2)$, positive and nonincreasing in $p^2 = p_1^2+p_2^2+\cdots+p_{d-1}^2$, then the sum

$$\sum_d = \sum_{(p_1,p_2,\cdots,p_{d-1})}^{+\infty} f(p_1^2+p_2^2+\cdots+p_{d-1}^2), \quad d \geqslant 2,$$

$$\sum_1 = f(0), \quad d=1, \tag{17}$$

can be bounded by

$$\sum_d \leqslant \binom{d-1}{0} S_d + \binom{d-1}{1} S_{d-1} + \cdots \binom{d-1}{k} S_{d-k} + \cdots \binom{d-1}{d-2} S_2 + \binom{d-1}{d-1} S_1, \tag{18}$$

where

$$S_d = \int_{-\infty}^{+\infty} f(p_1^2+p_2^2+\cdots+p_{p-1}^2) dp_1 \cdots dp_{d-1}, \tag{19}$$

$$S_1 = f(0). \tag{20}$$

This inequality results from the following decomposition: Σ_d being the sum over all sites of $f(p^2)$ in $\mathbb{Z}^{d-1}$, we call Σ_d' the sum over all sites of $f(p^2)$ in $\mathbb{Z}^{d-1}$ deprived of the sites which are on the $(d-1)$ hyperplanes of dimension $(d-2)$, forming the system of coordinates around the origin. Then it is clear that

$$\sum_d = \binom{d-1}{0} \sum_d' + \binom{d-1}{1} \sum_{d-1}' + \cdots \binom{d-1}{k} \sum_{d-k}' + \cdots \binom{d-1}{d-2} \sum_2' + \binom{d-1}{d-1} \sum_1, \tag{21}$$

with

$$\sum_1' = \sum_1. \tag{22}$$

Now (18) is simply the consequence of the fact that if $f(p^2)$ is positive nonincreasing then

$$\sum_d' \leqslant S_d. \tag{23}$$

Choosing for our lemma:

$$f(p^2) = \exp[-2\kappa(R^2+p^2)^{1/2}]/[R^2+p^2]^b, \tag{24}$$

we get immediately

$$A_- \frac{e^{-2\kappa R}}{2^b R^b} \leqslant A_+^2 \sum_{k=0}^{k=d-1} \binom{d-1}{k} S_{d-k}, \tag{25}$$

where

$$S_l = \int_{-\infty}^{+\infty} \frac{\exp[-2\kappa(R^2+p_1^2+\cdots+p_{l-1}^2)^{1/2}]}{[R^2+p_1^2+\cdots+p_{l-1}^2]^b} dp_1 \cdots dp_{l-1} \tag{26}$$

$$= \frac{\pi^{(l-1)/2}}{\Gamma\left(\frac{l-1}{2}\right)} R^{l-1-2b} \times \int_0^\infty \frac{\exp(-2\kappa R\sqrt{1+x})}{(1+x)^b} x^{(l-3)/2} dx. \tag{27}$$

In (27) set $t = \sqrt{1+x}$, then

$$S_l = \frac{\pi^{(l-1)/2}}{\Gamma[(l-1)/2]} R^{l-1-2b} \times 2\int_1^\infty e^{-2\kappa R t} t^{-2b+1} (t^2-1)^{(l-3)/2} dt. \tag{28}$$

Finally by setting $t = 1 + v/2\kappa R$ in (28), we get

$$S_l = \frac{\pi^{(l-1)/2}}{\Gamma[(l-1)/2]} \left(\frac{R}{\kappa}\right)^{(l-1)/2} \frac{e^{-2\kappa R}}{R^{2b}} J_b^l(\kappa R), \tag{29}$$

with

$$J_b^l(\kappa R) = \int_0^\infty e^{-v} v^{(l-3)/2} \left(1+\frac{v}{2\kappa R}\right)^{-2b+1} \times \left(1+\frac{v}{4\kappa R}\right)^{(l-3)/2} dv. \tag{30}$$

Therefore

$$\frac{A_-}{2^b A_+^2} \leqslant \frac{1}{R^b}\left\{1 + (d-1)\left(\frac{R}{\kappa}\right)^{\frac{1}{2}} J_b^2(\kappa R) + (d-2)(d-1)\frac{\pi}{2}\left(\frac{R}{\kappa}\right) J_b^3(\kappa R) \cdots + \binom{d-1}{p} \frac{\pi^{(d-p-1)/2}}{\Gamma[(d-p-1)/2]} \times \left(\frac{R}{\kappa}\right)^{(d-p-1)/2} J_b^{d-p}(\kappa R) + \cdots + \frac{\pi^{(d-1)/2}}{\Gamma[(d-1)/2]} \left(\frac{R}{\kappa}\right)^{(d-1)/2} J_b^d(\kappa R)\right\}. \tag{31}$$

Now for $l \geqslant 2$ and $2\kappa R \geqslant 1$, we can bound $J_b^l(\kappa R)$ by $\bar{J}^l$, because

$$1 \leqslant 1 + v/2\kappa R \leqslant 1 + v, \qquad 1 \leqslant 1 + v/4\kappa R \leqslant 1 + v, \tag{32}$$

and

$$\left(1+\frac{v}{2\kappa R}\right)^{1-2b} \leqslant (1+v) \text{ with } \begin{cases} b \geqslant 0, & 2\kappa R \geqslant 1, \\ v \geqslant 0, \end{cases} \tag{33}$$

and for $l > 1$,

$$\left(1+\frac{v}{4\kappa R}\right)^{(l-3)/2} < (1+v)^{|(l-3)/2|}. \tag{34}$$

Therefore,

$$\bar{J}^l = \int_0^\infty e^{-v} v^{(l-3)/2} (1+v)^{1+|(l-3)/2|} dv, \quad l \geqslant 2. \tag{35}$$

Finally,

$$\frac{A^-}{2^b A_+^2}$$

$$\leqslant \frac{1}{R^b}\left\{1 + (d-1)\left(\frac{R}{\kappa}\right)^{\frac{1}{2}}\bar{J}^2 + (d-2)(d-1)\frac{\pi}{2}\left(\frac{R}{\kappa}\right)\bar{J}^3 + \cdots\right.$$

$$+ \cdots + \begin{Bmatrix} d-1 \\ p \end{Bmatrix} \frac{\pi^{(d-p-1)/2}}{\Gamma[(d-p-1)/2]}\left(\frac{R}{\kappa}\right)^{(d-p-1)/2}\bar{J}^{d-p}$$

$$\left. + \cdots + \frac{\pi^{(d-1)/2}}{\Gamma[(d-1)/2]}\left(\frac{R}{\kappa}\right)^{(d-1)/2}\bar{J}^d\right\}. \tag{36}$$

If we let $R \to \infty$ in (36) and $b > (d-1)/2$, we find a contradiction, because the left-hand side of (36) is a finite strictly positive number, from our assumptions, while the right hand side will tend to zero.

A further improvement to this result has been suggested by A. Sokal.[9] The fundamental hypothesis (4) can be weakened to the following:

There exists $\kappa > 0$ and b such that for each $\epsilon > 0$, there exists $R_1(\epsilon) < \infty$ and $0 < A_-(\epsilon), A_+(\epsilon) < \infty \cdots$ such that

$$A_-(\epsilon)\frac{\exp(-\kappa|\alpha-\beta|)}{|\alpha-\beta|^{b+\epsilon}} \leqslant \langle\sigma_\alpha\sigma_\beta\rangle \leqslant A_+(\epsilon)\frac{\exp(-\kappa|\alpha-\beta|)}{|\alpha-\beta|^{b-\epsilon}} \tag{4'}$$

wherever $|\alpha - \beta| > R_1(\epsilon)$.

This change is possible because the proofs ultimately become just linear inequalities for b, e.g., Eqs. (9), (10), and (11) with $R \to \infty$, lead to $2b(\hat{R}) + 2\epsilon \geqslant b(\hat{R}) - \epsilon$ implies $b(\hat{R}) \geqslant -3\epsilon$. Since this result holds for $\epsilon > 0$, we have $b(\hat{R}) \geqslant 0$. Likewise for the other bound.

This argument allows one to extend our proof to the case where logarithmic corrections to the leading behavior exist. Equation (4') says briefly that

$$\lim_{|\alpha-\beta|\to\infty} \frac{\log[\exp(\kappa|\alpha-\beta|)\langle\sigma_\alpha\sigma_\beta\rangle]}{\log|\alpha-\beta|}$$

exists and equals $b(\hat{R})$.

We point our that our result is a very delicate one involving corrections to an exponential. In particular, it does not hold for the two-dimensional Ising model below T_c where the effective b (for the Ursell function rather than just the two-spin correlation function) is[3] 2 rather than $\frac{1}{2}$. Also in the two-dimensional model of McCoy and Perk,[10] where a single b, independent of direction is inappropriate, in one direction a b of 3/2 is found.

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On the reconstruction of the physical Hilbert spaces for quantum field theories with indefinite metric

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It is known that there may exist one or more Hilbert space structures corresponding to an indefinite metric quantum field theory. In this paper we prove that: (a) the existence of a Hilbert space structure is not needed in the construction of the physical Hilbert space(s); (b) different choices of the Hilbert space structure lead to physical Hilbert spaces isomorphic to that (those) mentioned in (a). Consequently, the physical content of the theory can be read off directly from the Wightman functions—in perfect analogy with the positive metric case. In this light we discuss a weaker form of the Wightman–Gårding–Strocchi axioms for indefinite metric quantum field theories.

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1. FORMULATION OF THE PROBLEM AND MAIN RESULTS

In order to fix the problem we are concerned with in this paper, let us recall the generalization of Wightman's reconstruction theorem for standard (positive metric) quantum field theories (QFT's) (see, e.g., Ref. 1) to indefinite metric QFT's.[2–4] For simplicity we consider an Hermitian scalar field, the generalization to multicomponent and non-Hermitian fields being straightforward. Wightman's functions are supposed to be distributions over an arbitrary nuclear test function space[5] denoted by $\mathcal{N}(\mathbb{R}^4)$. In order to incorporate into the discussion some physically interesting cases,[6] $\mathcal{N}(\mathbb{R}^4)$ is not necessarily assumed to be the Schwartz space $\mathcal{S}(\mathbb{R}^4)$. In analogy with Ref. 7, we introduce the algebra $\mathcal{N}$ defined as the topological direct sum

$$\mathcal{N} = \bigoplus_{n=0}^{\infty} \mathcal{N}_n,$$

where $\mathcal{N}_0 = \mathbb{C}$ and for $n \geqslant 1$, $\mathcal{N}_n = \mathcal{N}(\mathbb{R}^{4n})$. Any element $f \in \mathcal{N}$ can be represented as a sequence $(f_0, f_1, \ldots, f_n, \cdots)$, where $f_0 \in \mathbb{C}$, $f_n \in \mathcal{N}(\mathbb{R}^{4n})$ for $n \geqslant 1$, and all but finitely many f_n's are zero. Multiplication by scalars and addition in $\mathcal{N}$ are defined componentwise. The product of two elements and an involution $*$ are introduced respectively by

$$(f \times g)_n(x_1, \ldots, x_n) = \sum_{k=0}^{n} f_k(x_1, \ldots, x_k)\, g_{n-k}(x_{k+1}, \ldots, x_n),$$

$$(f^*)_n(x_1, \ldots, x_n) = \overline{f_n(x_1, \ldots, x_n)}.$$

In this way $\mathcal{N}$ becomes a topological $*$-algebra and the following reconstruction theorem holds[8]:

Theorem 1: (a) Let $\{w_n \mid w_n \in \mathcal{N}'(\mathbb{R}^{4n}),\ n = 1,2,\cdots\}$ be a sequence of translationally invariant distributions, i.e., for any $a \in \mathbb{R}^4$,

$$w_n(x_1 + a, \ldots, x_n + a) = w_n(x_1, \ldots, x_n), \tag{1}$$

satisfying the Hermiticity condition

$$w_n(x_1, \ldots, x_n) = \overline{w_n(x_n, \ldots, x_1)}. \tag{2}$$

Then there exist:

(i) a linear space D with a nondegenerate sequilinear form $\langle \cdot, \cdot \rangle$;

(ii) a vector $\Omega \in D$ with $\langle \Omega, \Omega \rangle = 1$;

(iii) a representation $f \mapsto \Phi(f)$ of the algebra $\mathcal{N}$ by linear and, in general, unbounded operators (called field operators) on D, such that for any $\varphi, \psi \in D$,

$$\langle \varphi, \Phi(f)\psi \rangle = \langle \Phi(f^*)\varphi, \psi \rangle$$

and $f \mapsto \langle \varphi, \Phi(f)\psi \rangle$ is continuous. Moreover,

$$D = \{ \Phi(f)\Omega \mid f \in \mathcal{N} \},$$

and, for all $f_n \in \mathcal{N}(\mathbb{R}^{4n})$,

$$\int d^4x_1 \cdots d^4x_n\, f_n(x_1, \ldots, x_n) w_n(x_1, \ldots, x_n) = \langle \Omega, \Phi(f_n)\Omega \rangle;$$

(iv) a representation $U(a)$ of the translation group, defined on D, under which the fields are covariant and such that for any $\varphi, \psi \in D$, for any $a \in \mathbb{R}^4$,

$$\langle U(a)\varphi, U(a)\psi \rangle = \langle \varphi, \psi \rangle \tag{3}$$

and

$$U(a)\Omega = \Omega. \tag{4}$$

The quadruple $\{D, \langle \cdot, \cdot \rangle, U(a), \Phi\}$ is determined by $\{w_n\}$ satisfying (1) and (2) up to isomorphism.

(b) If in addition to (1) and (2) the distributions $\{w_n\}$ obey the requirements

$$w_n(x_1, \ldots, x_i, x_{i+1}, \ldots, x_n) = w_n(x_1, \ldots, x_{i+1}, x_i, \ldots, x_n), \quad n = 2,3,\cdots, \tag{5}$$

for $(x_i - x_{i+1})$ spacelike, and

$$w_n(\Lambda x_1, \ldots, \Lambda x_n) = w_n(x_1, \ldots, x_n) \tag{6}$$

for any Λ belonging to the proper orthochronous Lorentz group $L^{\uparrow}_{+}$, then:

(i) $[\Phi(f), \Phi(g)] = 0$

for all $f, g \in \mathcal{N}(\mathbb{R}^4)$ and such that supp$f$ and supp$g$ are spacelike separated;

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(ii) there exists a representation $U(\Lambda)$ of $L_+^\uparrow$ leaving Ω and $\langle\cdot,\cdot\rangle$ invariant and transforming the fields covariantly.

The proof of the above theorem, when $\mathcal{N}(\mathbb{R}^4) = \mathcal{S}(\mathbb{R}^4)$, is given in Refs. 9 and 10 and can be generalized in a straightforward way to the case of arbitrary nuclear test function spaces. The reason why we have separated the formulation of Theorem 1 into two parts is that there exist physically important cases in which requirements (5) and (6) are violated. It has been proven[11] for example, that Lorentz invariance is spontaneously broken in any local formulation of the four-dimensional quantum electrodynamics (QED_4). On the other hand, all two-dimensional models involving at the same time the free massless scalar field and its dual field violate condition (5) (see, e.g., Ref. 12).

Now we are in the position to formulate the problems dealt with in the present paper. Comparing the Wightman–Gårding–Strocchi (WGS) axioms[2-4] to the quadruple $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$ reconstructed from $\{w_n\}$, one immediately realizes that the Hilbert space structure present in the former case is missing in $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$. Following Refs. 9 and 10, we adopt

Definition 1: The Hilbert space $\{\mathcal{H},(\cdot,\cdot)\}$ is called a Hilbert Space Structure (HSS) for $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$ if and only if:

(i) D is dense in $\{\mathcal{H},(\cdot,\cdot)\}$;

(ii) there exists a bounded, self-adjoint operator η (called metric operator) on $\mathcal{H}$, such that for any $\varphi,\psi\in D$

$$\langle\varphi,\psi\rangle = (\varphi,\eta\psi). \tag{7}$$

From point (ii) it follows that, for all $\varphi,\psi\in D$,

$$|\langle\varphi,\psi\rangle| \leqslant |\eta|\|\varphi\|\|\psi\| \tag{8}$$

($|\eta|$ is the norm of the metric operator), i.e., the form $\langle\cdot,\cdot\rangle$ is jointly continuous with respect to the Hilbert topology induced on D. Moreover, because of (i), the form $\langle\cdot,\cdot\rangle$ can be extended by continuity to the whole $\mathcal{H}$. For all $\varphi,\psi\in\mathcal{H}$ the extention, denoted by $\{\cdot,\cdot\}$ has the property:

$$|\{\varphi,\psi\}| \leqslant |\eta|\|\varphi\|\|\psi\|. \tag{9}$$

In the case $\mathcal{N}(\mathbb{R}^4) = \mathcal{S}(\mathbb{R}^4)$ necessary and sufficient conditions are known[9,10] for the existence of the HSS. When such a structure is fixed, one enters in the framework of the WGS axioms, where in particular the notion of physical space is defined. But two important and deeply connected problems remain unsolved:

P_1) how to define the physical space(s) corresponding to $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$ when it admits no HSS;

P_2) even when $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$ admits a HSS, this is in general not unique and the question arises whether different HSS's lead to inequivalent physical Hilbert spaces, or, in other words, have different physical content.

The above problems being specific for indefinite metric QFT's,[13] are far from being only of academic interest. Indeed, as it has been demonstrated in Ref. 4, local gauge theories, which currently dominate our understanding of elementary particle physics, are indefinite metric QFT's.

The main results of our analysis concerning P_1 and P_2 are:

(1) the existence of a HSS is not needed for the construction of the physical Hilbert space(s). The latter can be constructed only in terms of $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$;

(2) different HSS's lead to physical Hilbert spaces isomorphic to that (those) mentioned in (1).

On the basis of the above results it seems to us reasonable to weaken the WGS axioms in such a way that no use is made of the notion of HSS. We do not disregard the possibility, if it exists, of introducing a HSS: a suitable choice of a HSS gives in some cases technical advantages which can be used, being now sure that the physical content of the theory is not affected by the arbitrarity of the choice. In this light one can give an unambiguous meaning to the Fock representation of free indefinite metric quantum fields,[3,14] which always admit[15] a HSS.

2. CONSTRUCTION OF PHYSICAL HILBERT SPACES

The outline of this section is the following. We start with the case in which the quadruple $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$ obtained from $\{w_n\}$ admits a HSS $\{\mathcal{H},(\cdot,\cdot)\}$. Then, adopting the definition of physical Hilbert space of Ref. 4, we show that the latter can be constructed only in terms of $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$, namely without making use of $\{\mathcal{H},(\cdot,\cdot)\}$.

Definition 2: Let $\mathcal{H}'$ be a subspace of $\mathcal{H}$ with the following properties:

(i) $\{\varphi,\varphi\} \geqslant 0$ for any $\varphi\in\mathcal{H}'$; (10)

(ii) there exists a dense (in the Hilbert space topology) subspace $D'\subset\mathcal{H}'$, such that $D'\subset D$,

$$\Omega\in D', \tag{11}$$

and

$$U(a)D'\subset D' \quad \text{for any } a\in\mathbb{R}^4; \tag{12}$$

(iii) $\mathcal{H}'$ is maximal (with respect to inclusion) in $\mathcal{H}$ with the above properties, i.e., if $\mathcal{H}'_0\subset\mathcal{H}$ satisfies (i), (ii), and $\mathcal{H}'\subset\mathcal{H}'_0$, then $\mathcal{H}'_0 = \mathcal{H}'$.

Remarks: (a) We are not going to discuss now the physical motivations for conditions (i)–(iii) in Definition 2. We only anticipate that the assumption of the existence of the subspace D' dense in $\mathcal{H}'$ and $D'\subset D$ is sufficient to ensure that the action of a certain class of operators including $U(a)$ (the algebra $\mathcal{A}$ below), can be lifted on a domain dense in the physical Hilbert space corresponding to $\mathcal{H}'$. Note that in general the subspace D' obeying (ii) may not be unique.

(b) From the requirement of maximality of $\mathcal{H}'$ in $\mathcal{H}$, it follows that $\mathcal{H}'$ is closed in the Hilbert space topology. More precisely one has $\mathcal{H}' = \overline{D'}$, where the bar means the closure with respect to $(\cdot,\cdot)$.

(c) The following observation is useful for some considerations. Let $\{D'_\alpha|\alpha\in\mathbb{A}\}$ be the set of all subspaces of $\mathcal{H}'$ satisfying the requirements of point (ii) of Definition 2. As can be easily verified, $\{D'_\alpha|\alpha\in\mathbb{A}\}$ is a partially ordered set with respect to inclusion. Moreover, any linearly ordered subset of $\{D'_\alpha|\alpha\in\mathbb{A}\}$ has an upper bound. Therefore, by Zorn's lemma, $\{D'_\alpha|\alpha\in\mathbb{A}\}$ contains a maximal element (in $\mathcal{H}'$).

Let us consider furthermore the subspaces

$$\begin{aligned}\mathcal{H}'' &= \{\varphi\in\mathcal{H}'|\{\varphi,\varphi\} = 0\},\\ D'' &= \{\varphi\in D'|\langle\varphi,\varphi\rangle = 0\}\end{aligned} \tag{13}$$

and the factor spaces $\mathscr{H}'/\mathscr{H}''$ and D'/D'' equipped respectively with the sesquilinear forms

$$(\varphi_1,\psi_1)_1 = \{\varphi_1,\psi_1\}, \tag{14}$$

$$(\tilde{\varphi}_2,\tilde{\psi}_2)_2 = \langle\varphi_2,\psi_2\rangle. \tag{15}$$

Here φ_1, ψ_1 and φ_2, ψ_2 are arbitrary representatives of the equivalence classes $\varphi_1,\psi_1\in\mathscr{H}'/\mathscr{H}''$ and $\tilde{\varphi}_2,\tilde{\psi}_2\in D'/D''$ respectively. One easily verifies that the forms $(\cdot,\cdot)_i$, $i=1,2$, are well-defined scalar products, so that $\{\mathscr{H}'/\mathscr{H}'', (\cdot,\cdot)_1\}$ and $\{D'/D'', (\cdot,\cdot)_2\}$ are pre-Hilbert spaces. According to Ref. 4 we adopt the following:

Definition 3. The physical space $\mathscr{H}_{\text{phys}}(\mathscr{H}')$ corresponding to $\mathscr{H}'$ is given by:

$$\mathscr{H}_{\text{phys}}(\mathscr{H}') = \overline{\mathscr{H}'/\mathscr{H}''}, \tag{16}$$

where the bar means the completion with respect to $(\cdot,\cdot)_1$.

Remarks: (a) The space $\mathscr{H}'/\mathscr{H}''$ is complete in the topology induced by $(\cdot,\cdot)$ [see Remark (b) after Definition 2]. The space (16) is in general larger than $\mathscr{H}'/\mathscr{H}''$ and is the one appropriate to the physical interpretation of the theory.

(b) The unicity of the subspace $\mathscr{H}'$ with the properties (i)–(iii) of Definition 2, is not ensured by the WGS axioms. It may happen that there exist many such subspaces. In this case one can construct as many physical Hilbert spaces.

The reason why we consider the space $\{D'/D'',(\cdot,\cdot)_2\}$ parallel to $\{\mathscr{H}'/\mathscr{H}'',(\cdot,\cdot)_1\}$ becomes transparent when one tries to lift on $\mathscr{H}_{\text{phys}}(\mathscr{H}')$ the action of a certain type of operators defined on D. Note that the operators $U(a)$ and Φ, we are mainly interested in, are defined on D, and being in general unbounded, cannot be extended by continuity on $\mathscr{H}$, and correspondingly on $\mathscr{H}'$ and $\mathscr{H}_{\text{phys}}(\mathscr{H}')$.

So let $\mathscr{A}$ be the set of operators defined on D such that for any $A\in\mathscr{A}$:

$$D'\subset\mathscr{D}_{A^+}, \tag{17}$$

$$AD'\subset D', \quad A^+D'\subset D', \tag{18}$$

where A^+ is the $\langle\cdot,\cdot\rangle$-adjoint of A and $\mathscr{D}_{A^+}$ is its domain of definition. Because of the fact that $\langle\cdot,\cdot\rangle$ is nondegenerate on D, the operator A^+ is well defined on

$$\mathscr{D}_{A^+} = \{\psi\in D \mid \exists\chi\in D:\langle\psi,A\varphi\rangle = \langle\chi,\varphi\rangle\ \forall\varphi\in D\}. \tag{19}$$

The elements of $\mathscr{A}$ form an algebra, which, owing to (3) and (12), contains the operators $\{U(a)|a\in\mathbb{R}^4\}$. We stress that $\mathscr{A}$ is defined without making use of any HSS, differently from Refs. 3 and 16, where in the particular case of QED_4 an analog of $\mathscr{A}$, called the gauge invariant algebra,[3] is discussed.

For any $A\in\mathscr{A}$ let us consider the operator $\tilde{A}$ defined on D'/D'' in the following way:

$$\tilde{A}\tilde{\varphi} = \widetilde{A\varphi}, \tag{20}$$

where φ is an arbitrary representative of the class $\tilde{\varphi}\in D'/D''$. As a consequence of conditions (17) and (18), all elements of the set $\tilde{\mathscr{A}} = \{\tilde{A}\,|A\in\mathscr{A}\}$ are well defined operators on D'/D'', and $\tilde{\mathscr{A}}$ is an algebra such that the mapping

$$h:A\mapsto\tilde{A}, \tag{21}$$

defined by Eq. (20), is a $*$-homomorphism, i.e.,

$$\widetilde{\alpha_1A_1+\alpha_2A_2} = \alpha_1\tilde{A}_1+\alpha_2\tilde{A}_2,$$

$$\widetilde{A_1A_2} = \tilde{A}_1\tilde{A}_2 \quad \forall\alpha_1,\alpha_2\in\mathbb{C}, \quad \forall A_1,A_2\in\mathscr{A},$$

$$\tilde{A}^+ = \tilde{A}^*, \quad \forall A\in\mathscr{A},$$

where $*$ means $(\cdot,\cdot)_2$-conjugation.

A central role in what follows is played by

Lemma 1: There exists a dense subspace $\mathscr{D}\subset\mathscr{H}'/\mathscr{H}''$ isomorphic to D'/D''.

Proof: Consider the mapping

$$E:D'/D''\to\mathscr{H}'/\mathscr{H}'' \tag{22}$$

defined by

$$E:\tilde{\varphi}\to\varphi\to\underset{\sim}{\varphi},$$

where φ is an arbitrary representative of $\tilde{\varphi}$ and therefore belongs to D', i.e., to $\mathscr{H}'$. E is well defined because if $\varphi_1,\varphi_2\in\tilde{\varphi}$, then $\varphi_1-\varphi_2\in D''\subset\mathscr{H}''$ and therefore $\underset{\sim}{\varphi}_1 = \underset{\sim}{\varphi}_2$. Moreover, E is obviously linear and has the property

$$(\tilde{\varphi}_1,\tilde{\varphi}_2)_2 = (E(\tilde{\varphi}_1),E(\tilde{\varphi}_2))_1 \tag{23}$$

for any $\tilde{\varphi}_1,\tilde{\varphi}_2\in D'/D''$. Indeed

$$(\tilde{\varphi}_1,\tilde{\varphi}_2)_2 = \langle\varphi_1,\varphi_2\rangle = \{\varphi_1,\varphi_2\}$$
$$= (\underset{\sim}{\varphi}_1,\underset{\sim}{\varphi}_2)_1 = (E(\tilde{\varphi}_1),E(\tilde{\varphi}_2))_1.$$

One defines $\mathscr{D} = E(D'/D'')$. From (23) and the linearity of E, it follows that E is invertible. Therefore, E is an isomorphism between the pre-Hilbert spaces D'/D'' and $\mathscr{D}$, and what remains to be proved is that $\mathscr{D}$ is dense in $\mathscr{H}'/\mathscr{H}''$. Let $\underset{\sim}{\varphi}\in\mathscr{H}'/\mathscr{H}''$ and $\varphi\in\mathscr{H}'$ be an arbitrary representative of $\underset{\sim}{\varphi}$. Then, since D' is dense in $\mathscr{H}'$, there exists a sequence $\{\varphi_n\}\subset D'$ such that

$$\lim_{n\to\infty}\|\varphi-\varphi_n\| = 0.$$

Consider furthermore the sequence $\{\underset{\sim}{\varphi}_n\}\subset\mathscr{D}$. Using the estimates (9) and (10) one obtains

$$\lim_{n\to\infty}\|\underset{\sim}{\varphi}_n-\underset{\sim}{\varphi}\|_1^2 = \lim_{n\to\infty}\{\varphi_n-\varphi,\varphi_n-\varphi\}$$
$$= \lim_{n\to\infty}|\{\varphi_n-\varphi,\varphi_n-\varphi\}|$$
$$\leqslant|\eta|\lim_{n\to\infty}\|\varphi_n-\varphi\|^2 = 0,$$

which completes the proof of the lemma.

Now one performs the lifting on $\mathscr{D}$ of the action of $\mathscr{A}$, defining for any $A\in\mathscr{A}$,

$$\underset{\sim}{A} = E\circ h(A)\circ E^{-1}. \tag{24}$$

From Lemma 1 and (24) it follows that the elements of $\underset{\sim}{\mathscr{A}} = \{\underset{\sim}{A}\,/A\in\mathscr{A}\}$ form an algebra of operators with common domain $\mathscr{D}$ dense in $\mathscr{H}'/\mathscr{H}''$, and therefore, in $\mathscr{H}_{\text{phys}}(\mathscr{H}')$. Moreover the following theorem holds

Theorem 2: Let $\overline{D'/D''}$ be the completion of D'/D'' with respect to $(\cdot,\cdot)_2$. Then the Hilbert spaces $\mathscr{H}_{\text{phys}}(\mathscr{H}')$ and $\overline{D'/D''}$ are isomorphic and the isomorphism preserves the action of the algebras $\mathscr{A}$ and $\tilde{\mathscr{A}}$.

Proof: Owing to the fact that $\mathscr{D}$ is dense in $\mathscr{H}_{\text{phys}}(\mathscr{H}')$, the isomorphism

$$\mathscr{E}:\overline{D'/D''}\to\mathscr{H}_{\text{phys}}(\mathscr{H}')$$

is defined by extending the isomorphism

$$E:D'/D''\to\mathscr{D}\subset\mathscr{H}_{\text{phys}}(\mathscr{H}')$$

by continuity. $\mathscr{E}$ preserves the action of $\tilde{\mathscr{A}}$ and $\underset{\sim}{\mathscr{A}}$ by construction.

As a consequence of Theorem 2 one has that the structures $\{\mathscr{H}_{\rm phys}(\mathscr{H}'),\underset{\sim}{\mathscr{A}}\}$, $\{\overline{D'/D''},\tilde{\mathscr{A}}\}$ are equivalent. As $\{\overline{D'/D''},\tilde{\mathscr{A}}\}$ is built up only in terms of the quadruple $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$, without making use of the HSS $\{\mathscr{H},(\cdot,\cdot)\}$, the dependence of $\{\mathscr{H}_{\rm phys}(\mathscr{H}'),\underset{\sim}{\mathscr{A}}\}$ on $\{\mathscr{H},(\cdot,\cdot)\}$ is fictitious. Therefore the information about the physical Hilbert space(s) of any indefinite metric QFT is contained in $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi\}$ or equivalently, because of Theorem 1, in $\{w_n\}$.

3. A WEAKER FORM OF THE WGS AXIOMS

In this section we discuss a slight modification (see also Ref. 17) of the WGS axioms[2–4] without making use of the notion of HSS. For the reasons mentioned after Theorem 1 we adopt also a weaker form of the requirements of covariance, locality, and spectral condition. This weaker form, however, still ensure the physical interpretation of the theory.

So by indefinite metric QFT we mean a structure obeying the following axioms (A's) and definitions.

A_1: There exists a set of operator valued distributions $\{\Phi_i(f)|f\in\mathscr{N}(\mathbb{R}^4), i=1,...,n\}$ called fields and defined on a complex linear space D, equipped with a nondegenerate sesquilinear form $\langle\cdot,\cdot\rangle$. The polynomial algebra generated by $\{\Phi_i(f)|f\in\mathscr{N}(\mathbb{R}^4), i=1,...,n\}$ will be denoted by $\mathscr{F}$.

A_2: There exists a representation $\{U(a)|a\in\mathbb{R}^4\}$ of the translation group, defined on D and a vector $\Omega\in D$ with the properties:

(i) $\langle U(a)\varphi,U(a)\psi\rangle=\langle\varphi,\psi\rangle$ for any $\varphi,\psi\in D$ for any $a\in\mathbb{R}^4$;

(ii) $\langle\Omega,\Omega\rangle=1$ and $U(a)\Omega=\Omega$;

(iii) the fields Φ_i transform covariantly under $U(a)$.

A_3: There exists a subspace $D'\subset D$ such that:

(i) $\langle\varphi,\varphi\rangle\geqslant 0$ for any $\varphi\in D'$;

(ii) $\Omega\in D'$ and $U(a)D'\subset D'$ for any $a\in\mathbb{R}^4$;

(iii) D' is maximal (with respect to inclusion) in D with the above properties, i.e., if D'_0, satisfies A_3(i)–(ii) and $D\subset D'_0$, then $D'_0=D'$.

Definition 4: The physical Hilbert space corresponding to D' is defined by

$$\mathscr{H}_{\rm phys}(D')=\overline{D'/D''}.$$

Here $D''=\{\varphi\in D'|\langle\varphi,\varphi\rangle=0\}$ and the completion is taken with respect to the scalar product $(\cdot,\cdot)_2$ defined for any $\tilde{\varphi},\tilde{\psi}\in D'/D''$ by $(\tilde{\varphi},\tilde{\psi})_2=\langle\varphi,\psi\rangle$, φ and ψ being arbitrary representatives of $\tilde{\varphi}$ and $\tilde{\psi}$.

Definition 5: Let $\mathscr{A}$ be the algebra of operators defined on D and such that $\forall A\in\mathscr{A}$:

$$D'\subset\mathscr{D}_{A^\dagger},$$

$$AD'\subset D',\ A^\dagger D'\subset D'$$

($\dagger$ means $\langle\cdot,\cdot\rangle$-conjugation). By $\tilde{\mathscr{A}}$ one denotes the algebra of operators defined on $D'/D''\subset\mathscr{H}_{\rm phys}(D')$ as follows:

$$\tilde{A}\tilde{\varphi}=\widetilde{A\varphi}.$$

A_4: For any $\Phi,\Psi\in\mathscr{F}\cap\mathscr{A}$,

$$[\Phi(f),\Psi(g)]=0 \text{ for any } f,g\in\mathscr{N}(\mathbb{R}^4),$$

such that supp$f$ and supp$g$ are spacelike separated.

A_5: The operators $\{\tilde{U}(a)|a\in\mathbb{R}^4\}$ have the following spectral representation:

$$\tilde{U}(a)=\int e^{ipa}\,d\mu(p),\quad pa=p_0a_0-\sum_{i=1}^{3}p_ia_i,$$

where the spectral measure $\mu(p)$ has its support in the closure of the future light cone $\bar{V}_+=\{p\in\mathbb{R}^4|\,pp\geqslant 0, p_0\geqslant 0\}$.

Remarks: (a) The Axioms A_1–A_5 are formulated in terms of $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi_i\}$ which are the basic objects one obtains from $\{w_n\}$ by Theorem 1, i.e., like in the positive metric case there is a direct relationship between the reconstruction theorem and the axioms.

(b) The unicity of D' is not ensured by the requirements A_3(i)–(iii), in complete analogy with the case with $\mathscr{H}'$ in the framework of the WGS axioms [see Remark (b) after Definition 3].

(c) One can verify that Axioms A_1–A_5 are fulfilled by some exactly soluble models (see Ref. 15).

(d) Formulations of QED_4 which do not assume the existence of a HSS are discussed in Refs. 18–20.

In what follows we fix $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi_i\}$ satisfying axioms A_1–A_5. Let us denote furthermore by $\mathscr{B}=\{D'_\beta/\beta\in\mathbb{B}\}$ the set of all subspaces of D with the properties A_3(i)–(iii). Then one has

Lemma 2: Assume that $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi_i\}$ admits a HSS and let $\{\mathscr{H},(\cdot,\cdot)\}$ be such an arbitrary structure. Then: (a) For any $\beta\in\mathbb{B}$, the subspace $\mathscr{H}'_\beta\equiv\overline{D'_\beta}$, where the bar means the $(\cdot,\cdot)$-closure, obeys the requirements of Definition 2.

(b) For any $\mathscr{H}'\subset\mathscr{H}$ with the properties quoted in Definition 2, there exists a subspace $D'\subset\mathscr{H}'$ satisfying condition (ii) of Definition 2, and such that $D'\in\mathscr{B}$.

Proof: (a) One immediately verifies that $\mathscr{H}'_\beta\equiv D'_\beta$ satisfies (i) and (ii) of Definition 2. Concerning the maximality of $\mathscr{H}'_\beta$ in $\mathscr{H}$, suppose that there exists $\mathscr{H}''$ obeying (i)–(iii) of Definition 2 and such that

$$\mathscr{H}'_\beta\not\subseteq\mathscr{H}'. \tag{25}$$

Consider furthermore the subspace $D'\subset\mathscr{H}'$, $\overline{D'}=\mathscr{H}'$ which exists according to point (ii) of Definition 2 and has the properties listed therein. One has the following possibilities:

(1) $D'_\beta\not\subseteq D'$;

(2) $D'_\beta\supset D'$;

(3) neither (1) nor (2) are fulfilled.

The cases (1) and (2) are in contradiction with the maximality of D'_β in D [see A_3(iii)] and (25) respectively. Since $D'_\beta\subset\mathscr{H}'$ and $D'\subset\mathscr{H}''$ in the case (3), one has that $\mathscr{L}(D'_\beta\cup D')$ ($\mathscr{L}$ means linear envelope) obeys A_3(i)–(ii), but $\mathscr{L}(D'_\beta\cup D')\not\supseteq D'_\beta$, which is in contradiction with the maximality of D'_β.

(b) Let us fix an arbitrary subspace $\mathscr{H}''\subset\mathscr{H}$ satisfying the requirements of Definition 2 and let the corresponding subspace D' [see Definition 2(ii)] be maximal in $\mathscr{H}''$. Such a choice for D' is possible according to Remark (c) after Definition 2. We shall prove that $D'\in\mathscr{B}$. Indeed D' obeys A_3(i)–(ii) and therefore there exists $\beta_0\in\mathbb{B}$ such that $D'\subset D'_{\beta_0}$. Suppose

that

$$D' \not\subseteq D'_{\beta_0}, \tag{26}$$

and consider $\mathscr{H}'_{\beta_0} \equiv \overline{D'_{\beta_0}}$, where the bar means the $(\cdot,\cdot)$-closure. Then $\mathscr{H}'_{\beta_0}$ satisfies (i)–(iii) of Definition 2 [see the proof of point (a) of this lemma] and $\mathscr{H}' \subset \mathscr{H}'_{\beta_0}$. If we assume that $\mathscr{H}' = \mathscr{H}'_{\beta_0}$, we get a contradiction with (26) and the maximality of D' in $\mathscr{H}'$. Therefore, $\mathscr{H}' \not\subseteq \mathscr{H}'_{\beta_0}$, which on the other hand is in contradiction with the maximality of $\mathscr{H}'$ in $\mathscr{H}$. Therefore, $D = D'_{\beta_0} \in \mathscr{B}$.

Lemma 2 clarifies the relationship between the WGS axioms and A_1–A_5. Indeed one has

Corollary 1: In the case when $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi_i\}$ can be given a HSS $\{\mathscr{H},(\cdot,\cdot)\}$, the Axioms A_1–A_5 are equivalent to the WGS axioms, formulated in terms of $\{\mathscr{H},(\cdot,\cdot)\}$.

Finally the answer to the question posed by Problem P_2 (see Sec. 1) is given by the following corollary, being a consequence of Theorem 2 and Lemma 2(b).

Corollary 2:Let $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi_i\}$ admit at least one HSS. Then for any element of the family of physical Hilbert spaces obtained by both:

(i) possible different choices of $\mathscr{H}'$ for a given HSS, and

(ii) varying the HSS corresponding to $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi_i\}$, there is an isomorphic representative in the family

$$\{\overline{D'_\beta / D''_\beta}, \mathscr{A}_\beta | \beta \in \mathbb{B}\}, \tag{27}$$

where the bar means the completion with respect to $(\cdot,\cdot)_2$ (see Definition 4).

Since all elements of the family (27) are constructed only in terms of $\{D,\langle\cdot,\cdot\rangle, U(a),\Phi_i\}$, they are independent of the choice of a HSS. Moreover, the family (27) represents a complete classification of the physical Hilbert spaces corresponding to the indefinite metric QFT defined by $\{D,\langle\cdot,\cdot\rangle, U(a), \Phi_i\}$ or, equivalently (Theorem 1), by $\{w_n\}$.

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On quantum solitons and their classical relatives: II. "Fermion–boson reciprocity" and classical vs quantum problem for the sine-Gordon system [a]

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Both quantum and classical sine–Gordon fields can be built out of the fundamental free neutral massive excitations, which quantally obey the Bose–Einstein statistics. At the roots of the "boson-fermion reciprocity" invented by Coleman, lies the spin $\frac{1}{2}$ approximation of the underlying Bose system. By generalizing the coherent state methods to incorporate non-Fock quantum structures and to give account of the so-called boson transformation theory, we construct the carrier Hilbert space $\mathscr{H}_{SG}$ for quantum soliton operators. The $\hbar \to 0$ limit of state expectation values of these operators among pure coherent-like states in $\mathscr{H}_{SG}$ reproduces the classical sine–Gordon field. The related (classical and quantum) spin $\frac{1}{2}$ xyz Heisenberg model field is built out of the fundamental sine–Gordon excitations, and hence can be consistently defined on the appropriate subset of the quantum soliton Hilbert space $\mathscr{H}_{xyz}$. A correct classical limit is here shown to arise for the Heisenberg system: phase manifolds of the classical Heisenberg and sine–Gordon systems cannot be then viewed independently as a consequence of the quantum relation.

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1. A NONSINGULAR BOSON TRANSFORMATION

Suppose we have been given a classical scalar field, which obeys a differential equation:

$$\Lambda(\partial)\psi = F(\psi) \quad \Lambda(\partial) = -\nabla^2 + \partial^2/\partial x_0^2 + m^2, \tag{1.1}$$

and let $\varphi(\mathbf{x})$, $\pi(\mathbf{x})$ be the initial (time $t = 0$) data specifying an arbitrary free-field solution $\psi_0(\mathbf{x},t) = \psi_0(\mathbf{x},t,\varphi,\pi)$ of (1.1). By using the Yang–Feldman relation

$$\psi(\mathbf{x},t) = \psi_0(\mathbf{x},t) + \Lambda(\partial)^{-1}F(\mathbf{x},t,\psi_0), \tag{1.2}$$

we find that $\psi(\mathbf{x},t)$ is uniquely specified by fixing the initial free data

$$\begin{aligned}\psi(\mathbf{x},t) &= \psi(\mathbf{x},t,\varphi,\pi)\\ &= \psi_0(\mathbf{x},t,\varphi,\pi) + \Lambda(\partial)^{-1}F(\mathbf{x},t,\varphi,\pi).\end{aligned} \tag{1.3}$$

Whenever the data φ,π specify the conventional Fourier transformable plane wave solution ψ_0, we denote $\psi_0 = \psi_{in} = \psi_0(\varphi_{in},\pi_{in})$, called the in-field associated with ψ.

Let us now consider a quantum scalar (Heisenberg) field $\hat{\psi}$ satisfying an equation analogous to (1.1)

$$\begin{aligned}&\Lambda(\partial)\hat{\psi}(x) = F(x,\hat{\psi}) \quad x = (\mathbf{x},t)\\ &\hat{\psi}(x) = \hat{\psi}_0(x) + \Lambda(\partial)^{-1}F(x,\hat{\psi}_0),\end{aligned} \tag{1.4}$$

where we at once choose $\hat{\psi}_0(x) = \hat{\psi}_{in}(x)$, with $\hat{\varphi}_{in}(\mathbf{x}),\hat{\pi}_{in}(\mathbf{x})$ satisfying the (equal time) commutation relations

$$[\hat{\varphi}_{in}(\mathbf{x}),\hat{\pi}_{in}(\mathbf{y})]_- = \delta(\mathbf{x}-\mathbf{y})i\hbar. \tag{1.5}$$

Hence

$$\hat{\psi}(x) = \hat{\psi}_{in}(x) + \Lambda(\partial)^{-1}F(x,\hat{\varphi}_{in},\hat{\pi}_{in}), \tag{1.6}$$

which is understood as an equality among the matrix elements of the operators, calculated between the in-field (Fock space!) vectors. An expressions of $\hat{\psi}$ in terms of $\hat{\varphi}_{in},\hat{\pi}_{in}$ we call a *dynamical map*.[1-7] Armed with the plane wave quantum data $\hat{\varphi}_{in},\hat{\pi}_{in}$ obeying (1.5), we are able to construct these free (in) field states, which are generated from the vacuum by a classical current, the familiar coherent states

$$\begin{aligned}|\varphi,\pi) &= \hat{T}_{\varphi,\pi}|0)\\ &= \exp(i/\hbar)\int d^3x\,[\pi(\mathbf{x})\hat{\varphi}_{in}(\mathbf{x}) - \varphi(\mathbf{x})\hat{\pi}_{in}(\mathbf{x})]|0).\end{aligned} \tag{1.7}$$

Here an exponent can always be rewritten in terms of the canonical pair (no transition to momentum space) $a^*(\mathbf{x})$, $a(\mathbf{x})$ as $-(\alpha,a^*) + (\bar{\alpha},a)$, where the complex valued function $\alpha(\mathbf{x})$ is subject to the square integrability condition

$$(\bar{\alpha},\alpha) = \int d^3x\,\bar{\alpha}(\mathbf{x})\alpha(\mathbf{x}) = \|\alpha\|^2 < \infty, \tag{1.8}$$

with $\alpha(\mathbf{x}) = [\varphi(\mathbf{x}) + i\pi(\mathbf{x})]/\hbar\sqrt{2}$. Then

$$\begin{aligned}\hat{T}^{-1}_{\varphi,\pi}\hat{\varphi}_{in}(\mathbf{x})\hat{T}_{\varphi,\pi} &= \hat{\varphi}_{in}(\mathbf{x}) + \varphi(\mathbf{x}),\\ \hat{T}^{-1}_{\varphi,\pi}\hat{\pi}_{in}(\mathbf{x})\hat{T}_{\varphi,\pi} &= \hat{\pi}_{in}(\mathbf{x}) + \pi(\mathbf{x}),\end{aligned} \tag{1.9}$$

so that

$$\begin{aligned}\langle 0|\hat{T}^{-1}_{\varphi,\pi}\hat{\psi}(x)\hat{T}_{\varphi,\pi}|0\rangle &= \langle\varphi,\pi|\hat{\psi}(x)|\varphi,\pi)\\ &= \langle 0|\psi(x,\hat{\varphi}_{in} + \varphi,\hat{\pi}_{in} + \pi)|0\rangle,\end{aligned} \tag{1.10}$$

and hence a c-number field $\psi_{\varphi,\pi}(x)$ can be associated with $\hat{\psi}(x)$ according to

$$\langle 0|\hat{\psi}_{\varphi,\pi}(x)|0\rangle = \langle 0|\hat{T}^{-1}_{\varphi,\pi}\hat{\psi}(x)\hat{T}_{\varphi,\pi}|0\rangle = \psi_{\varphi,\pi}(x). \tag{1.11}$$

Because of (1.5), $\hat{\psi}_{\varphi,\pi}(x)$ can always be rearranged to a normal ordered form plus terms following from the contractions of the in-fields during the ordering procedure. These last, by virtue of (1.5) are proportional to $\hbar$, and hence, we can consider

$$\begin{aligned}\lim_{\hbar\to 0}\psi_{\varphi,\pi}(x) &= \lim_{\hbar\to 0}[\langle 0|{:}\hat{\psi}_{\varphi,\pi}(x){:}|0\rangle + O(\hbar)]\\ &= \langle 0|{:}\hat{\psi}_{\varphi,\pi}(x){:}|0\rangle = \phi(\mathbf{x},t,\varphi,\pi),\end{aligned} \tag{1.12}$$

[a] Main ideas of the paper are taken from my University of Alberta preprint under the title "On quantum solitons and their classical relatives."
[b] Permanent address.

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and quite analogously (notice that all $\hat{\psi}_{\varphi,\pi}(x)$ do commute among themselves under the sign :·: of the normal ordering)

$$\begin{aligned} \underset{\hbar\to 0}{\mathrm{m}} F_{\varphi,\pi}(x) &= \lim_{\hbar\to 0}\langle 0|\hat{F}_{\varphi,\pi}(x)|0\rangle \\ &= \lim_{\hbar\to 0}\left[\langle 0|{:}F(x,\hat{\psi}_{\varphi,\pi}){:}|0\rangle + O(\hbar)\right] \\ &= F(\mathbf{x},t,\phi(\varphi,\pi)) = F(x,\varphi,\pi). \end{aligned} \tag{1.13}$$

So that, after taking the $\hbar\to 0$ limit of the Fock vacuum expectation value of (1.4), we have transformed a quantum field equation into a corresponding classical Euler one. Everything is true under the assumption that the $\hbar\to 0$ limit exists at all,

$$\begin{aligned} &\lim_{\hbar\to 0}\langle 0|\Lambda(\partial)\hat{\psi}_{\varphi,\pi}(x)|0\rangle = \Lambda(\partial)\lim_{\hbar\to 0}\langle 0|\hat{\psi}_{\varphi,\pi}(x)|0\rangle \\ &= \Lambda(\partial)\phi(x,\varphi,\pi) = \lim_{\hbar\to 0}\langle 0|\hat{F}_{\varphi,\pi}(x)|\rangle = F(x,\phi) \\ &\Rightarrow \Lambda(\partial)\phi(x) = F(x,\phi). \end{aligned} \tag{1.14}$$

Let us recall that in the above, it was crucial to choose the classical data φ,π which are consistent with the square integrability condition (1.8). However such data do not at all exhaust the set of those allowed by the classical Euler equation (1.14). Hence it becomes of interest to establish whether such, say *singular*, data can be used (and in what sense) to generate operators of the form $\hat{\psi}_{\varphi,\pi}(x)$, and are consistent with the formula (1.14). The mapping (1.9) we call a *nonsingular boson transformation*.

2. A SINGULAR BOSON TRANSFORMATION

A nonsingular boson transformation maps a Fock space vector into a Fock space vector again, i.e., a vacuum $|0\rangle$ into a coherent state $|\varphi,\pi\rangle$, and this last can obviously be mapped into another coherent state, say $|\varphi',\pi'\rangle$ by a unitary transformation: $\hat{T}_{\varphi',\pi'}\hat{T}^{-1}_{\varphi,\pi}|\varphi,\pi\rangle = |\varphi',\pi'\rangle$.

In the above the square integrability condition (1.8) accounts for these classical data which are consistent with the unitarity requirement $\hat{T}^{-1}_{\varphi,\pi} = \hat{T}^{*}_{\varphi,\pi}$ and thus a good behavior at space infinity of the boson transformation parameters φ,π guarantees that $\hat{T}_{\varphi,\pi}$ is a nonsingular mapping.

To introduce a *singular boson transformation*, and to understand its meaning in the quantum theory (with the 1 +1 dimensional sine–Gordon perspective in mind) let us restrict the space dimensionality to one, and cover $\mathbb{R}^1$ by a countable sequence $\{\Delta_k\}_{k=0,\pm 1,\cdots}$ of the noninteresting, semi-open intervals each one with length (lattice spacing) Γ small enough. Let us introduce

$$\begin{aligned} a^{*}_k &= (1/\sqrt{\Gamma})\int \chi_k(x)a^{*}(x)\,dx, \\ a_k &= (1/\sqrt{\Gamma})\int \chi_k(x)a(x)\,dx, \end{aligned} \tag{2.1}$$

where $\chi_k(x) = \begin{matrix} 1 & x\in\Delta_k \\ 0 & x\notin\Delta_k \end{matrix}$ is a characteristic function of the set Δ_k. For any function $\lambda(x)$ on $\mathbb{R}^1$ we shall also introduce a sequence $\{\lambda_i = (1/\Gamma)\int\chi_i(x)\lambda(x)\,dx\}_{i=0,\pm 1,\cdots}$ approximating $\lambda(x)$ in the sense of $\lambda(x)\cong\Sigma_i\lambda_i\chi_i(x)$. Now let a sequence $\{a_k,a^{*}_k\}_{k=0,\pm 1,\cdots}$ generate a Fock representation of the CCR algebra

$$[a_i,a^{*}_j]_{-} = \delta_{ij},\quad [a_i,a_j]_{-} = 0,\quad a_i|0\rangle = 0\forall_i, \tag{2.2}$$

whose carrier (Fock) Hilbert space we designate IDPS ($|0\rangle$), according to the direct product convention.[8–13]

For each fixed value of $j = 0, \pm 1,\cdots$ a unitary transformation

$$\hat{T}^{\lambda}_j = \exp(\lambda_j a^{*}_j - \bar{\lambda}_j a_j) \tag{2.3}$$

realizes a boson transformation

$$\begin{aligned} &(\hat{T}^{\lambda}_j)^{-1}a_j\hat{T}^{\lambda}_j = a_j + \lambda_j, \\ &(\hat{T}^{\lambda}_j)^{-1}a^{*}_j\hat{T}^{\lambda}_j = a^{*}_j + \bar{\lambda}_j \end{aligned} \tag{2.4}$$

and under the condition $|\Sigma_i\lambda_j|^2 < \infty$, a global mapping

$$\hat{T}_{\lambda} = \prod_j \hat{T}^{\lambda}_j = \exp\left[\sum_j(\lambda_i a^{*}_j - \bar{\lambda}_j a_j)\right] \tag{2.5}$$

exists and is unitary. Moreover the previously considered $\hat{T}_{\varphi,\pi}$ (formally) emerges here as a continuum limit ($\Gamma\to 0$) of $\hat{T}_{\lambda}$.

Let h be a Hilbert space for an elementary quantum system, and let a^{*},a be the associated raising and lowering operators. Then the direct product construction leads to the direct product space $\mathscr{H} = \Pi^{\otimes}_j h_j$ where $h_j = h\forall_j$ and the representation $\{a^{*}_j,a_j,\mathscr{H}\}_{j=0,\pm 1,\cdots}$ is infinitely reducible. Recall that the generating vector $|0|$ for the (Fock) irreducibility sector IDPS ($|0\rangle$) reads $\Pi^{\otimes}_j(e_0)_j$, where $e_0\in h$ is the ground state of an elementary system. One easily finds that in the case $\Sigma_j|\lambda_j|^2 < \infty$, we get

$$\begin{aligned} \hat{T}_{\lambda}|0\rangle &= \prod_j \hat{T}^{\lambda}_j \prod_k{}^{\otimes}(e_0)_k = \prod_k{}^{\otimes}(\hat{T}^{\lambda}_k e_0)_k : \\ &= \prod_k{}^{\otimes}(|\lambda_k\rangle) = |\lambda\rangle\in\mathrm{IDPS}(|0\rangle), \end{aligned} \tag{2.6}$$

where for each $k = 0, \pm 1,\cdots$ $h\ni|\lambda_k\rangle$ is a coherent state: $a|\lambda_k\rangle = \lambda_k|\lambda_k\rangle$ specified by a parameter λ_k. It proves that the choice of any ill-behaving at $\pm\infty$ boson transformation parameter $\bar{\lambda}(x) = (1/\sqrt{2})[\varphi(x) + i\pi(x)]$ results in the failure of the $\Sigma_j|\lambda_j|^2 < \infty$ condition and hence the nonexistence of the global mapping operator $\hat{T}_{\lambda}$. This is just the singular case of interest for us.

Assume the series $\Sigma_j|\lambda_j|^2$ to diverge, and let us consider the vector $|\lambda\rangle\in\mathscr{H}$ given by

$$|\lambda\rangle = \prod_k{}^{\otimes}(\hat{T}^{\lambda}_k e_0) = \prod_k{}^{\otimes}|\lambda_k\rangle, \tag{2.7}$$

which by construction is unitarily inequivalent to $|0\rangle$, and hence orthogonal to it. As a consequence, $|\lambda\rangle$ generates a new irreducibility sector

$$\mathrm{IDPS}(|\lambda\rangle) = \mathscr{H}_{\lambda}\subset\mathscr{H} \tag{2.8}$$

for the representation $\{a^{*}_i,a_i\}_{i=0,\pm 1,\cdots}$ of the CCR algebra in $\mathscr{H}$. The representation is obviously a non-Fock one.

Assume now a quantum operator $\hat{F} = F(a^{*},a)$ $= F(\hat{\varphi}_{\mathrm{in}},\hat{\pi}_{\mathrm{in}})$ to map $|\lambda\rangle$ into a vector from IDPS ($|\lambda\rangle$) (otherwise $\hat{F}|\lambda\rangle$ would be orthogonal to $|\lambda\rangle$). Then

$$\begin{aligned} \langle\lambda|F(a^{*},a)|\lambda\rangle &= \langle 0|F(a^{*}+\bar{\lambda},a+\lambda)|0\rangle \\ &= \langle 0|F(\hat{\varphi}_{\mathrm{in}}+\varphi,\hat{\pi}_{\mathrm{in}}+\pi)|0\rangle = \langle 0|\hat{F}_{\lambda}|0\rangle, \end{aligned} \tag{2.9}$$

and the boson transformation is realized for each $\hat{\varphi}^{\mathrm{in}}_k$ or $\hat{\pi}^{\mathrm{in}}_k$

factor appearing in the explicit expression for $\hat{F}$. Notice that the discretization can be immediately removed by taking a continuum limit $\Gamma \to 0$.

A transformation

$$R_{\varphi,\pi}: F(\hat{\varphi}_{\rm in}, \hat{\pi}_{\rm in}) \to F(\hat{\varphi}_{\rm in} + \varphi, \hat{\pi}_{\rm in} + \pi), \tag{2.10}$$

with φ, π violating the condition $\|\lambda\|^2 < \infty$, we call a *singular boson transformation*. In this way, we have proved that a singular boson transformation necessarily induces a transition to a (different from the Fock one) irreducibility sector for the representation $\{\hat{\varphi}_{\rm in}, \hat{\pi}_{\rm in}\}$ of the CCR algebra in $\mathscr{H}$.

It is useful to know whether the two vectors $|\alpha\rangle$ and $|\gamma\rangle$, constructed according to (2.7)–(2.9) are unitarily inequivalent, i.e., whether a mapping: $\hat{F}_\lambda \to \hat{F}_\alpha$ is singular or not. For this purpose let us restrict considerations to a single quantum degree of freedom in the discretized (2.4) case. Namely, we have

$$|0\rangle = e_0, \quad |\alpha\rangle = \hat{T}_\alpha |0\rangle = \hat{T}_\alpha \hat{T}_\gamma^{-1} |\gamma\rangle = \hat{T}_{\alpha\gamma} |\gamma\rangle, \tag{2.11}$$

with

$$\begin{aligned} \hat{T}_\alpha &= \exp(\bar{\alpha} a - \alpha a^*) \\ &= \exp(|\alpha|^2/2)\exp(\bar{\alpha} a)\exp(-\alpha a^*) \\ &= \exp(-|\alpha|^2/2)\exp(-\alpha a^*)\exp(\bar{\alpha} a), \end{aligned} \tag{2.12}$$

and $\hat{T}_\gamma^{-1} = \hat{T}_{-\gamma}$ so that, by using the Baker–Hausdorff formula, we get

$$\begin{aligned} \hat{T}_\alpha \hat{T}_\gamma^{-1} &= \exp(\bar{\alpha} a - \alpha a^*)\exp(-\bar{\gamma} a + \gamma a^*) \\ &= \exp[(\bar{\alpha} - \bar{\gamma}) a - (\alpha - \gamma) a^*]\exp(\bar{\alpha}\gamma - \alpha\bar{\gamma})\tfrac{1}{2} \\ &= \exp[(\bar{\alpha} - \bar{\gamma}) a]\exp[(\gamma - \alpha) a^*] \\ &\quad \times \exp[(1/2)(|\alpha|^2 + |\gamma|^2 - 2\alpha\bar{\gamma})] \end{aligned} \tag{2.13}$$

i.e.,

$$|\langle 0|\hat{T}_\gamma^{-1}\hat{T}_\alpha|0\rangle|^2 = \exp(-|\alpha - \gamma|^2). \tag{2.14}$$

It proves that a necessary condition for the global mapping $\Pi_k \hat{T}^k_{\alpha\gamma}$ to be nonsingular, is

$$\sum_k |\alpha_k - \gamma_k|^2 < \infty, \tag{2.15}$$

whose continuum limit is simply

$$\begin{aligned} \int d^3x\, |\alpha(\mathbf{x}) - \gamma(\mathbf{x})|^2 = \tfrac{1}{2}\int d^3x\, \{ &[\varphi_\alpha(\mathbf{x}) - \varphi_\gamma(\mathbf{x})]^2 \\ &+ [\pi_\alpha(\mathbf{x}) - \pi_\gamma(\mathbf{x})]^2\} < \infty. \end{aligned} \tag{2.16}$$

In this limit a direct product $\Pi_i^{\otimes}$ becomes a continuous direct product. In that case only, a transition from $|\gamma\rangle$ to $|\alpha\rangle$ can be realized by a unitary transformation, within the same irreducibility sector IDPS ($|\alpha\rangle$), say. Otherwise quantum operators $F_\alpha(\hat{\varphi}_{\rm in}, \hat{\pi}_{\rm in}), F_\gamma(\hat{\varphi}_{\rm in}, \hat{\pi}_{\rm in})$ are associated with different (non-Fock) irreducibility $\mathscr{H}_\alpha$, $\mathscr{H}_\gamma$ respectively in $\mathscr{H}$, because we have

$$\sum_k |\alpha_k - \gamma_k|^2 \to \infty \Rightarrow \langle\gamma|\alpha\rangle \to 0, \tag{2.17}$$

i.e., an orthogonality property holds true for $|\alpha\rangle$, $|\gamma\rangle$ if a function $(\alpha - \gamma)(\mathbf{x})$ is not square integrable.

3. SINE–GORDON SOLITONS AND THE BOSON TRANSFORMATION PARAMETERS

A. Let us consider a classical sine–Gordon system in $1+1$ dimensions[14,15]

$$\begin{aligned} &\mathscr{L}(x,t) = (1/2)[\partial_x^2\psi - \partial_t^2\psi + 2m^2(1 - \cos\psi)](x,t), \\ &\partial^2\psi = m^2\sin\psi, \quad \partial^2 = \partial_x^2 - \partial_t^2, \end{aligned} \tag{3.1}$$

where $\hbar = c = 1$. The classical particle spectrum of (3.1) is well known to consist of the three kinds of elementary excitations: a fundamental neutral particle with mass m, a charged particle with mass $8m$, and a neutral particle with mass varying within an interval $[0, 16m]$. Except for fundamental particles, which can be identified through their counterpart to the total energy–momentum of the field only, the remaining two arise in the large time asymptotics of the so-called soliton solutions of the sine–Gordon equation, which we introduce via the formula

$$\begin{aligned} &\psi_N(x,t) = \arccos\{1 - (2/m^2)(\partial_x^2 - \partial_t^2)\ln f_N(x,t)\}, \\ &f_N(x,t) = \det(M_{ij}), \quad i,j = 1,2,\ldots,N \\ &M_{ij} = [2/(a_i + a_j^*)]\cosh[(\theta_i + \theta_j^*)/2]. \end{aligned} \tag{3.2}$$

The parameters a_i are allowed to be complex valued, provided that for each complex a_i in the sequence $\{a_1,\ldots,a_N\}$ there appears an associated a_j with the property $a_j = a_i^*$, a_i being real otherwise. The additional restrictions on a_i are as follows:

$$\begin{aligned} &a_i \neq a_j, \quad i \neq j, \\ &|a_i|^2 = (1 - v_i)/(1 + v_i), \quad |v_i| < 1. \end{aligned} \tag{3.3}$$

Moreover, if a_i is real, a corresponding θ_i is given by

$$\theta_i = \pm m\gamma_i(x - v_i t) + \delta_i = \theta_i(x,t), \tag{3.4}$$

where $\mathrm{sgn}(a_i)$ is chosen to coincide with the sign appearing in the expression for θ_i, and $\gamma_i^2 = (1 - v_i^2)^{-1}$.

If a_i is complex and then accompanied by $a_j = a_i^*$ in the parametric sequence $\{a_i\}_{i=1,\ldots,N}$, then we have

$$\begin{aligned} \theta_i &= \theta_j^* = \theta(a_j) = \theta_R + i\theta_I \\ &= (m\gamma/|a|)[a_R(x + vt) + ia_I(vx + t)] + \delta, \end{aligned} \tag{3.5}$$

where $\delta = \delta_i = \delta_R + i\delta_I$ is a complex phase, while $a = a_i = a_R + ia_I$, $\delta_i = \delta_j^*$.

One can easily verify that $\exp\theta_i(x,t) =: \lambda_i(x,t)$ with θ_i given by either (3.4) or (3.5), is a solution of the free-field equation

$$\partial^2\lambda(x,t) = m^2\lambda(x,t), \quad \partial^2 = \partial_x^2 - \partial_t^2. \tag{3.6}$$

Real solutions (not plane waves in general!) of (3.6) we identify with the mass m fundamental neutral fields associated with the sine–Gordon system. Notice that having λ complex, we have also $\bar{\lambda}$, and then $\frac{1}{2}(\lambda + \bar{\lambda})$ is the underlying mass m field.

Recall that to each real a_i there corresponds a one-soliton solution, while to each complex pair $a_i = a_j^*$ there corresponds a bound (bion, breather) solution, both in the large time asymptotics of $\psi_N(x,t) = \psi_N(a_1,\ldots,a_N,x,t)$. By looking at (3.2), and doing some algebra (with care however, as one must interchange infinite summations) one easily finds that after expanding $\psi_N(x,t)$ with respect to $\exp(\pm\theta)$ factors, for each θ_i a corresponding $\exp(-\theta_i)$ factor disappears,

and hence the following formal power series expansion is valid for the classical N-soliton field

$$\psi_N(x,\tau) = \sum_{n_1=0}^{\infty} \cdots \sum_{n_N=0}^{\infty} \psi^{n_1,\cdots,n_N} \exp(n_1\theta_1)\cdots\exp(n_N\theta_N)$$
$$= \sum_{n_1} \cdots \sum_{n_N} \psi^{n_1,\cdots,n_N} \lambda_1^{n_1}(x,t)\cdots\lambda_N^{n_N}(x,t), \tag{3.7}$$

with $\theta_i = \theta_i(x,t)$ for $i = 1,2,\ldots,N$ and $\psi^{n_1,\cdots,n_N}$ being the N-fold tensor coefficient, in which there are absorbed all the m, a_i dependent factors arising in the course of calculations, and $\psi_i(x,t) = \frac{1}{2}[\lambda_i(x,t) + \bar{\lambda}_i(x,t)]$ satisfies (3.6).

B. We are now at the point, in which considerations of the previous sections can be taken into account. Let $\hat{\psi}_{\text{in}}(x,t)$ be the quantum in-field (i.e., plane wave) solution of the equation

$$(\partial^2 - m^2)\hat{\psi}_{\text{in}}(x,t) = 0. \tag{3.8}$$

Let us furthermore consider the set of operator functional power series of the form

$$\hat{\psi}(x,t) = \psi(x,t,\hat{\varphi}_{\text{in}},\hat{\pi}_{\text{in}}),$$
$$F(x,t,\hat{\varphi}_{\text{in}},\hat{\pi}_{\text{in}}) = \hat{F}(x,t), \tag{3.9}$$

where $\hat{\varphi}_{\text{in}}(x)$, $\hat{\pi}_{\text{in}}(x)$ are the initial quantum data for $\hat{\psi}_{\text{in}}(x,t)$

$$[\hat{\varphi}_{\text{in}}(x),\hat{\pi}_{\text{in}}(y)]_- = i\hbar\delta(x-y). \tag{3.10}$$

We replace them by operators

$$a^*(x) = (1/\sqrt{2})[\hat{\varphi}_{\text{in}}(x) - i\hat{\pi}_{\text{in}}(x)],$$
$$a(x) = (1/\sqrt{2})[\hat{\varphi}_{\text{in}}(x) + i\hat{\pi}_{\text{in}}(x)], \tag{3.11}$$

which after the smearing operation (2.1) define a reducible in the direct product space $\mathscr{H}$ representation of the CCR algebra

$$[a_s,a_t^*]_- = \hbar\delta_{st},$$
$$[a_s,a_t]_- = 0 = [a_s^*,a_t^*]_-.$$

We say that an operator $\hat{\psi}(x,t) = \psi(a^*,a,x,t)$ satisfies the quantum sine–Gordon equation with the operator-valued source $\hat{F}(x,t) = F(a^*,a,x,t)$ if and only if an operator identity

$$\partial^2\hat{\psi}(x,t) = \hat{F}(x,t) \tag{3.12}$$

holds true in the sense

$$\langle 0|\partial^2\hat{\psi}(x,t)|0\rangle = \partial^2\langle 0|\hat{\psi}(x,t)|0\rangle = (0|\hat{F}(x,t)|0), \tag{3.13}$$

$$\lim_{\hbar\to 0}\partial^2\langle 0|\hat{\psi}(x,t)|0\rangle = \lim_{\hbar\to 0}\langle 0|\hat{F}(x,t)|0\rangle$$
$$= \partial^2\phi(x,t) = m^2\sin\phi(x,t), \tag{3.14}$$

where $|0)$ stands for the Fock vacuum for $\{\hat{\varphi}_{\text{in}},\hat{\pi}_{\text{in}}\} \equiv \{a^*,a\}$. It means that each particular solution $\phi(x,t)$ of (3.1) should arise as a vacuum expection value in the tree approximation of some corresponding quantum operator $\hat{\psi}_\phi(x,t)$

$$\phi(x,t) = \lim_{\hbar\to 0}\langle 0|\hat{\psi}_\phi(x,t)|0\rangle. \tag{3.15}$$

C. Because on the quantum level we deal with a single fundamental mass m "meson" in-field $\hat{\psi}_{\text{in}}(x,t)$, one easily finds by comparison with Secs. 1 and 2 that a sufficient condition for $\hat{\psi}_\phi(x,t)$ to generate power series expansions of the form (3.7), (3.9) in the sense of (3.13), (3.14) is the identity

$$\hat{\psi}_\phi(x,t) = \psi(x,t,\hat{\varphi}_{\text{in}} + \varphi,\hat{\pi}_{\text{in}} + \pi) =: \psi(x,t,a^* + \bar{\lambda},a + \lambda), \tag{3.16}$$

i.e.,

$$\langle 0|\hat{\psi}_\phi(x,t)|0\rangle =: \langle\lambda|\hat{\psi}(x,t)|\lambda\rangle \equiv \langle\varphi,\pi|\hat{\psi}(x,t)|\varphi,\pi), \tag{3.17}$$

which is a straightforward (albeit formal) generalization of the discrete procedures of Sec. 2.

Under an additional assumption that the whole classical N-soliton sector, N fixed, can be generated [via (3.12)–(3.17)] by using a *single quantum field* denoted $\hat{\psi}_N(x,t)$, the conditions (3.16), (3.17) are replaced by

$$\hat{\psi}_{N,\phi}(x,t) = \psi_N(x,t,a^* + \bar{\lambda}_N,a + \lambda_N), \tag{3.18}$$

with

$$\bar{\lambda}_N =: \sum_{i=1}^{N}\exp\theta_i = \lambda_N. \tag{3.19}$$

An operator $\hat{\psi}_N(x,t)$ we call a *quantum N-soliton operator*. Its domain in $\mathscr{H}$, i.e., the N-soliton sector in the state space, will be established below.

Recall that to have a comparison with arguments of Sec. 2, one should replace continuous translations $\bar{\lambda}(x),\lambda(x)$ by the approximating sequences $\{\bar{\lambda}_i,\lambda_i\}_{i=0,\pm 1,\pm 2,\cdots}$. But first, one should notice that $\varphi(x),\pi(x)$ arise as the initial classical data for the free field solution of $(\partial^2 - m^2)\psi(x,t) = 0$ of the form

$$\psi_N(x,t) = \sum_{i=1}^{N}\tfrac{1}{2}[\bar{\lambda}_i(x,t) + \lambda_i(x,t)]. \tag{3.20}$$

The consistency of the choice (3.20) of the boson transformation parameter was analytically checked in a slightly different framework in Ref. 5, see, e.g., also Ref. 3, for 1- and 2-solitons. An explicit form of the expansion coefficients $\psi^{n_1,\cdots,n_N}$ can easily be found for these particular fields.

D. In this way we have demonstrated that both quantum and classical soliton fields, can in principle be built out of the fundamental free neutral mass m excitations. Hence the three types of basic sine–Gordon excitations are only outwardly independent: All of them can be reduced to exhibit a more fundamental mass m neutral free field structure. This concept lies at the foundation of our studies of the Bose → Fermi metamorphosis in the whole series of papers[16–20] among which Ref. 20 is devoted to the study of spin $\frac{1}{2}$ approximation of the sine–Gordon system, and explanation of its relation to the spin $\frac{1}{2}$ xyz Heisenberg and Thirring models.

4. COHERENTLIKE DOMAINS FOR QUANTUM SOLITON OPERATORS

A. The time evolution of a quantum operator $\hat{\psi}_\phi(x,0) \to \hat{\psi}_\phi(x,t)$ must be consistent with the "classical limit" formula (3.15). Hence for a concrete N-soliton solution of (3.1), we can rewrite (3.15), as

$$\lim_{\hbar\to 0}\langle 0|\hat{\psi}_{N\phi}(x,t)|0\rangle = \lim_{\hbar\to 0}\langle\varphi,\pi,t|\hat{\psi}_N(x)|\varphi,\pi,t\rangle$$
$$= \lim_{\hbar\to 0}\langle\varphi,\pi|\hat{\psi}_N(x,t)|\varphi,\pi\rangle = \phi_N(x,t), \tag{4.1}$$

where $|\varphi,\pi,t\rangle$ differs from $|\varphi,\pi\rangle$ through replacing the initial data φ,π by the "time dependent" ones according to

$$\lambda_N = \lambda_N(x,t) = \sum_{i=1}^{N} \exp\theta_i(x,t). \tag{4.2}$$

$\theta_i(x,t)$ is fixed by specifying the $2N$ parameters $\{\underline{a},\underline{\delta}\} = \{a_1,...,a_N,\delta_1,...,\delta_N\}$ according to (3.2)–(3.5). Notice that the whole time dependence giving rise to a correct classical result, can be absorbed in the state vectors.

If we look at the difference $\lambda_N(x,t) - \lambda_N(x,0) = f(x,t)$ we see at once that $f(x,t)$ is not a square integrable function on $\mathbb{R}^1$ for $t \neq 0$, hence (see, e.g., Sec. 2) for neither instant of time $t \neq 0$, is a quantum state $|\varphi,\pi,t\rangle$ unitarily equivalent to $|\varphi,\pi\rangle$.[21-23] They both belong to the different (orthogonal) irreducibility sectors IDPS ($|\varphi,\pi\rangle$) and IDPS ($|\varphi,\pi,t\rangle$), respectively.

On the other hand, one finds immediately that a time development of $\theta_i(x)$ into $\theta_i(x,t)$ simply results in the time dependent phase shift of $\theta_i(x)$, which can thus be completely absorbed in the time dependent phase parameter

$$\delta_i \to \delta_i + \delta_i(t) \Rightarrow \theta_i \to \theta_i(x,t) = \theta_i(x) + \delta_i(t). \tag{4.3}$$

Consequently

$$\exp[\theta_i(x,t)] = \exp[\theta_i(x,t) + \delta_i(t)]. \tag{4.4}$$

Because for a fixed choice of soliton parameters $\{a_1,...,a_N\}$ the phases $\{\delta_1,...,\delta_N\}$ are still completely arbitrary, we have found that the quantum N-soliton time development

$$\hat{\psi}_N(x) \to \hat{\psi}_N(x,t), \tag{4.5}$$

can be described by giving a time dependent trajectory in the set of initial data

$$\psi_i(x,a,\delta) = x_i(x) \to \psi_i(x,t) = \psi_i(x,a,\delta'), \tag{4.6}$$
$$\delta' = \delta + \delta(t).$$

Hence for a given N-soliton solution $\phi_N(x,t)$ of (3.1) we have

$$|\varphi,\pi,t\rangle = |\varphi,\pi,\underline{a},\underline{\delta},t) = |\varphi,\pi,\underline{a},\underline{\delta}') \tag{4.7}$$

at a fixed instant of time t, with $\underline{a} = \{a_1,...,a_N\}$ so that

$$\langle\varphi,\pi|\hat{\psi}_N(x,t)|\varphi,\pi) = (\varphi',\pi'|\hat{\psi}_N(x)|\varphi',\pi') \tag{4.8}$$

at t fixed, and IDPS ($|\varphi,\pi\rangle$), IDPS ($|\varphi',\pi'\rangle$) being orthogonal. In the way we have replaced a time development problem for a quantum soliton operator $\hat{\psi}(x,t)$ by a transition through an infinity of unitarily inequivalent and non-Fock representations of the in-field canonical algebra. Each irreducible representation exists in its own IDPS ($|\varphi,\pi,\underline{a},\underline{\delta}\rangle$), where the $\underline{\delta}$ parametrization amounts to a time development, see, e.g., also Ref. 22.

Because for a fixed classical N-soliton $\phi_N(x,\underline{a},\underline{\delta})$ the soliton data $\underline{a}$ remain unchanged during the time evolution, it is convenient to collect all possible choices of $\underline{\delta}$'s for quantum solitons, by taking a direct integral.

$$\int_{\oplus}\cdots\int_{\oplus} d\mu(\delta_1,...,\delta_N)|\mathrm{IDPS}(|\varphi,\pi,\underline{a},\underline{\delta}\rangle):$$
$$= \mathrm{DPS}(|\varphi,\pi,\underline{a}\rangle), \tag{4.9}$$

where (i) the measure $d\mu(\underline{\delta})$ equals $d\delta_1\cdots d\delta_N$ if all $a_i, i = 1,2,...,N$ are real, (ii) if there is any conjugate pair $a_i = a_j^*$ in the set $\{a_1,...,a_N\}$ the integral $\int_{\oplus}\int_{\oplus} d\delta_i\, d\delta_j$ should be replaced by $\int\int_{\oplus} \delta(\delta_i - \delta_j^*)\, d\delta_i\, d\delta_j$, where the integration is carried out over a complex plane.

In the new Hilbert space (*nonseparable*) DPS($|\underline{a}\rangle$), a time evolution of the quantum operator $\hat{\psi}_\phi(x,t)$, $\phi = \phi(\underline{a})$ can be unitarily implemented.

B. In the above by using the notation DPS($|\underline{a}\rangle$), we have explictly indicated that all entering boson transformation parameters are considered at a fixed choice of the sequence $\underline{a} = \{a_1,...,a_N\}$. However we are allowed to vary the parameters $\{a_1,...,a_N\}$ at a fixed value of N, within the variability interval $(0,\infty) \ni |a_i|$ and under the demand that $a_i \neq a_j$ for $i \neq j$ which is a fundamental restriction used in producing any solution (3.2) of the classical sine–Gordon equation. While varying $\underline{a}$'s at N fixed, we are still within a classical N-soliton sector, while quantally we go through mutually orthogonal Hilbert spaces. Notice that states $|\underline{a},\underline{\delta})$, $|\underline{a}',\underline{\delta})$ are always orthogonal, despite how close two sets $\underline{a} = \{a_1,...,a_N\}, \underline{a}' = \{a_1',...,a_N'\}$ of soliton parameters are. In this connection see e.g. (3.4) and (3.5) and note that neither function of the form

$$f_{\lambda\lambda'}(x) = \exp(m\lambda x) - \exp(m\lambda' x) \tag{4.10}$$

is square integrable on the real line $\mathbb{R}^1$, when $\lambda \neq \lambda'$. As a consequence, each classical N-soliton sector gives rise to a quantum soliton sector consisting of the infinite family of mutually inequivalent and non-Fock irreducibility domains IDPS($|\underline{a},\underline{\delta}\rangle$) for the in-field algebra, each one being specified by giving the values of parameters $\underline{a}$ and $\underline{\delta}$, such that for all underlying $|\underline{a},\underline{\delta})$, $\lim_{k\to 0}(\underline{a},\underline{\delta}|\hat{\psi}_N(x,t)|\underline{a},\underline{\delta}) = \phi_N(x,t)$.

Let us now call a direct integral

$$\int_{\oplus} da\ \mathrm{DPS}(|a\rangle) = \mathscr{H}_1 \tag{4.11}$$

a *quantum one-soliton sector* for the sine–Gordon system. Here $|a| \in (0,\infty)$ and both 1-solitons and 1-antisolitons are included. The Hilbert space is by construction nonseparable, and the time evolution of quantum one-soliton is unitarily implemented in it. Let us consider a function

$$\epsilon^2(a_1,a_2) = \begin{cases} 1 & a_1 \neq a_2, \\ 0 & \text{otherwise}, \end{cases} \tag{4.12}$$

and then introduce a double direct integral

$$h_2^s := \int_{\oplus}\int da_1\, da_2\, \epsilon^2(a_1,a_2)\mathrm{DPS}(|a_1,a_2\rangle), \tag{4.13}$$

and the accompanying complex direct integral

$$h_2^b = \int_{\oplus}\int da_1\, da_2\, \delta(a_1 - a_2^*)\epsilon^2(a_1,a_2)\mathrm{DPS}(|a_1,a_2\rangle),$$
$$|a_1|,|a_2| \in (0,\infty). \tag{4.14}$$

The integral (4.13) gives acount of the asymptotically decomposable classical 2-solutions, while (4.14) gives account of the bound solitions (bions, breathers). The $\epsilon^2(a_1,a_2)$ factor in (4.13) is necessary to exclude the real coinciding parameters. The direct integral

$$h_2^s \oplus h_2^b = \mathscr{H}_2 \tag{4.15}$$

we call a *quantum 2-soliton* sector of the sine–Gordon system.

For any $N>2$, a classical soliton solution can arise for a number $r=\max\{r\leqslant N/2, r=1,2,3,\cdots\}$ of bion constituents. Therefore, a general *quantum N-soliton* sector of the sine–Gordon system reads as follows

$$\left\{\left[\int_{\oplus} da_1 \cdots \int_{\oplus} da_N\right] \oplus \left\{\sum_{(i,j)} \int_{\oplus} da_1 \cdots \left[\int_{\oplus}\int da_i\, da_j\, \delta(a_i - a_j^*)\right] \cdots \int_{\oplus} da_N\right\}\right.$$
$$\oplus \left\{\sum_{(i,j)}\sum_{(k,l)} \int_{\oplus} da_1 \cdots \left[\int_{\oplus}\int da_i\, da_j \delta(a_i - a_j^*)\right] \cdots \left[\int_{\oplus}\int da_k\, da_l \delta(a_k - a_l^*)\right] \cdots \int_{\oplus} da_N\right\}$$
$$\oplus \cdots \oplus \left\{\sum_{(i,j)}\sum_{(k,l)} \cdots \sum_{(m,n)} \int_{\oplus} da_1 \cdots \left[\int_{\oplus}\int da_i\, da_j \delta(a_i - a_j^*)\right]\right.$$
$$\left.\left. \cdots \left[\int_{\oplus}\int da_k\, da_l\, \delta(a_k - a_l^*)\right] \cdots \left[\int_{\oplus}\int da_m\, da_n \delta(a_m - a_n^*)\right] \cdots \int_{\oplus} da_N\right\}\right] [\epsilon^2(a_1,\cdots,a_N)\mathrm{DPS}(|a_1,\cdots,a_N\rangle)] = \mathscr{H}_N, \tag{4.16}$$

where the maximal number of double direct integrals in the N-fold one equals an integer $\max\{r\leqslant N/2\}$ and each double integral is carried over the complex area $|a_i|,|a_j|\in(0,\infty)$, while all single ones are carried over a real open interval $|a_i|\in(0,\infty)$.

C. Let us emphasize once more that the factor $\epsilon^2(a_1,\ldots,a_N)$ gives account of the specifics for classical solitons "exclusion principle" by virture of which neither parameter in the sequence $\{a_1,\ldots,a_N\}$ can coincide with any other.[24]

By taking a direct sum

$$\bigoplus_{N=1}^{\infty} \mathscr{H}_N = \mathscr{H}_{\mathrm{SG}}, \tag{4.17}$$

we get a particular subspace $\mathscr{H}_{\mathrm{SG}} \subset \mathscr{H}$ of the Bose in-field direct product space $\mathscr{H}$, which includes all possible *quantum soliton sectors* for the sine–Gordon system. $\mathscr{H}_{\mathrm{SG}}$ we call a *quantum soliton Hilbert space* for the sine–Gordon system in 1 +1 dimensions. For other approaches to the sectorial structures associated with nonlinear field equations see Refs.[25-27],

5. RELATION TO THE SPIN $\frac{1}{2}$ *xyz* HEISENBERG MODEL

A. The spin $\frac{1}{2}$ *xyz* Heisenberg chain arises naturally in the so-called[20] spin $\frac{1}{2}$ approximation of the sine–Gordon system [in the case of the lattice quantization of (3.1), under an assumption of the in-field structure of all the field operators]. Strictly speaking the Heisenberg chain Hamiltonian replaces the nearest neighbor coupling (gradient) term in the sine–Gordon chain Hamiltonian. The basic assumption was that all lattice field operators can be expressed in terms of the single-site generators $\{a_s^*, a_s\}_{s=0,\pm 1,\ldots}$ of the CCR algebra in the direct product space $\mathscr{H}$ constructed for a linear chain of quantum pendula. We identify these generators with the in-field ones introduced in the previous sections.

Recall that $\mathscr{H} = \Pi_s^{\otimes}(h)_s$ and the spin $\frac{1}{2}$ approximation appears by projecting on the lowest two energy levels of each single site (sth) Schröedinger problem in the linear chain

$$\mathfrak{S}_s^+ = P_s a_s^* P_s, \quad \mathfrak{S}_s^- = P_s a_s P_s,$$
$$P_s = :\exp(-a_s^* a_s): + a_s^* :\exp(-a_s^* a_s): a_s, \tag{5.1}$$
$$h \ni |\psi\rangle = \sum_{k=0}^{\infty} f_k |k\rangle \to P|\psi\rangle = \sum_{k=0,1} f_k |k\rangle .$$

The projection operation can be equivalently described by a simultaneously fulfilled sequence of single-site constraints:

$$\hat{n}_s(\hat{n}_s - 1)|\psi\rangle_s = 0, \quad \forall_s,$$
$$\hat{n}_s = a_s^* a_s, \quad \hat{n}_s|k)_s = k|k)_s. \tag{5.2}$$

Then the lattice sine–Gordon Hamiltonian

$$H = \sum_s \{[\pi_s^2 + 2m^2(1-\cos\phi_s)] - (\phi_s - \phi_{s+1})^2/\epsilon^2$$
$$= \sum_s (H_s + V_{s,s+n}), \tag{5.3}$$

if supplemented by the constraints (5.2) plus the periodic boundary conditions,[20] converts into

$$P\sum_s V_{s,s+1} P = P\left(H - \sum_s H_s\right)P = H_{xyz} = -\sum_{a,s} J_a \hat{S}_s^a \hat{S}_{s+1}^a, \tag{5.4}$$

with $P = \Pi_s P_s$ and H_{xyz} denoting the spin $\frac{1}{2}$ *xyz* Heisenberg model Hamiltonian. The coupling constants $\{J_a\}_{a=1,2,3}$ rely here on the explicit a_s^*, a_s dependence of the quantum lattice field $\hat{\phi}_s = \phi_s(a^*, a)$ entering the gradient term, see Ref. 20.

All the spin $\frac{1}{2}$ generators $\{\mathbf{S}_s\}_{s=0,\pm 1,\ldots}$ are obviously built out of the fundamental generators $\{a_s^*, a_s\}$,[18,19] and constitute an irreducible representation of the SU(2) algebra.

B. We wish to define the spin operators and the spin Hamiltonian on the domain $\mathscr{H}_{xyz}$ belonging to the carrier space $\mathscr{H}_{\mathrm{SG}}$ of quantum soliton operators. But for this purpose an irreducible spin $\frac{1}{2}$ realization of the H_{xyz} is inappropriate (no unique choice of the irreducibility domain in $\mathscr{H}_{\mathrm{SG}}$).

Let us introduce the following functions of $\{a_s^*, a_s\}$:

$$\hat{\underline{S}}_k^+ = (2s)^{1/2}(1 - a_k^* a_k/2s)^{1/2} a_k$$
$$\hat{\underline{S}}_k^- = (2s)^{1/2} a_k^* (1 - a_k^* a_k/2s)^{1/2} \tag{5.5}$$
$$\hat{\underline{S}}_k^3 = s - a_k^* a_k \quad s = 1|2,1,3|2,\ldots,$$

which satisfy in $\mathscr{H}$ the following operator identities

$$[\hat{\underline{S}}_i^+, \hat{\underline{S}}_j^-]_- = 2\hat{\underline{S}}_i^3 \delta_{ij}\hbar, \quad [\hat{\underline{S}}_i^3, \hat{\underline{S}}_j^{\pm}]_- = \pm 2\hat{\underline{S}}_i^3 \delta_{ij}\hbar. \tag{5.6}$$

It is the Holstein–Primakoff realization of the SU(2).[18,19] In the single site Hilbert space h_i, let us specify a proper sub-

space $P_s h_i$ by demanding that $P_s h_i$ (P_s is a projection) is a linear span of all eigenvectors $|n\rangle$ of $a_i^* a_i$ for which $a_i^* a_i |n\rangle = n|n\rangle$, $n \leqslant 2s$. One can easily check that the operator $\hat{\mathbf{S}}_i$ acts on $P_s h_i$ invariantly. Thus if restricted to $P_s h_i$, $\hat{\mathbf{S}}_i = P_s \hat{\mathbf{S}}_i P_s$ generates an irreducible spin $s = n/2$ representation of the SU(2) group Lie algebra.

Let us now introduce a coherent state domain in h_i, so that a single site coherent state $|\alpha\rangle_i$ is given. Then

$$\lim_{\hbar \to 0} {}_i\langle \alpha | \hat{\mathbf{S}}_i | \alpha \rangle_i = \mathcal{s}_i(\alpha), \tag{5.7}$$

where

$$\begin{aligned} \mathcal{s}_i^+(\alpha) &= (2s)^{1/2}(1 - |\alpha_i|^2/2s)^{1/2}\alpha_i, \\ \mathcal{s}_i^-(\alpha) &= (2s)^{1/2}(1 - |\alpha_i|^2/2s)^{1/2}\bar{\alpha}_i, \\ \mathcal{s}_i^3(\alpha) &= s - |\alpha_i|^2, \end{aligned} \tag{5.8}$$

and moreover because (5.7) and (5.8) holds true for all $i = 0, \pm 1, \ldots$, the direct product state expectation in terms of $|\alpha\rangle$ leads to:

$$\lim_{\hbar \to 0} \langle \alpha | H_{xyz} | \alpha \rangle = -\sum_{a,s} J_a \mathcal{s}_s^a(\alpha) \mathcal{s}_{s+1}^a(\alpha). \tag{5.9}$$

For the product state $|\alpha\rangle = \Pi_i |\alpha\rangle_i = |\alpha_1 s\rangle$ whose translation parameters satisfy

$$|\alpha_i|^2 \leqslant 2s \quad \forall i = 0, \pm 1, \cdots \tag{5.10}$$

the $\{\mathbf{s}_i(\alpha)\}$ admit the following parametrization

$$\begin{aligned} |\alpha_i|^2 &:= s(1 - \cos\Theta_i), \\ \mathrm{Re}\alpha_i &= \sin\Theta_i \cos\phi_i / [(1 + \cos\Theta_i)/s)]^{1/2}, \\ \mathrm{Im}\alpha_i &= \sin\Theta_i \sin\phi_i / [(1 + \cos\Theta_i)/s]^{1/2}, \end{aligned} \tag{5.11}$$

so that

$$\begin{aligned} \mathcal{s}_i^1 &= s\sin\Theta_i \cos\phi_i, \\ \mathcal{s}_i^2 &= s\sin\Theta_i \sin\phi_i, \\ \mathcal{s}_i^3 &= s\cos\Theta_i, \end{aligned} \tag{5.12}$$

and[28-32]

$$\lim_{s \to \infty} \lim_{\hbar \to 0} \langle \alpha, s | \frac{\hat{\mathbf{S}}_i}{s} | \alpha, s \rangle = \mathbf{s}_i, \tag{5.13}$$

$$\begin{aligned} &\lim_{s \to \infty} \lim_{\hbar \to 0} \langle \alpha, s | \frac{H_{xyz}}{s^2} | \alpha, s \rangle \\ &\quad = H_{xyz}^{\mathrm{cl}} = -\sum_{a,s} J_a s_s^a s_{s+1}^a, \end{aligned}$$

with

$$s^1 = \sin\Theta\cos\phi, \quad s^2 = \sin\Theta\sin\phi, \quad s^3 = \cos\Theta,$$

provided

$$|\alpha\rangle := |\alpha, s\rangle, \quad s = \tfrac{1}{2}, 1, \tfrac{3}{2}, \cdots.$$

C. The above procedures allow us to select a subset $\mathscr{H}_{xyz}$ in $\mathscr{H}_{\mathrm{SG}}$ which via $\hbar \to 0$ limit followed by the $s \to \infty$ limit of state expectations allows us to reproduce a classical level for the spin $\frac{1}{2}$ *xyz* Heisenberg model. The underlying soliton parameters (i.e., the boson transformation ones) are given by (5.11) with $s = \frac{1}{2}$.

In this way not only does the quantum sine–Gordon system recover the spin $\frac{1}{2}$ *xyz* model spectrum and the state space, the classical levels of both systems also exhibit the relation, as a consequence of the quantum one.

Remark 1: Because, after taking the continuum limit, the boson transformation parameters $\alpha(x,t)$ are themselves parametrized by the classical spins $\mathbf{s}(x,t)$, the sine–Gordon solitons can be viewed as functions of these spins also. It seems that classical motions on the phase manifold of the classical *xyz* Heisenberg system have their image in the corresponding submanifold of the sine–Gordon phase space, obviously if the respective α's obey (5.10)–(5.12).

Remark 2: In the above we have mainly discussed a discrete (lattice) version of the *xyz* model. Obviously, under an appropriate limiting operation, a continuous model can always be formally received. However, for the general case (i.e., with no restrictions on the coupling constants of the sine–Gordon system) the continuum limit may not exist on the quantum level (compare Refs. 19 and 20).

Remark 3: Let us comment that quite analgous application of the tree approximation for the Bose constructed Fermi system (however without a subsequent $s \to \infty$ limit as in the above) allows us to obtain an appropriate (commuting ring) *c*-number level for the Dirac field,[17] with no recourse to the Grassmann algebra methods. An analog of the infinite spin limit was then constructed for the Dirac system[33] at least on the level of relativistic quantum mechanics.

Remark 4: By taking advantage of the "psudoparticle"[34] structure of the Thirring model (the $N = \int dx \psi^+ \psi = 0$ sector)

$$\begin{aligned} H = \int dx \{ &-i(\psi_1^+ \partial_x \psi_1 - \psi_2^+ \partial_x \psi_2) \\ &+ m_0(\psi_1^+ \psi_2 + \psi_2^+ \psi_1) + 2g\psi_1^+ \psi_2^+ \psi_2 \psi_1 \}, \end{aligned} \tag{5.14}$$

$$\{\psi^+(x), \psi(y)\} = \delta(x - y)I, \quad \psi|0\rangle = \langle 0|\psi^+ = 0,$$

the eigenstates of H are found to be in the form

$$|\psi\rangle = \sum_{\{a\}} \int dx_1 \ldots dx_i \, \chi^{a, \cdots a_i}(x_1, \ldots, x_i) \psi_{a_1}^+(x_1) \cdots \psi_{a_i}^+(x_i)|0\rangle, \tag{5.15}$$

with $\chi^a(\underline{x})$ being the totally antisymmetric wavefunction. Because ψ, ψ^+ are the (free) pseudoparticle fields, we can at once repeat step by step all considerations of the papers[16,17] on quantization of spinor fields. Namely, the Thirring model can be considered as a spin $\frac{1}{2}$ approximation of the subsidiary two-component Bose system (field). The tree approximation, if applied to this mediating Bose level, immediately recovers the classical Thirring model (defined on the *c*-number commuting ring of spinor functions) by considering the associated-with-fermions Bose transformed operators and then taking the vacuum expectation values in the tree approximation. For this (non Grassmann) classical Thirring model complete integrability was proved and the soliton solutions found in Ref. 35. It neatly disproves the physical (!) utility of Grassmann algebra methods for the case of the Thirring model.

Remark 5: The above-mentioned two-component Bose field, (a four-component one in case of the Dirac system in 1 + 3 dimensions), acquires a physical meaning if considered in the framework of the "field-reservoir" interaction[19,20] where the spin $\frac{1}{2}$ approximation procedure for the sine–Gordon system does automatically involve an additional to the fundamental one $\{a_s^*, a_s\}_{s=0,\pm 1,\ldots}$, field of the reservoir $\{\tilde{a}_s^*, \tilde{a}_s\}_{s=0,\pm 1,\ldots}$, which all together give rise to ψ_1, ψ_1^+; ψ_2, ψ_2^+ in the continuum limit. Notice that $\{a_s^*, a_s\}$

describe elementary excitations of the sine–Gordon field, while $\{\tilde{a}_s^*, \tilde{a}_s\}$ describe those induced in the reservoir. Quantized ψ, ψ^+ are given in terms of the Bose constructed Fermi generators $b_\alpha = b_\alpha(a^*, a, \tilde{a}^*, \tilde{a})$, $b_\alpha^* = b_\alpha^*(a^*, a, \tilde{a}^*, \tilde{a})_{\alpha=1,2}$ so that the Lorentz invariance of the Thirring model becomes the Lorentz invariance of the field-reservoir system in the spin $\frac{1}{2}$ approximation.

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Dynamically variable internal symmetries

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The mathematical consequences of the ansatz that the generators of internal transformations, as well as the parameters, may be space–time-dependent is investigated. In addition to the Yang–Mills type fields, a transformation changing field must be introduced. The formalism developed is consistent. An appendix contains a derivation of the Fock–Ivanenko coefficient for the Dirac equation in general relativity that shows a connection between the ideas developed here and gauge fields.

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I. INTRODUCTION

The history of physics provides many examples where an increase in the generality of the transformation group, of the kinematical and dynamical variables, provided the mathematical basis for a more general theory.[1] As is well known, gauge fields are introduced as one goes from a global internal transformation group to a local one.[2] Similarly, the jump from Lorentz transformations to the four-dimensional manifold mapping group accompanies the change in theory from special to general relativity.[3] Other examples abound.[4]

All these pairs of theories have the feature that the more general one reduces to the less general one as the transformation group is properly specialized. In gauge theories, for example, some of the generators of the transformation group may be excluded and hierarchies of subgroups studied.

No theory, to the author's knowledge, allows the generators of the transformations to be dynamical variables: Most are based on an *a priorily* chosen Lie group (or, for supergravity, a graded Lie algebra). The purpose of this paper is to explore the possibility, the mathematical consistency, and some potential properties of a theory containing an internal transformation group that is dynamically determined. Thus both the generators and the parameters of the transformations will vary over space–time. In particular, when the transformation altering field (to be defined) is small or vanishes in some region then the field will not possess that transformation. This is independent of the values of the arbitrary parameters.

In Sec. II the transformation law and some geometrical objects will be studied. It will be seen that transformations are closely related to Yang–Mills gauge transformations, the difference being the addition of a symmetry changing field. Section III contains a sumary of the results and a brief discussion. The appendix features a derivation of the Fock–Ivanenko coefficient[5] that shows a link between the Yang–Mills approach, the formalism used here, and the Dirac equation.

II. FORMALISM

The standard gauge formalism[6] involves a multicomponent field ϕ whose internal transformation properties are given by

$$\bar{\delta}\phi = i\epsilon^a S_a \phi. \tag{1}$$

where the parameters of the transformation are the infinitesmal quantities ϵ^a and S_a are the generators of the Lie group used. While the ϵ^a are taken to be functions of position in space–time, the S_a are not.

Our generalization of Eq. (1) consists of considering the generators as being functions of space–time position. Let us rewrite Eq. (1) as

$$\bar{\delta}\phi = i\epsilon^A S_A \phi, \tag{2}$$

where the presence of capital Latin indices indicates this change of viewpoint. Note that while ϵ^A are functions of position, they are also infinitesmals. In addition, they are to be arbitrarily specifiable. Accordingly, an absorption of the space–time dependence of S_A into ϵ^A is not possible. This method allows for the possibility that the dynamics, in determining the space–time dependence of S_A, will delimit the transformation groups: allowing or excluding, "freezing-out." or weakening some transformations in different regions of space–time.

We shall consider, in a manner similar to that used with the vierbein, that S_A is given in terms of S_a by

$$S_A = h_A{}^a S_\alpha. \tag{3}$$

The field $h_A{}^a$ carries the desired space–time changes in the transformations. This enables us to determine the derivative of S_A:

$$S_{A,\mu} = h_A{}^a{}_{,\mu} S_a. \tag{4}$$

Taking g_{ab} to be the natural metric of the group generated by S_a, we define g_{AB} by

$$g_{AB} = h_A{}^a h_B{}^b g_{ab}. \tag{5}$$

Using these metrics to raise and lower their respective types of indices, we have

$$\begin{aligned} g^{ab} &= h_A{}^a h_B{}^b g^{AB}, \\ \delta_b{}^a &= h_A{}^a h_b{}^A, \\ \delta_B{}^A &= h_a{}^A h_B{}^a. \end{aligned} \tag{6}$$

Therefore, Eq. (4) is

$$S_{A,\mu} = h_A{}^a{}_{,\mu} h_a{}^B S_B. \tag{7}$$

To check that transformations (2) still form a group, we need to have the transform properties of $h_A{}^a$ and S_A. We require that

$$\bar{\delta}S_A = i\epsilon^B [S_B, S_A] - i\epsilon^B C_B{}^C{}_A S_C - S_{A,\mu}\xi^\mu. \tag{8}$$

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The first term comes from the fact that S_A is considered to be a matrix while ϕ in Eq. (2) is a column. The second term in Eq. (8) takes care of the transformation rule for the index C, and the last term is a transport term for space–time transformations with descriptor ξ_μ.

Since

$$[S_a,S_b] = C_a{}^c{}_b S_c, \tag{9}$$

where $C_a{}^c{}_b$ are the structure constants of the S_a group, if we define

$$C_A{}^C{}_B = h_A{}^a h_B{}^b h_c{}^C C_a{}^c{}_b, \tag{10}$$

then Eq. (8) will reduce to

$$\bar\delta S_A = -S_{A,\mu}\xi^\mu. \tag{11}$$

Next we need the transformation properties of $h_A{}^a$. We shall first show that parameters ϵ^a and ϵ^A, for transformations of the two types of indices, must be related. To do this, calculate $\bar\delta S_{A,\mu}$ two ways and equate the two results. We take

$$\bar\delta h_A{}^a = -i\epsilon^B C_B{}^C{}_A h_c{}^a + i\epsilon^b C_b{}^a{}_c h_A{}^c - h_A{}^a{}_{,\mu}\xi^\mu, \tag{12}$$

$$\bar\delta h_A{}^a = -h_A{}^a{}_{,\mu}\xi^\mu - i(\epsilon^B h_B{}^b - \epsilon^b)C_b{}^a{}_c h_A{}^c.$$

Now use Eqs. (7), (11), and (12) to calculate

$$\begin{aligned}\bar\delta S_{A,\mu} = &-[-h_A{}^a{}_{,\rho}h_a{}^B{}_{,\mu}\xi^\rho - i(\epsilon^B h_B{}^b - \epsilon^b)C_b{}^a{}_c h_A{}^c h_a{}^B{}_{,\mu}\\ &- h_A{}^a h_a{}^B{}_{,\rho\mu}\xi^\rho - h_A{}^a h_a{}^B{}_{,\rho}\xi^\rho{}_{,\mu}\\ &+ i(\epsilon^B h_B{}^b - \epsilon^b)_{,\mu}h_A{}^a C_b{}^c{}_a h_c{}^B\\ &+ i(\epsilon^B h_B{}^b - \epsilon^b)C_b{}^c{}_a h_A{}^a h_c{}^B{}_{,\mu}]S_B + h_A{}^a h_a{}^B{}_{,\mu}S_{B,\rho}\xi^\rho.\end{aligned}$$

Now from Eq. (11) directly

$$\bar\delta S_{A,\mu} = -h_A{}^a{}_{,\rho\mu}h_a{}^B S_B\xi^\rho - h_A{}^a{}_{,\rho}h_a{}^B S_B\xi^\rho{}_{,\mu}.$$

On equating the two values obtained for $\bar\delta S_{A,\mu}$, we obtain the condition

$$0 = -i(\epsilon^B h_B{}^b - \epsilon^b)_{,\mu}C_b{}^B{}_A S_B.$$

Therefore, ϵ^B and ϵ^b must be related with

$$\epsilon^b = \epsilon^B h_B{}^b + C^b, \tag{13}$$

where C^b is a space–time constant vector. To preserve the maximum freedom, we shall assume C^b is taken to be nonzero.

Now we may check that the transformations in Eq. (2) form a group. Calculate $\bar\delta_2\bar\delta_1\phi$ and find

$$\begin{aligned}\bar\delta_2\bar\delta_1\phi = &[-i\epsilon_1{}^A{}_{,\mu}\xi_2{}^\mu S_A\phi - i\epsilon_2{}^A{}_{,\mu}\xi_1{}^\mu S_A\phi - i\epsilon_1{}^A S_{A,\mu}\xi_2{}^\mu\phi\\ &- i\epsilon_2{}^A S_{A,\mu}\xi_1{}^\mu\phi - i\epsilon_2{}^A S_A\phi_{,\mu}\xi_1{}^\mu - i\epsilon_1{}^A S_A\phi_{,\mu}\xi_2{}^\mu\\ &+ \phi_{,\mu\nu}\xi_2{}^\nu\xi_1{}^\mu + \phi_{,\nu}(\xi_2{}^\nu{}_{,\mu}\xi_1{}^\mu + \xi_1{}^\nu{}_{,\mu}\xi^\mu)]\\ &- \phi_{,\mu}\xi_2{}^\mu{}_{,\nu}\xi_1{}^\nu - \epsilon_2{}^B\epsilon_1{}^C S_B S_C\phi.\end{aligned}$$

Construction of $\bar\delta_2\bar\delta_1\phi - \bar\delta_1\bar\delta_2\phi$ will result in the terms in the brackets cancelling. We obtain

$$\bar\delta_2\bar\delta_1\phi - \bar\delta_1\bar\delta_2\phi = i\epsilon_3{}^A S_A\phi - \phi_{,\mu}\xi_3{}^\mu, \tag{14}$$

where

$$\begin{aligned}\xi_3{}^\mu &= \xi_2{}^\mu{}_{,\nu}\xi_1{}^\nu - \xi_1{}^\mu{}_{,\nu}\xi_2{}^\nu,\\ \epsilon_3{}^A &= i\epsilon_2{}^B\epsilon_1{}^C C_B{}^A{}_C.\end{aligned} \tag{15}$$

Despite the possibility that the dynamics may force $h_A{}^a$ to be zero in some regions, we have a transformation group. The actual transformation group that applies in a region of space–time is dynamically determined.

Let us examine a special case in more detail before proceeding further with the formalism. Integrate Eq. (2) to finite transformations for the case of only one parameter, ϵ. Further, assume $h_A{}^a$ is diagonal with relevant component h and also that $(S_A)^2 = 1$. Then

$$\bar\delta\phi = \exp(i\epsilon h S_a)\phi = \cos\epsilon h\,)\phi + (\sin\epsilon h\,)S_a\phi. \tag{16}$$

Note that if h is unity, this is the standard transformation law that holds with gauge transformations. On the other hand, if h approaches zero, no finite value of ϵ (only finite transformations can be contemplated in experiments) will produce any transformation on ϕ. We have gained the possibility of dynamically weakening a transformation law so that entire subgroups may be eliminated.

If $h_A{}^a$ is not diagonal, mixing of terms will occur in the expansion of Eq. (16). For a single parameter ϵ, transformations will occur on ϕ that are as if a variety of parameters were present. This means that transformations may occur that were not expected on the basis of our selection of parameters.

Now continue the development to the Yang–Mills procedure. Require that the covariant derivative of $\phi,\phi_{;\mu}$, transform internally as ϕ does and as a space–time vector:

$$\bar\delta\phi_{;\mu} = i\epsilon^A S_A\phi_{;\mu} - \phi_{;\nu}\xi^\nu{}_{,\mu} - \phi_{;\mu,\nu}\xi^\nu. \tag{17}$$

Then the ansatz that

$$\phi_{;\mu} = \phi_{,\mu} + \Gamma_\mu\phi, \tag{18}$$

leads to the transformation law for Γ_μ

$$\begin{aligned}\bar\delta\Gamma_\mu = &-\Gamma_{\mu,\nu}\xi^\nu - \Gamma_\nu\xi^\nu{}_{,\mu} + i\epsilon^A[S_A,\Gamma_\mu]\\ &- i\epsilon^A{}_{,\mu}S_A - i\epsilon^A S_{A,\mu}.\end{aligned} \tag{19}$$

The last term vanishes in the gauge formalism. Now introduce fields $B_\mu{}^A$ and $B_\mu{}^a$ with

$$\Gamma_\mu = B_\mu{}^A S_A = B_\mu{}^A h_A{}^a S_a = B_\mu{}^a S_a. \tag{20}$$

After substituting Eq. (20) into Eq. (19), we obtain

$$\begin{aligned}\bar\delta B_\mu{}^A = &-B_\mu{}^A{}_{,\rho}\xi^\rho - B_\rho{}^A\xi^\rho{}_{,\mu} + i\epsilon^C C_C{}^A{}_B B_\mu{}^B\\ &- i(\epsilon^B h_B{}^a)_{,\mu}h_a{}^A,\end{aligned} \tag{21a}$$

$$\begin{aligned}\bar\delta B_\mu{}^a = &-B_\mu{}^a{}_{,\rho}\xi^\rho - B_\rho{}^a\xi^\rho{}_{,\mu} + i\epsilon^b C_b{}^a{}_c B_\mu{}^c\\ &- i(\epsilon^A h_A{}^a)_{,\mu}.\end{aligned} \tag{21b}$$

Now define $F_{\mu\nu}$ in terms of Γ_μ by

$$\phi_{;\mu\nu} - \phi_{;\nu\mu} = F_{\mu\nu}\phi = (\Gamma_{\mu,\nu} - \Gamma_{\nu,\mu} + \Gamma_\nu\Gamma_\mu - \Gamma_\mu\Gamma_\nu)\phi. \tag{22}$$

Calculation of $\bar\delta F_{\mu\nu}$ gives

$$\bar\delta F_{\mu\nu} = -F_{\mu\nu,\rho}\xi^\rho - F_{\rho\nu}\xi^\rho{}_{,\mu} - F_{\mu\rho}\xi^\rho{}_{,\nu} + i\epsilon^A[S_A,F_{\mu\nu}]. \tag{23}$$

Just as in the gauge formalism the nontensor transformation terms have cancelled out.

Setting $F_{\mu\nu} = F_{\mu\nu}{}^A S_A$ and substituting into Eqs. (22) and (23), we obtain

$$F_{\mu\nu}{}^A = B^a{}_{\mu,\nu}h_a{}^A - B^a{}_{\nu,\mu}h_a{}^A + B_\nu{}^c B_\mu{}^B C_c{}^A{}_B, \tag{24}$$

$$\begin{aligned}\bar\delta F_{\mu\nu}{}^A = &-F_{\mu\nu}{}^A{}_{,\rho}\xi^\rho - F_{\rho\nu}\xi^\rho{}_{,\mu} - F_{\mu\rho}\xi^\rho{}_{,\nu}\\ &+ i\epsilon^c C_c{}^A{}_B F_{\mu\nu}{}^B.\end{aligned} \tag{25}$$

Note that $F_{\mu\nu}{}^A$ transforms like a tensor but is constructed

out of a combination of $B_\mu{}^A$ and $h_A{}^a$ fields. If $h_A{}^a$ is the delta function, then the Yang–Mills case immediately follows.

Now search for objects that transform as tensors but are constructed solely from the $h_A{}^a$, their derivatives, and the metric. To obtain one such object, define h_μ by

$$h_\mu = h_A{}^a h_a{}^A{}_{,\mu}. \tag{26}$$

The calculation of $\bar{\delta} h_\mu$ reveals that h_μ is a vector. Scalars constructible in terms of $h_A{}^a$ and its derivatives include $h_\mu h^\mu, h_a{}^A{}_{,\mu} h_A{}^a{}_{,\nu} g^{\mu\nu}$, and $g_{AB,\mu} g^{AB}{}_{,\nu} g^{\mu\nu}$.

Let us begin to explore the possibility of a field theory built from these objects. First a Lagrangian density must be formed. This density, in order that it provide equations of motion for the $h_A{}^a$ field, must contain terms that are scalars, like those constructed above, multiplied by $\sqrt{\ } - g$. Let us leave the problem of the selection of the "correct" term for another time and investigate the kinds of results that are possible. Select the term $(\sqrt{\ } - g) g_{AB,\mu} g^{AB}{}_{,\nu} g^{\mu\nu}$ on an ad hoc basis and consider the Lagrangian density

$$= (\sqrt{\ } - g)[\kappa^{-1} R + \tfrac{1}{4} F_{\mu\nu}{}^A F_A{}^{\mu\nu} + L_\phi + g_{AB,\mu} g^{AB}{}_{,\nu} g^{\mu\nu}]. \tag{27}$$

Here R is the curvature scalar, and L_ϕ is a function of ϕ, $\phi_{,\mu}, B_\mu{}^A, h_A{}^a$, and S_a. Let us further specialize by fixing the metric, $g_{\mu\nu} = \eta_{\mu\nu}$. The independent variants are ϕ, $B_\mu{}^A$, and $h_A{}^a$: The S_a are fixed. Note that the imposition of the minimal coupling restriction on how the $B_\mu{}^A$ field couples to ϕ does not prevent the possibility of terms like $\phi^\dagger \gamma^\mu h_\mu \phi$ in L_ϕ (if ϕ is a spinor field). Other terms that are new include $\phi^\dagger h^\mu \phi_{,\mu}$. This type of term offers the possibility of forming equations that are first order in $\phi_{,\mu}$ even when ϕ is not a field with half-integral spin.[7]

III. DISCUSSION

It is not clear what the number of necessary "elementary" particles will prove to be.[8] As scattering experiments have been performed at higher energies, more particles have been discovered, and larger symmetry groups have been needed to describe them.

Nonlinear realizations of the SL $(2,C)$ group have attracted recent study because they offer new possibilities for the classification of elementary particles.[9] That work is exciting not only because new wave equations are obtained but also because nonlinear systems usually imply that particle number is not conserved.[10] The work in this paper is not directly related to those efforts, despite some similarities in the transformation equations.[11] This is because here the emphasis is on allowing the transformation group to be as general as possible: The symmetry group is the full covariance group because no absolute objects are allowed.[12] Since the Lagrangian is a dynamical function of all the fields, one may, *only after variation*, solve for $h_A{}^a$ and eliminate it in all the other equations. Then the transformations of some of the field variables will be of the nonlinear type.

No new physics is described in this paper. Rather an attempt has been made to generalize the gauge transformation idea while not requiring the *a priori* specification of a fixed internal transformation group as the basis for a theory. With the presence of vectors like h_μ, it is possible to construct new particle field equations. It is an open question whether any of these are consistent with experimental particle physics.

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APPENDIX

It is amusing to see that the Fock–Ivanenko coefficient[13] can be obtained for the Dirac field in general relativity by a Yang–Mills type of procedure. This is interesting to us in the present case because the parameters ϵ^A and the transformation matrices S_A are both functions of position. Taking

$$\bar{\delta}\psi = i\epsilon^A S_A \psi, \tag{A1}$$

we write the covariant derivative of ψ as

$$\psi_{;\mu} = \psi_{,\mu} + \Gamma_\mu \psi = \psi_{,\mu} + B_\mu{}^A S_A \psi. \tag{A2}$$

We assume that the Fock–Ivanenko coefficient Γ_μ can be written in terms of a $B_\mu{}^A$ field. Now the condition that the covariant derivative of the Dirac gamma matrices be zero implies

$$\gamma^\mu{}_{;\nu} = 0 = \gamma^\mu{}_{,\nu} + [\Gamma_\nu, \gamma^\mu] + \gamma^\rho \Gamma_{\rho\nu}{}^\mu. \tag{A3}$$

Of course,

$$\gamma_\mu \gamma_\nu = -\gamma_\nu \gamma_\mu + 2 g_{\mu\nu}. \tag{A4}$$

Now let the A index be shorthand for the $\rho\sigma$ index pair and define $S_A = \gamma_\rho \gamma_\sigma - \gamma_\sigma \gamma_\rho$. On substituting these equations into Eq. (A3), we find that it is possible to quickly solve for $B_\mu{}^A$. With $\gamma^\mu{}_{,\nu} = h^{\mu\rho'}{}_{,\nu} \gamma_{\rho'}$, where $\gamma_{\rho'}$ is a constant matrix, we obtain

$$\Gamma_\mu = \tfrac{1}{8}(\gamma_\sigma \gamma^\sigma{}_{;\mu} - \gamma^\sigma{}_{;\mu} \gamma_\sigma). \tag{A5}$$

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Bargmann–Wigner equations: Symmetries of multispinors and equations of motion [a)]

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A study of the Bargmann–Wigner wave equations (BWE) is carried out from the group theoretical point of view. Starting with totally symmetric multispinors of rank n and their expansion in terms of tensor coefficients, the general symmetry properties among them, the equation of motion and the Lorentz content of these tensors are derived for systems of arbitrary spin and nonzero mass. The same procedure is applied to multispinors of mixed symmetry corresponding to any Young diagram. Complete formulas are found for these multispinors, which are necessary in the construction of the first order Lagrangian for the BWE.

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I. INTRODUCTION

The wavefunctions in the BWE[1] are tensorial products of four-component spinors, which satisfy the Dirac equation for each of their spinorial indices. With respect to other relativistic wave equations of higher spin, the BWE have the advantage of representing particles with unique mass and spin. Their equivalence with Klein–Gordon, Proca, and Rarita–Schwinger equations for particles of spin 0, 1, and 3/2 respectively is well known.[1–4] Salam, Delbourgo, and Strathdee[5] used them in the representation of the supermultiplet models for heavy hadrons.

The study of free particles of higher spin can be attacked by group theoretical methods. When electromagnetic interactions are introduced, some physical problems appear. Velo and Zwanzinger[6] found that the equation for a particle of spin 3/2 with electromagnetic coupling leads to velocities higher than the velocity of light. Also Wightman[7] and Capri pointed out that the solution of this equation is stable when there are no imaginary eigenvalues in the mass spectrum, as is the case of the Pauli–Fierz equation when some external field is coupled.

Recent supersymmetry theories dealing with superfields which are related to higher spin fields, need wave equations for these fields, as in the work of Sokatchev,[8] Ogievetsky and Sokatchev,[9] Nieuwenhuizen,[10], Berends *et al.*,[11] where wave equations up to 5/2 spin are studied.

In this paper we have carried out the study of BWE for massive particles of arbitrary spin from the group theoretical point of view. In Sec. II we study symmetry properties of multispinors and their expansion in term of Lorentz tensors. We obtain closed expressions for any spin, and the equivalence between BWE and Pauli–Fierz equations for integer spin and the Rarita-Schwinger equation for half-integer spin. Afterwards, the Lorentz content of the tensor coefficients in the expansion is described in detail. In Sec. III the same program is applied to multispinors with arbitrary symmetry, their expansion, and the Lorentz content.

II. BARGMANN–WIGNER EQUATIONS FOR TOTALLY SYMMETRIC MULTISPINORS

A. Basic concepts and notation

Let B the space of spinors ψ^α, $\alpha = 1,2,3,4$, which transform according to the $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$ representation of $SL(2,\mathbb{C})$.[12] Using the charge conjugation matrix C[13] and the elements of the Dirac algebra, we can construct a basis for the direct product of the spaces $B\otimes B$, namely,

$$\{\Lambda_k\} = \{C^{-1}, \gamma^\mu C^{-1}, \sigma^{\mu\nu}C^{-1}, \gamma^5 C^{-1}, \gamma^\mu\gamma^5 C^{-1}\}, \tag{1}$$

where $\gamma^\mu C^{-1}, \sigma^{\mu\nu}C^{-1}$ are symmetric, and C^{-1}, $\gamma^5 C^{-1}$, $\gamma^\mu\gamma^5 C^{-1}$ are antisymmetric matrices.

Any multispinor of rank n can be expanded in the basis $\Lambda_{k_1}\otimes\cdots\otimes\Lambda_{k_r}$ if $n = 2r$, and in the basis $\Lambda_{k_1}\otimes\cdots\otimes\Lambda_{k_r}\otimes e_\alpha$ if $n = 2r+1$, where $\{e_\alpha\}$, $\alpha = 1,2,3,4$, is a basis for B. In the first case the coefficients of the expansion of a n-rank tensor are tensors under the Lorentz group. In the second case the coefficients are of the form $X^\alpha_{\mu_1\cdots\mu_r}$, where $\mu_1\cdots\mu_r$ are tensor indices and α is a spinor index.

The fundamental representation of the SU(2,2) group, when it is restricted to its subgroup SO(3,1) is decomposed as $(\frac{1}{2},0)\oplus(0,\frac{1}{2})$. Therefore, we can consider spinors as vectors in the carrier space of the fundamental representation of SU(2,2).

In order to obtain the decomposition of any irreducible representation of SU(2,2) when it is restricted to the (proper) Lorentz group, it is more convenient to use the weight diagrams associated with the irreducible representations of SU(4), since we can go easily from this representation to the (finite) irreducible representation of SU(2,2) by the standard technics of analytic continuations.[14] Due to the local ismorphism between SU(4) and SO(6), given an arbitrary representation of SO(6) of weight (m_1,m_2,m_3), we can obtain the SO(4) content with the help of the branching laws SO(6)→SO(5)→SO(4), and the result can be read off as the SO(3,1) content of the particular representation of SU(2,2) (see Table I).

[a)] This work contains part of the Doctoral Thesis of M. A. Rodriguez presented to the Facultad de Ciencias Físicas, Universidad Complutense de Madrid (Madrid, 1980).

[b)] One of the authors (M.A.R.) wishes to express his gratitude to the Ministerio de Educación y Ciencia for financial support.

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B. Symmetry properties and equations of motion

Let $\psi^{\{\alpha,\dots,\rho\}}$ be a multispinor of n-rank totally symmetric, associated with the Young diagram $[n]$. The BWE impose the conditions on each index:

$$(\gamma p)^{\tau}{}_{\tau'}\psi^{\{\alpha\cdots\tau'\cdots\rho\}} = m\psi^{\{\alpha\cdots\tau\cdots\rho\}}. \tag{2}$$

Bargmann and Wigner proved that this set of equations corresponds to an elementary system of unique spin $s = n/2$ and mass m.

Since $\psi^{\{\alpha\beta\cdots\rho\}}$ is totally symmetric, its expansion can only have the elements $\gamma^{\mu}C^{-1}$, $\sigma^{\mu\nu}C^{-1}$ and direct products of them. Since these elements are symmetric in pairs of indices, the rest of the symmetry properties of the multispinor impose more conditions in tensorial coefficients of the expansion.

For $n = 1,2,3$ the totally symmetric multispinors and their corresponding BWE lead to the Dirac, Proca, and Rarita–Schwinger equations, respectively.[15] For $n = 4$, the symmetry properties of the 4-rank multispinors lead to the following relation among the tensor coefficients that appear in the expansion:

$$X^{\mu\nu} = X^{\nu\mu}, \quad X^{\mu}{}_{\mu} = 0, \tag{3}$$

$$X^{[\mu\nu]\,[\rho\lambda]} = X^{[\rho\lambda]\,[\mu\nu]}, \quad X^{[\mu\nu]}{}_{[\mu\nu]} = 0,$$

$$\epsilon_{\mu\nu\rho\lambda}X^{[\mu\nu]\,[\rho\lambda]} = 0, \tag{4}$$

$$X^{[\mu\nu]}{}_{\nu} = 0, \quad \epsilon_{\mu\nu\rho\lambda}X^{[\nu\rho]\lambda} = 0, \tag{5}$$

$$X^{\mu\nu} = 4X^{[\mu\rho]}{}_{[\rho}{}^{\nu]}, \tag{6}$$

$$X^{[\mu\nu]\rho} = Y^{\rho[\mu\nu]}. \tag{7}$$

All the tensors can be obtained from $X^{[\mu\nu]\rho}$ and $X^{[\mu\nu]\,[\rho\lambda]}$. The 16 independent components of the first tensor and the 19 independent components of the second one are equal to the 35 independent components of the 4-rank multispinor. The BWE impose more conditions among the tensors, namely,

$$(p^2 - m^2)X^{\mu\nu} = 0, \quad p_{\mu}X^{\mu\nu} = 0, \tag{8}$$

$$X^{[\mu\nu]\rho} = -(i/2m)(p^{\mu}X^{\nu\rho} - p^{\nu}X^{\mu\rho}), \tag{9}$$

$$X^{[\mu\nu]\,[\rho\lambda]} = -(1/4m^2)[p^{\mu}(p^{\rho}X^{\nu\lambda} - p^{\lambda}X^{\nu\rho}) - p^{\nu}(p^{\rho}X^{\mu\lambda} - p^{\lambda}X^{\mu\rho})]. \tag{10}$$

TABLE I. YD = Young diagram, HW = Highest weight, N = Dimension of the representation.

YD	HW SU(4)	HW SO(6)	N	HW SO(5)	N	HW SO(4)	N
[1]	(3/4, − 1/4, − 1/4, − 1/4)	(1/2,1/2,1/2)	4	(1/2,1/2)	4	(1/2,1/2)	2
						(1/2, − 1/2)	2
[2]	(3/2, − 1/2, − 1/2, − 1/2)	(1, 1, 1)	10	(1, 1)	10	(1, 1)	3
						(1, 0)	4
						(1, − 1)	3
[1²]	(1/2,1/2, − 1/2, − 1/2)	(1, 0, 0)	6	(1, 0)	5	(1, 0)	4
						(0, 0)	1
				(0, 0)	1	(0, 0)	1
[3]	(9/4, − 3/4, − 3/4, − 3/4)	(3/2,3/2,3/2)	20	(3/2,3/2)	20	(3/2,3/2)	4
						(3/2,1/2)	6
						(3/2, − 1/2)	6
						(3/2, − 3/2)	4
[2,1]	(5/4,1/4, − 3/4, − 3/4)	(3/2,1/2,1/2)	20	(3/2,1/2)	16	(3/2,1/2)	6
						(3/2, − 1/2)	6
						(1/2,1/2)	2
						(1/2, − 1/2)	2
				(1/2,1/2)	4		
[1³]	(1/4,1/4,1/4, − 3/4)	(1/2,1/2, − 1/2)	4	(1/2,1/2)			
[4]	(3, − 1, − 1, − 1,)	(2, 2, 2)	35	(2, 2)	35	(2, 2)	5
						(2, 1)	8
						(2, 0)	9
						(2, − 1)	8
						(2, − 2)	5
[3,1]	(2, 0, − 1, − 1)	(2, 1, 1)	45	(2, 1)	35	(2, 1)	8
						(2, 0)	9
						(2, − 1)	8
						(1, 1)	3
						(1, 0)	4
						(1, 1)	3
				(1, 1)	10		
[2²]	(1, 1, − 1, − 1)	(2, 0, 0)	20	(2, 0)	14	(2, 0)	9
						(1, 0)	4
						(0, 0)	1
				(1, 0)	5		
				(0, 0)	1		
[2,1²]	(1, 0, 0, − 1)	(1, 1, 0)	15	(1, 1)	10		
				(1, 0)	5		
[1⁴]	(0, 0, 0, 0)	(0, 0, 0)	1	(0, 0)	1		

(8) together with (3) is equivalent to the Pauli–Fierz equations for a field of mass m and spin 2. Substituting (8), (9), and (10) in the expansion of the multispinor, we easily obtain

$$\psi^{\{\alpha\beta\gamma\delta\}} = \left[\frac{\gamma p + m}{m}\gamma^{\mu}C^{-1}\right]^{\alpha\beta}\left[\frac{\gamma p + m}{m}\gamma^{\nu}C^{-1}\right]^{\gamma\delta}X_{\{\mu\nu\}}, \quad (11)$$

a useful relation between the 4-rank multispinor and the traceless symmetric tensor of the Pauli-Fierz field of spin 2.[16]

For $n = 5$ we can carry out similar arguments, with the difference that the tensor coefficients should have a spinor index besides the normal tensor indices.

From the symmetry among the spinor indices one gets a set of relations similar to those of 4-rank multispinor [Eqs. (3)–(7)]. Besides, one obtains other constraints among the tensor coefficients, characteristic of odd-rank multispinors:

$$(\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{\{\mu\nu\}} = 0, \quad (\gamma^{\rho})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu\nu]\rho} = 0, \quad (12)$$

$$(\sigma^{\mu\nu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu\nu]\rho} = 0, \quad (13)$$

$$(\sigma^{\mu\nu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu\nu]\,[\rho\lambda\,]} = 0, \quad (14)$$

$$X^{\alpha}{}_{\{\nu\rho\}} = 2i(\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu\nu]\rho}, \quad (15)$$

$$X^{\alpha}{}_{[\nu\rho]\lambda} = 2i(\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu\lambda\,]\,[\nu\rho\,]}. \quad (16)$$

All these conditions can be derived from two of them, (14) and (16), which are 84 independent constraints. Thus we have finally $140 - 84 = 56$ independent components as it should correspond to a totally symmetric bispinor of rank 5.

The BWE gives similar results as in the case $n = 4$:

$$(p^2 - m^2)X^{\alpha}{}_{\mu\nu} = 0, \quad p^{\mu}X^{\alpha}{}_{\mu\nu} = 0, \quad (17)$$

$$X^{\alpha}{}_{[\mu\nu]\rho} = -(i/2m)(p_{\mu}X^{\alpha}{}_{\nu\rho} - p_{\nu}X^{\alpha}{}_{\mu\rho}) \quad (18)$$

$$X^{\alpha}{}_{[\mu\nu]\,[\rho\lambda\,]} = -(1/4m^2)[p_{\mu}(p_{\rho}X^{\alpha}{}_{\nu\lambda} - p_{\lambda}X^{\alpha}{}_{\nu\rho}) - p_{\nu}(p_{\rho}X^{\alpha}{}_{\mu\lambda} - p_{\lambda}X_{\mu\rho})] \quad (19)$$

All the tensors can be expressed in terms of the traceless symmetric tensor $X^{\alpha}{}_{\mu\nu}$. But (17) together with (2) is equivalent to the pair of equations

$$(\gamma p - m)^{\alpha}{}_{\beta}X^{\beta}{}_{\mu\nu} = 0, \quad (\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{\mu\nu} = 0, \quad (20)$$

which are the Rarita–Schwinger equations for a field of mass m and spin 5/2.

We can easily generalize the above results to the totally symmetric multispinors of rank n.

$n = 2r$

From the symmetries of the spinor indices, the symmetries of the tensor indices which appear in the expansion of the multispinor can be easily derived:

(i) $X_{\{\mu_1\cdots\mu_r\}}$ is a totally symmetric tensor and traceless for any pair of indices.

(ii) $X_{[\mu_1\mu_2]\cdots[\mu_{2k-1}\mu_{2k}]\{\mu_{2k+1}\cdots\mu_{r+k}\}}$, $k = 1,2,\ldots,r$

(a) is symmetric and traceless in the indices $\mu_{2k+1}\cdots\mu_{r+k}$,

(b) is antisymmetric in each pair of indices inside of any square bracket,

(c) is symmetric in the permutation of any pair of square brackets.

(iii) $X_{[\mu_1\mu_2]\cdots[\mu\nu]\cdots[\mu_{2k-1}\mu_{2k}]\{\mu_{2k+1}\cdots\mu_{r+k}\}} = 0.$ (21)

(iv) $\epsilon^{\lambda\mu\nu\rho}X_{[\mu_1\mu_2]\cdots[\mu\nu]\cdots[\mu_{2k-1}\mu_{2k}]\{\mu_{2k+1}\cdots\rho\cdots\mu_{r+k}\}} = 0.$ (22)

(v) $\epsilon^{\lambda\mu\nu\rho}X_{[\mu_1\mu_2]\cdots[\lambda\mu]\,[\nu\rho]\cdots[\mu_{2k-1}\mu_{2k}]\{\mu_{2k+1}\cdots\mu_{r+k}\}} = 0.$ (23)

All the tensor coefficients can be expressed, by contraction, in terms of the two independent tensors:

$X_{[\mu_1\mu_2]\cdots[\mu_{2r-3}\mu_{2r-2}]\mu_{2r-1}}$ and $X_{[\mu_1\mu_2]\cdots[\mu_{2r-1}\mu_{2r}]}$.

From the BWE we can obtain the general relations

$$(p^2 - m^2)X_{\{\mu_1\cdots\mu_r\}} = 0, \quad p^{\mu}X_{\{\mu\mu_2\cdots\mu_r\}} = 0, \quad (24)$$

$$X_{[\mu_1\mu_2]\{\mu_3\cdots\mu_{r+1}\}} = -(i/2m)(p_{\mu_1}X_{\{\mu_2\cdots\mu_{r+1}\}} - p_{\mu_2}X_{\{\mu_1\cdots\mu_{r+1}\}}), \quad (25)$$

$$X_{[\mu_1\mu_2]\{\mu_3\mu_4\}\{\mu_5\cdots\mu_{r+1}\}} = (-i/2m)^2[p_{\mu_1}(p_{\mu_3}X_{\{\mu_2\mu_4\cdots\mu_{r+2}\}} - p_{\mu_4}X_{\{\mu_2\mu_3\mu_5\cdots\mu_{r+2}\}})] - p_{\mu_2}(p_{\mu_3}X_{\{\mu_1\mu_4\cdots\mu_{r+2}\}} - p_{\mu_4}X_{\{\mu_1\mu_3\cdots\mu_{r+2}\}})], \quad (26)$$

$\cdots$

Equations (24) are equivalent to the Pauli–Fierz equation for a field of mass m and spin r. From (24) and (25) we can also prove by induction the relation between the totally symmetric multispinor of BWE and the totally symmetric tensor of Pauli–Fierz equations:

$$\psi^{\{\alpha_1\alpha_2\cdots\alpha_{2r}\}} = \prod_{k=1}^{r}\left[\frac{\gamma p + m}{m}\gamma^{\mu_k}C^{-1}\right]^{\alpha_{2k-1}\alpha_{2k}}X_{\{\mu_1\cdots\mu_r\}}. \quad (27)$$

$n = 2r + 1$

The symmetries of the tensorial indices $\mu_1\cdots\mu_{2r}$ are completely equivalent to those of tensor coefficients in the expansion of multispinors of rank $2r$; see Eqs. (21)–(23). For the symmetries of the multispinor index α_{2r+1}, we state the following result:

$$(\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{\{\mu\mu_2\cdots\mu_r\}} = 0, \quad (28)$$

$$(\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu_1\mu_2]\cdots[\mu_{2k-1}\mu_{2k}]\{\mu\mu_{2k+2}\cdots\mu_{k+r}\}} = 0, \quad 1\leqslant k\leqslant r-1, \quad (29)$$

$$(\sigma^{\mu\nu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu_1\mu_2]\cdots[\mu\nu]\cdots[\mu_{2k-1}\mu_{2k}]\{\mu_{2k+1}\cdots\mu_{k+r}\}} = 0, \quad 1\leqslant k\leqslant r, \quad (30)$$

$$X^{\alpha}{}_{\{\mu_1\cdots\mu_r\}} = 2i(\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu\mu_1]\{\mu_2\cdots\mu_r\}}, \quad (31)$$

$$X^{\alpha}{}_{[\mu_1\mu_2]\{\mu_3\cdots\mu_{r+1}\}} = 2i(\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{[\mu\mu_1]\,[\mu_1\mu_2]\{\mu_3\cdots\mu_{r+1}\}}, \quad (32)$$

$\cdots$

The BWE give rise to equivalent relations among the tensorial coefficients to those of multispinors of rank $2r$. See (24)–(26). It means that all the tensors can be expressed in terms of $X^{\alpha}{}_{\{\mu_1\cdots\mu_r\}}$. This tensor spinor satisfies

$$(\gamma p - m)^{\alpha}{}_{\beta}X^{\beta}{}_{\{\mu_1\cdots\mu_r\}} = 0, \quad (\gamma^{\mu})^{\alpha}{}_{\beta}X^{\beta}{}_{\{\mu\mu_2\cdots\mu_r\}} = 0,$$

which are the Rarita–Schwinger equation for a field of mass m and spin $s = r + \frac{1}{2}$. We have obtained a relation between the totally symmetric multispinor of rank $2r + 1$ and the symmetric traceless tensor-spinor of Rarita–Schwinger, namely,

$$\psi^{\{\alpha_1\cdots\alpha_{2r+1}\}} = \prod_{k=1}^{r}\left[\frac{\gamma p + m}{m}\gamma^{\mu_k}C^{-1}\right]^{\alpha_{2k-1}\alpha_{2k}}X^{\alpha_{2r+1}}{}_{\{\mu_1\cdots\mu_r\}}. \quad (33)$$

C. Lorentz content of multispinors

As we have said $\psi^{\{\alpha_1\cdots\alpha_n\}}$ can be considered as a tensor of a space in which acts some representation of the SU(2,2) group, with Young diagram $[n,0,0]$. The equivalent repre-

sentation of SO(4,2) will have the highest weight $(n/2, n/2, n/2)$. In the restriction of SO(4,2) to SO(3,1) this representation decomposes as follows:

$$(n/2,n/2)\oplus(n/2,n/2-1)\oplus\cdots\oplus(n/2,-n/2+1)\otimes(n/2,-n/2).$$

Our task is to know which of these representations of SO(3,1) is associated with the tensor coefficients in the expansion of multispinors.

We distinguish two cases

$n=2r$: Using the spinor notation[17] of the Lorentz group (k,l) the decomposition reads

$$[(r,0)\oplus(0,r)]\oplus[(r-\tfrac{1}{2},\tfrac{1}{2})\oplus(\tfrac{1}{2},r-\tfrac{1}{2})]\oplus\cdots\oplus\left[\left(\frac{r+1}{2},\frac{r-1}{2}\right)\oplus\left(\frac{r-1}{2},\frac{r+1}{2}\right)\right]\oplus\left(\frac{r}{2},\frac{r}{2}\right)$$

the tensor coefficients are associated with one or several irreducible representations (of the complete Lorentz group) of the above decomposition: $X_{\{\mu_1\cdots\mu_r\}}$ transforms under SO(3,1) according to the representation $(r/2,r/2)$:

$X_{[\mu_1\mu_2]\{\mu_3\cdots\mu_{r+1}\}}$ transforms according to

$$\left(\frac{r+1}{2},\frac{r-1}{2}\right)\oplus\left(\frac{r-1}{2},\frac{r+1}{2}\right),$$

$X_{[\mu_1\mu_2]\{\mu_3\mu_4\}\{\mu_5\cdots\mu_{r+2}\}}$ with

$$\vdots\quad\left[\left(\frac{r+2}{2},\frac{r-2}{2}\right)\oplus\left(\frac{r-2}{2},\frac{r+2}{2}\right)\right]\oplus\left(\frac{r}{2},\frac{r}{2}\right),$$

$X_{[\mu_1\mu_2]\cdots[\mu_{2r-3}\mu_{2r-2}]\mu_{2r-1}}$ with $[(r-\tfrac{1}{2},\tfrac{1}{2})\oplus(\tfrac{1}{2},r-\tfrac{1}{2})]\oplus\left[\left(r-\frac{3}{2},\frac{3}{2}\right)\oplus\left(\frac{3}{2},r-\frac{3}{2}\right)\right]$

$$\oplus\cdots\oplus\begin{cases}\left(\frac{r}{2},\frac{r}{2}\right) & \text{if } r \text{ is odd}\\ \left(\frac{r+1}{2},\frac{r-1}{2}\right)\oplus\left(\frac{r-1}{2},\frac{r+1}{2}\right) & \text{if } r \text{ is even,}\end{cases}$$

$X_{[\mu_1\mu_2]\cdots[\mu_{2r-1}\mu_{2r}]}$ with $[(r,0)\oplus(0,r)]\oplus[(r-1,1)\oplus(1,r-1)]\oplus\cdots$

$$\oplus\begin{cases}\left(\frac{r+1}{2},\frac{r-1}{2}\right)\oplus\left(\frac{r-1}{2},\frac{r+1}{2}\right) & \text{if } r \text{ is odd}\\ \left(\frac{r}{2},\frac{r}{2}\right) & \text{if } r \text{ is even.}\end{cases}$$

$n=2r+1$: In this case the Lorentz content of the totally symmetric multispinor is as follows:

$$[(r+\tfrac{1}{2},0)\oplus(0,r+\tfrac{1}{2})]\oplus[(r,\tfrac{1}{2})\oplus(\tfrac{1}{2},r)]\oplus\cdots\oplus[(r/2+1,r/2-\tfrac{1}{2})\oplus(r/2-\tfrac{1}{2},r/2+1)]\oplus[(r/2+\tfrac{1}{2},r/2)\oplus(r/2,r/2+\tfrac{1}{2})].$$

The Lorentz content of the tensor spinors is easily obtained and gives

$X^{\alpha}{}_{\{\mu_1\cdots\mu_r\}}$ transforms according to Δ_r,

$X^{\alpha}{}_{[\mu_1\mu_2]\{\mu_3\cdots\mu_{r+1}\}}$ transforms according to Δ_{r+1},

$\vdots$

$X^{\alpha}{}_{[\mu_1\mu_2]\cdots[\mu_{2r-3}\mu_{2r-2}]\mu_{2r-1}}$ transforms according to Δ_{2r-1},

$X^{\alpha}{}_{[\mu_1\mu_2]\cdots[\mu_{2r-1}\mu_{2r}]}$ transforms according to Δ_{2r},

where

$$\Delta_r=\left(\frac{r+1}{2},\frac{r}{2}\right)\oplus\left(\frac{r}{2},\frac{r+1}{2}\right),$$

$$\Delta_{r+1}=\left[\left(\frac{r+2}{2},\frac{r-1}{2}\right)\oplus\left(\frac{r-1}{2},\frac{r+2}{2}\right)\right]\oplus\Delta_r,$$

$$\Delta_{r+1}=\left[\left(\frac{r+2}{2},\frac{r-1}{2}\right)\oplus\left(\frac{r-1}{2},\frac{r+2}{2}\right)\right]\oplus\Delta_r,$$

$$\vdots$$

$$\Delta_{2r}=[(r+\tfrac{1}{2},0)\oplus(0,r+\tfrac{1}{2})]\oplus\Delta_{2r-1}.$$

III. BARGMANN–WIGNER EQUATIONS FOR MULTISPINORS OF MIXED SYMMETRIES

A. Uniqueness of mass and spin

In the case of not totally symmetric multispinors, due to the unimodularity of the SU(2,2) group, only those Young diagrams with three or less rows must be considered. But when we apply BWE to the multispinors with a Young diagram of three rows, we get zero solution. In fact, let ψ be a multispinor of n rank with three antisymmetric indices at least, in one column. In the rest system, the multispinor ψ satisfies

$$(\gamma^0\pm 1)^{\alpha}{}_{\alpha_i}\psi^{\alpha_1\cdots\alpha_i\cdots\alpha_n}=0. \tag{34}$$

Using a representation for γ's in which $\gamma^0=\mathrm{diag}(1,1,-1,-1)$, we immediately see that indices α_1, α_2, ..., α_n can take the values 1 or 2 in the case of positive energy solutions [lower sign of (34)], and 3 or 4 in the case of negative energy solutions [upper sign of (34)]. But when the Young diagram has three antisymmetric indices in one column, we have to use three different values which is impossible; therefore, the multispinor must vanish.

Thus we are left with multispinors the Young diagrams of which have only two rows. It is still possible to achieve more simplification. Let ψ be a multispinor of rank n corresponding to positive energy solutions. In the rest system ψ transforms as an irreducible representation of SU(2). Due to the unimodularity of this group, all the Young diagrams with two rows are equivalent to diagrams of one row, which are obtained by elimination of columns with two boxes.

For these reasons the multispinors of mixed symmetries also correspond to systems of unique spin as in the case of totally symmetric multispinors.

The uniqueness of mass of these multispinors with two rows in obvious from the BWE.

B. Symmetry properties and equations of motion

The simplest Young diagrams with mixed symmetry $[1^2]$ and [2,1] have been studied thoroughly.[18] For the diagram [3,1] the multispinor can be expanded in the Λ_k basis.

From the symmetry properties of the spinor indices and

$$\psi^{[\alpha_1\alpha_2]\{\alpha_3\alpha_4\}}+\psi^{[\alpha_2\alpha_3]\{\alpha_4\alpha_1\}}+\psi^{[\alpha_3\alpha_1]\{\alpha_2\alpha_4\}}=0, \tag{35}$$

one obtains the following relations among the tensorial coefficients[19]:

$$X^{\mu}=i\epsilon^{\mu\nu\rho\lambda}X_{5\nu[\rho\lambda]},\quad X_{5\mu}=2iX^{\rho}{}_{5[\rho\mu]}, \tag{36}$$

$$X^{[\mu\nu]}=-\tfrac{1}{2}\epsilon^{\lambda\tau\mu\nu}(X_{5[\lambda\tau]}+iY_{5\lambda\tau}),\quad Y_{5\mu}{}^{\mu}=0; \tag{37}$$

and from BWE, we get more conditions:

$$X_\mu = X_{[\mu\nu]} = 0, \tag{38}$$

$$Y_{5\mu\nu} = (1/m)p_\mu X_{5\nu}, \tag{39}$$

$$X_{5[\mu\nu]} = -(i/2m)(p_\mu X_{5\nu} - p_\nu X_{5\mu}), \tag{40}$$

$$X_{5\mu[\nu\rho]} = -(i/2m^2)p_\mu (p_\nu X_{5\rho} - p_\rho X_{5\nu}), \tag{41}$$

with

$$(p^2 - m^2)X_{5\mu} = 0, \quad p^\mu X_{5\mu} = 0. \tag{42}$$

Therefore all the coefficients can be expressed in terms of $X_{5\mu}$, which represents a field of spin 1. From (38)–(42) we can easily get the relation between the symmetric multispinor and the tensor $X_{5\mu}$, namely,

$$\psi^{[\alpha_1\alpha_2]\{\alpha_3\alpha_4\}} = \left[\frac{\gamma p + m}{m}\gamma^5 C^{-1}\right]^{\alpha_1\alpha_2} \times \left[\frac{\gamma p + m}{m}\gamma^\mu C^{-1}\right]^{\alpha_3\alpha_4} X_{5\mu}. \tag{43}$$

For the Young diagram [2,2] we have the following constrains for the 4-rank multispinor:

$$\psi^{[\alpha\beta][\gamma\delta]} + \psi^{[\alpha\gamma][\delta\beta]} + \psi^{[\alpha\delta][\beta\gamma]} = 0, \tag{44}$$

$$\psi^{[\alpha\beta][\gamma\delta]} = \psi^{[\gamma\delta][\alpha\beta]}. \tag{45}$$

From the symmetry of the spinor indices, we obtain

$$X_5 = Y_5, \quad X_{5\mu} = Y_{5\mu}, \quad X_{55\mu} = Y_{55\mu}, \quad X_{55\mu\nu} = X_{55\nu\mu}, \tag{46}$$

$$X + X_{55} - X_{55}{}^\mu{}_\mu = 0, \tag{47}$$

and, after the application of BWE, we get

$$X = X_5 = X_{5\mu} = 0, \tag{48}$$

$$X_{55\mu} = (1/m)p_\mu X_{55}, \quad X_{55\mu\nu} = (1/m^2)p_\mu p_\nu X_{55}, \tag{49}$$

$$(p^2 - m^2)X_{55} = 0. \tag{50}$$

Therefore the tensor X_{55} represents a field of zero spin, as expected. From (48)–(50) one easily obtains

$$\psi^{[\alpha_1\alpha_2][\alpha_3\alpha_4]} = \left[\frac{\gamma p + m}{m}\gamma^5 C^{-1}\right]^{\alpha_1\alpha_2} \times \left[\frac{\gamma p + m}{m}\gamma^5 C^{-1}\right]^{\alpha_3\alpha_4} X_{55}. \tag{51}$$

We can easily generalize the last equations for the bispinors with arbitrary Young diagram of two rows:

$$[s + 2r, s]: \psi^{[\alpha_1\alpha_2]\,[\alpha_{2s}\,\alpha_{2s}]\{\alpha_{2s+1}\cdots\alpha_{2(s+r)}\}} = \prod_{i=1}^{s}\left[\frac{\gamma p + m}{m}\gamma^5 C^{-1}\right]^{\alpha_{2i-1}\alpha_{2i}} \times \prod_{j=1}^{r}\left[\frac{\gamma p + m}{m}\gamma^{\mu_j} C^{-1}\right]^{\alpha_{2(s+j)-1}\alpha_{2(s+j)}} X_{5\cdots5\{\mu_1\cdots\mu_r\}}, \tag{52}$$

where $X_{5\cdots5\{\mu_1\cdots\mu_r\}}$ is a tensor totally symmetric and traceless in the tensor indices satisfying

$$(p^2 - m^2)X_{5\cdots5\{\mu_1\cdots\mu_r\}} = 0, \quad p^{\mu_1} X_{5\cdots5\{\mu_1\cdots\mu_r\}} = 0, \tag{53}$$

$$[s + 2r + 1, s]: \psi^{[\alpha_1\alpha_2]\cdots[\alpha_{2s}\,\alpha_{2s}]\{\alpha_{2s+1}\cdots\alpha_{2(s+r+1)}\}} = \prod_{i=1}^{s}\left[\frac{\gamma p + m}{m}\gamma^5 C^{-1}\right]^{\alpha_{2i-1}\alpha_{2i}} \times \prod_{j=1}^{r}\left[\frac{\gamma p + m}{m}\gamma^{\mu_j} C^{-1}\right]^{\alpha_{2(s+j)-1}\alpha_{2(s+j)}} X^{\alpha_{2(s+r)+1}}_{5\cdots5\{\mu_1\cdots\mu_r\}}, \tag{54}$$

where $X^\alpha{}_{5\cdots5\{\mu_1\cdots\mu_r\}}$ is a tensor spinor totally symmetric and traceless in its tensor indices, and satisfies the equation of motion

$$(\gamma p - m)X_{5\cdots5\{\mu_1\cdots\mu_r\}} = 0, \quad (\gamma^\mu)^\alpha{}_\beta X^\beta{}_{5\cdots5\{\mu\mu_2\cdots\mu_r\}} = 0, \tag{55}$$

corresponding to a field of spin $r + \frac{1}{2}$.

C. Lorentz content of the tensor coefficients

(a) Young diagram $[r,r]$. The SO(4,2) representation associated with this tableau is $(r,0,0)$, which decomposes, when it is restricted to SO(3,1), into

$$\left(\frac{r}{2},\frac{r}{2}\right) \oplus 2\left(\frac{r-1}{2},\frac{r-1}{2}\right) \oplus \cdots \oplus r(\tfrac{1}{2},\tfrac{1}{2}) \oplus (r+1)(0,0).$$

The following tensors transform according to the representation (0,0):

$$X, X_5, X_{55}, \ldots, \underbrace{X_{55\cdots5}}_{r\text{ times}},$$

which are equal among themselves. With respect to the representation $(\frac{1}{2},\frac{1}{2})$ we have the following tensors:

$$X_{5\mu}, X_{55\mu}, \ldots, \underbrace{X_{55\cdots5\mu}}_{r\text{ times}} \quad \text{and so on.}$$

Two tensors,

$$\underbrace{X_{55\cdots5\{\mu_1\cdots\mu_{r-1}\}}}_{r-1} \quad \text{and} \quad \underbrace{X_{55\cdots5\{\mu_1\cdots\mu_r\}}}_{r},$$

contain in their representations $[(r-1)/2, (r-1)/2]$, and finally the Lorentz content of $X_{\{\mu_1\cdots\mu_r\}}$ has among its components the representation $(r/2,r/2)$.

(b) Young diagram $[r,r-1]$. The weight is $(r - \frac{1}{2},\frac{1}{2},\frac{1}{2})$ which, when restricted to Lorentz group, decomposes into

$$\left[\left(\frac{r}{2},\frac{r-1}{2}\right) \oplus \left(\frac{r-1}{2},\frac{r}{2}\right)\right] \oplus 2\left[\left(\frac{r-1}{2},\frac{r-2}{2}\right) \oplus \left(\frac{r-2}{2},\frac{r-1}{2}\right)\right] \oplus \cdots \oplus (r-1)[(1,\tfrac{1}{2}) \oplus (\tfrac{1}{2},1)] \oplus r[(\tfrac{1}{2},0) \oplus (0,\tfrac{1}{2})].$$

$X^\alpha{}_{55\cdots5}$ transforms with $(\frac{1}{2},0) \oplus (0,\frac{1}{2})$, and we can carry out similar arguments as in (a) for the multiplicities of the representations.

(c) The diagram $[r,r-k]$, $0 < k < r$, k = even, are studied in a similar way.

(d) The diagram $[r,r,-k]$, $0 < k < r$, k = odd, follows techniques similar to case (b), but here the condition $(\gamma^\mu)^\alpha{}_\beta X^\beta{}_{5\cdots5} = 0$ eliminates representations of lower spin.

IV. CONCLUDING REMARKS

In the preceding chapters we have achieved a detailed analysis of the BWE from the group theoretical point of view: the decomposition of multispinors, carrying a irreducible representation of the conformal group, in terms of tensors of the Lorentz group contained in the conformal group; closed formulas for the symmetries of these tensors and the equations of motion of elementary systems associated with irreducible representations of the Poincaré group[20]; the relation between the BWE and the Pauli–Fierz equations for integer spin and the Rarita–Schwinger for half-integer spin particles. Although BWE are restricted to totally symmetric

multispinors, in our analysis they have been extended to multispinors of mixed symmetry corresponding to all allowed Young diagrams.

The above study is obviously necessary to attack the problem of covariant Lagrangians of elementary systems of arbitrary spin. The Lagrangian with first order derivatives of the tensor fields with the help of auxiliary field have been obtained by Singh and Hagen[21] for massive particles of arbitrary spin and by Fronsdal[22] for massless particles.

The Lagrangian in terms of the multispinors leading to the BWE has been worked out in the case of 3/2-spin particles by Guralnik and Kibble[23] with some minor errors corected by Gupta and Repko.[24] Another Lagrangian for zero spin in terms of 4-rank multispinor has been described by Larsen and Repko[24]; the same authors have introduced general principles for the construction of Lagrangians with the help of irreducible operators of the symmetric group, but no closed formulas have been proved for these Lagrangians. One thing becomes evident in their analysis: the need for mixed symmetry multispinors, the analysis of which has been worked out in our paper. Investigations in the complete study of the general Lagrangian for the BWE, and their relation to the Lagrangian obtained by Singh and Hagen, are in progress.

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$$k = \tfrac{1}{2}(m_1 + m_2), \quad l = \tfrac{1}{2}(m_1 - m_2)$$

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On the mass operators for multiquark systems

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The vector space of tensor operators transforming according to the adjoint representation of the unitary group is investigated for arbitrary (even infinite) dimension of the group. In particular, a natural basis consisting of generalized number operators is constructed and some properties are studied. The results are applied to the construction of mass operators for arbitrary multiquark systems with arbitrary dimsension of the one-quark flavor space. It is shown, also, how the proved properties of the spectrum simplify the obtaining of certain mass formulas.

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1. INTRODUCTION

In the original theory of unitary symmetry, the mass operator of the hadrons was assumed to be a linear combination of operators which were the images of certain tensor operators. These tensor operators transformed according to the adjoint or trivial representations of the group SU(3) (see, e.g., Ref. 1).

In the quark theory, the mass operator was constructed by means of a potential which includes all SU(3)-invariant combinations; this is in fact equivalent to the use of tensor operators of the same type (Sec. 5).

It is clear, however, that SU(3) tensor operators are not sufficient to describe the masses of the new (e.g., charmed) particles.

The aim of this paper is to investigate the analogous tensor operators for arbitrary dimension (even infinite) of the unitary group. More precisely, let H be a separable Hilbert space and let $\overline{H}$ be the space conjugate (anti-isomorphic) to H. These spaces can describe, for example, the one-quark flavor states.

We shall denote by

$$H^{N_1}\otimes\overline{H}^{N_2}:=H\otimes\cdots\otimes H\otimes\overline{H}\otimes\cdots\otimes\overline{H}\,,$$

the tensor space which we assume to describe the states of the system composed of N_1 quarks and N_2 antiquarks. The natural unitary representation U of the unitary (flavor) group $\mathrm{U}(H)$ acts in the space $H^{N_1}\otimes\overline{H}^{N_2}$:

$$\mathrm{U}(H)\ni v\to \mathrm{U}_v(x_1\otimes\cdots\otimes x_{N_1}\otimes\bar{y}_1\otimes\cdots\otimes\bar{y}_{N_2}):$$
$$=(vx_1)\otimes\cdots\cdots\otimes(\bar{v}\bar{y}_{N_2})\,,$$

where by bar we denote also the mapping $B(H)\ni A\to\overline{A}\in B(\overline{H})$ between the bounded operators on H and $\overline{H}$ which corresponds to the assumed anti-isomorphism, i.e., $\overline{A}\bar{y}:=\overline{Ay}, \bar{y}\in\overline{H}$.

Let K be a U-invariant (not necessarily irreducible) closed subspace of $H^{N_1}\otimes\overline{H}^{N_2}$ and let us denote the restriction of U to K also by U. We shall investigate the vector space $V(H,K)$ of all linear mappings

$$\mathfrak{N}:\ B(H)\to B(K),$$

which for any A in $B(H)$ and any v in $\mathrm{U}(H)$ satisfy

$$\mathfrak{N}(vAv^{-1})=\mathrm{U}_v\mathfrak{N}(A)\mathrm{U}_v^{-1}\,. \tag{1.1}$$

In other words, the elements of $V(H,K)$ intertwine the representation of $\mathrm{U}(H)$ in $B(H)$, defined by the conjugations $A\to vAv^{-1}$, with the analogous representation of $U(H)$, which is defined in $B(K)$ by means of U_v.

If $\dim H=n<\infty$, then the space $B(H)=H\otimes\overline{H}$ decomposes under the action of $\mathrm{U}(n)$ into the direct sum of the adjoint representation of $\mathrm{SU}(n)$ and the trivial representation. So it is clear that for any finite-dimensional H the space $V(H,K)$ consists exactly of the tensor operators mentioned above.

The simplest example of a mapping satisfying (1.1) for $\dim H\leqslant\infty$ is the tangent mapping to the representation U restricted to the subspace K. Let us notice that this tangent mapping, say $\tilde{\mathfrak{N}}$, can be decomposed as follows:

$$\tilde{\mathfrak{N}}=\sum_{i=1}^{N_1}\tilde{\mathfrak{N}}^i-\sum_{i=N_1+1}^{N_1+N_2}\tilde{\mathfrak{N}}^i\,,$$

where the mappings $\tilde{\mathfrak{N}}^i$ for $i=1,\ldots,N_1$ are given by the formula

$$B(H)\ni A\to\tilde{\mathfrak{N}}^i(A):=I\otimes\cdots\otimes I\otimes\overset{i}{A}\otimes I\otimes\cdots$$
$$\otimes I\otimes\overline{I}\otimes\cdots\otimes\overline{I}\,,$$

where $I:=I_H$ is the identity operator in H, and for $i=N_1+1,\ldots,N_1+N_2$ by the analogous formula with $\overline{A}$ instead of A. Of course (1.1) implies

$$\mathfrak{N}([A,B])=[\tilde{\mathfrak{N}}(A),\mathfrak{N}(B)]\,, \tag{1.1'}$$

for any $\mathfrak{N}$ in $V(H,K)$ and A,B in $B(H)$. Unlike the tangent mapping, the mappings $\tilde{\mathfrak{N}}^i$, $i=1,\ldots,N_1+N_2$, do not transform any U-invariant subspace of $H^{N_1}\otimes\overline{H}^{N_2}$ into itself. But by using the orthogonal projections onto U-invariant subspaces we can construct the elements of $V(H,K)$. Namely we have:

Lemma 1: Let the notation be as above, let L and M be U-invariant subspaces contained in K, and let us denote by the same capital letter the orthogonal projection onto the subspace. Then for arbitrary-dimension of H the mappings

$$(\mathfrak{LM})^i:\ B(H)\ni A\to(\mathfrak{LM})^i(A):=L\tilde{\mathfrak{N}}^i(A)M,\quad i=1\cdots N_1+N_2\,, \tag{1.2}$$

belong to the space $V(H,K)$.

Proof: Every mapping $\tilde{\mathfrak{N}}^i$ belongs to $V(H,H^{N_1}\otimes\overline{H}^{N_2})$ because it satisfies Eq. (1.1) on any simple tensor from the space $H^{N_1}\otimes\overline{H}^{N_2}$. This together with the fact that the orthogonal projections L and M commute with U implies

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the assertion.

In the case where $L=M$ the mapping $(\mathfrak{L}\mathfrak{L})^i$ shall be denoted just by $\mathfrak{L}^i$.

Now, let $\{x_j\}_{j=1}^{\dim H}$ be an orthonormal basis for H and let P_{x_j} be the orthogonal projection onto the vector x_j. By $\mathfrak{L}^i_j := \mathfrak{L}^i(P_{x_j})$ we shall denote the image of P_{x_j} under the mapping $\mathfrak{L}^i$. The symbols $(\mathfrak{L}\mathfrak{M})^i_j$, $\tilde{\mathfrak{N}}_j$, etc., shall have analogous meanings.

The content of the paper is the following: In Sec. 2 we obtain for $\dim H<\infty$ and for an arbitrary U-invariant subspace K the formula which express the dimension of the space $V(H,K)$ in terms of Young tableaux. In Sec. 3 we show for $\dim H\leqslant\infty$ which of the mappings $(\mathfrak{L}\mathfrak{M})^i$, $\mathfrak{L}^i$, etc., are linearly independent. Next using the results of Sec. 2 we prove that if $\dim H<\infty$ then these linearly independent mappings together with trivial mapping of type $B(H)\ni A\to \mathrm{Tr}(A)\cdot I$ form a basis for the space $V(H,K)$. In Sec. 5 we show how in the particular case $\dim H=3$ the mass operators can be expressed as linear combinations of the operators $\mathfrak{L}^i_j$ and $(\mathfrak{L}\mathfrak{M})^i_j+(\mathfrak{M}\mathfrak{L})^i_j$.

This form of mass operator enables us to interpret the mass of hadrons in terms of the number of quarks. Namely the images $\mathfrak{K}^i(P_x)$ of one-dimensional projections P_x in $B(H)$ have (for $\dim H\leqslant\infty$) the following interpretation: The expression $(\Psi|\mathfrak{K}^i(P_x)\Psi)$ is equal to the number of quarks (or antiquarks) in the state x which are contained in the multiparticle tensor state Ψ in K in the position labeled by i. Of course the total number of quarks and antiquarks in the state x is given by $\sum_{i=1}^{N_1+N_2}\mathfrak{K}^i(P_x)$. So we can say that the assumption that mass operators are built of tensor operators of the mentioned above type is equivalent to the assumption that the mass of a hadron is equal to the sum of the masses of labeled (by position) quarks where the mass of a labeled quark can depend on its label.

In our previous paper (Ref. 2) it was shown that the space $V(H,K)$ is closely connected with the notion of general number operators. In fact the mappings $\mathfrak{K}^i$ and $(\mathfrak{L}\mathfrak{M})^i+(\mathfrak{M}\mathfrak{L})^i$ are the general number operators. In other words, in addition to (1.1) they satisfy:

Lemma 2: Let the assumptions be as in Lemma 1. Then

(a) the mappings $\mathfrak{L}^i$, $\mathfrak{K}^i$, and $(\mathfrak{L}\mathfrak{M})^i$ are ultraweakly-weakly (even weakly-weakly) continuous.

(b) $\mathfrak{L}^i$, $\mathfrak{K}^i$, and $(\mathfrak{L}\mathfrak{M})^i+(\mathfrak{M}\mathfrak{L})^i$ are positivity preserving mappings.

(c) $\mathfrak{K}^i(I_H)=I_K$ and $((\mathfrak{L}\mathfrak{M})^i+(\mathfrak{M}\mathfrak{L})^i)(I_H)=0$.

Proof:

(a) Let $(A_k)_{k=1}^{\infty}$ converge weakly to A in $B(H)$. Then for any simple tensor Φ in $H^{N_1}\otimes\overline{H}^{N_2}$, $(\Phi|\tilde{\mathfrak{N}}^i(A_k)\Phi)\xrightarrow[k\to\infty]{}(\Phi|\tilde{\mathfrak{N}}^i(A)\Phi)$. So the $\tilde{\mathfrak{N}}^i$ are weakly-weakly continuous and hence also the mappings $\mathfrak{L}^i$, $\mathfrak{K}^i$, and $(\mathfrak{L}\mathfrak{M})^i$.

(b) and (c) follow immediately from the definitions of the mappings considered.

In this way we try to establish links between the unitary flavor group, the postulate of indistinguishability, and some postulates of quantum mechanics which we used in Ref. 2.to define the general number operators.

In Sec. 4 we investigate for irreducible L some properties of the spectrum of the operators $\mathfrak{L}^i_j$ and next in Sec. 5 we show how these properties simplify obtaining some mass formulas. In Sec. 6 we prove that every number operator acting in a U-invariant subspace $\mathfrak{K}$ of H^N ($\dim H=\infty$) is a linear combination of the mappings $\mathfrak{L}^i$, $\mathfrak{M}^i$, $(\mathfrak{L}\mathfrak{M})^i+(\mathfrak{M}\mathfrak{L})^i$, etc., $i=1,\ldots,N$.

2. THE DIMENSION OF THE SPACES $V(H,K)$ FOR $\dim H<\infty$

In this section we shall consider the case $1<\dim H=n<\infty$. It is well known that if $\dim H<\infty$, the natural representation of $\mathrm{U}(n)$ acting in a subspace of $H^{N_1}\otimes\overline{H}^{N_2}$, is equivalent to the direct sum of irreducible representations which act in the tensor space H^N with $N=N_1+(n-1)N_2$. (See Ref. 3). Each of these irreducible representations is given by the restriction of a representation of the type

$$\mathrm{U}(n)\ni v\to \mathrm{U}'_v := (\det v)^m \mathrm{U}_v\,, \tag{2.1}$$

with $m=-N_2$, where by U we denote the natural representation of $\mathrm{U}(n)$ in H^N. To avoid misunderstanding of the notation in this section, U shall denote only the representation in H^N. It is also clear that the subspace $K\subset H^N$ is U-invariant if and only if it is U′-invariant.

The integer power of the determinant shifts the images of the tangent mapping $\tilde{\mathfrak{N}}$. Namely if by $\tilde{\mathfrak{N}}^0$ we denote the mapping

$$B(H)\ni A\to\tilde{\mathfrak{N}}^0(A):=\mathrm{Tr}(A)\cdot I_{H^N}\,, \tag{2.2}$$

which obviously belongs to $V(H,H^N)$, then the tangent mapping $\tilde{\mathfrak{N}}'$ to the representation U′ is equal to

$$\tilde{\mathfrak{N}}'=\tilde{\mathfrak{N}}+m\cdot\tilde{\mathfrak{N}}^0\,. \tag{2.3}$$

The representations U and U′ define (by conjugation) the same representation in $B(H^N)$ and therefore for any $K\subset H^N$ the space $V(H,K)$ is equal to the analogous space of intertwiners obtained by means of the representation U′. Therefore if $\dim H<\infty$ it is sufficient to deal with the spaces H^N (N arbitrary).

Notice that in the finite-dimensional case $B(K)$ can be identified with $K\otimes\overline{K}$, and hence the representation of $\mathrm{U}(n)$ in $B(K)$ is equivalent to $\mathrm{U}|_K\otimes\overline{\mathrm{U}}|_{\overline{K}}$, where $\overline{\mathrm{U}}$ is the representation contragradient to U. Let $K=\oplus_{i=1}^{p}L_i$ where L_i are irreducible subspaces.

It is clear that to compute $\dim V(H,K)$ it is sufficient to know the dimensions of the vector spaces V_{ij} $(i,j=1,\ldots,p)$ consisting of all linear mappings which intertwine the representation of $\mathrm{U}(n)$ in $B(H)=H\otimes H$ with the representation acting in $L_i\otimes\overline{L}_j$.

In other words for any $\mathfrak{N}\in V_{ij}$ and $v\in\mathrm{U}(n)$ the following diagram should be commutative:

$$\begin{array}{ccc} H\otimes\overline{H} & \xrightarrow[\mathfrak{N}]{} & L_i\otimes\overline{L}_j \\ v\otimes\overline{v}\ \downarrow & & \downarrow\ \mathrm{U}_v|_{L_i}\otimes\overline{\mathrm{U}}_v|_{\overline{L}_j} \\ H\otimes\overline{H} & \xrightarrow[\mathfrak{N}]{} & L_i\otimes\overline{L}_j \end{array}\,. \tag{2.4}$$

The space $L_i\otimes\overline{L}_j$ is isomorphic with the set of all bounded operators from L_j to L_i. Therefore for any $\mathfrak{N}$ in V_{ij} we can define the mapping

$$\mathfrak{N}'\colon L_j\otimes H\otimes\overline{H}\to L_i\,,$$

by the formula

$$\mathfrak{N}'(\Psi\otimes x\otimes\overline{y}) := \mathfrak{N}(x\otimes\overline{y})\Psi,\quad x\in H,\overline{y}\in\overline{H},\Psi\in L_j\,.$$

The commutation property (2.4) of $\mathfrak{N}$ implies that the diagram

$$\begin{array}{ccc} L_j\otimes H\otimes\bar{H} & \xrightarrow{\mathfrak{N}'} & L_i \\ \mathrm{U}_v|_{L_j}\otimes v\otimes v \downarrow & & \downarrow \mathrm{U}_v|_{L_i} \\ L_j\otimes H\otimes\bar{H} & \xrightarrow{\mathfrak{N}'} & L_i \end{array} \tag{2.5}$$

is commutative.

On the other hand every linear mapping $\mathfrak{N}'$ which satisfies (2.5) determines by the formula

$$\mathfrak{N}(x\otimes\bar{y})\Psi := \mathfrak{N}'(\Psi\otimes x\otimes\bar{y}),$$

an element of V_{ij}. This means that to compute $\dim V_{ij}$ one should find how many times the irreducible representation $\mathrm{U}|_{L_i}$ is contained in the tensor product of three irreducible representations: $\mathrm{U}|_{L_j}$, the canonical representation in H and the one contragradient to it. This kind of approach to the problem is the generalization of an idea due to S. L. Woronowicz.

Let Y_{L_j} be the Young tableau (with N squares) corresponding to $\mathrm{U}|_{L_j}$. It is known that the irreducible components of $L_j\otimes H$ are described by all these Young tableaux which arise from Y_{L_j} by adding one square. On the other hand the representation of $\mathrm{U}(n)$ in $\bar{H}$ is equivalent to the irreducible subrepresentation in H^{n-1} given by formula (2.1) with $m=-1$. The Young tableau of that representation consists of one column with $(n-1)$ squares and one "negative" column of length n corresponding to $(\det v)^{-1}$. To decompose the tensor product of any irreducible representation, say acting in L, with the representation acting in $\bar{H}$ one should add to Y_L $(n-1)$ squares (each square to a different row) and next subtract one full (i.e., of length n) column.

We shall consider separately two cases:

(1) No square is added to the last row of Y_L. This can be done in a unique way with arbitrary Y_L.

(2) A square is added to the last row of Y_L. This can be done unless Y_L is a rectangle with n squares in each column. In the first case we have two possibilities.

(1a) Y_L contains no full column. Then we obtain the Young tableau which has one additional column with $n-1$ squares and one additional "negative" full column.

(1b) Y_L contains at least one full column. Then we obtain the Young tableau which arises from Y_L by subtracting one square from the last full column.

The second case provides, in general, a set of Young tableaux but all these tableaux arise from Y_L by subtracting one square from columns that are not full. In fact if we add one square to the last row then to obtain a proper Young tableau we have to add other squares in the same column until it becomes full. Next this column is subtracted and the other additional squares reproduce Y_L up to one square. So we see that $L\otimes\bar{H}$ contains all irreducible representations with the Young tableaux which arises from Y_L by subtracting one square and possibly the representation described in (1a). This result enables us to prove a lemma which generalizes the results of Ref. 2.

Lemma 3: Let $H^N\supset K=\oplus_{i=1}^p L_i$ and let $d(L_i)$ denote the number of different components in the signature of the irreducible representations $\mathrm{U}|_{L_i}$. Then $\dim V(H,K)=\sum_{i=1}^p\sum_{j=1}^p \dim V_{ij}$, where the dimensions of V_{ij} are given by the following formulas:

(i) If $\mathrm{U}|_{L_j}$ is equivalent to $\mathrm{U}|_{L_i}$ then $\dim V_{ij}=d(L_i)$.

(ii) If $\mathrm{U}|_{L_j}$ is not equivalent to $\mathrm{U}|_{L_i}$ then

(a) $\dim V_{ij}=1$ if Y_{L_i} arises from Y_{L_j} by shifting one square.

(b) $\dim V_{ij}=0$, otherwise.

Proof: As was already mentioned, $\dim V_{ij}$ is equal to the number of different possibilities of obtaining from Y_{L_j} the Young tableau Y_{L_i} by means of the procedure described above.

First let us notice that the representation obtained in (1a) is realized in the space $H^{(N+1)+(n-1)}\neq H^N$ and therefore it does not lead to any $\mathrm{U}|_{L_i}$.

So we can only add and subtract squares. There are exactly $d(L_j)$ different possibilities to add one square to Y_{L_j}. Each such possibility leads back to the same Young tableau only if we subtract the added square. Hence we obtain (i). By adding and subtracting one square we can shift at most one square. Moreover there is only one possibility to obtain from a given Y_{L_j} a Young tableau which differs from Y_{L_j} by the position of one square. This ends the proof of (ii).

Corollary: If $\dim H=n>N$, then $\dim V(H,K)$ does not depend on n.

Lemma 3 enables us to compute how many times the adjoint representation of $\mathrm{SU}(n)$ occurs in $\mathrm{U}|_K\otimes\bar{\mathrm{U}}|_{\bar{K}}$ for reducible $K=\oplus_{i=1}^p L_i$. Namely, let us denote this multiplicity by m_τ and let m_ω denote how many times the trivial representation of $\mathrm{U}(n)$ occurs in the above tensor product. Of course $\dim V(H,K)=m_\tau+m_\omega$. But m_ω can easily be computed because the trivial representation appears in $L_j\otimes\bar{L}_i$ only if $\mathrm{U}|_{L_i}\simeq\mathrm{U}|_{L_j}$; e.g., if all spaces L_i are different, then $m_\omega=p$.

So, Lemma 3 is a generalization of a result from Ref. 4.

3. THE TENSOR OPERATORS $\mathscr{L}^i$ AND $(\mathscr{L}\mathscr{M})^i$

In the case $\dim H=\infty$ the description of U-irreducible subspaces in $H^{N_1}\otimes\bar{H}^{N_2}$ was done in Ref. 5 by generalization of the classical results of Weyl.[3] Namely, besides the natural representation U of $\mathrm{U}(H)$ in $H^{N_1}\otimes\bar{H}^{N_2}$ there is a representation Γ of the Cartesian product of permutation groups $P_{N_1}\times P_{N_2}$ which commute with U:

$$\begin{aligned} P_{N_1}\times P_{N_2}\ni(\rho,\sigma)\to\Gamma^{-1}_{\rho,\sigma}(x_1\otimes\cdots\otimes x_{N_1}\otimes\bar{y}_{N_1+1}\otimes\cdots\otimes\bar{y}_{N_2}) \\ := x_{\rho 1}\otimes\cdots\otimes x_{\rho N_1}\otimes\bar{y}_{\sigma(N_1+1)}\otimes\cdots y_{\sigma N_2}. \end{aligned} \tag{3.1}$$

The representation Γ permutes labels of particles and antiparticles separately.

According to the results of Ref. 5, every U-invariant subspace $K\subset H^{N_1}\otimes\bar{H}^{N_2}$ has the form $K=K_1\otimes\bar{K}_2$, where $K_1\subset H^{N_1}$ (resp, $\bar{K}^2\subset\bar{H}^{N_2}$) is an invariant subspace under the natural action of $\mathrm{U}(H)$ in H^{N_1} (resp. in $\bar{H}^{N_2}$).

Any irreducible subspace $L=L_1\otimes\bar{L}_2$ in K is an image of a minimal Young projector which can be built by means of the representation Γ. So, L is labeled by *two Young diagrams*: one corresponding to an irreducible representation of P_{N_1} and the other to an irreducible representation of P_{N_2}. By the Young diagram of P_N we mean a Young tableau consisting of N squares which are labeled in an arbitrary way by integers $1,2,\ldots,N$.

Now notice that for $i=1,2,\ldots,N_1$ the images of the mappings $(\mathfrak{L}\mathfrak{N})^i$, $\mathfrak{L}^i$, etc. $(L,M\subset K)$, act trivially on $\bar{K}_2$ and for $i=N_1+1,\ldots,N_1+N_2$ they act trivially on K_1. Therefore independent of the dimension of H it is sufficient to investigate the properties of the intertwining

mappings $(\mathfrak{L}\mathfrak{M})^i, \mathfrak{L}^i$ only in the case $N_2=0$.

In what follows, K shall denote a U-invariant subspace of H^N ($\dim H \leq \infty$), Γ the representation of P_N in H^N, and Π the analogous representation of P_N in the space $B(H)^N := B(H)\otimes\cdots\otimes B(H)$:

$$P_N \ni \sigma \to \Pi_\sigma^{-1}(B_1\otimes\cdots\otimes B_N) = B_{\sigma 1}\otimes\cdots\otimes B_{\sigma N}, B_i \in B(H), \quad i=1,\ldots,N.$$

One can check that $\Pi_\sigma(B)=\Gamma_\sigma B\Gamma_\sigma^{-1}$, for $\sigma\in P_N$ and $B \in B(H)^N$. Now let J by any subset of the set $\{1,2,\ldots,N\}$, let $|J|$ denote the number of elements in J, and let P_J denote the corresponding subgroup of P_N.

By A_J (resp. S_J) we shall denote the antisymmetrizer (resp. symmetrizer) in the indices belonging to J:

$$A_J := \frac{1}{|J|!}\sum_{\sigma\in P_J}\operatorname{sgn}\sigma\cdot\Gamma_\sigma .$$

Similarly,

$$\mathfrak{A}_J := \frac{1}{|J|!}\sum_{\sigma\in P_J}\operatorname{sgn}\sigma\cdot\Pi_\sigma \quad (\text{resp. } \mathfrak{S}_J)$$

denotes the antisymmetrizer (resp. symmetrizer) acting in the space $B(H)^N$.

Lemma 4: For any B in $B(H)^N$ and any set $J\subset\{1,\ldots,N\}$

(a) $A_JBA_J = \mathfrak{S}_J(B)A_J = A_J\mathfrak{S}_J(B)$,

(b) $S_JBS_J = \mathfrak{S}_J(B)S_J = S_J\mathfrak{S}_J(B)$,

(c) $A_JBS_J = \mathfrak{A}_J(B)S_J = A_J\mathfrak{A}_J(B)$,

(d) $S_JBA_J = \mathfrak{A}_J(B)A_J = S_J\mathfrak{A}_J(B)$.

Proof: We shall prove only (d). The other proofs are entirely similar. For simplicity of notation let us assume that $J=\{1,2,\ldots,m\}$, $m\leq N$.

Let $B=B_1\otimes\cdots\otimes B_N$ and let $\Phi=x_1\otimes\cdots\otimes x_N$, where x_i is in H and $i=1,\ldots,N$.

Then by using the definition of (anti) symmetrizers we obtain

$$S_JBA_J\Phi = \frac{1}{m!}S_J\sum_{\sigma\in P_m}\operatorname{sgn}\sigma\cdot B_1x_{\sigma 1}\otimes\cdots\otimes B_mx_{\sigma m}\otimes B_{m+1}x_{m+1}\otimes\cdots\otimes B_Nx_N$$

$$= \frac{1}{m!}\frac{1}{m!}\sum_{\sigma\in P_m}\operatorname{sgn}\sigma\sum_{\rho\in P_m}B_{\rho 1}x_{\sigma\rho 1}\otimes\cdots\otimes B_{\rho m}x_{\sigma\rho m}\otimes B_{m+1}x_{m+1}\otimes\cdots\otimes B_Nx_N$$

$$= \frac{1}{m!}\sum_{\rho\in P_m}\operatorname{sgn}\rho\cdot B_{\rho 1}\otimes\cdots\otimes B_{\rho m}\otimes B_{m+1}\otimes\cdots\otimes B_N \cdot \frac{1}{m!}\sum_{\sigma\rho\in P_m}\operatorname{sgn}\sigma\cdot\operatorname{sgn}\rho\cdot x_{\sigma\rho 1}\otimes\cdots\otimes x_{\sigma\rho m}\otimes x_{m+1}\otimes\cdots\otimes x_N$$

$$= \mathfrak{A}_J(B)A_J\Phi .$$

But for the antisymmetrical tensor $\mathfrak{A}_J(B)$

$$\Gamma_\sigma\mathfrak{A}_J(B)\Gamma_\sigma^{-1} = \operatorname{sgn}\sigma\cdot\mathfrak{A}_J(B).$$

Hence we get

$$\mathfrak{A}_J(B)\cdot A_J = \frac{1}{m!}\sum_{\sigma\in P_m}\Gamma_\sigma\mathfrak{A}_J(B)\Gamma_\sigma^{-1}\Gamma_\sigma = S_J\mathfrak{A}_J(B) .$$

This simple combinatorial lemma enables us to prove the following:

Lemma 5: Let $K\subset H^N$ be the space of tensors antisymmetrical (resp. symmetrical) in indices belonging to the fixed set J, i.e., $K=A_J$ (resp. S_J). Then all mappings $\mathfrak{K}^i := K\tilde{\mathfrak{N}}^iK$ with i in J are equal, i.e., $i,j \in J$, then $\mathfrak{K}^i=\mathfrak{K}^j$.

Proof: For any A in $B(H)$ and any i,j in J,

$$\mathfrak{S}_J(\tilde{\mathfrak{N}}^i(A)) = \mathfrak{S}_J(\tilde{\mathfrak{N}}^j(A)) .$$

By using Lemma 4(a) [resp. (b)] with $A_J=K$ (resp. S_J) we obtain

$$\mathfrak{K}^i(A) = K\tilde{\mathfrak{N}}^i(A)K = \mathfrak{S}_J(\tilde{\mathfrak{N}}^i(A))\cdot K = \mathfrak{S}_J(\tilde{\mathfrak{N}}^j(A))K = \mathfrak{K}^j(A).$$

Let Y_L be the Young diagram corresponding to an irreducible representation acting in $L\subset H^N$. For any Y_L we can establish a natural one-to-one correspondence between the labeled squares of Y_L and the mappings $\mathfrak{L}^i$, $i=1,2,\ldots,N$. Let us divide Y_L vertically into the smallest possible number of rectangles.

Lemma 6: Let L be an irreducible subspace. Then the mappings $\mathfrak{L}^i$ corresponding to the squares from a given rectangle Y_L are equal.

Proof: From the construction of the Young projector onto L (e.g., first symmetrization and next antisymmetrization) it follows that the tensors in L are antisymmetrical in the indices corresponding to the labels of Y_L belonging to the same column. Hence by Lemma 5 we get that if i and j belong to the same column then $\mathfrak{L}^i=\mathfrak{L}^j$.

Now, let Y_L contain two columns of the same length. For simplicity we assume that the squares of these columns are labeled by $1,2,\ldots,m$ and by $m+1, m+2, \ldots, 2m$. The definition of the Young symmetrizer implies that

$$L\subset S_{\{1,m+1\}}\cdot S_{\{2,m+2\}}\cdots S_{\{m,2m\}} ,$$

where $S_{\{i,m+i\}}, i=1\cdots m$ denotes the symmetrizer in the indices i and $m+i$. Hence again by Lemma 5 we obtain, e.g., $\mathfrak{L}^1=\mathfrak{L}^{m+1}$ which completes the proof.

Our next aim is to show that for i belonging to different rectangles the mappings $\mathfrak{L}^i$ are linearly independent. To simplify the notation we shall give the proofs only for standard Young diagrams, i.e., first we label the squares of the first column, of the second column etc.[6]

Let be as given a standard Young diagram Y_L with columns of lengths $r_1\geq r_2\geq\cdots r_m\geq 0$. Let J be a set of labels corresponding to one rectangle of Y_L and let r be equal to the lengths of columns in that rectangle, i.e., $r=r_j$ for some j from $\{1,\ldots,m\}$.

Let us take r_1 orthonormal vectors from H, say x_1, $x_2,\ldots,x_{r_1}$, and let us build the following simple tensor from H^N.

$$\Phi = x_1\otimes x_2\otimes\cdots\otimes x_{r_1}\otimes x_1\otimes\cdots\otimes x_{r_2}\otimes\cdots\otimes x_{r_m} .$$

In what follows we refer to the vectors in the tensor product as factors, and will talk about their positions. For instance x_1 is to be found in the first r_1 plus first, etc., positions in Φ above.

Finally let P be the orthogonal projection onto x_r.

Lemma 7: Let L be the irreducible subspace corresponding to the standard Young diagram Y_L described above. Then for any i in J

$$\mathfrak{S}_J(\tilde{\mathfrak{N}}^i(P))\Phi = (1/r)\Phi .$$

Proof: The definitions of the vector Φ and the mappings $\tilde{\pi}^i$ imply that

$$\tilde{\pi}^i(P)\Phi = \begin{cases} \Phi \text{ if } i \text{ belongs to the last row of the chosen} \\ \text{rectangle.} \\ 0 \text{ otherwise.} \end{cases}$$

But from the definition of the symmetrizer S_J and Lemma 6 it follows that

$$S_J(\tilde{\pi}^i(P))\Phi = (c/|J|)\Phi ,$$

where c is the number of columns in our rectangle.

Lemma 8: Let L be irreducible. Then the mappings $\mathfrak{L}^i$ corresponding to squares belonging to different rectangles are linearly independent.

Proof: Let the notation be as in Lemma 7. Let q denote a number of rectangles in Y_L and let $\{\mathfrak{L}^{i_p}\}_{p=1}^q$ be the set of mappings corresponding to different rectangles. We want to prove that if $\sum_{p=1}^q a_p \mathfrak{L}^{i_p} = 0$ then all a_p are equal to zero.

Let us assume first that $a_1 \neq 0$, i.e.,

$$\mathfrak{L}^{i_1} = \frac{1}{a_1} \sum_{p=2}^{q} a_p \mathfrak{L}^{i_p} .$$

We shall show that this leads to a contradiction. To this end let us introduce the nonzero tensor $\Psi := C_L \Phi$, where C_L is the Young symmetrizer corresponding to Y_L. One can easily check that if by $A_{J_1}, \ldots, A_{J_m}$ we denote the antisymmetrizers corresponding to different columns of Y_L then $\Psi = A_{J_1} \cdot A_{J_2} \cdots A_{J_m} \Phi$.

Now, let P_1 be the projection onto x_{r_1} and let J_1 be a set of labels belonging to the first rectangle. From the definition of the tensor Ψ it follows that x_{r_1} can appear as a factor only in positions labeled by J_1. Therefore, since the x_i are orthogonal we get

$$\sum_{p=2}^{q} a_p \mathfrak{L}^{i_p}(P_1)\Psi = 0 .$$

On the other hand by using Lemmas 4, 6, and 7 we obtain

$$\begin{aligned} \mathfrak{L}^{i_1}(P_1)\Psi &= L S_{J_1}(\tilde{\pi}^{i_1}(P_1)) A_{J_1} \cdots A_{J_m} \Phi \\ &= L A_{J_1} \cdot \cdots \cdot A_{J_m} S_{J_1}(\tilde{\pi}^{i_1}(P_1))\Phi = (1/r_1)\Phi . \end{aligned}$$

So we have a contradiction; and $a_1 = 0$. Next in a similar way we examine the equation $\mathfrak{L}^{i_2} = (1/a_2)\sum_{p=3}^{q} a_p \mathfrak{L}^{i_p}$, and instead of the projection onto x_{r_1} we take the projection onto x_{r_j} where r_j is equal to the lengths of columns in the second rectangle. Going on we obtain the result in q steps.

Lemma 9: Let $\dim H = n < \infty$ and let L be an irreducible subspace of H^N.

(a) If the length r_1 of the first column in Y_L is equal to n then the mappings of $\mathfrak{L}^i$, where i corresponds to squares belonging to different rectangles, form a basis in the space $V(H,L)$.

(b) If $r_1 < n$ then the space $V(H,L)$ is spanned by the mappings $\mathfrak{L}^i$ mentioned in (a) and $\mathfrak{L}^0$ given by the restriction of $\tilde{\pi}^0$ [see Eq. (2.2)] to L.

Proof: Using the results of Lemma 3 part (i) we see that in the case (a) $\dim V(H,L)$ is equal to the number of rectangles in Y_L and in the case (b) we need one mapping more. But if $r_1 < n$ then there exists a vector x in H which is orthogonal to all vectors $x_1, x_2, \ldots, x_{r_1}$ which are used in Lemma 8 to build the vector Ψ. Let P denote the projection onto x. Then for any i, $\mathfrak{L}^i(P)\Psi = 0$ whereas $\mathfrak{L}^0(P)\Psi = \Psi$. Hence it is clear that in the case (b) $\mathfrak{L}^0$ is linearly independent of all $\mathfrak{L}^i$.

Now we shall consider the reducible case. Without loss of generality we can assume that $K = L + M$ where L and M carry irreducible representations. According to the results of Lemma 3 part (ii)-(a), it is sufficient to consider the case where Y_L differs from Y_M by shifting one square and to construct besides the mappings $\mathfrak{L}^i$ and $\mathfrak{M}^j$ two linearly independent elements from $V(H,K)$.

To simplify the notation we shall describe the result in the following case. Let Y_L be a standard Young diagram and let Y_M be a Young diagram which arises from Y_L by shifting up one of its squares (together with the label of the square). Let s be the label of the shifted square and let r be the number of the row in Y_L to which this square belongs.

Lemma 10: Let $\dim H \leq \infty$ and let the notation be as above. Then

(a) $(\mathfrak{L}\mathfrak{M})^s$ and $(\mathfrak{M}\mathfrak{L})^s$ are nonzero mappings belonging to $V(H,K)$.

(b) The set of mappings $(\mathfrak{L}\mathfrak{M})^s, (\mathfrak{M}\mathfrak{L})^s, \mathfrak{L}^i, \mathfrak{M}^j$, where i (resp j) labels the squares which belong to different rectangles of Y_L (resp. Y_M), is linearly independent.

Proof: Let Φ be the vector constructed in Lemma 7, let P denote the projection onto x_r, and let C_L (resp. C_M) denote the Young symmetrizer corresponding to Y_L (resp. Y_M). We shall show that

$$(C_M\Phi \,|\, (\mathfrak{M}\mathfrak{L})^s(P) C_L \Phi) = 1 . \tag{3.2}$$

To this end let us denote by A_{J_0} the antisymmetrizer corresponding to the column which contains the label s and let $J_0' := J_0 - \{s\}$. Now note that

$$\tilde{\pi}^i(P) A_{J_0}\Phi = A_{J_0'}\Phi .$$

Hence by using Lemma 4 we obtain

$$\begin{aligned} &(\mathfrak{M}\mathfrak{L})^s(P) C_L \Phi \\ &= M\tilde{\pi}^i(P) A_{J_1} \cdots A_{J_0} \cdots A_{J_m}\Phi \\ &= M A_{J_1} \cdots A_{J_0'} \cdots A_{J_m}\Phi = M\Phi . \end{aligned}$$

The last equation holds because the tensors from M are antisymmetrical exactly in the indices corresponding to $J_1, \ldots J_0', \ldots J_m$. So, the left-hand side of (3.2) is equal to $(C_M\Phi \,|\, M\Phi) = (C_M\Phi \,|\, \Phi)$. But $C_M\Phi = A_M S\Phi$, where by A_M we denote the product of all antisymmetrizers corresponding to columns of Y_M and by S we denote the symmetrizer corresponding to the row of Y_M to which the square was shifted. The expression $S\Phi$ is equal to a linear combination of different simple tensors of which all but one (equal to Φ) have the following property: The factors in the position labeled by s are vectors orthogonal to x_r. Also the action of A_M on these simple tensors cannot put in the position labeled by s the vector x_r, because we have shifted one square up and A_M can put in this position only factor vectors x_j with $j < r$. Therefore

$$(C_M\Phi \,|\, \Phi) = (A_M\Phi \,|\, \Phi)$$

Similarly with A_M, since every nontrivial permutation of factors x_j in Φ which arises under the ac-

tion of A_M leads to a product which is orthogonal to Φ. Hence

$$(A_M\Phi \mid \Phi) = (\Phi \mid \Phi).$$

Now, because L and M are Hermitian projectors it is clear that

$$(C_L\Phi \mid (\mathfrak{L}\mathfrak{M})^s(P)C_M\Phi) = 1,$$

which ends the proof of Lemma 10 part (a). Now, because L is orthogonal to M, (b) follows from (a) and Lemma 9.

The Lemma 10 and Lemma 3 part (ii) imply the following corollary.

Corollary: If $\dim H < \infty$, then the mappings $(\mathfrak{L}\mathfrak{M})^s$, $(\mathfrak{M}\mathfrak{L})^s, \mathfrak{L}^0, \mathfrak{M}^0, \mathfrak{L}^i, \mathfrak{M}^j$, where i (resp. j) correspond to different rectangles of Y_L (resp, Y_M), span the space $V(H,K)$.

It is also clear that all other mappings $(\mathfrak{L}\mathfrak{M})^k$, with $k \neq s$, are proportional to $(\mathfrak{L}\mathfrak{M})^s$, i.e., $(\mathfrak{L}\mathfrak{M})^k = c_{ks}(\mathfrak{L}\mathfrak{M})^s$. It seems to be awkward to find explicit formulas for the c_{ks}. In general some of the constants are equal to zero. However, because L is orthogonal to M, $\sum_{k=1}^{N}(\mathfrak{L}\mathfrak{M})^k = 0$ on the space K. This sometimes enables one to compute the c_{ks} by using the generalization of Lemma 6 for the reducible case.

4. THE SPECTRUM OF THE MAPPINGS $\mathfrak{L}^i_j$

Let K be a U-invariant subspace of H^N ($\dim H \leqslant \infty$) and let P_x be a projection onto an arbitrary direction x in H^N. According to Eq. (1.1), the spectrum of all operators $\mathfrak{K}^i(P_x)$, where i is fixed and x runs through all H^N, does not depend on the particular choice of x. Moreover one can easily check that to know the eigenvalues of $\mathfrak{K}^i(P_x)$ it is sufficient to investigate the spectrum of its restriction to some finite-dimensional subspace of K.

In what follows we shall look at the properties of the spectrum of operators $\mathfrak{L}^i_j := L\tilde{\mathfrak{M}}^i(P_{x_j})L$, $i = 1, \ldots, N$, $j = 1, \ldots, n$, where L carries an irreducible representation of $U(n)$, and $\{x_j\}_{j=1}^n$ is an orthonormal basis in H.

Let $\alpha = (\alpha_1, \ldots, \alpha_n)$, where $\alpha_1 \geqslant \alpha_2 \geqslant \cdots \alpha_n \geqslant 0$ and $\sum_{i=1}^n \alpha_i = N$, be the signature of the representation $U|_L$ corresponding to the basis $\{x_j\}_{j=1}^n$, i.e., α is a functional on the vector space consisting of $(n \times n)$ matrices which are diagonal in the basis $\{x_j\}_{j=1}^n$ (choice of a Cartan subalgebra).[6]

Without loss of generality we can assume that $\alpha_n = 0$. In fact, such a situation can always be obtained if L arises by restriction from the infinite-dimensional case. On the other hand, if $\dim H < \infty$ and $\alpha_n > 0$, then the spectra of the $\mathfrak{L}^i_j$ arise from the case $\alpha_n = 0$ by shifting by an integer [compare (2.3)].

Let L_β denote a weight subspace of L corresponding to the weight $\beta = (\beta_1, \ldots, \beta_n)$. By using the definition of the weight space and the property (1.1′) one can see that every operator $\mathfrak{L}^i_j$ is reduced by all orthogonal projections L_β onto weight spaces L_β.

Moreover, it seems that for any i the spectrum of $\mathfrak{L}^i_j$ is rational. We shall prove this assertion only for a particular case, but the generalization seems to be only a technical problem.

Lemma 11: For any irreducible representation $U|_L$ of $U(n)$ with signature α where $\alpha_i \geqslant 0$ and $\sum_{i=1}^n \alpha_i = N$, the spectrum of all $\mathfrak{L}^i_j$, $i = 1, \ldots, N, j = 1, \ldots, n$ is rational at least on the weight spaces L_β with $\dim L_\beta < 3$.

Proof: Let Y_L be a standard Young diagram corresponding to α. For any $\beta = (\beta_1, \ldots, \beta_n)$ we take β_1 basic vectors x_1, β_2 basic vectors x_2, etc., and for a fixed $j = s$ we build a simple tensor $\Phi \in H^N$ with two properties:

(i) the positions of factor vectors x_s in Φ are labeled first by labels of the last row of the first rectangle in Y_L, next by labels of the last row of the second rectangle, etc., until all available β_s copies of the vector x_s have been used up.

(ii) the vectors x_j with $j \neq s$ are distributed in such a way that for the Young symmetrizer C_L it is true that $\Psi := C_L\Phi \neq 0$.

In other words the vector Ψ is built according to the Young diagram Y_L with the additional requirement that vectors x_s are positioned on the bottom of Y_L (see Fig. 1). One can easily check that for any β at least one such vector can be constructed and that $\Psi \in L_\beta \subset L$. It is also clear that to obtain Ψ it is sufficient to symmetrize the rows in which vectors x_s occur only in those parts which lie at the bottom of a rectangle. This is because two identical vectors may not lie in the same column, for the antisymmetrizer will annihilate such a contribution,

So, $\Psi = C_L\Phi = A_L S_L \Phi = A_L \cdot S'_L\Phi$ where S_L is the product of symmetrizers corresponding to rows of Y_L, and S'_L is the smaller symmetrizer described above. Now, let J be the set of labels from one rectangle and let $J' \subset J$ contain the labels of the last row of our rectangle. Using parts (a) and (b) of Lemma 9 we obtain:

$$\sum_{i\in J}\tilde{\mathfrak{M}}^i_s\Phi = A_L\sum_{i\in J}\tilde{\mathfrak{M}}^i_s S'_L\Phi = A_L\sum_{i\in J'}\tilde{\mathfrak{M}}^i_s S'_L\Phi$$
$$= A_L S'_L\sum_{i\in J'}\tilde{\mathfrak{M}}^i_s\Phi = mA_L S'_L\Phi = m\Psi,$$

where m is the number of places in the rectangle occupied by factor vectors x_s. Figure 1 shows the case where m is less than the length of the bottom of the right most rectangle containing some x_s. This is a generalization of Lemma 7.

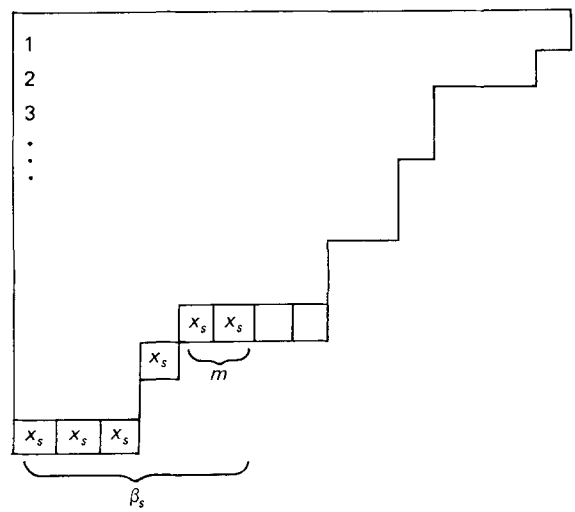

FIG. 1. β_s is the number of factor vectors x_s in ϕ, m, the number of places occupied by x_s in the right most rectangle containing some x_s.

On the other hand, for i in J Lemma 6 implies

$$\mathfrak{L}^i_s = \frac{1}{|J|} L \sum_{j\in J} \tilde{\mathfrak{N}}^j_s L\Psi = \frac{m}{|J|}\Psi .$$

So in every weight space K_β there exists at least one eigenvector with a rational eigenvalue.

If $\dim L_\beta = 2$ then we know that the vector $\Psi^\perp$ which is orthogonal to Ψ is also an eigenvector: Hence (for $\|\Psi^\perp\| = 1$) we have

$$\lambda = (\Psi^\perp | L\tilde{\mathfrak{N}}^i_s \Psi^\perp) = \|\tilde{\mathfrak{N}}^i_s \Psi^\perp\|^2 .$$

But the vector $\Psi^\perp$ can be obtained by orthonormalization from Ψ and an arbitrary (linearly independent from Ψ) vector $\Psi_1 = C_L \Phi_1$, where Φ_1 is a simple tensor which is built from β_1 vectors x_1, β_2 vectors x_2, etc. Next one can check that this construction always leads to a rational λ. The next Lemma is very useful for computation of eigenvalues of $\mathfrak{L}^i_j$.

Lemma 12: Let the notation be as in Lemma 11.

(a) Let W be the Weyl group acting on the weights as follows: for $w \in W \simeq P_n$, $w\beta := (\beta_{w^{-1}(1)}, \ldots, \beta_{w^{-1}(n)})$. Then for a fixed i and any $w \in W$ the set of eigenvalues of all operators $\mathfrak{L}^i_j, j = 1, \ldots, N$ connected with the space L_β is equal to the analogous set connected with the space $L_{w\beta}$.

(b) Define, for any A in $B(L)$, $\mathrm{Tr}_\beta(A) := \mathrm{Tr}(L_\beta A L_\beta)$. Then $\sum_{j=1}^n \mathrm{Tr}_\beta(\mathfrak{L}^i_j) = \dim L_\beta$, $i = 1, \ldots, N$.

(c) For any weight β, let $\beta^W := \{w\beta : w \in W\}$ denote the orbit of β under the action of W. Let $|\beta^W|$ be the number of elements in β^W, let $L^W_\beta := \oplus_{w\beta\in\beta^W} L_{w\beta}$, and let $\mathrm{Tr}^W_\beta(A) := \mathrm{Tr}(L^W_\beta A L^W_\beta)$.

Then for any i and j

$$n \cdot \mathrm{Tr}^W_\beta(\mathfrak{L}^i_j) = |\beta^W| \dim L_\beta .$$

(d) Let $\dim H = n > 2$ and let $\dim L_\beta = 1$. Let $\Psi_{w\beta}$ in $L_{w\beta}$ denote the normalized vectors corresponding to the orbit β^W. Then for any i and j

$$\sum_{w\in W} \mathrm{sgn}(w)(\Psi_{w\beta} | \mathfrak{L}^i_j \Psi_{w\beta}) = 0 .$$

Proof:

(a) The definition of the weight space implies that L_β is spanned by simple tensors from H^N in which the basic vector x_j is contained as a factor β_j times ($j = 1, \ldots, n$). Hence for any w in W the operator $\mathfrak{L}^i_j$ has on L_β the same eigenvalues as $L^i_{w(j)}$ on $L_{w\beta}$. The assertion is implied because w determines a bijection between coordinates of β and $w\beta$.

(b) The equation follows from $\sum_{j=1}^n \mathfrak{L}^i_j = \mathfrak{L}^i(I_H) = I_{H^N}$.

(c) First we shall prove that for any j and k the operators $\mathfrak{L}^i_j$ and $\mathfrak{L}^i_k$ have the same spectrum on the space L^W_β. In fact, for any j and k there exists a w_0 in W such that $j = w_0(k)$. But for any w in W the spectrum of $\mathfrak{L}^i_k$ on the weight space $L_{w\beta}$ is equal to the spectrum of $\mathfrak{L}^i_j = \mathfrak{L}^i_{w_0(k)}$ on the space $L_{w_0 w\beta}$ [compare (a)]. Moreover, if w runs through all the group W so does $w_0 w$. Hence we get

$$n \cdot \mathrm{Tr}^W_\beta(\mathfrak{L}^i_j) = \mathrm{Tr}^W_\beta\left(\sum_{k=1}^n \mathfrak{L}^i_k\right) = \mathrm{Tr}^W_\beta(I_{H^N}) = \dim L^W_\beta = |\beta^W| \cdot \dim L_\beta .$$

(d) We know that if $\dim L_\beta = 1$ then for any i and j

$$(\Psi_{w\beta} | \mathfrak{L}^i_j \Psi_{w\beta}) = (\Psi_\beta | \mathfrak{L}^i_{w^{-1}(j)} \Psi_\beta) .$$

Now, if $n > 2$, then for given j the permutation group $P_n \simeq W$ can be divided into pairs in such a way that for any pair, say (w_1, w_2) it is true that $w_1^{-1}(j) = w_2^{-1}(j)$ and $\mathrm{sgn}(w_1) = -\mathrm{sgn}(w_2)$. Therefore, independent of the eigenvalues of the operators $\mathfrak{L}^i_{w^{-1}(j)}$,

$$\sum_{w\in W} \mathrm{sgn}(w)(\Psi_\beta | \mathfrak{L}^i_{w^{-1}(j)} \Psi_\beta) = 0 .$$

In the next section we shall see that for $\dim H = 3$ Lemma 12 part (c) immediately implies the Gell-Mann mass formula, whereas (d) yields the Coleman-Glashow mass formulas (see, e.g., Ref. 7).

However, if we want to consider similar mass formulas for multiquark systems with $\dim H > 3$ then we need some generalization of Lemma 12 part (c) and (d).

Let W' be any subgroup of the Weyl group W and let $\beta^{W'}$, $L^{W'}_\beta$, etc., have similar meanings to the symbols connected with W. Using the isomorphism between W and P_n let us divide the set $\{1, 2, \ldots, n\}$ into two disjoint parts J_1 and J_2, where J_2 consists of these numbers which are *not* permuted by elements from W'. Of course J_2 can be an empty set even if W' is a proper subgroup of W. On the other hand if W' consists only of the identity, then J_1 is empty.

(c′) Let the notation be as above and let $\mathfrak{L}^i_m$ be equal to zero on $L^{W'}_\beta$ for any m in J_2 and any $i = 1, 2, \ldots, N$. Let n_1 denote the number of elements in J_1. Then for any j in J_1 and any $i = 1, \ldots, N$,

$$n_1 \cdot \mathrm{Tr}^{W'}_\beta(\mathfrak{L}^i_j) = \dim L^{W'}_\beta = |\beta^{W'}| \cdot \dim L_\beta .$$

Proof: In the same way as in Lemma 12(c) we prove that for any j and k in J_1 the spectra of the operators $\mathfrak{L}^i_j$ and $\mathfrak{L}^i_k$ are equal on the space $L^{W'}_\beta$. Next using the assumption about the operators $\mathfrak{L}^i_m$ with m in J_2 we obtain the result as in Lemma 12(c).

The assumption about $\mathfrak{L}^i_m$ with m in J_2 holds if in all weights $w\beta$ with w in W' the coordinates labeled by elements from J_2 are equal to zero. In fact, in such a case the operators $\tilde{\mathfrak{N}}_m$ are equal to zero on the space $L^{W'}_\beta$, and hence also the operators $\mathfrak{L}^i_m$, $i = 1, \ldots, N$.

The last Lemma implies also a generalization of (d) from Lemma 12.

(d′) Let W_1 be a subgroup of W which is isomorphic to some permutation group, i.e., $W_1 = P_{n_1}$. Let $n_1 > 2$, let J_1, J_2 have the similar meaning as above, and let $\mathfrak{L}^i_m$ with m in J_2 be equal to zero on $L^{W_1}_\beta$ for any $i = 1, \ldots, N$. Finally let $\dim L_\beta = 1$, and let $\Psi_{w\beta}$ denote vectors corresponding to the orbit β^{W_1}. Then for j in J_1 and arbitrary i,

$$\sum_{w\in W_1} \mathrm{sgn}(w)(\Psi_{w\beta} | \mathfrak{L}^i_j \Psi_{w\beta}) = 0 .$$

Proof: Let W' be the subgroup of W_1 consisting of all even permutations. The assumption $n_1 > 2$ implies that W' is not trivial. Then according to Lemma 12 (c′) we have for j in J_1 and arbitrary w_0 in W_1,

$$\mathrm{Tr}^{W'}_\beta(\mathfrak{L}^i_j) = \frac{\dim L^{W'}_\beta}{n_1} = \frac{\dim L^{W'}_{w_0\beta}}{n_1} = \mathrm{Tr}^{W'}_{w_0\beta}(\mathfrak{L}^i_j), \quad i = 1, \ldots, N \tag{4.1}$$

Hence for $\dim L_\beta = 1$ and an odd permutation w_0 from W_1 we obtain

$$\sum_{w\in W_1} \operatorname{sgn}(w)(\Psi_{w\beta}\,|\,\mathfrak{L}^i_j \Psi_{w\beta}) = \operatorname{Tr}^{W'}_{\beta}(\mathfrak{L}^i_j) - \operatorname{Tr}^{W'}_{w_0\beta}(\mathfrak{L}^i_j) = 0\,.$$

Let us note that Eq. (4.1), which holds for any dimension of L_β, can be used for a generalization of the Coleman-Glashow formula for weight spaces L_β with $\dim L_\beta > 1$.

As was mentioned in the beginning of this section all the results can be extended to the infinite-dimensional case ($\dim H = \infty$). In such a case we start with the permutation group P_n (with sufficiently large n) which permutes n ordered basic vectors from H. This group gives rise to the Weyl group if we restrict an irreducible representation of $U(H)$ acting in $L \subset H^N$ to tensors which are built only by means of the n chosen basic vectors. In this way we can obtain for $\dim H = \infty$ equations similar to those in Lemma 12 holding on some finite-dimensional subspaces of L.

5. THE MASS OPERATORS

In this section we shall show how to express some mass operators used in the theory of unitary symmetry or in the quark model by means of general number operators and next how this form of the mass operators simplifies the deduction of some mass formulas.

We assume that the orthonormal basic vectors in H, say $\{x_i\}_{i=1}^{\dim H}$, correspond to the different quarks; e.g., if $\dim H = 4$ the vectors x_1, x_2, x_3, x_4 correspond to the quarks u, d, s, c. In other words we describe the quarks u, d, etc., as different flavor one-particle states.

For any representation (multiplet of particles) K in $H^{N_1}\otimes \bar{H}^{N_2}$, the operator of baryon number is proportional to the identity operator

$$B = [(N_1 - N_2)/3]\cdot I_K\,,$$

and the operators of charge, third component of isospin, strangeness, and charm can be expressed in terms of operators related to the number of quarks in the following way:

$$Q = \mathfrak{N}_1 - B,\quad I_3 = \tfrac{1}{2}(\mathfrak{N}_1 - \mathfrak{N}_2),\quad S = \mathfrak{N}_3,\quad C = \mathfrak{N}_4\,. \tag{5.1}$$

First we shall consider the baryon case; i.e., let L be an irreducible subspace of H^N. We claim that the Gell-Mann mass operator with electromagnetic corrections can be expressed in terms of general number operators as follows:

$$G = \sum_{j=1}^{\dim H}\sum_{i=1}^{N} m^i_j \mathfrak{L}^i_j\,, \tag{5.2}$$

where to the constant m^i_j can be given the interpretation of the mass of the quark in the state x_j which is contained in the multiparticle tensor state from L in the position labeled by i (compare Sec. 1).

The formula (5.2) can be used even if $\dim H = \infty$ because the properties of the spectra of the operators $\mathfrak{L}^i_j$ imply that the infinite sum is convergent, e.g., in the strong topology.

For the established baryons ($N = 3, \dim H = 3$) we see that formula (5.2) contains 9 constants, whereas the usual Gell-Mann mass operator with electromagnetic corrections contains at most 5 constants.

In what follows we shall reduce the number of constants in (5.2) and shall show that, in general, agreement with the experimental data can be obtained only if the mass of a labeled (by position) quark depends on its label and the choice of the space L (i.e., is different, e.g., for octet and decuplet of baryons).

Although the operator G given by (5.2) contains so many constants we prefer to start with this form because it does not distinguish any direction in H and any kind of labeling in Young tableaux corresponding to L. We shall show also that formula (5.2) enables us to obtain very easily the Gell-Mann and Coleman–Glashow mass formulas.

Finally, as was mentioned in Sec. 1, it has a simple interpretation in terms of the number of labeled quarks.

In the case of an octet of baryons ($\dim H = 3, N = 3$) the reduction in the number of constants can be done as follows. If to describe the octet of baryons we use the subspace L corresponding to the standard Young diagram

1	3
2	

then according to Lemma 6 the mappings $\mathfrak{L}^1$ and $\mathfrak{L}^2$ are equal. Hence by using the property $\mathfrak{L}^i(I_H) = I_L$ we can transform the operator G, for example, into the form

$$G = c_1\mathfrak{L}^1_1 + c_2\mathfrak{L}^1_3 + c_3\mathfrak{L}^3_1 + c_4\mathfrak{L}^3_3 + c_5 I_L\,, \tag{5.3}$$

where

$$c_1 = m^1_1 + m^2_1 - m^1_2 - m^2_2,\quad c_2 = m^1_1 + m^2_3 - m^1_2 - m^2_2\,,$$
$$c_3 = m^3_1 - m^3_2,\quad c_4 = m^3_3 - m^3_2,\quad c_5 = m^1_2 + m^2_2 - m^3_2\,.$$

From Lemma 9 we know that in the considered case the mappings $\mathfrak{L}^1$, $\mathfrak{L}^3$, and $\mathfrak{L}^0(\cdot) := \operatorname{Tr}(\cdot) I_L$ are linearly independent tensor operators from the space $V(H, L)$ Moreover, the relations (1.1′) and (5.1) imply that the operators $\mathfrak{L}^1_1$ and $\mathfrak{L}^3_1$ transform like the charge operator whereas the operators $\mathfrak{L}^1_3$ and $\mathfrak{L}^3_3$ transform like the hypercharge operator. Therefore G given by (5.3) is equal to the Gell-Mann mass operator with electromagnetic corrections. Using (5.3) one can easily check that to obtain agreement with the experimental data one should assume in the octet case, for example, that $m^1_1 \neq m^1_3$.

If we neglect electromagnetic effects then the formula

$$G' = c_1'\mathfrak{L}^1_3 + c_2'\mathfrak{L}^3_3 + c_3' I_L \tag{5.4}$$

gives us the classical Gell-Mann operator. Of course the operators G and G' commute with the operators Q, I_3, S, etc. [see (1.1′)]. One should, however, remember that in general $[\mathfrak{L}^i_j, \mathfrak{L}^i_k] \neq 0$ for $j \neq k$. (See an example in Ref. 2). On the other hand if $\dim V(H, L) \leq 3$ then for any i, m, and j it is true that $[\mathfrak{L}^i_j, \mathfrak{L}^m_j] = 0$. In fact, in such a case (according to Lemma 9) we can build a basis in the space $V(H, L)$ by using the mapping $\mathfrak{L}^0$ and at most two of the mappings $\mathfrak{L}^i$, $i = 1, \ldots, N$. Let us denote these two mappings by $\mathfrak{L}'$ and $\mathfrak{L}''$. Then on the space L $\mathfrak{N} = a_0\mathfrak{L}^0 + a'\mathfrak{L}' + a''\mathfrak{L}''$, where for the case (a) of Lemma 9, $a_0 = 0$.

Now, because $[\mathfrak{L}'_j, \mathfrak{N}_j] = [\mathfrak{L}''_j, \mathfrak{N}_j] = 0$ and $\mathfrak{L}^0_j = I_L$, we get $[\mathfrak{L}'_j, \mathfrak{L}''_j] = 0$ and hence $[\mathfrak{L}^i_j, \mathfrak{L}^m_j] = 0$ for any i, m, and j.

One can easily check that for any three-quark ($N=3$) or quark-antiquark system ($N_1=N_2=1$) the dimension of the space $V(H,L)$ is smaller than 3 independent of the dimension of the space H. Therefore the components of the classical Gell-Mann operator commute.

We shall show now that Lemma 12 gives a "mathematical background" for the Gell-Mann and the Coleman–Glashow mass formulas. Namely, Lemma 12(c) implies that for any weight β

$$\frac{\mathrm{Tr}^W_\beta(G)}{\dim L^W_\beta}=\frac{1}{n}\sum_{j=1}^{n}\sum_{i=1}^{N} m_j^i . \tag{5.5}$$

The left-hand side of (5.5) is equal to the average mass of particles which are connected with the orbit β^W. So we get the following rule:

For given L the average mass of particles connected with different orbits does not depend on the orbit.

For example in the octet case for the signature $\alpha=(2,1,0)$ $\dim L^W_{(210)}=6$ and for the weight $\beta=(1,1,1)$, $\dim L^W_{(1,1,1)}=2$. Hence we obtain the Gell-Mann mass formula with electromagnetic corrections:

$$m_P+m_N+m_{\Sigma^+}+m_{\Sigma^-}+m_{\Xi^0}+m_{\Xi^-}=3(m_{\Lambda^0}+m_{\Sigma^0}) . \tag{5.6}$$

Putting in (5.6) $m_P=m_N, m_{\Sigma^+}=m_{\Sigma^-}=m_{\Sigma^0}, m_{\Xi^-}=m_{\Xi^0}$ or equivalently using the operator G' instead of G, we get the classical Gell-Mann mass formula.

Similarly, for an octet of baryons Lemma 12 part (c) implies

$$\sum_{w\in P_3}\mathrm{sgn}(w)(\Psi_{w(2,1,0)})G\Psi_{w(2,1,0)})=0 ,$$

which is equivalent to the Coleman–Glashow formula

$$m_P-m_N+m_{\Sigma^-}-m_{\Sigma^+}+m_{\Xi^0}-m_{\Xi^-}=0 . \tag{5.7}$$

Of course using Lemma 12 case (c') with W' consisting of even permutations of P_3 we obtain immediately ($n_1=n=3$)

$$\frac{m_P+m_{\Sigma^-}+m_{\Xi^0}}{3}=\frac{m_N+m_{\Sigma^+}+m_{\Xi^-}}{3}=\frac{m_{\Sigma^0}+m_{\Lambda^0}}{2} , \tag{5.8}$$

which is equivalent to (5.6) and (5.7).

Applying Lemma 12 case (c') and (d') one can easily prove that analogous mass formulas hold independently of $\dim H$. For example, if we include quark with charm and assume that the mass operator is given by (5.2) then for a "twentyplet" of baryons [i.e., $\alpha=(2100)$]. Lemma 12 case (c') implies that equations analogous to (5.8) hold separately four times: first for 8 particles with charm $C=0$, next for 8 particles with $S=0$, etc. It is clear that Lemma 12 parts (c) and (d) cannot give any new relations. In the case of a decuplet of baryons [i.e., $\alpha=(3,0,0)$]we have $\mathfrak{L}^1=\mathfrak{L}^2=\mathfrak{L}^3$. Therefore the operator G can be reduced to

$$G=b_1\mathfrak{L}^1_1+b_2\mathfrak{L}^1_3+b_3\mathfrak{L}\cdot I_L . \tag{5.9}$$

Because in the decuplet case the operator $\tilde{\mathfrak{N}}_j|_L$, which gives the total number of quarks in the state x_j, is proportional to $\mathfrak{L}^1_j$ we obtain the rule of equidistance of the mass between isospin multiplets and a similar rule inside the isospin multiplets. In this case Lemma 12 does not give any new relations.

Now, let us consider the meson case. We shall discuss only the case $K=H\otimes\bar{H}=L\oplus M$, where $\dim L=n^2-1$ ($n>2$) and $\dim M=1$, but all the results can be easily extended to any reducible subspace K of $H^{N_1}\otimes\bar{H}^{N_2}$.

We claim that the operator of mass (or of the squared mass) for vector (or pseudoscalar) mesons which is used in the quark theory can be expressed in terms of general number operators in the following way

$$G=\sum_{j=1}^{n}\sum_{i=1}^{2}[\lambda^i_j\mathfrak{L}^i_j+\mu^i_j\mathfrak{M}^i_j+\nu^i_j((\mathfrak{L}\mathfrak{M})^i_j+(\mathfrak{M}\mathfrak{L})^i_j)] , \tag{5.10}$$

where the mappings $(\mathfrak{L}\mathfrak{M})^i$ are given by (1.2) and the mappings $\mathfrak{L}^i$ and $\mathfrak{M}^i$ by the same formula with $L=M$. Note that for the representation L [i.e., $\alpha=(1,0,\ldots,0,-1)$] the mappings $\mathfrak{L}^1$ and $\mathfrak{L}^2$ are linearly independent. The assumption that the mass of a particle is equal to the mass of its antiparticle is fulfilled iff

$$\lambda^1_j=\lambda^2_j=:\lambda_j,\quad \mu^1_j=\mu^2_j=:\mu_j,\quad \nu^1_j=\nu^2_j=:\nu_j . \tag{5.11}$$

Therefore we obtain

$$G=\sum_{j=1}^{n}\lambda_j\mathfrak{L}_j+\mu_j\mathfrak{M}_j+\nu_j\widehat{(\mathfrak{L}\mathfrak{M})}_j , \tag{5.12}$$

where the image of the projection P_{x_j} under the mapping $\mathfrak{L}:=\mathfrak{L}^1+\mathfrak{L}^2$ (resp. $\mathfrak{M}=\mathfrak{M}^1+\mathfrak{M}^2$) counts the total number of quarks and antiquarks in the state x_j which are contained in a multiquark state from the space L (resp. M), while the operators $(\mathfrak{L}\mathfrak{M})_j:=(\mathfrak{L}\mathfrak{M})^1_j+(\mathfrak{L}\mathfrak{M})^2_j+(\mathfrak{M}\mathfrak{L})^1_j+(\mathfrak{M}\mathfrak{L})^2_j$ describe a mixing between the subspaces L and M. The assumption (5.11) implies also that in this case the Coleman–Glashow formula is fulfilled in the trivial way: $0\equiv 0$.

As in the baryon case we can make a further reduction of constants, and if, moreover, we neglect the electromagnetic terms then (5.12) can be transformed into the following form

$$G=b_1(\mathfrak{L}_3+\mathfrak{M}_3)+b_2I_L+b_3I_M+b_4(\mathfrak{L}\mathfrak{M})_3 . \tag{5.13}$$

One can easily check that the mass operator used in the quark theory for mesons (see, e.g., Ref. 8, Chap. 8, Sec. 1) is equivalent to (5.13). It is also clear that the constant $b_1=\Delta=m_s-m_u$, b_2 is equal to the mass of the pure octet state, b_3 to the mass of the pure singlet state, and that b_4 describes a mixing.

For vector mesons we have ideal mixing, i.e., $b_2=b_3=:b$ and $b_4=\Delta$. Therefore (5.13) reduces to

$$G=\Delta\mathfrak{K}_3+b\cdot I_K , \tag{5.14}$$

where $K=L\oplus M$, and we see that the mass operator is built by means of the total number operator $\mathfrak{K}=\tilde{\mathfrak{N}}^1+\tilde{\mathfrak{N}}^2$.

In a similar way one can consider the mass operator for mesons with charm, and without complicated calculations try to predict connections between masses of new particles (compare Ref. 9).

6. GENERAL NUMBER OPERATORS FOR $\dim H=\infty$

In the case where $\dim H=\infty$ and K is a U-invariant subspace of H^N, the space $B(H)$ [resp. $B(K)$] is not isomorphic to $H\otimes\bar{H}$ (resp. $K\otimes\bar{K}$). Therefore we are not able to compute the dimension of the space $V(H,K)$ as was done in Sec. 2. It is clear, however, that $\dim V(H,$

K) cannot be smaller than the number of linearly independent mappings $\mathfrak{L}^i, \mathfrak{M}^i, (\mathfrak{L}\mathfrak{M})^i, (\mathfrak{M}\mathfrak{L})^i$, etc., where $i = 1,2,\ldots,N$, and L,M, etc., are irreducible subspaces of K. But by using the results of Sec. 2 this number can easily be computed even if $\dim H = \infty$.

In what follows we shall show that if a mapping from the space $V(H,K)$ is a general number operator, i.e., if it satisfies the assertion of Lemma 2, then it is equal to a linear combination of the mappings $\mathfrak{L}^i, \mathfrak{M}^i, (\mathfrak{L}\mathfrak{M})^i + (\mathfrak{M}\mathfrak{L})^i$, etc., with $i = 1,\ldots,N$.

This statement is a generalization of the result obtained in Ref. 10 and its proof is based on the same idea.

Lemma 13: Let K be a U-invariant subspace of H^N ($\dim H = \infty$), and let $\mathfrak{N}$ be a mapping from $V(H,K)$ satisfying the following additional properties:

(a) $\mathfrak{N}(I_H) = c \cdot I_K$ where c is a constant.

(b) For any closed subspace D of H, $\mathfrak{N}(\hat{I}_D) \geq 0$ where by definition $\hat{I}_D$ acts as the identity on D and is equal to zero on $D^\perp$ (the orthocomplement of D in H).

(c) $\mathfrak{N}$ is an ultraweakly-weakly continuous mapping.

Then $\mathfrak{N}$ is a linear combination of the mappings $\mathfrak{L}^i, \mathfrak{M}^i, (\mathfrak{L}\mathfrak{M})^i, (\mathfrak{M}\mathfrak{L})^i$, etc., with $i = 1,\ldots,N$, where L,M, etc., are irreducible constituents of K.

If moreover the mapping $\mathfrak{N}$ satisfies:

(d) $\mathfrak{N}$ is a positivity preserving mapping, then the constants which are in front of the mappings $(\mathfrak{L}\mathfrak{M})^i$ and $(\mathfrak{M}\mathfrak{L})^i$ are equal one to another.

Proof: Let F be a closed subspace of H^N. Considering F^N as the subspaces of H^N we can define the subspace $K_F := K \cap F^N$. Using for reducible K the same trick which was used in Ref. 10 for irreducible spaces one sees easily that for any A in $B(H)$ which is reduced by F and for any $\mathfrak{N}$ in $V(H,K)$ the image $\mathfrak{N}(A)$ is reduced by K_F.

Therefore the formula $\mathfrak{N}^F(B) := K_F \mathfrak{N}(\hat{B}) K_F$, where B is in $B(F)$ and $\hat{B}$ is given by

$$\hat{B}x = \begin{cases} Bx, & \text{for } x \text{ in } F, \\ 0, & \text{for } x \text{ in } F^\perp, \end{cases}$$

defines a mapping belonging to $V(F,K_F)$.

Now, if we assume that $\dim F = n < \infty$ then K_F is a direct sum of U(n)-irreducible subspaces, say L_F, M_F, etc., Hence according to the results of Sec. 3 the mapping $\mathfrak{N}^F$ is in general a linear combination of the mappings $(\mathfrak{L}_F)^i, (\mathfrak{M}_F)^i$, etc., where $i = 0,1,\ldots,N$, and the mappings $(\mathfrak{L}_F\mathfrak{M}_F)^i, (\mathfrak{M}_F\mathfrak{L}_M)^i$, etc., where $i = 1,\ldots,N$.

Choosing another finite-dimensional subspace E of H such that F is contained in E one can check that if n was sufficiently large then the constants in the linear combination mentioned above do not depend on F. Let us denote them by c_L^i, c_M^i, $i = 0,1,\ldots,N$, etc. Next we use the assumptions (a) and (b) with $D = F^\perp$ and we obtain for a normalized vector Φ in K_F:

$$c = (\Phi \,|\, \mathfrak{N}(I_H)\Phi) \geq (\Phi \,|\, \mathfrak{N}(\hat{I}_F)\Phi) = (\Phi \,|\, \mathfrak{N}^F(I_F)\Phi). \tag{6.1}$$

But for $i = 0$,

$$c_L^0 \mathfrak{L}_F^0(I_F) = c_L^0 \cdot \dim F \cdot I_{L_F}, \quad c_M^0 \cdot \mathfrak{M}_F^0(I_F) = c_M^0 \dim F \cdot I_{M_F},$$

and, for big $\dim F$, (6.1) leads to a contradiction unless the constants c_L^0, c_M^0, etc., are equal to zero. It is also clear that the assumption (d) implies that the constants in front of $(\mathfrak{L}_F\mathfrak{M}_F)^i$ and $(\mathfrak{M}_F\mathfrak{L}_F)^i$ must be equal.

So we get that our mapping $\mathfrak{N}$ restricted to any finite-dimensional F is equal to a linear combination of a desired form. Now, because $\dim F$ was arbitrary and finite-rank operators are ultraweakly dense in $B(H)$ the assertion follows from the assumption (c).

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Asymptotics of atomic ground states: The relation between the ground state of helium and the ground state of He^+

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The asymptotic behavior of ground states of two-electron atoms is investigated. Suppose $\psi(x_1,x_2)$ is the ground state of helium, $\rho(x_1) = \int \psi^2(x_1,x_2)\, dx_2$ the corresponding electron density, and $\Phi(x_2)$ the ground state of He^+. We show that in the $L^2(dx_2)$-sense, $\lim_{|x_1|\to\infty} \psi(x_1,x_2)[\rho(x_1)]^{-1/2} = \Phi(x_2)$, and that $\psi[\rho(x_1)]^{-1/2}$ solves for large $|x_1|$ the Schrödinger equation for He^+ in the quadratic form sense. The rate of convergence of these limits is also discussed.

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I. INTRODUCTION

We consider the asymptotic behavior of the ground state of a two-electron atom described by the Hamiltonian

$$H = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \tag{1.1}$$

where Z denotes the nuclear charge, $r_i = |x_i|$, $x_i \in \mathbb{R}^3$, $i = 1,2$, $r_{12} = |x_1 - x_2|$. The ground state ψ which we assume normalized satisfies $(H - E)\psi = 0$, where E denotes the ground state energy. ψ is taken to be positive and is in fact with this convention bounded away from zero on compacts.[1] We denote by $\Phi(x_2)$ the normalized, positive ground state of the corresponding one-electron system satisfying

$$(-\Delta_2/2 - Z/r_2 - E_0^{(1)})\Phi(x_2) = 0, \tag{1.2}$$

where $E_0^{(1)} = -Z^2/2$ denotes the ground state energy. The ionization energy is defined by

$$\epsilon = E_0^{(1)} - E. \tag{1.3}$$

In this paper we investigate the relation between $\psi(x_1,x_2)$ and $\Phi(x_2)$. To provide motivation, let us give first a simple physical picture. Suppose we look at $\psi(x_1,x_2)$ with r_1 very large and r_2 small. Then the second electron should not "feel" the first electron anymore. Hence the wavefunction itself should factorize in some sense for r_1 very large like

$$\psi \sim \Phi(x_2)\chi(x_1) \tag{1.4}$$

for some funtion $\chi(x_1)$.

The purpose of this article is to make (1.4) precise. We shall prove the two following results. Let $\rho(x_1) = \int \psi^2\, dx_2$ denote the electron density; then

$$\lim_{r_1\to\infty} \frac{\psi(x_1,x_2)}{\sqrt{\rho(x_1)}} = \Phi(x_2), \quad \text{in } L^2(dx_2)\text{-sense}, \tag{1.5}$$

and

$$\lim_{r_1\to\infty} \int \frac{\psi}{\sqrt{\rho(x_1)}}\left(-\frac{\Delta_2}{2} - \frac{Z}{r_2} - E_0^{(1)}\right)\frac{\psi}{\sqrt{\rho(x_1)}}\, dx_2 = 0. \tag{1.6}$$

The proof of (1.5) and (1.6) will be based on recently obtained upper and lower bounds on the electron density.[2] In Sec. II we shall summarize some of these bounds and give a proof of (1.5) based on differential inequality techniques. We shall also show that $\Phi(x_2)\, u(x_1)$ solves the Schrödinger equation in the asymptotic region r_1 large, x_2 fixed, where $u(x_1)$ is a function exhibiting the same asymptotic behavior as $\sqrt{\rho}$. In Sec. III and IV we shall prove (1.5) and (1.6) together with an estimate on the rate of convergence of the limits. There we use together with the bounds to ρ which serve as an input, a partitioning technique and some spectral analysis related to the work of Combes and Thomas[3] and Deift *et al.*[4] on decay properties of boundstate wavefunctions.

Independently and simultaneously Elliott Lieb and Barry Simon[5] proved something equivalent to (1.4) for positive ground states of many particle systems using Brownian motion ideas. They need as an input also upper and lower bounds.[6,7] For helium their result reads

$$\lim_{r_1\to\infty} \frac{\psi(x_1,x_2')}{\psi(x_1,x_2)} = \frac{\Phi(x_2')}{\Phi(x_2)}, \tag{1.7}$$

which is equivalent to (1.4). While we get (1.7) [as a consequence of (1.5)] only almost everywhere, their result is pointwise. For potentials of compact support they recover (1.5) and obtain an exponential rate of this limit.

II. COMPARISON METHODS

In this section we give a simple proof of (1.5) based on differential inequalities. As an aside we also show that there is a function

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$$u(x_1) = \int \Phi(x_2)\psi(x_1,x_2)\,dx_2, \tag{2.1}$$

such that for any fixed x_2

$$|[1/\Phi(x_2)u(x_1)]\,[(H-E)\Phi(x_2)u(x_1)]| = O(1/r_1^{3/2}) \tag{2.2}$$

as $r_1 \to \infty$.

For the proof of (1.5) and (2.2) it is necessary to describe some of the bounds obtained in Ref. 2 together with some remarks on their proof. In Refs. 2 and 8 the following differential inequalities for $\sqrt{\rho}$ and u were derived:

$$\left(-\frac{\Delta}{2} - \frac{Z-1}{r} + \epsilon - \frac{d}{r^2}\right)\sqrt{\rho} \leqslant 0, \quad r \geqslant r_0 > 0. \tag{2.3}$$

Here d is some positive constant. For $u(x_1)$ one obtains from

$$\int \Phi(x_2)(H-E)\psi(x_1,x_2)\,dx_2$$

$$= \left(-\frac{\Delta_1}{2} - \frac{Z}{r_1} + \epsilon\right)u + \int \frac{\Phi\psi}{r_{12}}\,dx_2 = 0, \tag{2.4}$$

by estimating the integral $\int (\Phi\psi/r_{12})\,dx_2$ for $r_1 \geqslant r_0 > 0$ from above,

$$\left(-\frac{\Delta_1}{2} - \frac{Z-1}{r_1} + \epsilon + \frac{d'}{r_1^{3/2}}\right)u(x_1) \geqslant 0, \tag{2.5}$$

where d' is a suitable positive constant. Note that $u(x_1)$ is positive by the positivity of ψ and Φ, and $u \leqslant \sqrt{\rho}$ by Cauchy–Schwarz.

To extract from (2.3) and (2.5) upper and lower bounds to $\sqrt{\rho}$ and u, we need the following well known

Lemma 2.1: Let Ω be an open subset of $\mathbb{R}^n$, and if

(a) $f,g \in C^0(\bar{\Omega})$, $f \geqslant 0$, $f,g \to 0$ as $|x| \to \infty$ in Ω

(b) $f \geqslant g \;\forall x \in \partial\Omega$

(c) $(-\Delta + W_1)g \leqslant 0$, $(-\Delta + W_2)f \geqslant 0$ in Ω in the distributional sense

(d) $0 \leqslant W_2 \leqslant W_1$

then $f \geqslant g$ in all of Ω.

For a proof see, e.g., Deift *et al.*[4]

Remark 2.1: Under mild additional assumptions on f, g, (d) can be replaced by $W_2 < W_1$ almost everywhere.[9]

The application of Lemma 2.1 leads now to the required bounds. We only have to find functions v_1, v_2 such that

$$\left(-\frac{\Delta_1}{2} - \frac{Z-1}{r_1} + \epsilon - \frac{d}{r_1^2}\right)v_1(x_1) \geqslant 0, \quad r_1 \geqslant r_0, \tag{2.6}$$

with $v_1(r_0) \geqslant [\rho(r_0)]^{1/2}$ and r_0 sufficiently large such that $-(Z-1)/r_0 + \epsilon - d/r_0^2 > 0$; and analogously

$$\left(-\frac{\Delta_1}{2} - \frac{Z-1}{r_1} + \epsilon + \frac{d'}{r_1^{3/2}}\right)v_2(x_1) \leqslant 0, \quad r_1 \geqslant r_0, \tag{2.7}$$

with $v_2(r_0) \leqslant u(r_0)$ and r_0 sufficiently large. Note that ρ and u are radially symmetric functions. This leads to

Theorem 2.1[2,8]: For $r > a$, a sufficiently large

$$C_- r^\gamma (1 - d_1/\sqrt{r}) e^{-2\sqrt{\epsilon}r} \leqslant u \leqslant \sqrt{\rho} \leqslant C_+ r^\gamma (1 - d_2/r) e^{-\sqrt{2\epsilon}r}, \tag{2.8}$$

with d_1 and d_2 some positive constants and

$$\gamma = (Z-1)/\sqrt{2\epsilon} - 1,$$

$$C_- = \frac{u(a)}{a^\gamma(1 - d_1/\sqrt{a})} e^{\sqrt{2\epsilon}a}, \quad C_+ = \frac{[\rho(a)]^{1/2}}{a^\gamma(1 - d_2/a)} e^{\sqrt{2\epsilon}a}. \tag{2.9}$$

Since u and $\sqrt{\rho}$ are strictly positive functions this implies

$$1 \leqslant \sqrt{\rho}/u \leqslant \kappa \tag{2.10}$$

for some constant κ.

Remark 2.2: In Ref. 2 also upper and lower bounds to ψ itself are given which differ only in the pre-exponential factors. The upper bounds to $\sqrt{\rho}$ hold also for n-electron atoms described by

$$H^{(n)} = \sum_{i=1}^{n}\left(-\frac{\Delta_i}{2} - \frac{Z}{r_i}\right) + \sum_{i<j}^{n}\frac{1}{r_{ij}}, \tag{2.11}$$

with γ replaced by $[Z - (n-1)]/\sqrt{2\epsilon} - 1$ and $\rho(x_1) = \int |\psi^{(n)}(x_1 \cdots x_n)|^2\,dx_2 \cdots dx_n$. Also the lower bounds in (2.9) and (2.11) hold for mathematical ground states (no Pauli principle) of atoms, if $u(x_1)$ is redefined by $u(x_1) = \int \psi^{(n-1)}(x_2 \cdots x_n)\psi^{(n)}(x_1 \cdots x_n)\,dx_2 \cdots dx_n$. In these bounds ϵ is given by $E^{(n-1)} - E^{(n)}$. Everything we shall prove in this article can be readily extended to these "bosonic atoms." But since real atoms obey Fermi statistics these extensions are only of academic interest.

We proceed to prove (1.5). First we derive a differential inequality to $\sqrt{\rho}$ which is related to (2.3).

Lemma 2.2: Let $E_1^{(1)}$ be the first excited eigenvalue of the ionized system described by the Hamiltonian given in (1.2); then

$$-(\Delta_1/2)[\rho(x_1)]^{1/2} + (E_1^{(1)} - E_0^{(1)})(1 - u^2/\rho)\sqrt{\rho} - (Z/r_1)[\rho(x_1)]^{1/2} + \epsilon[\rho(x_1)]^{1/2} \leqslant 0 \tag{2.12}$$

holds in the distributional sense.

We follow essentially the strategy of Ref. 10 to derive this inequality. First we write $\int \psi(H-E)\psi\,dx_2 = 0$ as follows:

$$\int \psi(x_1,x_2)\left(-\frac{\Delta_2}{2} - \frac{Z}{r_2} - E_0^{(1)}\right)\psi(x_1,x_2)\,dx_2 + \int \psi(x_1,x_2) \times \left(-\frac{\Delta_1}{2} - \frac{Z}{r_1} + \frac{1}{r_{12}} + \epsilon\right)\psi(x_1,x_2)\,dx_2 = 0. \tag{2.13}$$

Now let P be the projection operator on $L^2(\mathbb{R}^6)$ defined by

$$Pf(x_1,x_2) = \Phi(x_2)\int \Phi(x_2)f(x_1,x_2)\,dx_2,$$

and let $Q = I - P$. Since

$$-\Delta_2/2 - Z/r_2 - E_0^{(1)} \geqslant Q(E_1^{(1)} - E_0^{(1)})$$

in the quadratic form sense, we get

$$\int \psi(x_1,x_2)\left(-\frac{\Delta_2}{2} - \frac{Z}{r_2} - E_0^{(1)}\right)\psi(x_1,x_2)\,dx_2 \geqslant (E_1^{(1)} - E_0^{(1)})\int \psi Q\psi\,dx_2 = (E_1^{(1)} - E_0^{(1)})(\rho - u^2).$$

The second integral in (2.13) is estimated using the positivity of the electronic repulsion term and

$-\sqrt{\rho}\Delta_1\sqrt{\rho} \leqslant -\int \psi(x_1,x_2)\Delta_1\psi(x_1,x_2)\,dx_2$.[10] This leads to

$$(E_1^{(1)} - E_0^{(1)})(\rho - u^2) + \rho^{1/2}(-\Delta_1/2 - Z/r_1 + \epsilon)\sqrt{\rho} \leqslant 0, \tag{2.14}$$

from which (2.12) follows by dividing by $\sqrt{\rho}$.

In order to prove (1.5) it suffices to show

$\lim_{r\to\infty}(1 - u/\sqrt{\rho}) = 0$ for $\int [\psi/\sqrt{\rho} - \Phi(x_2)]^2\,dx_2$ $= 2(1 - u/\sqrt{\rho})$. First we show that

$$\liminf_{r\to\infty}(1 - u/\sqrt{\rho}) = 0. \tag{2.15}$$

We already remarked that u and $\sqrt{\rho}$ are radially symmetric. Suppose now that $\inf_{r>a}(1 - u^2/\rho) = \delta > 0$ for some $a \geq 0$. Then Lemma 2.1 implies that $\sqrt{\rho} \leqslant f(r)\exp[-\sqrt{2(\epsilon+\delta)}\,r]$ where f is a polynomially bounded function. But this leads to a contradiction to the lower bound to $\sqrt{\rho}$ given in Theorem 2.1, thus proving (2.15).

To show $\limsup(1 - u^2/\rho) = 0$ we just apply the bounds (2.8) and (2.9). By (2.15) there is for any $\delta > 0$ an arbitrarily large a_δ such that $u(a_\delta)/[\rho(a_\delta)]^{\frac{1}{2}} \geqslant 1 - \delta$. Hence using (2.8) and (2.9), we get

$$\begin{aligned}\lim_{r_1\to\infty} \frac{u}{\sqrt{\rho}} &\geqslant \lim_{r_1\to\infty} \frac{u(a_\delta)(1 - d_2/a_\delta)(1 - d_1/\sqrt{r_1})}{\sqrt{\rho(a_\delta)}\,(1 - d_1/\sqrt{a_\delta})\,(1 - d_2/r_1)} \\ &= (1-\delta)\frac{1 - d_2/a_\delta}{1 - d_1/\sqrt{a_\delta}}.\end{aligned} \tag{2.16}$$

Since we can choose a_δ arbitrarily large, we get $\lim_{r\to\infty} u/\sqrt{\rho} \geqslant 1 - \delta$ for any $\delta > 0$ and (1.5) is proven.

Remark 2.3: There are certain shortcomings in the proof of (1.5) as we give it in this section. First, we do not get any estimate on the rate of convergence of (1.5). This will be achieved with more powerful (but also more complicated) techniques in the next section (Theorem 3.1). Secondly, we use explicitly the radial symmetry of ρ and u. For instance we have no proof of (1.5) in the case of the hydrogen molecule with two fixed nuclei. Accordingly it would be desirable to have also bounds on the rate at which $\sqrt{\rho}$ becomes spherically symmetric in the case of molecules with fixed nuclei. Theorem (3.1) however implies some result (see Remark 3.2).

To conclude this section we want to show (2.2). First we note that by (2.4),

$$(H - E)u\Phi = \Phi\left(\frac{u}{r_{12}} - \int \frac{\Phi\psi}{r_{12}}\,dx_2\right). \tag{2.17}$$

But it was already shown in Ref. 2 that for r_1 large enough and x_2 fixed,

$$\int \frac{\Phi\psi}{r_{12}}\,dx_2 \leqslant \frac{u}{r_1} + \frac{d'}{r_1^{3/2}}u, \tag{2.18}$$

d' some positive constant, and therefore

$$\Phi\left(\frac{u}{r_{12}} - \int \frac{\Phi\psi}{r_{12}}\,dx_2\right) \geqslant -\frac{d''}{r_1^{3/2}}\Phi u \quad \text{for fixed } x_2, \tag{2.19}$$

d'' some positive constant. To show an asymptotic bound in the other direction we estimate $\int(\Phi\psi/r_{12})\,dx_2$ by the following chain of inequalities:

$$\begin{aligned}\int \frac{\Phi\psi}{r_{12}}\,dx_2 &\geqslant \int \frac{\Phi\psi}{r_1 + r_2}\,dx_2 \geqslant \int_{r_2 \leqslant \sqrt{r_1}} \frac{\Phi\psi}{r_1 + r_2}\,dx_2 \\ &\geqslant \frac{1}{r_1 + \sqrt{r_1}}\left(u(r_1) - \int_{r_2 \geqslant \sqrt{r_1}} \psi\Phi\,dx_2\right) \\ &\geqslant \frac{1}{r_1 + \sqrt{r_1}}\left[u - \sqrt{\rho}\left(\int_{r_2 \geqslant \sqrt{r_1}} \Phi^2 dx_2\right)^{1/2}\right] \\ &\geqslant \frac{1}{r_1 + \sqrt{r_1}}\left[u - \sqrt{\rho}\left(\Phi(\sqrt{r_1})\int \Phi dx_2\right)^{1/2}\right] \\ &\geqslant \frac{1}{r_1 + \sqrt{r_1}}\{u[1 - c\exp(-\beta\sqrt{r_1})]\},\end{aligned} \tag{2.20}$$

where c and β are suitable positive constants. In the last step we used (2.10) and the decay of $\Phi(x_2)$. From (2.20) we get immediately $\int(\Phi\psi/r_{12})\,dx_2 \geqslant (1/r_1 - d/r_1^{3/2})u$ for sufficiently large r_1 and a suitable d which proves (2.2).

Remark: The $r^{-3/2}$ in (2.2) can be improved to $r^{-\alpha}$, $\alpha < 2$.

III. PARTITIONING METHODS

In this and the next section our strongest version of (1.5) and (1.6) will be proven. We have

Theorem 3.1: For $\lim r_1 \to \infty$,

$$\int\left[\frac{\psi}{\sqrt{\rho}} - \Phi(x_2)\right]^2 dx_2 = O\left(\frac{1}{r_1^2}\right), \tag{3.1}$$

$$\int \frac{\psi}{[\rho(x_1)]^{\frac{1}{2}}}\left(-\frac{\Delta_2}{2} - \frac{Z}{r_2} - E_0^{(1)}\right)\frac{\psi}{[\rho(x_1)]^{\frac{1}{2}}}\,dx_2 = O\left(\frac{1}{r_1^2}\right). \tag{3.2}$$

The proof of (3.1) and (3.2) will require many steps which, however, might be of interest by themselves. One of them follows from some ideas of Refs. 3 and 4 (Sec. IV).

Let

$$u_0(x_1) = (1 + r_1)^\gamma e^{-\sqrt{2\epsilon}\,r_1}, \quad \gamma = (Z - 1)/\sqrt{2\epsilon} - 1. \tag{3.3}$$

By Theorem 2.1 we have $\kappa_- u_0 \leqslant u \leqslant \sqrt{\rho} \leqslant \kappa_+ u$ for some positive constants κ_-, κ_+. For $\alpha \in \mathbb{R}$ consider the unitary group on $L^2(\mathbb{R}^6)$:

$$W(\alpha)f = e^{i\alpha \ln u_0} f, \quad f \in L^2(\mathbb{R}^6), \tag{3.4}$$

and

$$\begin{aligned}H(\alpha) &= W(\alpha)HW(\alpha)^{-1} \\ &= \tfrac{1}{2}\left(i\nabla_1 + \alpha\frac{\nabla u_0}{u_0}\right)^2 - \frac{\Delta_2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}.\end{aligned} \tag{3.5}$$

Now let

$$g(x_1) = (\nabla_1 u_0/u_0)(x_1) = (-\sqrt{2\epsilon} + \gamma(1 + r_1)^{-1})x_1/r_1. \tag{3.6}$$

By Proposition 4.1 (see Sec. IV) the family of operators $[QH(\alpha)Q\text{-}E]^{-1}$ is analytic in a ball $|\alpha| < 1 + \beta$, for some $\beta > 0$, Here Q is defined as in the proof of Lemma 2.2. By projecting the Schrödinger equation for ψ into the ranges of P and Q respectively, we get

$$Q\psi = (E - QHQ)^{-1}Q(1/r_{12})P\psi. \tag{3.7}$$

Applying $W(\alpha)$, $\alpha\in\mathbb{R}$, to (3.7) we get

$$W(\alpha)Q\psi = [E - QH(\alpha)Q]^{-1}Q(1/r_{12})\Phi u u_0^{i\alpha}, \tag{3.8}$$

where u is given by (2.1). We want to show that rhs of (3.8) has a continuous continuation in $L^2(\mathbb{R}^6)$ up to $|\alpha| = 1$ and that $Q\psi/u_0\in L^2(\mathbb{R}^6)$. First we show that

$$Q(1/r_{12})\Phi(x_2) = Q(1/r_{12} - 1/r_1)\Phi(x_2)\in L^2(\mathbb{R}^6). \tag{3.9}$$

(3.9) is implied by the following estimates. We split the integral

$$\int\left(\frac{1}{r_1} - \frac{1}{r_{12}}\right)^2\Phi(x_2)\,dx_1dx_2 = \int_{r_1<2r_2} + \int_{r_1\geq 2r_2}. \tag{3.10}$$

Now

$$\int_{r_1\leq 2r_2}\left(\frac{1}{r_1} - \frac{1}{r_{12}}\right)^2 dx_1 \leq \int_{r_1<2r_2}\left(\frac{1}{r_1^2} + \frac{1}{r_{12}^2}\right)dx_1$$
$$\leq 2\int_{r_1<3r_2}\frac{dx_1}{r_1^2} = \kappa r_2$$

for some constant κ. But $\Phi(x_2)$ decreases exponentially showing that the first integral on the rhs of (3.10) is finite. For the second integral on the rhs of (3.10) we use

$$\int_{r_1\geq 2r_2}\left(\frac{1}{r_1} - \frac{1}{r_{12}}\right)^2 dx_1$$
$$\leq \int_{r_1\geq 2r_2}\max\left[\left(\frac{1}{r_1} - \frac{1}{r_1+r_2}\right)^2, \left(\frac{1}{r_1-r_2} - \frac{1}{r_1}\right)^2\right]dx_1.$$

By a simple argument these integrals can be shown to behave like κr_2 which again implies the finiteness of the second integral on the rhs. of (3.10) due to the decay of $\Phi(x_2)$.

The above stated analyticity property of $[QH(\alpha)Q - E]^{-1}$ implies that it is uniformly continuous in $|\alpha|\leq 1$ in operator norm.

Theorem 2.1 implies that $uu_0^{i\alpha}$ is uniformly pointwise bounded and continuous in $|\alpha|\leq 1$.

With the aid of (3.9) and the last two remarks it follows from (3.8) that $(Q\psi/u_0)\in L^2(\mathbb{R}^6)$ and that

$$u_0^{-1}Q\psi = [E - QH(-i)Q]^{-1}Q(1/r_{12})\Phi u/u_0. \tag{3.11}$$

Given this we proceed to prove (3.1) and (3.2) and postpone the proof of the analyticity properties of $[E - QH(\alpha)Q]^{-1}$ to Sec. IV.

Let

$$\zeta_0(x_1,x_2) = (1/r_{12} - 1/r_1)\Phi(x_2)u(x_1)/u_0(x_1), \tag{3.12}$$

$$\zeta \equiv Q\psi/u_0 = \psi/u_0 - [u(x_1)/u_0(x_1)]\Phi(x_2). \tag{3.13}$$

We have $[E - QH(-i)Q]^{-1}\zeta = Q\zeta_0$. First we prove

Lemma 3.1: (a) The family of self-adjoint operators $\{H(\alpha):\alpha\in\mathbb{R}\}$ can be analytically continued to an analytic family of type A.[11]

(b) $\zeta\in W^{2,2}(\mathbb{R}^6)$, where $W^{2,2}$ denotes the usual Sobolev space.[12]

Proof: For $\alpha\in\mathbb{R}$ we have according to (3.5) and (3.6),

$$H(\alpha) - H = \tfrac{1}{2}\alpha^2|g|^2 + i\alpha g\cdot\nabla_1 + \tfrac{1}{2}\alpha\,\mathrm{div}g, \tag{3.14}$$

which is readily seen to be a relatively bounded perturbation of $-\Delta_1$ with arbitrarily small relative bound. Since the domain of H satisfies $\mathscr{D}(H) = \mathscr{D}(-\Delta_1 - \Delta_2) = W^{2,2}(\mathbb{R}^6) \subseteq \mathscr{D}((-\Delta_1\times I), H(\alpha) - H$ is also H-bounded with arbitrarily small relative bound. Accordingly $\mathscr{D}(H(\alpha)) = \mathscr{D}(H) = W^{2,2}(\mathbb{R}^6)$, and since (3.14) obviously acts analytically on $W^{2,2}(\mathbb{R}^6)$ analyticity of type A in $\mathbb{C}$ follows.

To prove (b) we note first that by (3.9), (3.11), and $P\zeta = 0$,

$$\|[QH(-i)Q + PH(-i)P]\zeta\| < \infty. \tag{3.15}$$

Now

$$\|H(-i)\zeta\| \leq \|[QH(-i)Q + PH(-i)P]\zeta\| + \|P(1/r_{12})Q\zeta\|.$$

But $P(1/r_{12})Q$ is bounded relatively to $-\Delta_1/2 - \Delta_2/2$ (which we call H_0 from now on) with arbitrarily small bound and hence, by (a), also with respect to $H(-i)$. This implies $\zeta\in\mathscr{D}(H(-i)) = W^{2,2}(\mathbb{R}^6)$.

Remark 3.1: For further reference we note that $P(1/r_{12})Q$ is a H_0-compact operator. (This is well known and proven, e.g., in a more general setting in Combes.[13])

We proceed to prove (3.1). First we note the following essentially one-dimensional result.

Lemma 3.2: Suppose $f\in W^{2,1}(\mathbb{R}^3)$ and f is radially symmetric; then $|f|\leq c/r$ for $r\geq a$, a positive, c some constant.

Proof: This follows from the one-dimensional estimate[14] $\|y\|_\infty^2 \leq \|y\|\,\|dy/dx\|$, where y denotes an absolutely continuous funtion $y:R^+\to R$. Since f is radially symmetric we note that by standard arguments[15] $rf(r)$ is absolutely continuous and we get $\int|\nabla f|^2\,dx = \int|\partial(rf)/\partial r|^2\,dr\,d\Omega$, where $d\Omega$ denotes integration over the surface of the unit sphere. This implies that $r^2|f|^2\leq\kappa\|f\|\,\|\nabla f\|$ for some constant κ which proves the assertion.

From Lemma 3.1 and 3.2, Theorem 3.1 now follows readily: Since $(\rho/u^2 - 1)u^2/u_0^2 = \int\zeta^2\,dx_2$ and $\kappa_1\leq u/u_0\leq\kappa_2$ for some positive constants according to Theorem 2.1, it suffices to show $(\int\zeta^2\,dx_2)^{1/2}\leq c/r_1$. Now $\int\zeta^2\,dx_2$ is obviously radially symmetric since ρ, u, and u_0 are. We get

$$\int|\nabla_1(\int\zeta^2\,dx_2)^{1/2}|^2\,dx_1 = \int\left|\frac{\int\zeta\nabla_1\zeta\,dx_2}{(\int\zeta^2\,dx_2)^{1/2}}\right|^2 dx_1$$
$$\leq \int|\nabla_1\zeta|^2\,dx_1dx_2 < \infty,$$

since $\zeta\in W^{2,2}(\mathbb{R}^6)$. We used Cauchy–Schwarz in the last step. Therefore, $(\int\zeta^2dx_2)^{1/2}$ is according to Lemma 3.2 bounded by c/r_1 and (3.1) is proven.

To prove (3.2) we proceed analogously. We have

$$\int\left|\nabla_1\left(\int|\nabla_2\zeta|^2\,dx_2\right)^{1/2}\right|^2 dx_1$$
$$= \int\left|\frac{\partial}{\partial r_1}\left(\int|\nabla_2\zeta|^2\,dx_2\right)^{1/2}\right|^2 dx_1$$
$$= \int\left|\frac{\int|\nabla_2\zeta|\,\partial/\partial r_1|\nabla_2\zeta|\,dx_2}{(\int|\nabla_2\zeta|^2\,dx_2)^{1/2}}\right|^2 dx_1$$
$$\leq \int\left|\frac{\partial}{\partial r_1}\nabla_2\zeta\right|^2 dx_1dx_2 < \infty,$$

since $\zeta\in W^{2,2}(\mathbb{R}^6)$. Hence $(\int|\nabla_2\zeta|^2dx_2)^{1/2}\leq c/r_1$ by Lemma 3.2. But

$$\int \frac{\psi}{\sqrt{\rho}}\left(-\frac{\Delta_2}{2}-\frac{Z}{r_2}-E_0\right)\frac{\psi}{\sqrt{\rho}}\,dx_2$$
$$=\frac{u_0}{\sqrt{\rho}}\left(\int\frac{|\nabla_2\zeta|^2}{2}\,dx_2-\int\frac{Z}{r_2}\zeta^2\,dx_2-E_0^{(1)}\int\zeta^2\,dx_2\right).$$

Since $\int\zeta^2 dx_2$ has been estimated already by c/r_1^2, this bound to $\int|\nabla_1\zeta|^2 dx_2$ implies (3.2).

Remark 3.2: Since Theorem 2.1 holds also for two-electron molecules with fixed nuclei, (3.1) and (3.2) have to be weakened for this case to lhs of (3.1) and (3.2) $\in L^1(dx_1)$.

IV. SOME SPECTRAL PROPERTIES OF ATOMIC HAMILTONIANS

For the proof of Theorem 3.1 we still have to show that $[E-QH(-i)Q]^{-1}Q$ is a bounded operator on $L^2(\mathbb{R}^6)$. In order to prove this we have to do some spectral analysis of the operator family $\{H(\alpha):\alpha\in\mathbb{C}\}$. In connection with decay properties of bound states Combes and Thomas[3] and Deift *et al.*[4] already investigated spectral properties of a general class of operators $H[f]=e^{if}He^{-if}$, with f some complex valued function. Unfortunately their analysis does not cover our case $f=i\ln u_0$ with u_0 given by (3.3). However, with some modifications which we present below the methods of Deift *et al.*[4] can be adapted to this situation.

We first state the main result of this section

Proposition 4.1: (i) $\sigma_{\rm ess}[H(\alpha)]\subset\{z\in\mathbb{C}:$ $\mathrm{Re}z\geqslant E_0^{(1)}-(\mathrm{Im}\alpha)^2\epsilon\}$.

(ii) Let $\delta=E_1^{(1)}-E_0^{(1)}$; then

$\sigma_{\rm ess}[H(\alpha)+\delta P]\subset\{z\in\mathbb{C}:$ $\mathrm{Re}z\geqslant\min(E_0^{(1)},E_1^{(1)}-(\mathrm{Im}\alpha)^2\epsilon)\}$.

(iii) $[E-QH(\alpha)Q]^{-1}$ is analytic in α for $|\alpha|<1+\beta$ for some $\beta>0$, β sufficiently small.

Remark: We define the essential spectrum following Ref. 4: Let A be a closed operator on a Hilbert space $\mathscr{H}$ with resolvent set $\rho(A)$ and spectrum $\sigma(A)$. $\sigma_{\rm disc}(A)$ = set of all isolated eigenvalues of A with finite algebraic multiplicities. $\sigma_{\rm ess}(A)=\sigma(A)\setminus\sigma_{\rm disc}(A)$.

The proof of (i) and (ii) is heavily based on results of Ref. 4 (Sec. 3 of their paper). The necessary definitions and lemmata are collected in Appendix A. The analyticity properties of $[E-QH(\alpha)Q]^{-1}Q$, which we need for the proof of Theorem 3.1, follow then readily from (ii). But first we give an immediate consequence of Lemma A1.

Lemma 4.1: Let A be a closed operator on $\mathscr{H}$ with nonempty resolvent set and let $\Theta(A)=\{\lambda\in\mathbb{C}:$ there exist $\phi\in\mathscr{D}(A)$ with $(\phi,A\phi)=\lambda$, $\|\phi\|=1\}$ denote the numerical range of A. Then

$$N_{\rm ess}(A)\subset\sigma_{\rm ess}(A)\subset\overline{\Theta(A)}. \tag{4.1}$$

Proof: Following Kato[11] (p. 267, 571) this follows easily: For suppose $\lambda\in N_{\rm ess}(A)$; then Definition A.1 implies $\lambda\in\overline{\Theta(A)}$. But since $\Theta(A)$ is convex (4.1) follows from Lemma A.1 (ii).

Remark. Actually $\sigma_{\rm ess}(A)\subset\overline{\Theta(A)}$ is stated in Kato's book,[11] but Kato's definition of $\sigma_{\rm ess}$ differs from the one we use here.

Next we consider the following class of operators on $L^2(\mathbb{R}^6)$. Let $\tilde H$ denote $H(\alpha)$, $H(\alpha)+\delta P$, or $H_{D_3}(\alpha)$, where

$$H_{D_3}(\alpha)\equiv\tfrac12(i\nabla_1-\alpha\sqrt{2\epsilon}x_1/r_1)^2+V_{01}-\tfrac12\Delta_2+1/r_{12}, \tag{4.2}$$

with

$$V_{01}=\tfrac12(i\nabla_1+\alpha g)^2-\tfrac12(i\nabla_1-\alpha\sqrt{2\epsilon}x_1/r_1)^2. \tag{4.3}$$

Note that V_{01} is $-\Delta_1$-compact. We shall show that Lemma A2 applies to $\tilde H$. For this we consider the two-cluster decompositions of our three particle system (the nucleus is labeled by 0): $D_1=\{(0,1),(2)\}$, $D_2=\{(0,2),(1)\}$, $D_3=\{(0),(1,2)\}$, and introduce the related partition on $\mathbb{R}^6$ (see Def. A3) $\{\chi_0,\chi_{D_1},\chi_{D_2},\chi_{D_3}\}$ with support of χ_D contained in a region where $|x_i-x_j|>1$ if i and j are in different clusters of D.

Note that P respectively V_{01} are non-multiplicative interactions between the particles 0 and 2 respectively 0 and 1.

Lemma 4.2:

$$N_{\rm ess}(\tilde H)=N_\infty(\tilde H)=\cup_D N_\infty^D(\tilde H), \tag{4.4}$$

where N_∞ and N_∞^D are defined in Appendix A.

Proof: we have to check that the assumptions of Lemma A2 are verified in our case. The resolvent set of $\tilde H$ is obviously nonempty since $\tilde H$ is obtained from H_0 by adding relatively bounded perturbations with arbitrarily small bound. This implies that $\mathscr{D}(\tilde H)=\mathscr{D}(H_0)=W^{2,2}(\mathbb{R}^6)$, and also that $C_0^\infty(\mathbb{R}^6)$ is a core for $\tilde H$, since the norms $\|\tilde H\phi\|+\|\phi\|$, $\|H_0\phi\|+\|\phi\|$ are equivalent and $C_0^\infty(\mathbb{R}^6)$ is a core for H_0.

Next we show (i) of Lemma A2. Note first that $\rho(\tilde H)\subset\rho(H_0)$. Hence for $z\in\rho(\tilde H)$ we get

$$\chi_0(z-\tilde H)^{-1}$$
$$=\chi_0(z-H_0)^{-1}+\chi_0(z-H_0)^{-1}(\tilde H-H_0)(z-\tilde H)^{-1}. \tag{4.5}$$

$\chi_0(z-H_0)^{-1}$ is obviously compact and $(\tilde H-H_0)(z-\tilde H)^{-1}$ is bounded with implies the required compactness of $\chi_0(z-\tilde H)^{-1}$.

The requirement (ii) of Lemma A2 follows by standard arguements[4]; essentially by working out the commutators and by noting that the norms $\|\tilde H\phi\|+\|\phi\|$, $\|H_0\phi\|+\|\phi\|$ are equivalent $[\phi\in\mathscr{D}(H_0)=\mathscr{D}(\tilde H)]$.

According to the different cluster decompositions we consider now the operators $\tilde H_D$, where $\tilde H_D$ is obtained from $\tilde H$ by removing the interactions v_d between different clusters in D; $\tilde H_D=\tilde H-v_D$.

Remark: For amplification see also (4.2), (4.12), and (4.15).

Lemma 4.3:

$$N_{\rm ess}(\tilde H)\subset\cup_D\sigma_{\rm ess}(\tilde H_D). \tag{4.6}$$

Proof: By Lemma 4.2 we have $N_{\rm ess}(\tilde H)=\cup_D N_\infty^D(\tilde H)$. Now suppose $\lambda\in N_\infty^D(\tilde H)$ and let $\{u_n\}$ be a corresponding Weyl sequence. We have

$$\|(\lambda-\tilde H_D)u_n\|\leqslant\|(\lambda-\tilde H)u_n\|+\|v_Du_n\|. \tag{4.7}$$

It is straightforward to show that $\|v_Du_n\|\underset{n\to\infty}{\longrightarrow}0$ for

$\mathrm{supp} u_n \subset \mathrm{supp}\chi_D^n$: For the multiplicative terms $v_{ij}(y)$ of v_D (y is either x_1, x_2, or r_{12}) this follows from $v_{ij}(y) \to 0$ for $|y| \to \infty$. For the projector P it is implied by the exponential decay of $\Phi(x_2)$, and finally for V_{01} it holds since $1/(1+r_1) \to 0$ for $r_1 \to \infty$ and since $(1+r_1)V_{01}$ is a $-\Delta_1$-bounded operator with arbitrarily small relative bound. Hence

$$N_{\mathrm{ess}}(\tilde{H}) \subset \bigcup_D N_\infty^D(\tilde{H}_D) \subset \bigcup_D N_{\mathrm{ess}}(\tilde{H}_D), \tag{4.8}$$

from which by Lemma A1 the assertion follows.

Armed with Lemma 4.1 and 4.3 we proceed now to prove (i) and (ii) of Proposition 4.1. First we consider the operator $\frac{1}{2}(i\nabla_1 + \alpha g)^2$ with g given by (3.6). The already remarked $-\Delta_1$-compactness of V_{01} implies

$$N_{\mathrm{ess}}(\tfrac{1}{2}(i\nabla_1 + \alpha g)^2) = N_{\mathrm{ess}}\left[\tfrac{1}{2}(i\nabla_1 - \alpha\sqrt{2\epsilon}\, x_1/r_1)^2\right]. \tag{4.9}$$

Lemma 4.1 implies

$$\sigma_{\mathrm{ess}}(\tfrac{1}{2}(i\nabla_1 + \alpha g)^2) \subset \{z \in \mathbb{C}: \mathrm{Re}z \geqslant -(\mathrm{Im}\alpha)^2\epsilon\}. \tag{4.10}$$

Note that by considering the numerical range of $\frac{1}{2}(i\nabla_1 + \alpha g)^2$ directly we would run into difficulties because we would get a γ-dependent result.

Standard analyticity arguments imply now that there is no eigenvalue of $\frac{1}{2}(i\nabla_1 + \alpha g)^2$ outside the essential spectrum since otherwise by letting $|\alpha|$ decrease to zero this eigenvalue would be in the spectrum of $-\Delta_1$. So we get

$$\sigma(\tfrac{1}{2}(i\nabla_1 + \alpha g)^2) \subset \{z \in \mathbb{C}: \mathrm{Re}z \geqslant -(\mathrm{Im}\alpha)^2\epsilon\}, \tag{4.11}$$

We consider now

$$H_{D_1}(\alpha) = \tfrac{1}{2}(i\nabla_1 + \alpha g)^2 - Z/r_1 - \tfrac{1}{2}\Delta_2. \tag{4.12}$$

By Ichinose's Lemma we have

$$\sigma[H_{D_1}(\alpha)] = \sigma[\tfrac{1}{2}(i\nabla_1 + \alpha g)^2 - Z/r_1] + \mathbb{R}^+. \tag{4.13}$$

The analysis is as before except that now $\frac{1}{2}(i\nabla_1 + \alpha g)^2 - Z/r_1$ can have eigenvalues above $E_0^{(1)}$, so

$$\sigma[H_{D_1}(\alpha)] \subset \{z \in \mathbb{C}: \mathrm{Re}z \geqslant \min(E_0^{(1)}, -(\mathrm{Im}\alpha)^2\epsilon)\}. \tag{4.14}$$

Analogously we find for

$$H_{D_2}(\alpha) = \tfrac{1}{2}(i\nabla_1 + \alpha g)^2 + (-\Delta_2/2 - Z/r_2), \tag{4.15}$$

$$\sigma[H_{D_2}(\alpha)] \subset \{z \in \mathbb{C}: \mathrm{Re}z \geqslant E_0^{(1)} - (\mathrm{Im}\alpha)^2\epsilon\}. \tag{4.16}$$

We note that

$$\sigma(H_{D_2}(\alpha) + \delta P) = \sigma([H(\alpha) + \delta P]_{D_2}) \subset \{z \in \mathbb{C}: \mathrm{Re}z \geqslant E_1^{(1)} - (\mathrm{Im}\alpha)^2\epsilon\}. \tag{4.17}$$

Finally we consider

$$\begin{aligned} H_{D_3}(\alpha) &= \tfrac{1}{2}(i\nabla_1 + \alpha g)^2 - \tfrac{1}{2}\Delta_2 + 1/r_{12} \\ &= \tfrac{1}{2}(i\nabla_1 - \alpha\sqrt{2\epsilon}\, x_1/2)^2 + V_{01} - \tfrac{1}{2}\Delta_2 + 1/r_{12} \\ &\equiv H_{12}(\alpha) + V_{01}. \end{aligned}$$

To this operator we apply again Lemma 4.3 and obtain

$$\sigma_{\mathrm{ess}}[H_{D_3}(\alpha)] \subset \sigma_{\mathrm{ess}}[\tfrac{1}{2}(i\nabla_1 + \alpha g]^2 - \tfrac{1}{2}\Delta_2) \cup \sigma_{\mathrm{ess}}[H_{12}(\alpha)]. \tag{4.18}$$

Now by the positivity of $1/r_{12}$ we get $\Theta[H_{12}(\alpha)] \subset \{z \in \mathbb{C}: \mathrm{Re}z > -(\mathrm{Im}\alpha)^2\epsilon\}$ and hence by (4.11),

$$\sigma[H_{D_3}(\alpha)] \subset \{z \in \mathbb{C}: \mathrm{Re}z \geqslant -(\mathrm{Im}\alpha)^2\epsilon\}. \tag{4.19}$$

Combining (4.13), (4.15), and (4.19), Lemma 4.3 gives (i) of Proposition 4.1. Proposition 4.1 (ii) follows by noting that the cluster decomposition of $H(\alpha) + \delta P$ are the same as for $H(\alpha)$ except for D_2 which is covered by (4.17). Therefore, (4.13), (4.17), and (4.19) imply (ii).

Finally we show that (ii) implies (iii) of Proposition 4.1. By Lemma 3.1a, $\{H(\alpha), \alpha \in C\}$ is an analytic family of type A. Now

$$H(\alpha) = QH(\alpha)Q + PH(\alpha)P + [P(1/r_{12})Q + Q(1/r_{12})P]. \tag{4.20}$$

According to Remark 3.1 the term in brackets is H_0-compact and therefore $QH(\alpha)Q + PH(\alpha)P$ is also an analytic family of type A; the same holds obviously for $Q\{H(\alpha)Q + P[H(\alpha) + \delta P]P\}$. By Weyl's criterion we have $N_{\mathrm{ess}}[QH(\alpha)Q + P(H(\alpha)P + \delta P] = N_{\mathrm{ess}}[H(\alpha) + \delta P]$; so (ii) of Proposition 4.1 implies that $[QH(\alpha)Q + PH(\alpha)P + \delta P - Z]^{-1}$ is meromorphic in α for $\mathrm{Re}z < \min([E_0^{(1)}, E_1^{(1)} - (\mathrm{Im}\alpha)^2\epsilon]$ with poles when $z \in \sigma_{\mathrm{disc}}[QHQ + PH(\alpha)P + \delta P]$. Actually since the group $W(\alpha)$, $\alpha \in \mathbb{R}$ commutes with P and Q we have for $\alpha \in \mathbb{R}$, $PH(\alpha)P + QH(\alpha)Q = W(\alpha)(PHP + QHQ)W^{-1}(\alpha)$. From this it follows that isolated eigenvalues of $PH(\alpha)P + QH(\alpha)Q$ remain independent of $\alpha \in \mathbb{C}$ as long as they are not absorbed in the essential spectrum. In particular,

$$\{E - [QH(\alpha)Q + PH(\alpha)P + \delta P]\}^{-1}Q = [E - QH(\alpha)Q]^{-1}Q$$

is analytic in α for $E < E_1^{(1)} - (\mathrm{Im}\alpha)^2\epsilon$ — which obviously includes $|\alpha| \leqslant 1$— provided $E \notin \sigma_{\mathrm{disc}}[QHQ + PHP]$. This follows from the Rayleigh–Ritz principle according to which $E \leqslant \min[\inf\sigma(PHP), \inf\sigma(QHQ)] = \inf\sigma(QHQ + PHP)$; equality cannot be attained unless $P\psi = \psi$ or $Q\psi = \psi$. Now $P\psi = \psi$ would mean $\sqrt{\rho} = u$ which corresponds to the trivial case of a two-electron atom without electronic repulsion. $Q\psi = \psi$ implies $u = 0$ contradicting Theorem 2.1. The same arguement applies for $QHQ + PHP + \delta P$. Hence we have shown that (ii) implies (iii). This finally completes the proof of Theorem 3.1.

Remarks: (1) With a little more effort it should be possible to give a complete characterization of $\sigma_{\mathrm{ess}}(H(\alpha))$ as a union of paraboloids centered at the various thresholds. This more precise result is not necessary however for our investigations. Notice that this characterization of $\sigma_{\mathrm{ess}}(H(\alpha))$ is not an immediate consequence of Theorem 4.1 of Ref. 4, since the function g given by (3.6) is not $C^\infty(\mathbb{R}^6)$ outside some finite ball in $\mathbb{R}^6$, but rather in $\mathbb{R}^3$.

(2) As already mentioned in Remark 2.2, Theorem 3.1 and the methods of Sec. 4 extend readily to "bosonic" atoms. In fact the method of Sec. 4 is applicable to more general situtions but since for such cases we have no bounds as given in Theorem 2.1 these results are not very interesting for the moment.

(3) Finally we should mention that if we replace the $1/r_{12}$ in (1.1) by $-\lambda(1/r_{12})$ with λ positive and sufficiently large, Theorem 3.1 is not necessarily true. See Ref. 5 for a discussion of the factorizability of ground state wavefuncitons as indicated in (1.4).

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APPENDIX

Here we collect the definitions and results of Deift *etal.*[4] which we needed in Sec. IV.

Definition A1: Let A be a closed operator on a Hilbert space $\mathscr{H}$. $N_{\rm ess}(A) = \{\lambda\in\mathbb{C}$: there exists a sequence $u_n\in\mathbb{D}(A)$ such that $\|u_n\| = 1$, $u_n\to 0$ (weakly) and $\|(\lambda - A)u_n\|\to 0\}$.

Lemma A 1: Let A be a closed operator on $\mathscr{H}$ with nonempty resolvent set $\rho(A)$. Then

(i) $N_{\rm ess}(A)\subset\sigma_{\rm ess}(A)$

(ii) Boundary of $\sigma_{\rm ess}(A)\subset N_{\rm ess}(A)$.

Definition A2: Let A be a closed operator on $L^2(\mathbb{R}^\nu)$ (ν some positive integer) having $C_0^\infty(\mathbb{R}^\nu)$ as a core. $N_\infty(A)$ $= \{\lambda\in\mathbb{C}$: there exists a sequence $u_n\in C_0^\infty(\mathbb{R}^\nu)$ such that $\|u_n\| = 1$, $\text{supp}u_n\cap K$ empty for each compact $K\subset\mathbb{R}^\nu$, and n sufficiently large, and $\|(\lambda - A)u_n\|\to 0$ as $n\to\infty\}$. Such a sequence will be called Weyl's sequence for A and λ.

Definition A3: A partition of unity in $\mathbb{R}^\nu$ is a finite set $\chi_0,\chi_1\cdots\chi_s$ of C^∞ functions with bounded derivatives obeying $0\leqslant\chi_i\leqslant 1$, $\sum_{i=0}^{s}\chi_i = 1$. $\chi_0\in C_0^\infty(\mathbb{R}^\nu)$ with $\chi_0 = 1$ on some neighborhood of 0. For $0 < d < \infty$, χ_i^d denotes the function $\chi_i(x/d)$, and also the corresponding multiplication operator.

Definition A4: Let $\chi_0,\cdots,\chi_s$ be a partition of unity on $\mathbb{R}^\nu$. For $i = 1,\ldots,s$ we define $N^i{}_\infty(A) = \{\lambda\in\mathbb{C}$: there exists a Weyl sequence u_n for A and g with $\text{supp}u_n\subset\text{supp}\chi_i^n\}$.

Lemma A2: Let A be a closed operator on $L^2(\mathbb{R}^\nu)$ with nonempty resolvent set having $C_0^\infty(\mathbb{R}^\nu)$ as a core. Let $\chi_0,\cdots,\chi_s$ be a partion of unity and suppose

(i) For each d, $\chi_0^d(z - A)^{-1}$ is compact for $z\in\rho(A)$.

(ii) For all $u\in C_0^\infty(\mathbb{R}^\nu)$ and $i = 0,\ldots,s$, $\|[A,\chi_i^d]u\|\leqslant\epsilon(d)(\|Au\| + \|u\|)$ with $\epsilon(d)\to 0$ as $d\to\infty$. Then

$$N_{\rm ess}(A) = N_\infty(A) = \bigcup_{i=1}^{s} N^i{}_\infty(A). \tag{A1}$$

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Exact solution of the Dicke model for the interaction of one atom with the electromagnetic field

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A formal solution is found for the probability amplitude of emission of a photon by an atom coupled with the electromagnetic radiation, without the assumption of the rotating wave approximation.

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I. INTRODUCTION

The problem of the interaction of a two-level atom with the electromagnetic field was solved more than a decade ago,[1,2] using the Dicke model[3] under the rotating-wave approximation (RWA). This approximation involves only locally energy-conserving terms, i.e., every time a photon is emitted, the atom decays to its lower level and vice versa. This assumption results in a probability of emission that varies periodically in time and there is a periodical transfer of energy from the atom to the field back and forth.[2]

In the present work within the electric dipole interaction, we do not neglect the counter-rotating terms. In other words we consider the virtual processes such as the creation of a photon and the simultaneous creation of a quantum of energy in the atom, as well as the annihilation of a photon and a quantum of energy in the atom. These terms, usually neglected in quantum optics, appear naturally in Dicke's model.

II. THE MODEL

Consider a two-level atom interacting with the electromagnetic field. The Hamiltonian describing this system can be written as[3]:

$$\mathscr{H} = \hbar\omega a^\dagger a + \hbar\omega_0\sigma_3 + \hbar K(a + a^\dagger)(\sigma^+ + \sigma^-), \quad (2.1)$$

where ω is the frequency of a single mode radiation field, $\hbar\omega_0$ is the energy separation of the levels, K the coupling constant, a and $a^\dagger$ the annihilation and creation operators for the field, and σ_3, σ^+, and σ^- the Pauli spin matrices representing the two-level atom. These operators obeys the standard commutation rules:

$$[\sigma_3,\sigma^\pm] = \pm\sigma^\pm; \quad [\sigma^+,\sigma^-] = 2\sigma_3, \quad [a,a^\dagger] = 1. \quad (2.2)$$

The RWA consists in neglecting the terms $a^\dagger\sigma^+$ and $a\sigma^-$ in Eq. (2.1). The usual argument given to neglect these terms is the following[4]: For $K = 0$ the Heisenberg operators have a time dependence given by $a(t) = a(0)\exp(-i\omega t)$, $a^\dagger(t) = a^\dagger(0)\exp(i\omega t)$, and $\sigma^+(t) = \sigma^+(0)\exp(i\omega_0 t)$. Near resonance ($\omega \simeq \omega_0$) the interaction terms $a\sigma^+$ and $a^\dagger\sigma^-$ are practically d-c terms as compared with $a\sigma^-$ and $a^\dagger\sigma^+$ that vary rapidly in time at frequencies $(\omega + \omega_0)$ and average to zero. This approximation is equivalent to decomposing a linearly polarized electromagnetic wave into opposite circularly polarized waves and keeping only the one rotating in the same sense as the precession of the two-level spin-atom.

Other authors have previously worked on this problem, with special interest in the Block–Siegert frequency shift,[5] which arises because of the presence of counter-rotating terms in the Hamiltonian. Hioe and Eberly[6] included these terms to calculate the Block–Siegert shift using a perturbation approach (up to the eighth order) by means of the Bargmann representation. Their results are in agreement with the earlier work done by Shirley[7] and with the work of Stedholm,[8] who derived a continuous fraction expression for this shift from a semiclassical theory. A comparison between semiclassical and quantum approaches was made by Swain.[9]

In the present work both rotating and counter-rotating terms are included in the Hamiltonian. An exact formal solution is found in the next section.

III. THE SOLUTION

The probability amplitude for the transition from an initial state $|i\rangle = |n\rangle|\frac{1}{2}\rangle$ to a final state $|f\rangle = |n+1\rangle|-\frac{1}{2}\rangle$ is given by

$$\phi = \langle f|\exp(-i\mathscr{H}t/\hbar)|i\rangle = \sum_{p=0}^{\infty}(-i\omega t)^p\langle f|(\mathscr{H}')^p|i\rangle/p!, \quad (3.1)$$

where

$$\mathscr{H}' = a^\dagger a + \sigma_3 + (K/\omega)(a + a^\dagger)(\sigma^+ + \sigma^-), \quad (3.2)$$

and exact resonance ($\omega = \omega_0$) has been assumed.

The term $\langle f|(\mathscr{H}')^p|i\rangle$ can be written as follows:

$$\langle f|(\mathscr{H}')^p|i\rangle = \sum_{\lambda_1,\lambda_2,\ldots\lambda_p}\langle f|\mathscr{H}'|\lambda_1\rangle\langle\lambda_1|\mathscr{H}'|\lambda_2\rangle\cdots\langle\lambda_{p-1}|\mathscr{H}'|i\rangle, \quad (3.3)$$

where

$$|\lambda_q\rangle \equiv |n_q; \pm\tfrac{1}{2}\rangle. \quad (3.4)$$

Each term in (3.3) corresponds to a set of states λ_r with $\lambda_0 = f$, $\lambda_p = i$, and $r = 1,2,\ldots,p-1$. The set $\{\lambda_r\}$ contains a subset $\{\lambda'_s\}$ where $\lambda'_s \neq \lambda'_r \forall s \neq r$, with $s = 1,2,\ldots,s_m \leqslant p$. In other words, every term in the summation (3.3) contains s_m different states. This subset defines a graph with s_m vertices and $s_m - 1$ branches in a unique way, and each vertex is uniquely associated to a given state in such a way that each branch corresponds to a nondiagonal element $\langle\lambda_q|\mathscr{H}'|\lambda_{q'}\rangle$ and each vertex corresponds to a diagonal element $\langle\lambda_q|\mathscr{H}'|\lambda_q\rangle$.

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For a fixed value of p, only those graphs with a number[10] of vertices less or equal than $\max(s_m) = \mathrm{INT}[(p+3)/2]$ contributes to the sum (3.3). The corresponding maximum number of branches is $\mathrm{INT}[(p+1)/2]$. Each graph can be travelled in many different ways, which we call paths. Each path starts at state $|i\rangle$, goes through the vertices or states λ_1 to λ_{p-1}, and finally arrives at state $|f\rangle$. We will say that a factor $\langle\lambda_i|\mathscr{H}'|\lambda_j\rangle$ in (3.3) corresponds to a "stop" at the vertex λ_i if $\lambda_i = \lambda_j$, and to a "step" from λ_i to λ_j if $\lambda_i \neq \lambda_j$.

In order to simplify the notation we denote the state $|i\rangle = |n;\frac{1}{2}\rangle$ by $|0\rangle$ and the state $|f\rangle = |n+1;-\frac{1}{2}\rangle$ by $|1\rangle$. The remaining states in the graph will be associated to an integer number according to the scheme shown in Fig. 1. The maximum value of this integer is $N \geqslant 1$ and its minimum value is $M \leqslant 0$. The pair (N,M) defines a graph uniquely, and since $N - M$ is the number of branches of this graph, the following condition is satisfied:

$$1 \leqslant N - M \leqslant \mathrm{INT}[(p+1)/2]. \tag{3.5}$$

There are many possible paths in a given graph satisfying (3.5). Any of these paths can be partially specified by the number of steps, which we call m, and the number of stops, $p - m$. Notice that for the initial and final states, $|i\rangle$ and $|f\rangle$, given above nonzero contributions exists only for m odd. For given values of p, N, and M the possible values of m are limited by

$$m_B = 2(N-M) - 1 \leqslant m \leqslant (p,p-1), \tag{3.6}$$

where $(p,p-1)$ is equal to p or $p-1$ according to whether p is odd or even, respectively.

The number of times a given path goes through a given state j is called the number of stations corresponding to the state j and this number is denoted by l_j. As an illustration consider Fig. 2(a) where a typical path is shown in the graph $(N=2, M=0)$. In this particular example the number of stations is given by the set $\{l_0 = 2, l_1 = 4, l_2 = 2\}$.

A given path defines the set $\{l_j\}$ uniquely. However the reciprocal statement is not true. This is shown by comparing Figs. 2(a) and 2(b). For given set $\{l_j\}$ there are many possible paths. The number of paths for given number of stations is a given graph will be denoted by $W(\{l_j\})$. It can be easily

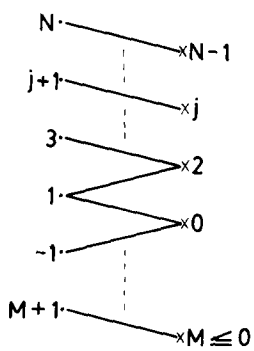

FIG. 1. Typical graph with dots (·) indicating the state $|\sigma_z\rangle = |-\frac{1}{2}\rangle$ and crosses (×) the state $|\sigma_z\rangle = |+\frac{1}{2}\rangle$. The vertex j corresponds to the state $|n+j;\sigma_z\rangle$. N and M define this graph uniquely. Note that N and M may correspond to either a dot or a cross.

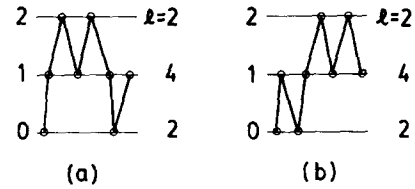

FIG. 2 (a). A typical path corresponding to a graph $(N=2, M=0)$ with the set of stations $\{l_0 = 2, l_1 = 4, l_2 = 2\}$. (b) Another possible path in the same graph and with the same set $\{l_0, l_1, l_2\}$, as in Fig. 2(a). The set of numbers $\{l_0, l_1, l_2\}$ corresponds to the number of stations at the states 0, 1, 2. A given path determines this set uniquely. The reciprocal statement is not true.

shown that set $\{l_j\}$ in the graph (N,M) satisfies the constraint

$$\sum_{j=M}^{N} l_j = m + 1. \tag{3.7}$$

Another trivial constraint to be satisfied by the set $\{l_j\}$ is $l_M \geqslant 1$, $l_N \geqslant 1$, $l_j \geqslant 2$ for $j \neq N, M$.

With the above considerations one can easily see that the sum in (3.3) can be rewritten as

$$\langle f|(\mathscr{H}')^p|i\rangle = \sum_{(N,M)} \sum_{\substack{m=m_B \\ \text{odd}}}^{(p,p-1)} \sum_{\{l_j\}} W(\{l_j\}) \prod_{j=M+1}^{N} a_j^{S_j} \sum_{q_1} \cdots \sum_{q_{m+1}} \mathscr{A}_1^{q_1} \cdots \mathscr{A}_{m+1}^{q_{m+1}}, \tag{3.8}$$

where in the last summation the indices are subject to the constraint $q_1 + q_2 + \cdots + q_{m+1} = p - m$, $a_j = K(n+j)^{\frac{1}{2}}/\omega$, and s_j is the number of steps between the states $j-1$ and j. $\mathscr{A}_t$ denotes a diagonal element of $\mathscr{H}'$ at the station t, where $1 \leqslant t \leqslant m+1$.

Explicit expressions for $W(\{l_j\})$, s_j and the summation over the q's are obtained in Appendices A and B. Replacing these results in (3.8) one obtains

$$\langle f|(\mathscr{H}')^p|i\rangle = \sum_{M=M_1}^{0} \sum_{N=1}^{N_1+M} \sum_{\substack{m=m_B \\ \text{odd}}}^{p,p-1} \sum_{\{l_j\}} \frac{Z_0!(Z_0-1)!}{(2Z_0-1)!} \times \prod_{j=M+1}^{N} \frac{(Z_{j-1}+Z_j-1)!}{(Z_j)!(Z_{j-1}-1)!} a_j^{s_j} \times \frac{\sum_{\eta=\mu}^{\nu} (A_\eta)^p A_\eta / 2^{1-\kappa_\eta} \binom{p}{\kappa_\eta - 1}}{2^m \prod_{\substack{\eta'=\mu \\ \neq\eta}}^{\nu} (\eta - \eta')^\kappa \eta}, \tag{3.9}$$

where $N_1 = \mathrm{INT}[(p+1)/2]$, $M_1 = -n$ or $1 - N_1$ depending on which number is larger, $\nu = \mathrm{INT}(N/2)$, $\mu = \mathrm{INT}(M/2)$, $\eta = \mathrm{INT}(j/2)$, $\kappa_n = l_{2\eta} + l_{2\eta+1}$, and $A_\eta = n + \frac{1}{2} + 2\eta$. Also

$$Z_j = \sum_{q=0}^{N-j} (-1)^q l_{j+q} \quad \text{for } j > 0,$$
$$Z_j = \sum_{q=0}^{j-M} (-1)^q l_{j-q} \quad \text{for } j \leqslant 0, \tag{3.10}$$

and $s_j = 2Z_j$, for $j \neq 1$ and $s_1 = 2Z_1 - 1$.

After inserting (3.10) in (3.1), we can invert the summation over p with all the summations appearing in (3.10), as it is shown in Appendix C. This allows us to perform the sum-

mation over p as follows:

$$\sum_{p=m}^{\infty}(-i\omega t)^p\binom{p}{\kappa_\eta-1}A_\eta^{p-\kappa_\eta+1}/p!$$
$$=A_\eta^{m-\kappa_\eta+1}\frac{(-i\omega t)^m}{(\kappa_\eta-1)!}\sum_{q=0}^{\infty}\frac{(-i\omega tA_\eta)^q}{(q+m+1-\kappa_\eta)!},$$

which can be readily written as

$$\frac{(-i\omega t)^m}{m!}\binom{m}{\kappa_\eta-1}A_\eta^{m-\kappa_\eta+1}\,{}_1F_1(1,m+2-\kappa_\eta;-i\omega A_\eta t), \tag{3.11}$$

where ${}_1F_1$ is the confluent hypergeometric function.

The final result for the probability amplitude ϕ is given by

$$\phi=\sum_{M=-n}^{0}\sum_{N=1}^{\infty}\sum_{\substack{m=m_B\\ \text{odd}}}^{\infty}\frac{(-i\tau)^m}{m!}\sum_{\{l_j\}}Z_0!(Z_0-1)!/(2Z_0-1)!$$
$$\times\prod_{j=M+1}^{N}(Z_j+Z_{j-1}-1)!/[Z_j!(Z_{j-1}-1)!]\}(n+j)^{s_j/2}$$
$$\times\sum_{\eta=\mu}^{\nu}(A_\eta/2)^{m-\kappa_\eta+1}(\kappa_\eta^m)\,{}_1F_1(1,m+2-\kappa_\eta;-i\omega A_\eta t)/$$
$$\prod_{\substack{\eta'=\mu\\ \neq\eta}}^{\nu}(\eta-\eta')^{\kappa_\eta}, \tag{3.12}$$

where $\tau=Kt$.

By restricting the calculation to 1-branch graphs this formula can be used to obtain the RWA result. This is done in Appendix D.

APPENDIX A

We consider the problem of determining the number of paths in a given graph (N,M), for which the number of stations at each state, the set $\{l_j\}$, is completely known. In order to proceed with the calculation we suppose that the number of steps between the states 0 and 1 is known. This number is called s_1, and it will later be shown that it is wholly determined from $\{l_j\}$. Then at this point the number of stations at $j=0$ is Z_0 and $Z_1=Z_0$ at $j=1$. Notice that $s_1=2Z_1-1$. Initially with have no other step in the whole graph (see Fig. 3). In order to form *one* path in the graph we proceed as follows. Consider one station at state 1, say the first station. We split this station into two stations 1 and 1′ and insert $2n_1$ steps between these stations and state 2, as shown in Fig. 3, adding in this way n_1 stations at state 2 and n_1 extra stations at state 1. We can follow the same procedure with the remaining stations at state 1, and find that the given number of stations at state 1, i.e., l_1, is given by

$$l_1=Z_1+Z_2,\quad\text{where}\quad Z_2=\sum_{i=1}^{Z_1}n_i.$$

By means of the same procedure we can reach states 3, 4, etc. up to state N, and therefore write the set of equations

$$\begin{aligned}
&l_1=Z_1+Z_2,\\
&l_2=Z_2+Z_3,\\
&\quad\vdots\\
&l_j=Z_j+Z_{j+1},\\
&l_{N-1}=Z_{N-1}+Z_N,\\
&l_N=Z_N.
\end{aligned}\tag{A1}$$

In the same manner we may proceed "downwards" up to state M and find the set of equations

$$\begin{aligned}
&l_0=Z_0+Z_{-1},\\
&l_{-1}=Z_{-1}+Z_{-2},\\
&\quad\vdots\\
&l_{M+1}=Z_{M+1}+Z_M,\\
&l_M=Z_M.
\end{aligned}\tag{A2}$$

Solving these equations for the Z_j's, we find

$$\begin{aligned}
Z_j&=\sum_{q=0}^{N-j}(-1)^q l_{j+q},\quad\text{for}\quad j>0\\
&=\sum_{q=0}^{j-M}(-1)^q l_{j-q},\quad\text{for}\quad j\leqslant 0.
\end{aligned}\tag{A3}$$

We notice that the number of steps between the states $j-1$ and j is by $s_j=2Z_j$ for $j\neq 1$, and $s_1=2Z_1-1$. The set $\{l_j\}$ is subject to three different constraints. The first two are

$$\sum_{j=M}^{N}l_j=m+1, \tag{A4}$$

and

$$l_M\geqslant 1,\quad l_N\geqslant 1,\quad\text{and}\quad l_j\geqslant 2\quad\text{for}\ j\neq N,M. \tag{A5}$$

The third constraint is obtained from

$$\sum_{j=M+1}^{N}s_j=m. \tag{A6}$$

From (A3) it can be easily shown that

$$\sum_{j=1}^{N}s_j=\sum_{j=1}^{N}[1+(-1)^{j-1}]l_j-1, \tag{A7}$$
$$\sum_{j=0}^{M+1}s_j=\sum_{j=-1}^{M}[1+(-1)^{j-1}]l_j,$$

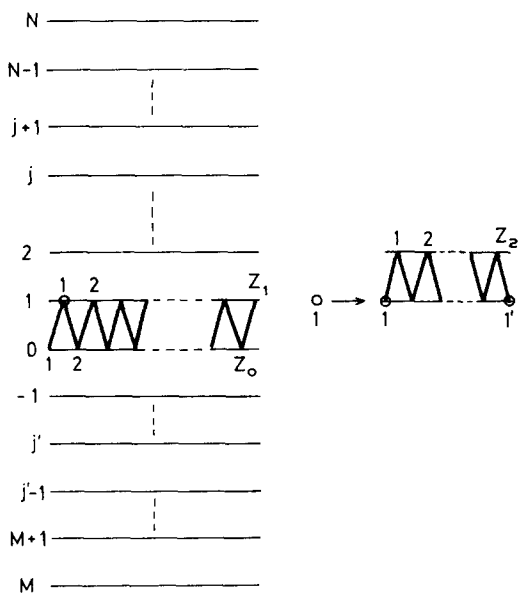

FIG. 3. Illustration of the insertion technique. Station 1 is splitted into 1 and 1′ and $2Z_2$ steps are inserted between states 1 and 2, creating Z_2 stations at state 2 and adding Z_2 stations at state 1.

Adding these two equations we obtain the third constraint to be satisfied by the l_j's:

$$\sum_{j=M}^{N}(-1)^{j-1}l_j = 0. \tag{A8}$$

Now we consider $W(\{l_j\})$. We notice that at the state i we can insert the Z_{i+1} extra stations in the Z_i original stations in

$$(Z_i + Z_{i+1} - 1)!/[Z_i!(Z_{i+1} - 1)!],$$

different manners, from which we readily obtain

$$W(\{l_j\}) = \prod_{j'=0}^{M+1}\frac{(Z_{j'} + Z_{j'-1} - 1)!}{Z_{j'-1}!(Z_{j'} - 1)!} \times \prod_{j=1}^{N-1}\frac{(Z_j + Z_{j+1} - 1)!}{Z_{j-1}!(Z_j - 1)!}, \tag{A9}$$

which can also be written as

$$W(\{l_j\}) = \frac{Z_0!(Z_0 - 1)!}{(2Z_0 - 1)!}\prod_{j=M}^{N-1}\frac{(Z_j + Z_{j+1} - 1)!}{Z_{j+1}!(Z_j - 1)!}. \tag{A10}$$

APPENDIX B

We first show the relation:

$$I_m(p') = \sum_{q_m}\sum_{q_{m-1}}\cdots\sum_{q_1}\mathscr{A}_m^{q_m}\mathscr{A}_{m-1}^{q_{m-1}}\cdots\mathscr{A}_1^{q_1} = \sum_{i=1}^{m}\mathscr{A}_i^{p'+m}/\prod_{\substack{j=1\\ \neq i}}^{m}(\mathscr{A}_i - \mathscr{A}_j), \tag{B1}$$

where $\mathscr{A}_i \neq \mathscr{A}_j \forall i \neq j$, and the q's are subject to the constraint

$$q_m + q_{m-1} + \cdots + q_1 = p'. \tag{B2}$$

Equation (B1) can be proved by induction. It can[11] easily be verified for $m = 1$ or 2. We start by assuming the validity of (B1) and then form $I_{m+1}(p')$:

$$I_{m+1}(p') = \sum_{q_{m+1}}\sum_{q_m}\sum_{q_{m-1}}\cdots\sum_{q_1}\mathscr{A}_{m+1}^{q_{m+1}}\mathscr{A}_m^{q_m}\mathscr{A}_{m-1}^{q_{m-1}}\cdots\mathscr{A}_1^{q_1},$$

where the indices are subject to a constraint similar to (B2):

$$q_{m+1} + q_m + q_{m-1} + \cdots + q_1 = p' \tag{B3}$$

Then we can write

$$I_{m+1}(p') = \sum_{q=0}^{p'}\mathscr{A}_{m+1}^{q} I_m(p' - q),$$

where we have set $q_{m+1} = q$. Now by means of (B1) we obtain

$$\begin{aligned} I_{m+1}(p') &= \sum_{q=0}^{p'}\mathscr{A}_{m+1}^{q}\sum_{i=1}^{m}\mathscr{A}_i^{p'-q+m}/\prod_{\substack{j=1\\ \neq i}}^{m}(\mathscr{A}_i - \mathscr{A}_j) \\ &= \sum_{i=1}^{m}\mathscr{A}_i^{p'+m+1}/\prod_{\substack{j=1\\ \neq i}}^{m}(\mathscr{A}_i - \mathscr{A}_j) \\ &\quad - \mathscr{A}_{m+1}^{p'+1}\sum_{i=1}^{m}\mathscr{A}_i^{m}/(\mathscr{A}_i - \mathscr{A}_{m+1}) \\ &\quad \times \prod_{\substack{j=1\\ \neq i}}^{m}(\mathscr{A}_i - \mathscr{A}_j), \end{aligned} \tag{B4}$$

However the last summation of (B4) is the partial fraction expansion of

$$-\mathscr{A}_{m+1}^{m}/\prod_{\substack{j=1\\ \neq i}}^{m+1}(\mathscr{A}_{m+1} - \mathscr{A}_j),$$

hence setting $p' = p - m$, (B4) reduces to

$$I_{m+1}(p') = \sum_{i=1}^{m+1}\mathscr{A}_i^{p+1}/\prod_{\substack{j=1\\ \neq i}}^{m+1}(\mathscr{A}_i - \mathscr{A}_j), \tag{B5}$$

and the proof of (B1) is completed.

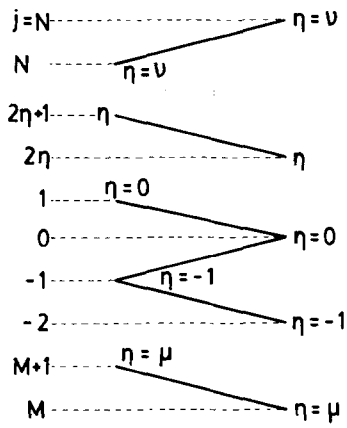

FIG. 4. This diagram illustrates the relation between indices j and η.

Now recall that the indices $i = 1,...,m+1$ denote the stations in a path through the graph (N,M) as shown in Fig. 4. We notice that for the states $j = 2\eta$ and $j = 2\eta + 1$, the value of the diagonal element $\mathscr{A}_j$ is the same for all the $\kappa_\eta = l_{2\eta} + l_{2\eta+1}$ stations at these two states and equal to $\mathscr{A}_\eta = n + \frac{1}{2} + 2\eta$, where $\eta = \mathrm{INT}(j/2)$ for $M \leqslant j \leqslant N$. We then set the first κ_μ elements equal to A_μ where $\mu = \mathrm{INT}(M/2)$, the next $\kappa_{\mu+1}$ elements equal to $A_{\mu+1}$ and so on. Then the first κ_μ terms in the summation (B5) can be written as

$$(A_\mu - A_{\mu+1})^{-\kappa_{\mu+1}}(A_\mu - A_{\mu+2})^{-\kappa_{\mu+2}}\cdots(A_\mu - A_\nu)^{-\kappa_\nu} \lim_{\substack{\mathscr{A}_i \to A_\mu\\ A_j \to A_\mu}}\sum_{i=1}^{\kappa_\mu}\mathscr{A}_i^{p}/\prod_{\substack{j=1\\ \neq i}}^{\kappa_\mu}(\mathscr{A}_i - \mathscr{A}_j),$$

where $\nu = \mathrm{INT}(N/2)$.

However, by means of (B1), with $m = \kappa_\mu$ and $p' = p - m$, the last sum is equal to

$$\lim_{\substack{\mathscr{A}_i \to A_\mu\\ 1 \leqslant i \leqslant \kappa_\mu}}\sum_{q_1}\sum_{q_2}\cdots\sum_{q_{\kappa_\mu}}\mathscr{A}_1^{q_1}\mathscr{A}_2^{q_2}\cdots\mathscr{A}_{\kappa_\mu}^{q_{\kappa_\mu}}, \tag{B6}$$

where the indices satisfy the constraint: $q_1 + \cdots + q_{\kappa_\mu} = p - \kappa_\mu + 1$. After taking the limit (B6) reduces to

$$A_\mu^{p-\kappa_\mu+1}\sum_{q_1}\sum_{q_2}\cdots\sum_{q_{\kappa_\mu}}1 = \binom{p}{\kappa_\mu - 1}A_\mu^{p-\kappa_\mu+1}.$$

The same procedure can be used for the remaining $m + 1 - \kappa_\mu$ terms in (B5), and thus, with $A_\eta - A_{\eta'} = 2(\eta - \eta')$, we finally obtain

$$\sum_{q_1}\sum_{q_2}\cdots\sum_{q_{m+1}}\mathscr{A}_1^{q_1}\mathscr{A}_2^{q_2}\cdots\mathscr{A}_m^{q_m}$$

$$=\sum_{\eta=\mu}^{\nu}2^{\kappa_\eta-m-1}A_\eta^{p-\kappa_\eta+1}\binom{p}{\kappa_\eta-1}\Big/\prod_{\substack{\eta'=\mu\\\neq\eta}}^{\nu}(\eta-\eta')^{\kappa}\eta'. \quad \text{(B7)}$$

APPENDIX C

In this appendix we show that the following summation inversion can be performed:

$$\sum_{p=0}^{\infty}\sum_{M=M_1}^{N_1+M}\sum_{\substack{m=m_B\\\text{odd}}}^{p,p-1}F(p,M,N,m)$$

$$=\sum_{M=-n}^{0}\sum_{N=1}^{\infty}\sum_{\substack{m=m_B\\\text{odd}}}^{\infty}\sum_{p=m}^{\infty}F(p,M,N,m). \quad \text{(C1)}$$

Let

$$G(p,M)=\sum_{N=1}^{N_1+M}\sum_{\substack{m=m_B\\\text{odd}}}^{p,p-1}F(p,M,N,m).$$

If we order this array by columns of constant M, we will notice that total number of columns is $n+1$, and that the smallest value of p is $-2M+1$. Therefore

$$\sum_{p=0}^{\infty}\sum_{M=M_1}^{0}G(p,M)=\sum_{M=-n}^{0}\sum_{p=-2M+1}^{\infty}G(p,M). \quad \text{(C2)}$$

Now consider

$$\sum_{p=-2M+1}^{\infty}G(p,M)=\sum_{p=-2M+1}^{\infty}\sum_{N=1}^{N_1+M}G'(p,N).$$

Then for constant N, the lowest value of p is $2(N-M)-1=m_B$; hence

$$\sum_{p=-2M+1}^{\infty}\sum_{N=1}^{N_1+M}G'(p,N)=\sum_{N=1}^{\infty}\sum_{p=m_B}^{\infty}G'(p,N). \quad \text{(C3)}$$

Finally we consider

$$\sum_{p=m_B}^{\infty}G'(p,N)=\sum_{p=m_B}^{\infty}\sum_{\substack{m=m_B\\\text{odd}}}^{p,p-1}F(p,M,N,m).$$

For a fixed value of m the smallest value of p is m, hence

$$\sum_{p=m_B}^{\infty}\sum_{\substack{m=m_B\\\text{odd}}}^{p,p-1}F(p,M,N,m)=\sum_{\substack{m=m_B\\\text{odd}}}^{\infty}\sum_{p=m}^{\infty}F(p,M,N,m). \quad \text{(C4)}$$

Collecting the results (C2), (C3), and (C4) we find (C1).

APPENDIX D

For one-branch graphs, i.e., $M=0$, $N=1$, $\Sigma\{l_j\}$ contains only one terms, i.e., $l_0=l_1=(m+1)/2$. In this case $W(\{l_j\})=1$. We also notice that there is only one possible value for η, i.e., $\eta=0$, for which value $A_\eta=n+\frac{1}{2}$. Also $s_j=s_1=m$ and $a_1=K(n+1)^{\frac{1}{2}}/\omega$. Replacing this results in (C1) we obtain

$$\kappa_\eta=m+1,\quad m_B=1,$$
$${}_1F_1(1,1;-i\omega(n+\tfrac{1}{2})t)=\exp[-i\omega(n+\tfrac{1}{2})t],$$

and

$$\phi=\sum_{m=1}^{\infty}\frac{(-i\tau)^m}{m!}(n+1)^{m/2}\exp[-i\omega(n+\tfrac{1}{2})t]$$
$$=-i\sin[\tau(n+1)^{\frac{1}{2}}]\exp[-i\omega(n+\tfrac{1}{2})t].$$

(see also Ref. 11). This is the usual result from the RWA.

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[10] By INT(α) we mean the highest integer number less than or equal to α.
[11] For $m=1$ (B1) reduces to an identity.

The expansion of cylindrical fiber modes in a spherical coordinate

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Rigorous expansions of cylindrical fiber modes in a spherical coordinate are obtained. The expansions are possible not only for the case in which the origin of the spherical coordinates is located just on the center axis of the fiber but also for the case in which the origin is in an arbitrary position in the transverse cross-sectional plane including the exterior cladding region where the fields are of the evanescent type.

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I. INTRODUCTION

Expansions of the Gaussian beam wave in terms of the spherical functions have been studied in connection with the problem of scattering of Gaussian beam wave by a spherical object.[1–5] Works on the two-dimensional version of this subject have also been available.[6–8] To the authors' knowledge, however, the expansions of the cylindrical fiber modes in a spherical coordinate have not yet been derived so far.

The expansion formulas derived in the present paper enable us to treat a wide variety of scattering and/or mode conversion problems of cylindrical modes due to spherical objects analytically as a conventional boundary value problem, although we need to use, in the practical application of these formulas, the approximation with respect to the boundary condition on the cylindrical boundary–neglect of multiple scattering between the object and the cylindrical boundary in the first stage. In fact, for example, the scattering and mode conversion of guided modes in a step-index optical fiber caused by a spherical obstacle have been analyzed successfully[9] by using the results obtained in the present paper.

The purpose of this paper is to obtain the rigorous expansions of the fiber modes in a spherical coordinate. The expansion coefficients are given in closed form for either electric or magnetic field.

II. MODES OF THE STEP-INDEX OPTICAL FIBER

Let us consider the so-called "LP" (linearly polarized) modes of the step-index optical fiber.[10] Let the origin of the spherical coordinates be located at a point O_1 on the x axis apart from the origin O by a distance l_0, as shown in Fig. 1 in which the z axis corresponds to the fiber axis. Then, the electric field of the guided modes in the core region with y-polarized electric field can be expressed in terms of the elementary cylindrical wave function $\overset{(1)}{\psi}_i{}^{(2)}(\mathbf{r}_i,s)$ $(i=1,2)$ as follows[9]:

$$\mathbf{E}^{(2)}=\sum_{s=0}^{\infty}\left(1-\frac{\delta_{s0}}{2}\right)\left[P^{(2)}(s)\overset{(1)}{\psi}_1{}^{(2)}(\mathbf{r}_1,s)+Q^{(2)}\overset{(1)}{\psi}_2{}^{(2)}(\mathbf{r}_1,s)\right], \tag{1}$$

where

$$\overset{(1)}{\psi}_1{}^{(2)}(\mathbf{r}_1,s)=\mathbf{i}_y J_s(h\rho_1)\exp\{-j\beta z\}\begin{matrix}\cos\\ \sin\end{matrix} s\phi_1,$$

$$\overset{(1)}{\psi}_2{}^{(2)}(\mathbf{r}_1,s)=\mathbf{i}_z J_s(h\rho_1)\exp(-j\beta z)\begin{matrix}\sin\\ \cos\end{matrix} s\phi_1, \tag{2}$$

and

$$\overset{(1)}{P}{}^{(2)}(s)=A\left[J_{\nu-s}(hl_0)\pm(-1)^s J_{\nu+s}(hl_0)\right],$$

$$\overset{(1)}{Q}{}^{(2)}(s)=\frac{jA}{\beta l_0}\left[\pm(\nu-s)J_{\nu-s}(hl_0)-(-1)^s(\nu+s)J_{\nu+s}(hl_0)\right]. \tag{3}$$

In these equations, δ_{mn} indicates Kronecker's delta, $\mathbf{i}_y$ and $\mathbf{i}_z$ represent the unit vectors directed along the positive y and z axes, respectively, and A is the mode amplitude coefficient. $J_s(\cdot)$ is the Bessel function of sth order, $h=\sqrt{(k_1^2-\beta^2)}$, $k_1=\omega\sqrt{\epsilon_1\mu_0}=n_1k_0$, where k_0 is the free-space wave number, β is the propagation constant, and $n_1(=\sqrt{\epsilon_1/\epsilon_0})$ is the refractive index of the core region. The superscripts (1) and (2) on the left-hand side of Eqs. (2) and (3) correspond to the upper and lower functions [Eq. (2)] and signs [Eq. (3)] on the right-hand sides, respectively. If we replace h by $j\gamma$ in Eq. (2), and A and $J_\nu(hl_0)$ by $AJ_\nu(hR)/H_\nu^{(1)}(j\gamma R)$ and $H_\nu^{(1)}(j\gamma l_0)$, respectively, in Eq. (3), we can obtain the electric fields of the

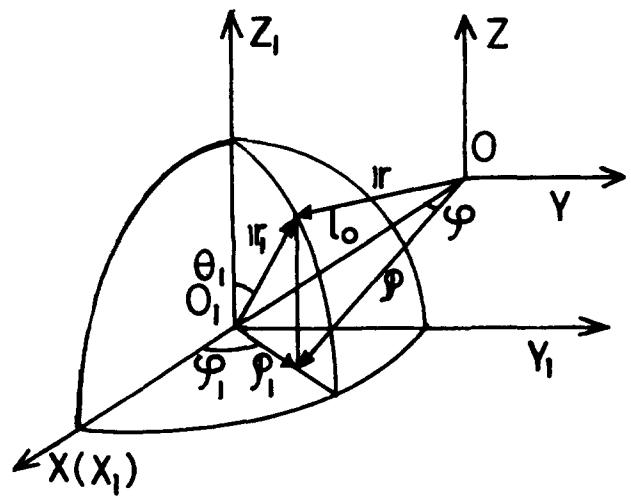

FIG. 1. System of coordinates used for the analysis.

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same mode in the cladding region, where $H_\nu^{(1)}(\cdot)$ is the νth order Hankel function of the first kind, R is the core radius, $\gamma = \sqrt{(\beta^2 - k_2^2)}$, where $k_2 = n_2 k_0$, and n_2 is the refractive index of the cladding region.

III. EXPANSIONS OF ELEMENTARY FUNCTIONS ψ_i IN TERMS OF SPHERICAL VECTOR WAVE FUNCTIONS

Using the expression of the cylindrical wave function in spherical coordinates,[11] the elementary function ψ_i given by Eq. (2) can be expressed in the spherical coordinates about the polar axis z_1 as follows:

$$\overset{(1)}{\psi}_1{}^{(2)}(\mathbf{r}_1,s) = \overset{(1)}{\psi}{}^{(2)}(\mathbf{i}_{r_1}\sin\theta_1\sin\phi_1 + \mathbf{i}_{\theta_1}\cos\theta_1\sin\phi_1 + \mathbf{i}_{\phi_1}\cos\phi_1), \tag{4}$$

$$\overset{(1)}{\psi}_2{}^{(2)}(\mathbf{r}_1,s) = \overset{(2)}{\psi}{}^{(1)}(\mathbf{i}_{r_1}\cos\theta_1 - \mathbf{i}_{\theta_1}\sin\theta_1), \tag{5}$$

with

$$\overset{(1)}{\psi}{}^{(2)} = \sum_{\eta=0}^{\infty} \Theta_\eta P_\eta^s(\cos\theta_1)\begin{matrix}\cos\\ \sin\end{matrix} s\phi_1, \tag{6}$$

where

$$\Theta_\eta = (-j)^{\eta - s}(2\eta+1)\frac{(\eta - s)!}{(\eta + s)!} P_\eta^s(\cos\alpha)\mathscr{J}_\eta(k_1 r_1), \tag{7}$$

and $\cos\alpha = \beta/k_1$, and where $P_\eta^s(\cdot)$ and $\mathscr{J}_\eta(\cdot)$ denote the associated Legendre function and the spherical Bessel function, respectively. Equation (4)–(7) hold also in the cladding region, although $\cos\alpha$ becomes apparently greater than 1.

Our next step is to expand ψ_i in terms of the spherical vector wave functions $\mathbf{M}$ and $\mathbf{N}$

$$\overset{(1)}{\psi}_1{}^{(2)} = \sum_{n=0}^{\infty}\sum_{m=0}^{n}\sum_{\sigma=e,0}\left(-j\frac{\omega}{k_1}C'^{(1)}_{(2)\sigma mn}\mathbf{M}^{(1)}_{\sigma mn} + D'^{(1)}_{(2)\sigma mn}\mathbf{N}^{(1)}_{\sigma mn}\right), \tag{8}$$

$$\overset{(1)}{\psi}_2{}^{(2)} = \sum_{n=0}^{\infty}\sum_{m=0}^{n}\sum_{\sigma=e,0}\left(-j\frac{\omega}{k_1}C''^{(1)}_{(2)\sigma mn}\mathbf{M}^{(1)}_{\sigma mn} + D''^{(1)}_{(2)\sigma mn}\mathbf{N}^{(1)}_{\sigma mn}\right). \tag{9}$$

The functions $\mathbf{M}$ and $\mathbf{N}$ are defined by[12,13]

$$\mathbf{M}^{(i)}_{\substack{e\\o}mn} = \mathrm{rot}\left[\mathbf{i}_r r z_n^{(i)}(kr)P_n^m(\cos\theta)\begin{matrix}\cos\\ \sin\end{matrix} m\phi\right],$$

$$\mathbf{N}^{(i)}_{\substack{e\\o}mn} = \frac{1}{k}\mathrm{rot}\mathbf{M}^{(i)}_{\substack{e\\o}mn}, \tag{10}$$

where $z_n^{(i)}$ represents the spherical Bessel functions $\mathscr{J}_n$, $\mathscr{N}_n$, $\mathscr{H}_n^{(1)}$, and $\mathscr{H}_n^{(2)}$ for $i = 1, 2, 3$, and 4, respectively. The coefficients $C_{\sigma mn}$ and $D_{\sigma mn}$ can be determined by using the orthogonality properties of $\mathbf{M}$ and $\mathbf{N}$.

A. Determination of $C'_{\sigma mn}$ and $C''_{\sigma mn}$

$C'^{(1)}_{(2)\sigma mn}$ can be calculated from

$$C'^{(1)}_{(2)\sigma mn} = \frac{j2k_1\mathscr{J}_n(k_1 r_1)}{(1+\delta_{m0})\omega\mathscr{B}^{(1)}_{mn}(r_1)} \times \sum_{\eta=0}^{\infty}\Theta_\eta(-mI_1^{(1)(2)} - I_2^{(1)(2)}), \tag{11}$$

where

$$\mathscr{B}^{(i)}_{mn}(r) = \frac{4\pi n(n+1)}{2n+1}\frac{(n+m)!}{(n-m)!}[z_n^{(i)}(k_1 r)]^2, \tag{12}$$

and

$$I_1^{(1)} = \int_0^{2\pi}\begin{matrix}\cos\\ \sin\end{matrix} s\phi_1 \begin{matrix}\sin\\ \cos\end{matrix} \phi_1 \begin{matrix}\sin\\ \cos\end{matrix} m\phi_1\, d\phi_1 \times \int_0^{\pi} P_\eta^s(\cos\theta_1)P_n^m(\cos\theta_1)\cos\theta_1\, d\theta_1, \tag{13}$$

$$I_2^{(1)} = \int_0^{2\pi}\begin{matrix}\cos\\ \sin\end{matrix} s\phi_1 \begin{matrix}\cos\\ \sin\end{matrix} \phi_1 \begin{matrix}\cos\\ \sin\end{matrix} m\phi_1\, d\phi_1 \times \int_0^{\pi} P_\eta^s(\cos\theta_1)\frac{dP_n^m(\cos\theta_1)}{d\theta_1}\sin\theta_1\, d\theta_1, \tag{14}$$

$I_1^{(2)}$ is the same as $I_1^{(1)}$ with $\cos s\phi_1$ being replaced by $\sin s\phi_1$ and $I_2^{(2)}$ is the same as $I_2^{(1)}$ with the same replacement. The integration with respect to ϕ_1 can easily be performed, yielding $I_1^{(2)} = I_2^{(2)} = 0$ and

$$I_1^{(1)} = \frac{\pi}{2}\int_0^{\pi} P_\eta^s(\cos\theta_1)P_n^m(\cos\theta_1)\cos\theta_1\, d\theta_1 \times [\delta_{s,m-1}(1+\delta_{m1}) - \delta_{s,m+1}(1-\delta_{m0})], \tag{15}$$

$$I_2^{(1)} = \frac{\pi}{2}\int_0^{\pi} P_\eta^s(\cos\theta_1)\frac{dP_n^m(\cos\theta_1)}{d\theta_1}\sin\theta_1\, d\theta_1 \times [\delta_{s,m-1}(1+\delta_{m1}) + \delta_{s,m+1}(1+\delta_{m0})], \tag{16}$$

From $I_1^{(2)} = I_2^{(2)} = 0$, we get

$$C'^{(2)}_{emn} = 0. \tag{17}$$

Let us introduce the functions J_a and J_b defined by

$$J_a(\eta,n,m) = \int_0^{\pi} P_\eta^{m-1}(\cos\theta_1)P_n^m(\cos\theta_1)\cos\theta_1\, d\theta_1, \tag{18}$$

$$J_b(\eta,n,m) = \int_0^{\pi} P_\eta^{m+1}(\cos\theta_1)P_n^m(\cos\theta_1)\cos\theta_1\, d\theta_1, \tag{19}$$

$I_1^{(1)}$ can then be expressed as

$$I_1^{(1)} = \frac{\pi}{2}[\delta_{s,m-1}(1+\delta_{m1})J_a(\eta,n,m) - \delta_{s,m+1}(1-\delta_{m0})J_b(\eta,n,m)]. \tag{20}$$

Using the recurrence and the integral formulas of the associated Legendre function, $I_2^{(1)}$ can be reduced to

$$I_2^{(1)} = \frac{\pi}{2}\left[\delta_{s,m-1}(1+\delta_{m1})\left(\delta_{n\eta}\frac{2(n+m-1)!(n+m)}{(n-m)!(2n+1)} - mJ_a(\eta,n,m)\right) + \delta_{s,m+1}(1+\delta_{m0}) \times\left(mJ_b(\eta,n,m) - \delta_{n\eta}\frac{2(n+m+1)!}{(n-m-1)!(2n+1)}\right)\right]. \tag{21}$$

Using Eqs. (20) and (21), $C'^{(1)}_{emn}$ becomes

$$C'^{(1)}_{emn} = (1+\delta_{s0})\Upsilon_1 - \Upsilon_2, \tag{22}$$

where

$$\Upsilon_1 = \delta_{s,m+1}\frac{(n-s)!}{(n+s)!}\Upsilon_0, \quad \Upsilon_2 = \delta_{m,s-1}\frac{(n-s+1)!}{(n+s-1)!}\Upsilon_0,$$
$$\Upsilon_0 = (k_1/\omega)g_n(-j)^{n-s+1}P_\eta^s(\cos\alpha), \tag{23}$$

$$g_n = (2n+1)/[2n(n+1)]. \tag{24}$$

It should be noted that neither $J_a(\eta,n,m)$ nor $J_b(\eta,n,m)$ is included in Eq. (22) any more.

$C'^{(1)}_{(2)0mn}$ can be calculated from

$$C'^{(1)}_{(2)0mn} = \frac{j2k_1 \not{j}_n(k_1r_1)}{(1+\delta_{m0})\omega \mathscr{B}^{(1)}_{mn}(r_1)} \sum_{\eta=0}^{\infty} \Theta_\eta (mI_3^{(1)(2)} - I_4^{(1)(2)}), \tag{25}$$

where $I_3^{(1)(2)}$ is the same as $I_1^{(1)(2)}$ with $\sin m\phi_1$ replaced by $\cos m\phi_1$ and $I_4^{(1)(2)}$ is the same as $I_2^{(1)(2)}$ with $\cos m\phi_1$ replaced by $\sin m\phi_1$. By steps similar to those leading to the expressions for C'_{emn} given by Eqs. (17) and (22), we can derive the expressions for C'_{0mn}:

$$C'^{(1)}_{0mn} = 0, \tag{26}$$

$$C'^{(2)}_{0mn} = (1-\delta_{s0})\Upsilon_1 - (1-\delta_{s1})\Upsilon_2. \tag{27}$$

C''_{emn} and C''_{0mn} can easily be calculated. The results are

$$C''^{(2)}_{emn} = C''^{(1)}_{0mn} = 0, \tag{28}$$

$$C''^{(2)}_{0mn} = \delta_{ms} 2s\Upsilon_0 (n-s)!/(n+s)!, \tag{29}$$

$$C''^{(1)}_{emn} = -(1-\delta_{s0}) C''^{(2)}_{0mn}. \tag{30}$$

B. Determination of D'_{emn} and D''_{emn}

$D'^{(1)}_{(2)emn}$ can be calculated from

$$D'^{(1)}_{(2)emn} = \frac{2k_1}{(1+\delta_{m0})\mathscr{D}^{(1)}_{mn}(r_1) r_1} \times \sum_{\eta=0}^{\infty} \Theta_\eta \left(n(n+1) \not{j}_n(k_1r_1) I_5^{(1)(2)} + \frac{d[r_1 \not{j}_n(k_1r_1)]}{dr_1} [I_6^{(1)(2)} - mI_7^{(1)(2)}] \right), \tag{31}$$

where

$$\mathscr{D}^{(i)}_{mn}(r) = \frac{4\pi k_1^2 n(n+1)}{(2n+1)^2} \frac{(n+m)!}{(n-m)!} \times \{(n+1)[z^{(i)}_{n-1}(k_1r)]^2 + n[z^{(i)}_{n+1}(k_1r)]^2\}, \tag{32}$$

and

$$I_5^{(1)} = \int_0^{2\pi} \sin\phi_1 \cos m\phi_1 \cos s\phi_1 \, d\phi_1 \times \int_0^{\pi} P^s_\eta(\cos\theta_1) P^m_n(\cos\theta_1) \sin^2\theta_1 \, d\theta_1, \tag{33}$$

$$I_6^{(1)} = \int_0^{2\pi} \sin\phi_1 \cos m\phi_1 \cos s\phi_1 \, d\phi_1 \times \int_0^{\pi} P^s_\eta(\cos\theta_1) \frac{dP^m_n(\cos\theta_1)}{d\theta_1} \cos\theta_1 \sin\theta_1 \, d\theta_1, \tag{34}$$

$$I_7^{(1)} = \int_0^{2\pi} \cos\phi_1 \sin m\phi_1 \cos s\phi_1 \, d\phi_1 \times \int_0^{\pi} P^s_\eta(\cos\theta_1) P^m_n(\cos\theta_1) \, d\theta_1. \tag{35}$$

$I_5^{(2)}$, $I_6^{(2)}$, and $I_7^{(2)}$ are of the same forms as $I_5^{(1)}$, $I_6^{(1)}$, and $I_7^{(1)}$, respectively, except that $\cos s\phi_1$ is replaced by $\sin s\phi_1$. Since

$$I_5^{(1)} = I_6^{(1)} = I_7^{(1)} = 0, \quad D'^{(1)}_{emn} = 0. \tag{36}$$

After some manipulations, $I_5^{(2)}$, $I_6^{(2)}$, and $I_7^{(2)}$ can be reduced to

$$I_5^{(2)} = (\pi/2)[-\delta_{s,m-1}(1-\delta_{s0}) F_a(\eta,n,m) + \delta_{s,m+1}(1+\delta_{s1}) F_b(\eta,n,m)], \tag{37}$$

$$I_6^{(2)} = \frac{\pi}{2} \Big[\delta_{s,m-1}(1-\delta_{s0}) \Big(mJ_a(\eta,n+1,m) + (n+m)(n+m-1)(n+1) F_a(\eta,n,m-2) - \delta_{\eta,n+1} \frac{2(n+m)!(n+m)(n+1)}{(n-m+2)!(2n+3)} \Big) + \delta_{s,m+1} \times (1+\delta_{s1}) \Big(\frac{m(n-m+1)}{n+m+1} J_b(\eta,n+1,m) + (n+1)(F_b(\eta,n,m) - \delta_{\eta,n+1} \times \frac{2(n+m+2)!(n+1)}{(n-m)!(2n+3)(n+m+1)} \Big) \Big], \tag{38}$$

$$I_7^{(2)} = \frac{\pi}{2} \Big[\delta_{s,m-1}(1-\delta_{s0}) \Big(J_a(\eta,n-1,m) + \delta_{\eta,m-1} \times \frac{2(n+m-2)!(n+m-1)}{(n-m)!(2n-1)} \Big) + \delta_{s,m+1}(1-\delta_{m0}) \times \Big(\frac{n-m+1}{n+m+1} J_b(\eta,n+1,m) + \delta_{\eta,n+1} \times \frac{2(n+m)!(n+m+2)}{(n-m)!(2n+3)} \Big) \Big], \tag{39}$$

where

$$F_a(\eta,n,m) = \int_0^{\pi} P^{m-1}_\eta(\cos\theta_1) P^m_n(\cos\theta_1) \sin^2\theta_1 \, d\theta_1 = (\delta_{\eta,n-1} - \delta_{\eta,n+1}) \frac{2(n+m)!}{(n-m)!(2\eta+1)(2n+1)}, \tag{40}$$

$$F_b(\eta,n,m) = \int_0^{\pi} P^{m+1}_\eta(\cos\theta_1) P^m_n(\cos\theta_1) \sin^2\theta_1 \, d\theta_1 = (\delta_{\eta,n+1} - \delta_{\eta,n-1}) \frac{2(n+m+1)!}{(n-m-1)!(2\eta+1)(2n+1)}. \tag{41}$$

Using Eqs. (37)–(41) and the relation

$$J_a(\eta,n+1,m) - J_a(\eta,n-1,m) = \delta_{\eta,n+1} \frac{2(n+m)!}{(n-m+1)!(2n+3)} + \delta_{\eta,n-1} \frac{2(n+m-1)!}{(n-m)!(2n-1)}, \tag{42}$$

we obtain, after some manipulations,

$$D'^{(2)}_{emn} = (1-\delta_{s0})\Delta_1 + \Delta_2, \tag{43}$$

where

$$\Delta_1 = \delta_{m,s+1} \Delta_0 \Big(\frac{\Lambda_1 P^s_{n-1}(\cos\alpha)}{(n-s)(n-s+1)} + \frac{\Lambda_2 P^s_{n+1}(\cos\alpha)}{(n+s)(n+s+1)} \Big),$$

$$\Delta_2 = \delta_{m,s-1}\Delta_0[\Lambda_1 P^s_{n-1}(\cos\alpha) + \Lambda_2 P^s_{n+1}(\cos\alpha)],$$
$$\Delta_0 = g_n(-j)^{n-s+1}(n-s+1)!/(n+s-1)!,$$
$$\Lambda_1 = (n+1)\mathscr{f}^2_{n-1}(k_1r_1)/\Lambda_0, \quad \Lambda_2 = n\mathscr{f}^2_{n+1}(k_1r_1)/\Lambda_0,$$
$$\Lambda_0 = (n+1)\mathscr{f}^2_{n-1}(k_1r_1) + n\mathscr{f}^2_{n+1}(k_1r_1). \tag{44}$$

$D'^{(1)}_{0mn}{}^{(2)}$ can be calculated from

$$D'^{(1)}_{0mn}{}^{(2)} = \frac{2k_1}{(1+\delta_{m0})\mathscr{D}^{(1)}_{mn}(r_1)r_1} \times \sum_{\eta=0}^{\infty}\Theta_\eta\left(n(n+1)\mathscr{f}_n(k_1r_1)I_8{}^{(1)}_{(2)} + \frac{d[r_1\mathscr{f}_n(k_1r_1)]}{dr_1}\left[I_9{}^{(1)}_{(2)} + mI_{10}{}^{(1)}_{(2)}\right]\right), \tag{45}$$

where $I_8{}^{(1)}_{(2)}$ and $I_9{}^{(1)}_{(2)}$ are the same as $I_5{}^{(1)}_{(2)}$ and $I_6{}^{(1)}_{(2)}$, respectively, with $\cos m\phi_1$ replaced by $\sin m\phi_1$, and $I_{10}{}^{(1)}_{(2)}$ is the same as $I_7{}^{(1)}_{(2)}$ with $\sin m\phi_1$ replaced by $\cos m\phi_1$. Since the terms associated with θ_1 in I_8, I_9 ands I_{10} are just the same as those in I_5 I_6, and I_7, respectively, D'_{0mn} can be calculated following the same procedure by which D'_{emn} was calculated. The results are

$$D'^{(1)}_{0mn} = -(1+\delta_{s0})\Delta_1 - (1-\delta_{s1})\Delta_2, \tag{46}$$
$$D'^{(2)}_{0mn} = 0. \tag{47}$$

$D''^{(1)}_{emn}{}^{(2)}$ can be calculated from

$$D''^{(1)}_{emn}{}^{(2)} = \frac{2k_1}{(1+\delta_{m0})\mathscr{D}^{(1)}_{mn}(r_1)r_1}\sum_{\eta=0}^{\infty}\Theta_\eta \times\left(n(n+1)\mathscr{f}_n(k_1r_1)I_{11}{}^{(1)}_{(2)} - \frac{d[r_1\mathscr{f}_n(k_1r_1)]}{dr_1}I_{12}{}^{(1)}_{(2)}\right), \tag{48}$$

where

$$I^{(1)}_{11} = \int_0^{2\pi}\cos m\phi_1\sin s\phi_1\,d\phi_1 \times\int_0^{\pi}P^s_\eta(\cos\theta_1)P^m_n(\cos\theta_1)\cos\theta_1\sin\theta_1\,d\theta_1, \tag{49}$$

$$I^{(1)}_{12} = \int_0^{2\pi}\cos m\phi_1\sin s\phi_1\,d\phi_1 \times\int_0^{\pi}P^s_\eta(\cos\theta_1)\frac{dP^m_n(\cos\theta_1)}{d\theta_1}\sin^2\theta_1\,d\theta_1, \tag{50}$$

and $I^{(2)}_{11}$ and $I^{(2)}_{12}$ are the same as $I^{(1)}_{11}$ and $I^{(1)}_{12}$, respectively, with $\cos m\phi_1$ replaced by $\sin m\phi_1$. Since $I^{(1)}_{11} = I^{(1)}_{12} = 0$,

$$D''^{(1)}_{emn} = 0. \tag{51}$$

Following the similar procedure as before, we obtain

$$I^{(2)}_{11} = 2\pi\delta_{sm}(1+\delta_{s0})\left(\delta_{\eta,n+1}\frac{(n+m+1)!}{(n-m)!(2n+3)(2n+1)} + \delta_{\eta,n-1}\frac{(n+m)!}{(n-m-1)!(2n-1)(2n+1)}\right), \tag{52}$$

$$I^{(2)}_{12} = 2\pi\delta_{sm}(1+\delta_{s0})\left(\delta_{\eta,n+1}\frac{(n+m+1)!n}{(n-m)!(2n+3)(2n+1)} - \delta_{\eta,n-1}\frac{(n+m)!(n+1)}{(n-m-1)!(2n-1)(2n+1)}\right). \tag{53}$$

Consequently, we get

$$D''^{(2)}_{emn} = -2\delta_{ms}\Delta_0\left(\frac{\Lambda_1}{n-s+1}P^s_{n-1}(\cos\alpha) - \frac{\Lambda_2}{n+s}P^s_{n+1}(\cos\alpha)\right). \tag{54}$$

It can easily be shown that $D''^{(1)}_{0mn}$ becomes

$$D''^{(1)}_{0mn} = (1-\delta_{s0})D''^{(2)}_{emn}, \tag{55}$$
$$D''^{(2)}_{0mn} = 0. \tag{56}$$

Thus, all the coefficients in the expansion of ψ_1 and ψ_2 have been determined. The coefficients of the corresponding expansions in the cladding region can be obtained from those for ψ_1 and ψ_2 by only replacing k_1 and k_2.

IV. EXPANSION OF GUIDED MODES IN THE STEP-INDEX OPTICAL FIBER

A typical example of applications of the expansions for the elementary functions ψ_1 and ψ_2 is the expansion of guided modes in the step-index optical fiber in terms of spherical vector wave functions.

In the case of $l_0 \neq 0$, the expansion for the electric field given by Eq. (1) becomes

$$\mathbf{E}^{(1)(2)} = \sum_{n=0}^{\infty}\sum_{m=0}^{n}\left(-j\frac{\omega}{k_1}C^{(1)}_{(2)mn}\mathbf{M}^{(1)}_{\substack{e\\o}mn} + D^{(1)}_{(2)mn}\mathbf{N}^{(1)}_{\substack{o\\e}mn}\right), \tag{57}$$

where

$$-j\frac{\omega}{k_1}C^{(1)}_{(2)mn} = -\Gamma_{mn}W^{(1)}_{(2)mn},$$
$$D^{(1)}_{(2)mn} = j\Gamma_{mn}(F^{(1)}_{(2)mn}\Lambda_1 + G^{(1)}_{(2)mn}\Lambda_2),$$
$$\Gamma_{mn} = (-j)^{n-m+1}(n-m)!/(n+m)!, \tag{58}$$
$$W^{(1)}_{mn} = U_1(m-1)\cdot B_1 + U_1(m+1)\cdot B_2 + U_2(m)\cdot B_3,$$
$$W^{(2)}_{mn} = V_1(m-1)\cdot(1-\delta_{m1})B_1 + (1-\delta_{m0})V_1(m+1)\cdot B_2 + V_2(m)\cdot B_3, \tag{59}$$
$$B_1 = P^{m-1}_n(\cos\alpha)\cdot(n-m+1)(n+m),$$
$$B_2 = P^{m+1}_n(\cos\alpha), \tag{60}$$
$$B_3 = 2mP^m_n(\cos\alpha),$$
$$F^{(1)}_{mn} = U_1(m-1)\cdot D_1 - U_1(m+1)\cdot(1-\delta_{m0})D_2 - 2U_2(m)\cdot(1-\delta_{m0})D_3,$$
$$F^{(2)}_{mn} = -V_1(m-1)\cdot(1-\delta_{m1})D_1 + V_1(m+1)\cdot D_2 + V_2(m)\cdot(2-\delta_{m0})D_3, \tag{61}$$
$$D_1 = P^{m+1}_{n-1}(\cos\alpha)\cdot(n+m-1)(n+m),$$
$$D_2 = P^{m+1}_{n-1}(\cos\alpha), \tag{62}$$
$$D_3 = P^m_{n-1}(\cos\alpha)\cdot(n+m),$$
$$G^{(1)}_{mn} = U_1(m-1)\cdot T_1 - U_1(m+1)\cdot(1-\delta_{m0})T_2 + 2U_2(m)\cdot(1-\delta_{m0})T_3,$$

$$G^{(2)}_{mn} = -V_1(m-1)\cdot(1-\delta_{m0})T_1 + V_1(m+1)\cdot T_2 - V_2(m)\cdot(2-\delta_{m0})T_3, \tag{63}$$

$$T_1 = P^{m-1}_{n+1}(\cos\alpha)\cdot(n-m+2)(n-m+1),$$
$$T_2 = P^{m+1}_{n+1}(\cos\alpha),$$
$$T_3 = P^{m}_{n+1}(\cos\alpha)\cdot(n-m+1), \tag{64}$$
$$U_1(m) = g_n P^{(1)}(m),$$
$$U_2(m) = -jg_n Q^{(1)}(m),$$
$$V_1(m) = g_n P^{(2)}(m),$$
$$V_2(m) = jg_n Q^{(2)}(m). \tag{65}$$

The above expansions are also applicable for the cladding region, except that h, A, and $J_\nu(hl_0)$ must be replaced by $j\gamma$, $AJ_\nu(hR)/H^{(1)}_\nu(j\gamma R)$, and $H^{(1)}_\nu(j\gamma l_0)$, respectively.

In the case of $l_0 = 0$, it would be better to start from the following equation:

$$\mathbf{E}^{(1)}_{(2)} = A\psi^{(1)}_{1\,(2)}(\mathbf{r},\nu) \pm j\frac{Ah}{2\beta}\left(\psi^{(1)}_{2\,(2)}(\mathbf{r},\nu+1) + \psi^{(1)}_{2\,(2)}(\mathbf{r},\nu-1)\right). \tag{66}$$

The results are written in the similar forms as Eqs. (57)–(65), but W_{mn}, F_{mn}, and G_{mn} must be replaced by the following:

$$W^{(1)}_{mn} = Ag_n[\delta_{\nu,m-1}(1+\delta_{m1})B_1 + \delta_{\nu,m+1}B_2 + (h/2\beta)fB_3],$$
$$W^{(2)}_{mn} = Ag_n[\delta_{\nu,m-1}(1-\delta_{m1})B_1 + \delta_{\nu,m+1}(1-\delta_{m0})B_2 + (h/2\beta)fB_3], \tag{67}$$

$$F^{(1)}_{mn} = Ag_n[\delta_{\nu,m-1}(1+\delta_{m1})D_1 - \delta_{\nu,m+1}(1-\delta_{m0})D_2 - (h/\beta)(1-\delta_{m0})fD_3],$$
$$F^{(2)}_{mn} = Ag_n[-\delta_{\nu,m-1}(1-\delta_{m1})D_1 + \delta_{\nu,m+1}D_2 + (h/\beta)fD_3], \tag{68}$$
$$G^{(1)}_{mn} = Ag_n[\delta_{\nu,m-1}(1+\delta_{m1})T_1 - \delta_{\nu,m+1}(1-\delta_{m0})T_2 - (h/\beta)(1-\delta_{m0})fT_3],$$
$$G^{(2)}_{mn} = Ag_n[-\delta_{\nu,m-1}(1-\delta_{m1})T_1 + \delta_{\nu,m+1}T_2 - (h/\beta)fT_3], \tag{69}$$

where

$$f = (1+\delta_{\nu 0})\delta_{\nu,m-1} + \delta_{\nu,m+1}. \tag{70}$$

Thus far, we have derived the expansion formulas of the guided modes whose transverse electric field is polarized linearly in the y direction and have assumed that the expansion center is on the x axis. However, we can treat the more general case where the expansion center is located at an arbitrary position in the transverse (xy) plane by superposing the x- and y-polarized modes. The electric field of the guided mode in the core region whose transverse electric field component is polarized linearly in the x direction is, for the case of $l_0 \neq 0$,

$$\hat{\mathbf{E}}^{(1)}_{(2)} = \sum_{n=0}^{\infty}\sum_{m=0}^{n}\left[-j\frac{\omega}{k}\hat{C}^{(1)}_{(2)mn}\mathbf{M}^{(1)}_{\substack{o\\e}mn} + \hat{D}^{(1)}_{(2)mn}\mathbf{N}^{(1)}_{\substack{e\\o}mn}\right], \tag{71}$$

where

$$-j\frac{\omega}{k_1}\hat{C}^{(1)}_{(2)mn} = -\Gamma_{mn}\hat{W}^{(1)}_{(2)mn},$$

$$\hat{D}^{(1)}_{(2)mn} = j\Gamma_{mn}(\hat{F}^{(1)}_{(2)mn}A_1 + \hat{G}^{(1)}_{(2)mn}A_2), \tag{72}$$
$$\hat{W}^{(1)}_{mn} = U_1(m-1)\cdot B_1 + (1-\delta_{m0})U_1(m+1)\cdot B_2 - U_3(m)\cdot B_3,$$
$$\hat{W}^{(2)}_{mn} = V_1(m-1)\cdot(1-\delta_{m1})B_1 - V_1(m+1)\cdot B_2 + V_3(m)\cdot B_3, \tag{73}$$

$$\hat{F}^{(1)}_{mn} = U_1(m-1)\cdot D_1 + U_1(m+1)\cdot D_2 - U_3(m)\cdot D_3(2-\delta_{m0}),$$
$$\hat{F}^{(2)}_{mn} = V_1(m-1)\cdot(1-\delta_{m1})D_1 + V_1(m+1)\cdot(1-\delta_{m0})D_2 - 2V_3(m)\cdot(1-\delta_{m0})D_3, \tag{74}$$

$$\hat{G}^{(1)}_{mn} = U_1(m-1)\cdot T_1 + U_1(m+1)\cdot T_2 + U_3(m)\cdot(2-\delta_{m0})T_3,$$
$$\hat{G}^{(2)}_{mn} = V_1(m-1)\cdot(1-\delta_{m1})T_1 + V_1(m+1)\cdot(1-\delta_{m0})T_2 + 2V_3(m)\cdot(1-\delta_{m0})T_3, \tag{75}$$

$$U_3(m) = -g_n R^{(1)}(m),$$
$$V_3(m) = -g_n R^{(2)}(m), \tag{76}$$

$$R^{(1)}_{(2)}(m) = (j\hat{A}h/2\beta)\times\{[J_{\nu+1-m}(hl_0) - J_{\nu-1-m}(hl_0)] \pm (-1)^m[J_{\nu+1+m}(hl_0) - J_{\nu-1+m}(hl_0)]\}. \tag{77}$$

The expansion formulas in the cladding region can also be written in the same form except that h, A, and $J_\nu(hl_0)$ are replaced by $j\gamma$, $AJ_\nu(hR)/H^{(1)}_\nu(j\gamma R)$, and $H^{(1)}_\nu(j\gamma l_0)$, respectively.

The expansion formulas for the magnetic field can automatically be obtained from those for the electric field using Maxwell's equations. So, we need not obtain both of them. However, we may get first the formulas for the magnetic field instead of the electric field, but these results do not completely coincide with those obtained through the expansion formulas for the electric field because the LP modes of the fiber do not strictly satisfy Maxwell's equations: the difference is, of course, negligibly small in the numerical sense.

V. CONCLUDING REMARKS

The rigorous expansion formulas for the guided mode of the step-index optical fiber in terms of the spherical vector wave functions were derived for an arbitrary polarized mode and for an arbitrary location of the expansion center. The radiation mode can also be expanded in terms of the spherical vector wave functions in a similar fashion, since the difference between radiation mode and guided mode is not essential in obtaining the expansion.

Lastly, it would be worth mentioning that the expansions for the electric field of the guided mode in both the core and cladding regions have numerically been calculated for fairly wide ranges of parameters and the results have been confirmed to agree very well with those obtained from the original expressions.

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A family of differential equations arising from multi-ion electrodiffusion

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The system of Nernst–Planck equations and Gauss's law describing an arbitrary mixture of ions in steady-state drift and diffusion is shown to be equivalent to a single ordinary differential equation of order equal to the number of distinct ionic charges in the system.

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INTRODUCTION

The theory of electrodiffusion is a macroscopic description of the transport of charged particles through material barriers by a combination of diffusional and migrational fluxes. From its origin in the liquid-junction theory of Nernst and Planck[1] it became the basis of Bernstein's[2] membrane theory of nerve potentials. It has been used extensively in the description of biological membranes and the artificial membranes designed to model them.[3–9] Applications in condensed-matter systems include space-charge-limited currents in solid dielectrics.[10–14] Related formulations have appeared in the study of the drift-dissipative instability in plasma physics.[15] The Nernst–Planck formulation continues to be important in electrochemistry.[16]

This paper deals with a steady-state one-dimensional electrodiffusion regime with no restriction on the number and type of ion species present. (Because the term "carrier" has different meanings in solid-state physics and membrane biophysics, the work "ion" is here used to designate a charged particle of any type.) Its purpose is to report the existence of a family of ordinary nonlinear differential equations that arises from this formulation. The first two members of this family, a first-order differential equation describing ions of the same charge[8,10–13] and a second-order differential equation for a system with ions of two different charges,[17,18] have already appeared in the literature. Differential equations of the type reported here govern stationary electrodiffusion regimes of arbitrary complexity, the order of the equation being equal to the number of different ionic charges present in the system.

STATEMENT OF THE PROBLEM

As Schlögl[19] showed, it is convenient to divide the ions present in a drift-diffusion system into classes all of the same charge, q_i. The different species belonging to a given charge class will be indexed by j. The two equations comprising the steady-state electrodiffusion system are the Nernst–Planck equation

$$J_{ij} = -q_i u_{ij}\theta \frac{dN_{ij}}{dX} + u_{ij} q_i^2 E N_{ij}, \tag{1}$$

which states that the current density J_{ij} due to ion ij consists of a diffusion and a migration component, and Gauss's law

$$\frac{dE}{dX} = \frac{4\pi}{\epsilon} \sum_{i=1}^{m} \sum_{j=1}^{k_i} q_i N_{ij}. \tag{2}$$

Here X is the coordinate normal to the planar boundaries, E the electric field, N_{ij} the number density of the ion ij and u_{ij} its mobility, ϵ the dielectric constant and θ the temperature in energy units (i.e., $\theta = k_B T$), the latter three quantities being assumed uniform across the membrane. In the steady state, and in the absence of sources or sinks, here assumed, the J_{ij} are also independent of X. Implicit in Eq. (1) is the assumption of Einstein's equation, $D_{ij} = u_{ij}\theta$, which relates the mobility to the diffusion coefficient. The total number of ion species is $\Sigma_{i=1}^{m} k_i$.

Interactions between ions of different species are not present in Eq. (1) (with scalar u_{ij}), but arise from electrostatic coupling, through Gauss's law. In membrane studies the quantities of interest in comparisons with experimental data are the electrical potential difference

$$V = -\int_0^L E\, dX, \tag{3}$$

where L is the membrane thickness, and the net current.

It is the principal object of this paper to show that the system of $m + 1$ coupled differential equations of Eqs. (1) and (2) can be reduced to a single differential equation of order m in the single dependent variable E.

THE SCALING PROPERTY

Equations (1) and (2) constitute a nonlinear system, so the solutions are not subject to superposition or multiplication by an arbitrary constant. However, they are unified by a general scaling property.[8] For an arbitrary nonzero real number α, let the transformation T_α be defined by the following (subscripts ij are omitted for simplicity):

$$\left.\begin{aligned} X &\to \alpha^{-1} X \\ V &\to V \\ E &\to \alpha E \\ N &\to \alpha^2 N \\ J &\to \alpha^3 J \end{aligned}\right\} T_\alpha. \tag{4}$$

It is readily seen that the system defined by Eqs. (1)–(3) is invariant to T_α so that from any given solution an infinity of further solutions can be generated. The set of transformations T_α forms an Abelian group with successive transformations $T_\alpha T_\beta = T_{\alpha\beta}$ as the (commutative) binary operation, T_1 the identity, and $T_{1/\alpha}$ the inverse of T_α.

DIMENSIONLESS FORM

Equations (1) and (2) will now be cast into dimensionless form, with the simultaneous suppression of the index j.

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(The fact that this can be done shows that the behavior of the system reflects charge classes rather than individual ion species present,[19] although the latter must be accounted for in the boundary conditions.) Let q_0 be the unit of charge, taken as the proton charge. Then

$$\nu_i = q_i/q_0 \tag{5}$$

is the (signed) valency of the ion. The index i is assigned such that q_i (and ν_i) for different i are unequal.

For an arbitrary unit of ion density N_0 the Debye length is defined

$$\lambda = \left(\frac{\epsilon\theta}{4\pi q_0^2 N_0}\right)^{1/2}. \tag{6}$$

Let

$$n_i = N_0^{-1}\sum_{j=1}^{k_i} N_{ij}, \tag{7}$$

$$c_i = \frac{\lambda}{N_0 q_i \theta}\sum_{j=1}^{k_i}\left(\frac{J_{ij}}{u_{ij}}\right), \tag{8}$$

$$p = (q_0\lambda/\theta)E, \tag{9}$$

$$x = (X/\lambda) + x_1, \tag{10}$$

where x_1 is a constant to be defined.

In these dimensionless units, Eqs. (1) and (2) become

$$\frac{dn_i}{dx} = \nu_i p n_i - c_i, \quad i = 1,2,...,m\ , \tag{11}$$

$$\frac{dp}{dx} = \sum_{i=1}^{m}\nu_i n_i. \tag{12}$$

THE ONE- AND TWO-CHARGE CASES

The single-ion case was solved by Borgnis[20] in 1936, and Fan introduced the more convenient Airy–function form of the solution in 1948.[10] Leuchtag and Swihart pointed out that the single-ion solution can be generalized to the case of ions of one charge, called the homovalent case.[8] The individual ion densities can be regained by use of a formula obtained by Schlögl.[8,19]

With $m = 1$, Eqs. (11) and (12) become

$$n_1' = \nu p n_1 - c, \tag{13}$$

$$p' = \nu n_1, \tag{14}$$

where primes denote x-derivatives. Elimination of n_1 from the nonlinear term and integration yields

$$n_1 = \tfrac{1}{2}p^2 - cx, \tag{15}$$

where the x_1 in Eq. (10) has been used to absorb the constant of integration. Thus the differential equation equivalent to the system of Eqs. (13) and (14) is

$$p' = \tfrac{1}{2}\nu p^2 - \nu c x. \tag{16}$$

This equation is the first member of the family of differential equations described here. (Reconversion to physical variables is omitted.)

For a system containing ions of two different valencies, $m = 2$, Eqs. (11) and (12) become

$$n_1' = \nu_1 p n_1 - c_1, \tag{17}$$

$$n_2' = \nu_2 p n_2 - c_2, \tag{18}$$

$$p' = \nu_1 n_1 + \nu_2 n_2. \tag{19}$$

The equation obtained by summing (17) and (18), substituting (19), and integrating,

$$n_1 + n_2 = \tfrac{1}{2}p^2 - cx, \tag{20}$$

where $c = c_1 + c_2$, is solved for n_2 and substituted into (19). Between the resulting equation,

$$p' = \tfrac{1}{2}\nu_2 p^2 + (\nu_1 - \nu_2)n_1 - \nu_2 c x$$

and Eq. (17), n_1 is eliminated to give the desired differential equation in p,

$$p'' - (\nu_1 + \nu_2)pp' + \tfrac{1}{2}\nu_1\nu_2 p^3 - \nu_1\nu_2 cxp + \nu_1 c_1 + \nu_2 c_2 = 0. \tag{21}$$

This is the second member of our family of differential equations. It was derived for one positive and one negative ion by Bruner in 1965.[17] With ions of equal and opposite charges, the second term in Eq. (21) vanishes; this version (for ± 1) was derived by Bass[18] in 1964 and by Cohen and Cooley[21] in 1965. A related integrodifferential equation recently appeared in a study of enzymatic surface layers.[22]

THE GENERAL REGIME

The procedure for a system with an arbitrary number of different ionic charges is a straightforward generalization of these special cases. As before, we sum Eq. (11) on i, use Gauss's law, Eq. (12), to eliminate the $\nu_i n_i$ from the product term and integrate, using the previously incorporated constant of integration [see Eq. (10)]. The result is the general first integral,

$$\sum_{i=1}^{m} n_i = \tfrac{1}{2}p^2 - x\sum_{i=1}^{m} c_i, \tag{22}$$

of which Eqs. (15) and (20) are special cases.

To eliminate the n_i requires m relations between them, of which Eqs. (22) and (12) constitute two. We multiply Eq. (11) through by ν_i^{n-1}, where n is an arbitrary integer ranging from 1 to m, to obtain

$$\sum_{i=1}^{m}\nu_i^n n_i = \frac{1}{p}\left[\frac{d}{dx}\left(\sum_{i=1}^{m}\nu_i^{n-1}n_i\right) + \sum_{i=1}^{m}\nu_i^{n-1}c_i\right]. \tag{23}$$

Now define

$$f_n(x) = \sum_{i=1}^{m}\nu_i^{n-1}n_i(x) \tag{24}$$

and

$$A_n = \sum_{i=1}^{m}\nu_i^{n-1}c_i \tag{25}$$

to write Eq. (23) as a recursion relation for the function $f_n(x)$

$$f_{n+1}(x) = \frac{1}{p(x)}\left[f_n'(x) + A_n\right]. \tag{26}$$

This recursion relation can be used to derive the entire set of f's from its first two members, Eqs. (22) and (12), as functions of p and its derivatives, and x:

$$f_1 = \tfrac{1}{2}p^2 - A_1 x, \tag{27}$$

$$f_2 = (f_1' + A_1)/p = p', \tag{28}$$

$$f_3 = (f_2' + A_2)/p = (p'' + A_2)/p, \tag{29}$$

$$f_4 = (f_3' + A_3)/p = p'''/p^2 - (p'' + A_2)p'/p^3 + A_3/p, \tag{30}$$

...

The general expression is

$$f_n = \sum_{k=0}^{n-3} A_{n-k-1} \left(\frac{1}{p}\frac{d}{dx}\right)^k \left(\frac{1}{p}\right) + \left(\frac{1}{p}\frac{d}{dx}\right)^{n-2} \frac{dp}{dx}, \quad n = 3,4,...,m. \tag{31}$$

Thus the m linear combinations of n_i,

$$\begin{aligned} &n_1 + n_2 + \cdots + n_m = f_1, \\ &\nu_1 n_1 + \nu_2 n_2 + \cdots + \nu_m n_m = f_2, \\ &\nu_1^2 n_1 + \nu_2^2 n_2 + \cdots + \nu_m^2 n_m = f_3, \\ &\quad\cdots \\ &\nu_1^{m-1} n_1 + \nu_2^{m-1} n_2 + \cdots + \nu_m^{m-1} n_m = f_m \end{aligned} \tag{32}$$

are known functions of x, p, and the first $m + 1$ derivatives of p, and can be solved for the n_i.

The existence of solutions for the ion concentrations n_i follows from the nonvanishing of the determinant of the coefficients,

$$\Delta_m = \begin{vmatrix} 1 & 1 & \cdots & 1 \\ \nu_1 & \nu_2 & \cdots & \nu_m \\ \nu_1^2 & \nu_2^2 & \cdots & \nu_m^2 \\ \cdots & & & \cdots \\ \nu_1^{m-1} & \nu_2^{m-1} & \cdots & \nu_m^{m-1} \end{vmatrix}, \tag{33}$$

which in turn is a consequence of the unique assignment of the valencies, assumed above [below Eq. (5)].

The solution for n_1 is

$$n_1 = \Delta_m^{-1} \begin{vmatrix} f_1 & 1 & \cdots & 1 \\ f_2 & \nu_2 & \cdots & \nu_m \\ \cdots & & & \cdots \\ f_m & \nu_2^{m-1} & \cdots & \nu_m^{m-1} \end{vmatrix} = \sum_{n=1}^{m} B_{n1} f_n \Big/ \sum_{n=1}^{m} \nu_1^{n-1} B_{n1} \tag{34}$$

and that for the general concentration n_i $(i = 1,2,...,m)$ is

$$n_i = \sum_{n=1}^{m} B_{ni} f_n \Big/ \sum_{n=1}^{m} \nu_i^{n-1} B_{ni}, \tag{35}$$

where the integers B_{ni} are the cofactors of the ni element of Δ_m, Eq. (33).

The substitution of Eq. (34) into Eq. (11), for $i = 1$, generates the equation

$$\sum_{n=1}^{m} B_{n1}(f_n' - \nu_1 p f_n + \nu_1^{n-1} c_1) = 0. \tag{36}$$

With the functional values of f_n given in Eqs. (27)–(31) in terms of p and its derivatives and x, Eq. (36) can be seen to be an ordinary differential equation of order m and first degree. A general solution of the equation is a function of the form $p = p(x)$, containing as parameters the m current densities c_i, the m valencies ν_i, and m constants of integration. To obtain the concentrations n_i, one uses $p(x)$ and its first $m - 1$ derivatives to obtain the f_n from Eqs. (27)–(31); these are then substituted into Eq. (35).

EXPLICIT FORMS FOR THREE- AND FOUR-CHARGE CASES

The method may be easily illustrated by deriving a differential equation for an electrodiffusion system with three different valencies.

Noting that, for $m = 3$, $B_{21}/B_{31} = -(\nu_2 + \nu_3)$ and $B_{11}/B_{31} = \nu_2\nu_3$, we may write Eq. (36) in the form

$$\begin{aligned} &f_3' - \nu_1 p f_3 - (\nu_2 + \nu_3)(f_2' - \nu_1 p f_2) + \nu_2\nu_3(f_1' - \nu_1 p f_1) \\ &\quad + [\nu^2{}_1 - \nu_1(\nu_2 + \nu_3) + \nu_2\nu_3]c_1 = 0. \end{aligned} \tag{37}$$

With Eqs. (27)–(29) and (25), this becomes

$$\begin{aligned} &pp''' - p'p'' - (\nu_1 + \nu_2 + \nu_3)p^2p'' + (\nu_1\nu_2 + \nu_1\nu_3 + \nu_2\nu_3)p^3p' \\ &\quad - (\nu_1 c_1 + \nu_2 c_2 + \nu_3 c_3)p' - \tfrac{1}{2}\nu_1\nu_2\nu_3 p^5 \\ &\quad + \nu_1\nu_2\nu_3(c_1 + c_2 + c_3)xp^3 - [(\nu_2 + \nu_3)\nu_1 c_1 \\ &\quad + (\nu_1 + \nu_3)\nu_2 c_2 + (\nu_1 + \nu_2)\nu_3 c_3]p^2 = 0. \end{aligned} \tag{38}$$

Similarly, for $m = 4$, the differential equation for the field p is

$$\begin{aligned} &B_{41}[p^2p^{(4)} - (3pp' + \nu_1 p^3)p''' - (pp'' - 3p'^2 - \nu_1 p^2 p') \\ &\quad \times(p'' + A_2) - A_3(p^2p' + \nu_1 p^4)] \\ &\quad + B_{31}[p^3p''' - p^2p'p'' - \nu_1 p^4 p'' - A_2 p^2(p' + \nu_1 p^2)] \\ &\quad + B_{21}p^4(p'' - \nu_1 pp') + B_{11}p^4(pp' - \tfrac{1}{2}\nu_1 p^3 \\ &\quad + \nu_1 A_1 xp - A_1) + Bc_1 p^4 = 0, \end{aligned} \tag{39}$$

where

$$\begin{aligned} B_{41} &= -[\nu_2^2(\nu_4 - \nu_3) - \nu_3^2(\nu_4 - \nu_2) + \nu_4^2(\nu_3 - \nu_2)], \\ B_{31} &= \nu_2^3(\nu_4 - \nu_3) - \nu_3^3(\nu_4 - \nu_2) + \nu_4^3(\nu_3 - \nu_2), \\ B_{21} &= -[\nu_2^3(\nu_4^2 - \nu_3^2) - \nu_3^3(\nu_4^2 - \nu_2^2) + \nu_4^3(\nu_3^2 - \nu_2^2)], \\ B_{11} &= -\nu_2\nu_3\nu_4 B_{41}, \\ B &= \sum_{n=1}^{4} \nu_1^{n-1} B_{n1}, \end{aligned}$$

and the A's are as defined for $m = 4$ in Eq. (25).

DISCUSSION

The complexity of the steady-state behavior of an electrodiffusion system depends on the number of distinct charges present. The system of Eqs. (1) and (2), for m charges, is described by the m–order differential equation, Eq. (36). The first four members of this infinite family of differential equations are given in Eqs. (16), (21), (38), and (39).

Equation (16) is a Riccati equation whose solution is well known, both in terms of Bessel functions of fractional $(\pm\frac{1}{3}, \pm\frac{2}{3})$ order[11,12,20] and in terms of the equivalent but more convenient Airy functions.[8,10,13] A numerical method for solving the two-point boundary problem generates the current-voltage curves for this case.[23] [The conversion to the notation in Refs. (8) and (23) is: $s = (x - x_1)/\sqrt{2}$; $e = p/\sqrt{2}$; $n_i = n_i$; $j_i = \sqrt{2}c_i$.] Equation (21), with $\nu_2 = -\nu_1$, is reducible to the second transcendent of Painlevé,[18,22,24] which has been generated from Airy functions by exact modified Korteweg-de Vries equation theory.[25] Since Eqs. (38) and (39) have (to my knowledge) not been published before, there are clearly no known solutions for them.

The scaling property, Eq. (4), may, of course, be written in terms of the dimensionless variables, with $\{X, E, N_i, J_i\}$

$\rightarrow\{x, p, n_i, c_i\}$; the A_n transform like the c_i. A quick check reveals that Eqs. (16), (21), (38), and (39) are homogeneous with respect to the scaling transformation.

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Integral inequalities for optical constants

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Some upper bound integral inequalities are derived for various optical constants. Weight functions which damp out the high frequency spectral domain are given special emphasis. The implications for testing experimental data are discussed.

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I. INTRODUCTION

The purpose of this paper is to consider integral inequalities of the form

$$\int_{\alpha}^{\beta} W(\omega_0,\omega)\mathcal{O}(\omega)d\omega < A(\alpha,\beta,\omega_0), \tag{1}$$

where $\mathcal{O}(\omega)$ denotes a particular optical constant and $W(\omega_0,\omega)$ is some convenient weight function. In the present work the interval $[\alpha,\beta]$ will be taken as $[0,\infty)$ and $A(0,\infty,\omega_0)$ will be abbreviated to $A(\omega_0)$. The situation for general limits α and β, which is certainly a case of considerable interest and practical application, appears somewhat more difficult if a discussion free of additional assumptions about the specific nature of the medium is required. The topic is currently under investigation.

The motivation for this study was twofold. A considerable amount of work has been carried out on sum rules for optical constants.[1-7] Almost all these results may be written in the form

$$\int_0^{\infty} w(\omega_0,\omega)\mathcal{O}(\omega)d\omega = B(\omega_0). \tag{2}$$

There are severe restrictions on the choice of weight function $w(\omega_0,\omega)$ which allow $B(\omega_0)$ to be determined explicitly. In order for a relationship like Eq. (2) to be useful in the analysis of experimental data, it is highly desirable that, for values of the optical constants which are experimentally inaccessible, the resulting contributions to the integral be as small as possible. Usually, the most inacessible spectral range for optical constant measurements is the high energy domain.

Problems in data analysis could be reduced to a minimum by the simple expedient of choosing a weight function vanishing very rapidly at high frequencies; for example, an appropriate gaussian function would be suitable. This has the effect of producing for the optical constant of interest what is essentially a "band-limited" function. Unfortunately, for weight functions of this particular form, the function $B(\omega_0)$ cannot be determined (at least by the procedures used in Refs. 1–7).

A commonly employed approach is to augment the available experimental data with semiempirical extrapolations to the high frequency range. In those particular cases where the spectral range for the optical data is rather restricted, which is common in practice, it becomes somewhat difficult to ascertain whether any inaccuracy in satisfying Eq. (2) rests with the experimental data or the extrapolation procedure, or both. In such cases Eq. (2) is of restricted utility for testing experimental data.

The alternative viewpoint, which is taken in this work, is to start with a highly damped weight function and then determine the upper bound $A(\omega_0)$. Errors arising from neglect of experimental data beyond some upper frequency can be reduced significantly by choosing weight functions which vanish rapidly as $\omega\to\infty$. The utility of Eq. (1) is then governed by the magnitude of the deviation between the constant $A(\omega_0)$ and the true value of the integral in question. When such deviations are small for a particular choice of weight function, Eq. (1) may be more useful in practical applications than Eq. (2), for reasons mentioned above.

The constant $A(\omega_0)$ is not in general determined as the best possible bound in this work. Work to determine the best possible bounds would certainly clarify the relative advantages of Eq. (1) and (2) in data analysis.

II. INEQUALITIES FOR THE REFRACTIVE INDEX

In this work we have restricted the assumptions on the mathematical properties of the optical constants to those employed in the derivation of Eq. (2). Stated briefly, the generalized optical constant is an analytic function in an appropriate domain, and some assumption about the asymptotic behavior as $\omega\to\infty$ is used to derive Eq. (2). Usually the asymptotic behavior is taken from the free electron gas model. With such general assumptions on the behavior of the optical constants, it is to be expected that there are relatively few general inequality relations.

If we denote the real and imaginary parts of the generalized refractive index by $n(\omega)$ and $\kappa(\omega)$, respectively, then

$$\int_0^{\infty} \omega^{1/2}\kappa(\omega)^{1/2}\exp(-\pi^3\omega^2/128\omega_0^2)\,d\omega \leqslant \omega_0^{1/2}\omega_p \tag{3}$$

and

$$\int_0^{\infty} [\omega\kappa(\omega)n(\omega)]^{1/2}\exp(-\pi^3\omega^2/128\omega_0^2)\,d\omega \leqslant \omega_0^{1/2}\omega_p, \tag{4}$$

where ω_p is the plasma frequency and ω_0 is some arbitrary frequency. Equation (3) is derived in the following manner. Starting from the Buniakowsky–Schwartz inequality, and for some weight function $W(\omega_0,\omega)$,

$$\int_0^{\infty} \omega^{1/2}\kappa(\omega)^{1/2}W(\omega_0,\omega)\,d\omega \leqslant \left[\int_0^{\infty}\omega\kappa(\omega)\,d\omega\int_0^{\infty}W(\omega_0,\omega)^2\,d\omega\right]^{1/2}. \tag{5}$$

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If we choose

$$W(\omega_0,\omega) = \exp(-\pi^3\omega^2/128\omega_0^2) \tag{6}$$

and use the result[2]

$$\int_0^\infty \omega\kappa(\omega)\,d\omega = \tfrac{1}{4}\pi\omega_p^2, \tag{7}$$

then Eq. (3) follows directly. An equivalent procedure yields Eq. (4) if the sum rule[2]

$$\int_0^\infty \omega\kappa(\omega)n(\omega)\,d\omega = \tfrac{1}{4}\pi\omega_p^2 \tag{8}$$

is employed.

In Eq. (3) the gaussian weight function is very highly damped as $\omega\to\infty$, so errors resulting from omission of data should be negligible for the high frequency spectral range. It should also be noted that Eq. (3) has an advantage over Eq. (4), since only experimental data for a single optical constant is required to utilize Eq. (3), whereas Eq. (4) requires both the dispersive and dissipative data for the generalized refractive index. Inequality constraints like Eq. (4) therefore do not provide information on the quality of the experimental data for the dispersive and dissipative modes separately.

An inequality similar to Eq. (3) can be derived for the refractive index. The first step is to introduce a second weight function of the form $(\omega^2+\omega_\alpha^2)^{-1/2}$. A related idea is well known in the derivation of certain types of integral inequalities, such as generalizations of Carlson's inequality.[8] We have

$$\int_0^\infty n(\omega)^{1/2}W(\omega_0,\omega)\,d\omega$$

$$= \int_0^\infty [(\omega^2+\omega_\alpha^2)^{1/2}W(\omega_0,\omega)n(\omega)^{1/2}\,d\omega/(\omega^2+\omega_\alpha^2)^{1/2}]$$

$$\leqslant \left\{\int_0^\infty (\omega^2+\omega_\alpha^2)W(\omega_0,\omega)^2\,d\omega \int_0^\infty [n(\omega)\,d\omega/(\omega^2+\omega_\alpha^2)]\right\}^{1/2}. \tag{9}$$

If we make use of the relation[6]

$$\int_0^\infty \frac{n(\omega)\,d\omega}{\omega^2+\omega_\alpha^2} - \frac{\pi}{2\omega_\alpha} = \frac{1}{\omega_\alpha}\int_0^\infty \frac{\omega\kappa(\omega)\,d\omega}{\omega^2+\omega_\alpha^2}, \tag{10}$$

then

$$\int_0^\infty n(\omega)^{1/2}W(\omega_0,\omega)\,d\omega$$

$$\leqslant \left[\int_0^\infty (\omega^2+\omega_\alpha^2)W(\omega_0,\omega)^2\,d\omega(\pi/2\omega_\alpha)(1+\omega_p^2/2\omega_\alpha^2)\right]^{1/2}, \tag{11}$$

where the inequality

$$\int_0^\infty \omega\kappa(\omega)\,d\omega/(\omega^2+\omega_\alpha^2) < \pi\omega_p^2/4\omega_\alpha^2 \quad (\omega_\alpha>0) \tag{12}$$

has been employed. For the choice

$$W(\omega_0,\omega) = e^{-\omega^2/2\omega_0^2}, \tag{13}$$

$$\int_0^\infty n(\omega)^{1/2}W(\omega_0,\omega)\,d\omega$$

$$< (\pi^{3/4}/4\omega_\alpha)[(\omega_0/\omega_\alpha)(2\omega_\alpha^2+\omega_0^2)(2\omega_\alpha^2+\omega_p^2)]^{1/2} \quad (\omega_\alpha>0). \tag{14}$$

Since ω_0 is arbitrary in Eq. (13), we may choose $\omega_0=\omega_\alpha$ and obtain

$$\int_0^\infty n(\omega)^{1/2}W(\omega_\alpha,\omega)\,d\omega < \frac{3^{1/2}}{4}\pi^{3/4}(2\omega_\alpha^2+\omega_p^2)^{1/2}, \tag{15}$$

with weight function $W(\omega_\alpha,\omega) = \exp(-\omega^2/2\omega_\alpha^2)$. The case $\omega_\alpha=\omega_p$ leads to the simple bound

$$\int_0^\infty n(\omega)^{1/2}\exp(-\omega^2/2\omega_p^2)\,d\omega < \tfrac{3}{4}\pi^{3/4}\omega_p. \tag{16}$$

The best possible bound for Eq. (14) can be obtained by determining the minimum of the right-hand side with respect to ω_α. We find the sharpest bound when ω_α is given by

$$\omega_\alpha = \tfrac{1}{2}\{\omega_p^2+\omega_0^2+[\omega_p^4+\omega_0^4+14\omega_p^2\omega_0^2]^{1/2}\}^{1/2}.$$

The above derivation may be carried through in an analogous manner with $n(\omega)^{1/2}$ replaced by $[\omega\kappa(\omega)]^{1/2}$ to yield

$$\int_0^\infty [\omega\kappa(\omega)]^{1/2}\exp(-\omega^2/2\omega_\alpha^2)\,d\omega$$

$$< (3^{1/2}/4)\pi^{3/4}\omega_\alpha^{1/2}\omega_p. \tag{17}$$

The above approach leads to a final result similar to that discussed at the start of this section; however, the final bound is less sharp. This is immediately apparent on writing Eq. (17) in the equivalent form

$$\int_0^\infty [\omega\kappa(\omega)]^{1/2}\exp(-\pi^3\omega^2/128\omega_0^2)\,d\omega < (\tfrac{3}{2})^{1/2}\omega_0^{1/2}\omega_p. \tag{18}$$

This is not surprising, since the procedure of introducing the additional weight factor $(\omega^2+\omega_\alpha^2)^{-1/2}$ does not lead to optimum bounds.

For the particular choice of weight function

$$W(\omega_0,\omega) = (\omega^2+\omega_\alpha^2)^{-1} \tag{19}$$

the following simple inequality for the refractive index is obtained:

$$\int_0^\infty [n(\omega)\,d\omega/(\omega^2+\omega_0^2)] < (\pi/2\omega_0)n(0) \quad (\omega_0>0), \tag{20}$$

where $n(0)$ is the refractive index at zero frequency. The bound indicated is of interest only for the case of insulators, since for conductors $n(\omega)\sim\omega^{-1/2}$ as $\omega\to 0$. The proof of Eq. (20) follows directly from the Kramers–Kronig relation connecting the real and imaginary parts of the refractive index:

$$n(\omega_0) - 1 = (2/\pi)P\int_0^\infty [\omega\kappa(\omega)\,d\omega/(\omega^2-\omega_0^2)] \tag{21}$$

and for $\omega_0=0$

$$n(0) - 1 = (2/\pi)\int_0^\infty [\kappa(\omega)\,d\omega/\omega]$$

$$> (2/\pi)\int_0^\infty [(\omega\kappa(\omega)\,d\omega/(\omega^2+\omega_0^2)], \tag{22}$$

and using Eq. (10) leads to Eq. (20). It is to be noted that inequality (20) involves only a single optical constant and is therefore suitable for analysis of experimental data.

The inequality (20) can be used to derive the following inequality (using the approach indicated above):

$$\frac{[\int_0^\infty W(\omega_0,\omega)n(\omega)^{1/2}\,d\omega]^2}{\int_0^\infty W^2(\omega_0,\omega)(\omega^2+\omega_\alpha^2)\,d\omega} < \frac{\pi n(0)}{2\omega_\alpha}, \quad \omega_\alpha > 0, \tag{23}$$

where $W(\omega_0,\omega)$ is any suitable weight function. Equation (23) depends on only one optical constant, and the final result is independent of the plasma frequency.

III. INEQUALITY FOR THE REFLECTANCE

If we know that the optical constant satisfies

$$0 \leqslant \mathscr{O}(\omega) \leqslant \mathscr{A} \tag{24}$$

for the interval $[0,\infty)$, and we consider a weight function $W(\omega)$ which is decreasing on the same interval, then

$[\mathscr{A} - \mathscr{O}(\omega)][W(\omega) - W(\omega')]$ is positive for ω on the interval $[0,\omega']$

and

$\mathscr{O}(\omega)[W(\omega') - W(\omega)]$ is positive for ω on the interval $[\omega',\infty)$.

Hence,

$$\int_0^{\omega'} [\mathscr{A} - \mathscr{O}(\omega)][W(\omega) - W(\omega')]\,d\omega + \int_{\omega'}^\infty \mathscr{O}(\omega)[W(\omega') - W(\omega)]\,d\omega \geqslant 0. \tag{25}$$

Equation (25) can be rewritten as

$$F(\omega') \equiv \mathscr{A}\int_0^{\omega'} W(\omega)\,d\omega + W(\omega')\left[\int_0^\infty \mathscr{O}(\omega)\,d\omega - \mathscr{A}\omega'\right] \geqslant \int_0^\infty \mathscr{O}(\omega)W(\omega)\,d\omega. \tag{26}$$

The optimum upper bound is determined from the minimum of $F(\omega')$. Hence,

$$\frac{\partial F(\omega')}{\partial \omega'} = \left[\int_0^\infty \mathscr{O}(\omega)\,d\omega - \omega\mathscr{A}\right]\frac{\partial W(\omega')}{\partial \omega'} = 0 \tag{27}$$

and therefore

$$\omega' = (1/\mathscr{A})\int_0^\infty \mathscr{O}(\omega)\,d\omega. \tag{28}$$

Equation (26) may be written in the following form:

$$\int_0^\infty \mathscr{O}(\omega)W(\omega)\,d\omega \leqslant \mathscr{A}\int_0^{\omega'} W(\omega)\,d\omega \tag{29}$$

with ω' given by Eq. (28). Equation (29) is a variant of Steffensen's inequality,[9] and the above derivation is related to a procedure of Apéry.[10] Equation (29) would be potentially very useful if the appropriate upper bounds on the various optical constants were available. Unfortunately, except for one important case, such upper bounds are unknown.

Consider the special case of Eq. (29) for the reflectance $R(\omega)$,

$$\mathscr{O}(\omega) \equiv R(\omega), \tag{30}$$

$$\mathscr{A} = 1, \tag{31}$$

$$\omega' = \int_0^\infty R(\omega)\,d\omega, \tag{32}$$

and choose a convenient weight function

$$W(\omega) = e^{-\omega/\omega_0}, \tag{33}$$

where ω_0 is some arbitrary frequency. Combining Eqs. (29)–(33) yields

$$(1/\omega_0)\int_0^\infty R(\omega)e^{-\omega/\omega_0}d\omega \leqslant 1 - e^{-\omega'/\omega_0}. \tag{34}$$

This is clearly a refinement on the obvious inequality

$$(1/\omega_0)\int_0^\infty e^{-\omega/\omega_0}R(\omega)\,d\omega < 1 \tag{35}$$

and will be a substantial improvement when $(1/\omega_0)\int_0^\infty R(\omega)\,d\omega$ is much less than 1.

IV. DISCUSSION

The procedures discussed in Sec. II can be applied to the dispersive and absorptive parts of the generalized dielectric constant, to yield exactly analogous inequalities to those reported for the real and imaginary parts of the generalized refractive index. The approach also applies to most of the optical constants if appropriate equations analogous to Eqs. (7) and (10) can be established.

It is to be stressed that the reported inequalities are necessary constraints only. In those cases where experimental data lead to a violation of one of the inequalities, then that data is to be regarded as inaccurate. Nothing can be said about the accuracy of the data when the inequalities are satisfied, since offsetting inaccuracies may still exist in the experimental data.

For some of the inequalities derived herein, we have not made use of the precise asymptotic behavior of the optical constant under investigation, although it is implicitly assumed that it is such that all integrals under discussion converge. This contrasts with the situation for the derivation of some exact sum rules, where the asymptotic behavior must be precisely known.

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Some properties of static general relativistic stellar models. II [a)]

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We expand here the study of the type of identity which has been successfully used to prove the necessity of spherical symmetry in static black holes and uniform density stellar models. We show how the system of partial differential equations, whose solutions correspond to these identities, can be decoupled and partially integrated for fluids with an arbitrary equation of state. The problem of finding such identities is reduced thereby to the problem of finding the solutions to a single ordinary differential equation, plus quadratures.

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I. INTRODUCTION

At the present time, the program to determine from general relativity theory its predictions, concerning the properties of the equilibrium states of astrophysical objects (stars and black holes), is far from complete. One aspect of that program, to confirm our intuitive belief that static (i.e., stationary and nonrotating) stellar models and black holes must necessarily have spherical symmetry, has been partially completed. It has been shown that isolated static black holes[1–3] and uniform density stellar models[4] must have spherical symmetry. The crucial element in the arguments which lead to those results is the existence of certain identities satisfied by the static solutions of Einstein's equations. In this paper we discuss identites of this type which apply in the interior regions of stellar models having arbitrary equations of state. We show how the procedure which was developed to derive these identities[4] can be significantly simplified. In particular, we show how the system of partial differential equations, whose solutions correspond to these identities, can be decoupled and partially integrated. The problem of finding identities for fluids with arbitrary equations of state is reduced thereby to finding the solutions of a single ordinary differential equation, plus some quadratures. Since identities of this type have played such a crucial role in the understanding of static black holes and uniform density stellar models, it seems likely that the simplifications presented here will bring us a step closer to the complete proof that all static stellar models must be spherical.

II. REVIEW

In the first paper of this series (Ref. 4; hereafter referred to as Paper I) we described how useful identities for static stellar models could be obtained by solving an appropriate system of partial differential equations. We review now the results of that work.

A static stellar model is a metric,

$$ds^2 = -V^2dt^2 + g_{ab}dx^a dx^b, \tag{1}$$

(where the scalar V and 3-metric g_{ab} are independent of the coordinate t) which satisfies Einstein's equations:

$$\nabla^a\nabla_a V = 4\pi V(\rho + 3p), \tag{2}$$

$$R_{ab} = V^{-1}\nabla_a\nabla_b V + 4\pi(\rho - p)g_{ab}. \tag{3}$$

In these equations R_{ab} and ∇_a are the Ricci curvature and covariant derivative of g_{ab}, while ρ and p are the density and pressure of the fluid. The density and pressure are assumed to be related by a given equation of state $\rho = \rho(p)$, and as a consequence of Eqs. (2) and (3) must also satisfy Euler's equation:

$$\nabla_a p = -V^{-1}(\rho + p)\nabla_a V. \tag{4}$$

In Paper I it was shown that identities of the form

$$\nabla_a[K_1(V, W)\nabla^a V + K_2(V, W)\nabla^a W] = \tfrac{1}{4}K_2(V, W)V^4W^{-1}R_{abc}R^{abc} + \left(\frac{\partial K_2(V, W)}{\partial W} + \frac{3}{4}W^{-1}K_2(V, W)\right)|\nabla_a W - F\nabla_a V|^2 \tag{5}$$

will exist if the functions $K_1(V, W)$ and $K_2(V, W)$ satisfy the following system of partial differential equations:

$$\frac{\partial K_1}{\partial V} = F^2\frac{\partial K_2}{\partial W} - 4\pi K_1 VW^{-1}(\rho + 3p) - \left(16\pi^2V^2W^{-1}(\rho + 3p)^2 - \tfrac{3}{4}W^{-1}F^2 + 8\pi V\frac{d}{dV}(\rho + p)\right)K_2, \tag{6}$$

$$\frac{\partial K_2}{\partial V} = -2F\frac{\partial K_2}{\partial W} - \frac{\partial K_1}{\partial W} - \left[V^{-1} - 4\pi VW^{-1}(\rho + 3p) + \tfrac{3}{2}W^{-1}F\right]K_2. \tag{7}$$

In the above equations W is defined as $W = \nabla^a V\nabla_a V$; $F = F(V, W)$ is a function chosen so that a spherical model would satisfy $\nabla_a W = F\nabla_a V$; $R_{abc}R^{abc}$ is the square of the three-dimensional conformal tensor which vanishes if and only if the stellar model is spherical (see Paper I); and ρ and p are taken to be the known functions of V determined by the equation of state and Eq. (4).

Another useful function, introduced in Paper I, is

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$W_0 = W_0(V)$: the function to which W would be equal if the model were spherical. This function satisfies the second order differential equation

$$\frac{d^2W_0}{dV^2} = \frac{1}{V}\frac{dW_0}{dV} + \frac{3}{4}\frac{1}{W_0}\left(\frac{dW_0}{dV}\right)^2 - 8\pi\frac{V}{W_0}\frac{dW_0}{dV}(\rho + 3p) + 16\pi^2\frac{V^2}{W_0}(\rho + 3p)^2 + 8\pi V\frac{d}{dV}(\rho + p). \tag{8}$$

For a detailed discussion of these results, the reader should consult Paper I.

III. A SIMPLIFIED PROCEDURE FOR FINDING IDENTITIES

In this section we show how the procedure for finding identities in the form of Eq. (5) can be simplified by decoupling and partially integrating the system of partial differential equations (6), (7). The first step in this procedure is to change dependent variables to the set: $A(V, W) = K_1(V, W) + F(V, W)K_2(V, W)$ and $B(V, W) = K_2(V, W)$. We next take appropriate linear combinations of Eqs. (6), (7), expressed in these new variables, to obtain the following system:

$$\frac{\partial A}{\partial V} + F\frac{\partial A}{\partial W} + 4\pi VW^{-1}(\rho + 3p)A = \left(\frac{\partial F}{\partial V} + F\frac{\partial F}{\partial W} - \frac{F}{V} - \frac{3}{4}\frac{F^2}{W} + 8\pi\frac{V}{W}F(\rho + 3p) - 16\pi^2\frac{V^2}{W}(\rho + 3p)^2 - 8\pi V\frac{d}{dV}(\rho + p)\right)B, \tag{9}$$

$$\frac{\partial B}{\partial V} + F\frac{\partial B}{\partial W} - \left(\frac{\partial F}{\partial W} - \frac{1}{V} + 4\pi\frac{V}{W}(\rho + 3p) - \frac{3}{2}\frac{F}{W}\right)\times B + \frac{\partial A}{\partial W} = 0. \tag{10}$$

The next step is to take advantage of the arbitrariness in the choice of the function F. The only restriction which F must satisfy is that, when the star is spherical (i.e., when $W = W_0$), F must satisfy $\nabla_a W = F\nabla_a V$; this is equivalent to requiring that $F(V, W_0) = dW_0/dV$. At this point, however, we are free to choose how F will behave for $W \neq W_0$. To make that choice specific, let us require that F satisfy the following partial differential equation:

$$\frac{\partial F}{\partial V} + F\frac{\partial F}{\partial W} = \frac{F}{V} + \frac{3}{4}\frac{F^2}{W} - 8\pi\frac{V}{W}F(\rho + 3p) + 16\pi^2\frac{V^2}{W}(\rho + 3p)^2 + 8\pi V\frac{d}{dV}(\rho + p). \tag{11}$$

Since Eq. (11) reduces to Eq. (8) on the surface $W = W_0$ when $F = dW_0/dV$, it follows that Eq. (11) admits solutions which satisfy our criterion $F(V, W_0) = dW_0/dV$. With this choice of F, the system of equations (9), (10) decouples. The coefficient of B in Eq. (9) vanishes, so that this equation can be used to determine A. Given the solution for A, Eq. (10) can be integrated to determine B.

To proceed further, it is necessary to change independent variables from the set (V, W) to a more appropriate set, which we call (X, Y). The new variables $X = X(V, W)$ and $Y = Y(V, W)$ are defined by the following equations:

$$X(V, W) = V, \tag{12}$$

$$\left(\frac{\partial}{\partial V} + F(V, W)\frac{\partial}{\partial W}\right)Y(V, W) = 0. \tag{13}$$

For the discussion that follows, it will be most helpful to treat V and W as the functions of X and Y given by the inverse of the transformation defined by Eqs. (12) and (13). The differentials of these variables are related by

$$\frac{\partial}{\partial X} = \frac{\partial}{\partial V} + F\frac{\partial}{\partial W}, \tag{14}$$

$$\frac{\partial}{\partial Y} = \frac{\partial W}{\partial Y}\frac{\partial}{\partial W}. \tag{15}$$

We note that it follows from Eq. (14) that $F = \partial W/\partial X$. With this choice of variables, the equations for A and B become

$$\frac{\partial A}{\partial X} + 4\pi\frac{X}{W}(\rho + 3p)A = 0, \tag{16}$$

$$\frac{\partial B}{\partial X} - \left[\left(\frac{\partial W}{\partial Y}\right)^{-1}\frac{\partial^2 W}{\partial X\partial Y} - \frac{1}{X} + 4\pi\frac{X}{W}(\rho + 3p) - \frac{3}{2}\frac{1}{W}\frac{\partial W}{\partial X}\right]B + \left(\frac{\partial W}{\partial Y}\right)^{-1}\frac{\partial A}{\partial Y} = 0. \tag{17}$$

It is straightforward now to completely reduce Eqs. (16) and (17) to quadratures. We define the function

$$\Psi(X, Y) = \exp\left\{-4\pi\int^X \frac{X'[\rho(X') + 3p(X')]dX'}{W(X', Y)}\right\}. \tag{18}$$

If follows that

$$A(X, Y) = a(Y)\Psi(X, Y), \tag{19}$$

$$B(X, Y) = \left[b(Y) - \int^X X'W^{3/2}\left(\frac{\partial W}{\partial Y}\right)^{-2}\frac{\partial A}{\partial Y}\Psi(X', Y)dX'\right]\frac{\partial W}{\partial Y}\Big/[XW^{3/2}\Psi], \tag{20}$$

where $a(Y)$ and $b(Y)$ are completely arbitrary C^1 functions of Y. These quadratures [Eqs. (18)–(20)] can be performed as soon as one determines the function $W(X, Y)$. Since $F = \partial W/\partial X$, as we have seen, the real problem lies in determining the function F from Eq. (11). This problem can be expedited by changing to the variables (X, Y) discussed above, and making the substitution $F = \partial W/\partial X$ in Eq. (11):

$$\frac{\partial^2 W}{\partial X^2} - \frac{1}{X}\frac{\partial W}{\partial X} - \frac{3}{4}\frac{1}{W}\left(\frac{\partial W}{\partial X}\right)^2 + 8\pi\frac{X}{W}\frac{\partial W}{\partial X}(\rho + 3p) - 16\pi^2\frac{X^2}{W}(\rho + 3p)^2 - 8\pi X\frac{d}{dX}(\rho + p) = 0. \tag{21}$$

We note that only the independent variable X appears explicitly in Eq. (21). Therefore, the equation to determine $W(X, Y)$ is an *ordinary* differential equation. In fact this is the same differential equation used to determine W_0, Eq. (8). The only difference between W_0 and W then is one of boundary conditions. The boundary conditions on W_0 are uniquely deter-

mined by the asymptotic flatness conditions and appropriate smoothness conditions at the surface of the star (see Paper I). On the other hand, $W(X, Y)$ is a one-parameter family of solutions to Eq. (21). Since Eq. (21) is a second order equation, there are in principle two free parameters in the most general solution. Therefore, there is considerable freedom still available in the choice of the function $W(X, Y)$.

To summarize, we have succeeded in reducing the problem of finding identities from that of solving the system of partial differential equations (6), (7) to that of solving the single ordinary differential equation (21) plus the quadratures in Eqs. (18)–(20).

IV. EXAMPLES: NEW VACUUM IDENTITIES

To illustrate the generality and usefulness of the simplifications which have been presented here, we show now how every previously discussed identity for vacuum and uniform density spaces is a special case of the results presented here. Also, we explicitly write down the most general vacuum identity of this type. These vacuum identities are significantly more general than those presented elsewhere[1–4] and may possibly provide the way to show that no multiple static vacuum black hole solutions exist.

Turning to the uniform density case first, we find that a one-parameter family of solutions to Eq. (21) is given by

$$W = W_0(X) + Y, \tag{22}$$

$$W_0 = \tfrac{8}{3}\pi\rho X(3X_s - X) + \tfrac{2}{3}\pi\rho(1 - 9X_s^2), \tag{23}$$

where ρ is the density of the star and X_s is the value of X at the surface of the star. Given these integrals of Eq. (21), it is straightforward to evaluate the quadratures in Eqs. (18)–(20). In particular, we find

$$A(X, Y) = a(Y)W^{-3/2}, \tag{24}$$

$$B(X, Y) = X^{-1}\left[b(Y) - \int^X X'\left(\frac{da}{dY}W - \frac{3}{2}a\right)W^{-5/2}dX'\right]. \tag{25}$$

The integral indicated here is simple to perform [using Eqs. (22), (23)], but the result is lengthy and unenlightening. The uniform density identity presented in Paper I is the special case of the above with $a(Y) = 0$.

For vacuum spaces, it is possible to explicitly evaluate the most general integral of Eq. (21). In particular, we find that the general solution is given by

$$W(X, Y) = [g(Y)X^2 + h(Y)]^4, \tag{26}$$

where g and h are arbitrary functions of Y. It is also straightforward now to perform the quadratures in Eqs. (18)–(20). If $dg/dY \equiv g' \neq 0$, we find

$$A(X, Y) = a(Y), \tag{27}$$

$$B(X, Y) = \frac{4(g'X^2 + h')}{XW^{3/4}}\left[b(Y) + \frac{a'}{32g'(g'X^2 + h')}\right], \tag{28}$$

where $a' = da/dY$, etc. When $g' = 0$, we get Eq. (27) and

$$B(X, Y) = \frac{4h'}{XW^{3/4}}\left[b(Y) - \frac{a'X^2}{32h'^2}\right]. \tag{29}$$

Specific examples of these vacuum identities have been given by Israel,[1] Robinson,[3] and in Paper I. One example given in Paper I is $g(Y) = -h(Y) = -\frac{1}{2}M^{-1/2}Y^{1/4}$, where M is the constant which is the asymptotically defined mass of the star (or black hole). The identities of Israel and Robinson are special cases of this example, as was shown in Paper I. Another example given in Paper I (except for typographical errors) is $g(Y) = -\frac{1}{2}M^{-1/2}$ and $h(Y) = \frac{1}{2}M^{-1/2} + Y$. Clearly a large number of other possibilities also exist for other choices of g and h. Perhaps some of these identities can be used to eliminate the possibility of multiple static vacuum black holes.

Note added in proof: An error has been discovered in Sec. V of Paper I. The argument given there, that uniform density static stellar models must be spherical, is not correct. One can only conclude, from an argument such as that presented there, that any nonspherical uniform density model must have $W/W_0 < 1$ everywhere (including spatial infinity). This implies, for example that the constants of a nonspherical model must satisfy the inequality $32\pi\rho M^2 > 3(1 - V_s^2)^3$.

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