Irreducible tensor method for a chain $SU_2 \supset \cdots \supset G'' \supset G' \supset G$ and molecular physics

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Three things are discussed in this note around two results in the theory of angular momentum. First, certain Clebsch–Gordan coefficients of a compact topological group, which has a representation generalizing the antisymmetric representation $[1^n]$ of S_n, are shown to possess an interesting symmetry property. Second, for physical purpose this property is applied to the octahedral group $O \approx S_4$ and its double (i.e., covering) group O^* (i.e., $O^*/S_2 \approx O$) considered as subgroups of SO_3 and SU_2, respectively. We take this opportunity for briefly connecting some papers on the representation theory of SU_2 recently published in this journal with some previous works by the author on the Wigner–Racah algebra of a noncanonical chain $SU_2 \supset G$. Third, the material is used for rationalizing the well-known ($j = 1$)- and less known ($j = 1/2$)-isomorphisms of molecular physics in terms of isoscalar factors for the chains $SO_3 \subset O$ and $SU_2 \subset O^*$, respectively.

1. PRELIMINARIES

Result 1: An elementary calculation shows that[1] the matrix of the angular momentum J within the subspace spanned by

$$B_2 \equiv \{-(1/\sqrt{2})\,|2-1\rangle - (1/\sqrt{2})\,|21\rangle,\ (i/\sqrt{2})\,|2-1\rangle - (i/\sqrt{2})\,|21\rangle, -(1/\sqrt{2})\,|2-2\rangle + (1/\sqrt{2})\,|22\rangle\}$$

is equal to the matrix of $-J$ within

$$B_1 \equiv \{(1/\sqrt{2})\,|1-1\rangle - (1/\sqrt{2})\,|11\rangle, (i/\sqrt{2})\,|1-1\rangle + (i/\sqrt{2})\,|11\rangle, |10\rangle\}.$$

(As usual, $|jm\rangle$ denotes a normalized eigenvector of J^2 and J_z.) Of course, the preceding equality still holds when the basis B_j, $j = 2$ and 1, undergo the same unitary transformation. Therefore, in what precedes we may replace the Cartesian basis B_2 and B_1 by the pseudospherical basis

$$B_2' \equiv \{|2-1\rangle, -(1/\sqrt{2})\,|2-2\rangle + (1/\sqrt{2}\,|22\rangle, -|21\rangle\}$$

and

$$B_1' \equiv \{|11\rangle, |10\rangle, |1-1\rangle\},$$

respectively.[2–4] This first result turns out to be very useful in molecular physics and more specifically in ligand field theory.[1–5]

Result 2: In the same spirit, it is straightforward to verify that[1,5] the matrix of J within the subspace

$$B_{5/2} \equiv \left\{\left(\frac{5}{6}\right)^{1/2}\left|\frac{5}{2}-\frac{3}{2}\right\rangle - \left(\frac{1}{6}\right)^{1/2}\left|\frac{5}{2}\frac{5}{2}\right\rangle, -\left(\frac{1}{6}\right)^{1/2}\left|\frac{5}{2}-\frac{5}{2}\right\rangle + \left(\frac{5}{6}\right)^{1/2}\left|\frac{5}{2}\frac{3}{2}\right\rangle\right\}$$

is equal to the matrix of $-\frac{5}{3}J$ within

$$B_{1/2} \equiv \{|\tfrac{1}{2}\tfrac{1}{2}\rangle, |\tfrac{1}{2}-\tfrac{1}{2}\rangle\}.$$

A formal proof of Result 1 has been given by Griffith[3] through the using of Clesbsch–Gordan coefficients (CGc's) for the octahedral group O. More recently, Buch[6] has reconsidered this proof in terms of isoscalar factors for the chain $SO_3 \supset O$. The proof by Griffith and thus by Buch lies in a symmetry property for some particular CGc's of O (a subgroup of SO_3!). Reasonably, a similar property for the CGc's of the spinor octahedral group O^* (a subgroup of SU_2!) should lead to a proof of Result 2.

The aim of this article is to investigate Results 1 and 2, as well as their extensions to other subspaces than B_2 and $B_{5/2}$,[1,3,4] in the light of the Wigner–Racah algebra (WRa) of the chains $SO_3 \supset O$ and $SU_2 \supset O^*$, respectively. Section 2 is devoted to a particular symmetry property for the CGc's of a given family (including O and O^*) of groups. In Sec. 3 some basic considerations, useful to our problem, on the WRa of an arbitrary chain $SU_2 \supset \cdots \supset G'' \supset G' \supset G$ are reviewed. In addition, these considerations are connected to some (apparently distant) papers recently published in this journal. Finally, we go back to our physical problem in Sec. 4 by combining Secs. 3 and 2.

2. ON THE SYMMETRY OF CERTAIN CLEBSCH–GORDAN COEFFICIENTS

Notations: Let G be a compact topological group. We use Γ to denote an irreducible representations class (IRC) of G. For each IRC Γ, we make a choice of a unitary matrix representation

$$D^\Gamma = \{D^\Gamma(R) : R \in G\},$$

the matrix elements of $D^\Gamma(R)$ being $D^\Gamma(R)_{\gamma\gamma'}$, with γ, $\gamma' = 1, 2, \ldots, \dim\Gamma$. We take the G irreducible tensorial sets (ITS's) that we deal with in the standard form. That is to say, an ITS associated to Γ spans D^Γ rather than a representation equivalent to D^Γ. We choose a set of CGc's compatible with our set

$$\{D^\Gamma\text{: all possible } \Gamma\text{'s}\}.$$

Finally, the notation $(\Gamma_1\Gamma_2\gamma_1\gamma_2|\beta\Gamma\gamma)$, where β is an internal multiplicity label, is employed for the CGc's of G.

Special hypothesis: As first hypothesis, we assume that G possesses a one-dimensional representation $D^{\tilde{\Gamma}_0}$ distinct from the identity representation D^{Γ_0}. Clearly, the inner Kronecker product $\Gamma \otimes \tilde{\Gamma}_0$ is an IRC. We

convene to denote $\Gamma\otimes\tilde{\Gamma}_0$ as $\tilde{\Gamma}$ once and only once $\Gamma\otimes\tilde{\Gamma}_0 \neq \Gamma$. As second hypothesis, we assume our set $\{D^\Gamma$: all possible Γ's$\}$ to be constructed in such a way that $D^{\tilde{\Gamma}} \equiv D^\Gamma \otimes D^{\tilde{\Gamma}_0}$.

Theorem: If Γ is contained once and only once in $\Gamma_1\otimes\Gamma_2$, and if $\Gamma_1\otimes\Gamma_0 \neq \Gamma$ and $\Gamma\otimes\tilde{\Gamma}_0 \neq \Gamma$, we have

$$(\tilde{\Gamma}_1\Gamma_2\gamma_1\gamma_2|\tilde{\Gamma}\gamma) = t(\Gamma_1\Gamma_2\Gamma)(\Gamma_1\Gamma_2\gamma_1\gamma_2|\Gamma\gamma), \tag{1}$$

where $t(\Gamma_1\Gamma_2\Gamma)$ is a phase factor which does not depend on γ_1, γ_2, and γ.

Outline of proof and discussion: The proof is immediate when specializing Gaunt's formula[7]

$$\int_G D^\Gamma(R)_{\gamma\gamma'} {}^* D^{\Gamma_1}(R)_{\gamma_1\gamma_1'} D^{\Gamma_2}(R)_{\gamma_2\gamma_2'} d\mu(R)$$

$$= [\int_G d\mu(R)/\dim\Gamma] \sum_\beta (\Gamma_1\Gamma_2\gamma_1\gamma_2|\beta\Gamma\gamma)(\Gamma_1\Gamma_2\gamma_1'\gamma_2'|\beta\Gamma\gamma')^*$$

to our particular case. [The integration in $\int_{\hat{G}} \cdots d\mu(R)$, where $d\mu$ is the relevant Haar measure, is to be performed over the topological space $\hat{G}$ of G.] Therefore, we get the relation

$$(\tilde{\Gamma}_1\Gamma_2\gamma_1\gamma_2|\tilde{\Gamma}\gamma)(\tilde{\Gamma}_1\Gamma_2\gamma_1'\gamma_2'|\tilde{\Gamma}\gamma')^* = (\Gamma_1\Gamma_2\gamma_1\gamma_2|\Gamma\gamma)(\Gamma_1\Gamma_2\gamma_1'\gamma_2'|\Gamma\gamma')^*$$

from which the announced theorem is easily deduced. Moreover, we may always arrange that the factor $t(\Gamma_1\Gamma_2\Gamma)$ in Eq. (1) be equal to 1. Note that a relation similar to Eq. (1) holds when $\tilde{\Gamma}_1\Gamma_2$ is replaced by $\Gamma_1\tilde{\Gamma}_2$. Note also that Eq. (1) may be extended to the cases where $\Gamma_1\otimes\tilde{\Gamma}_0$ and/or $\Gamma\otimes\tilde{\Gamma}_0$ are equal to Γ_1 and/or Γ, respectively; the corresponding formulas are complicated and not interesting for our physical purpose, so we shall not present them here. These matters generalize the particular symmetry properties of the V coefficients for some simply reducible groups[3] of interest in molecular physics.

Examples: The group S_n is particularly adequate for illustrating the preceding ideas. In that case Γ_0 corresponds to the partition $[n]$ and the unique $\tilde{\Gamma}_0$ corresponds to $[1^n]$. Furthermore, $[a]$ standing for an arbitrary IRC of S_n, the IRC's $[a]\otimes[1^n]$ and $[a]$ are customarily said to be associate or conjugate. According to our convention, we use the notation $[a]\otimes[1^n]=\widetilde{[a]}$ only when $[a]\otimes[1^n] \neq [a]$, a fact which slightly differs from the literature on S_n. To be more specific let us consider $S_4 \approx O$. The five IRC's [4], [31], [22], $[21^2]=\widetilde{[31]}$, and $[1^4]=\widetilde{[4]}$ for S_4 are generally denoted by the chemical physicists as A_1, T_2, E, T_1, and A_2 for O, respectively. The theorem gives

$$([31][a]\gamma_1\gamma_2|[31]\gamma) = ([21^2][a]\gamma_1\gamma_2|[21^2]\gamma) \quad \forall\, \gamma_1, \gamma_2, \gamma, \text{ and } [a]$$

which can be rewritten as

$$(T_2\Gamma\gamma_2\gamma|T_2\gamma_1) = (T_1\Gamma\gamma_2\gamma|T_1\gamma_1) \quad \forall\, \gamma_2, \gamma, \gamma_1, \text{and } \Gamma. \tag{2}$$

Equation (2) specializes to the relation[3,6]

$$V\begin{pmatrix} T_2 & T_2 & T_1 \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix} = V\begin{pmatrix} T_1 & T_1 & T_1 \\ \gamma_1 & \gamma_2 & \gamma \end{pmatrix} \quad \forall\, \gamma_1, \gamma_2, \text{ and } \gamma$$

that actually explains Result 1.[3,6]

As another example, let us consider O*. This group has seven IRC's: A_1, T_1, E, $T_2=\tilde{T}_1$, $A_2=\tilde{A}_1$ (the five single-valued classes of O) and E', U', $E''=\tilde{E}'$ (the three double-valued classes of O). According to the theorem, we have

$$(E''\Gamma\gamma_2\gamma|E''\gamma_1) = (E'\Gamma\gamma_2\gamma|E'\gamma_1) \quad \forall\, \gamma_2, \gamma, \gamma_1, \text{ and } \Gamma \tag{3}$$

which will be proved to explain Result 2.

3. WIGNER–RACAH ALGEBRA FOR A CHAIN $SU_2 \supset \cdots \supset G'' \supset G' \supset G$

Trivialities: Let G be a subgroup of SU_2. We shall use the notations of Sec. 2 for denoting the IRC's, irreducible unitary matrix representations, and related CGc's of G. The restriction to G of each IRC (j) of SU_2 $(j=0, \frac{1}{2}, 1, \cdots)$ yields a generally reducible representations class of G. This means that the standard irreducible matrix representation $\mathcal{D}^{(j)}$ of SU_2 restricted to G is equivalent to a completely reduced representation $\oplus_\Gamma \sigma(\Gamma|j)D^\Gamma$ of G, where $\sigma(\Gamma|j)$ is the frequency of Γ in (j). In other words, there exists a unitary matrix U^j, whose elements are denoted as $U^j_{m,a\Gamma\gamma}$, such that

$$\sum_{mm'} U^j_{m,a\Gamma\gamma} {}^* \mathcal{D}^{(j)}(R)_{mm'} U^j_{m',a'\Gamma'\gamma'} = \delta(a'a)\delta(\Gamma'\Gamma) D^\Gamma(R)_{\gamma\gamma'} \quad \forall\, R \in G,$$

where $m, m' = -j, -j+1, \ldots, j$ and the symbol a is an external multiplicity label necessary only when $\sigma(\Gamma|j) > 1$. Note that a may be a simple numeral taking the values $1, 2, \ldots, \sigma(\Gamma|j)$ or a complicated symbol containing IRC's of the groups $G', G'', \cdots$ such that $SU_2 \supset \cdots \supset G'' \supset G' \supset G$. It is thus possible to construct G ITS's from the SU_2 ITS's of vectors $\{|\alpha jm)$: $m=-j, -j+1, \ldots, j\}$ and operators $\{T^k_q$: $q=-k, -k+1, \ldots, k\}$. For instance,

$$\left\{ |\alpha ja\Gamma\gamma) = \sum_m |\alpha jm) U^j_{m,a\Gamma\gamma} \text{: } \gamma = 1, 2, \ldots, \dim\Gamma \right\}$$

is a G ITS spanning D^Γ. The same thing is true for

$$\left\{ T^{k a\Gamma}_\gamma = \sum_q T^k_q U^k_{q,a\Gamma\gamma} \text{: } \gamma = 1, 2, \ldots, \dim\Gamma \right\}.$$

The f function: The function f defined via

$$f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma \end{pmatrix} = (2j_1+1)^{-1/2}(-1)^{2j} \sum_{m_2 m m_1} U^{j_2}_{m_2,a_2\Gamma_2\gamma_2} \times U^j_{m,a\Gamma\gamma}(j_2 j m_2 m | j_1 m_1) U^{j_1}_{m_1,a_1\Gamma_1\gamma_1} {}^*,$$

where $(j_2 j m_2 m | j_1 m_1)$ is a standard SU_2 CGc, proved to be very useful in the field of molecular physics.[8-10] The properties (existence conditions, selection rules, symmetry properties, orthogonality properties, $\cdots$) of the f coefficients have been extensively studied.[8-11] We shall only report here the factorization formula[10]

$$f\begin{pmatrix} j_1 & j_2 & j \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma \end{pmatrix} = (2j_1+1)^{-1/2}(-1)^{2j}$$

$$\times\sum_{\beta}(j_2a_2\Gamma_2+ja\Gamma\,|\,j_1a_1\beta\Gamma_1)^*(\Gamma_2\Gamma\gamma_2\gamma\,|\,\beta\Gamma_1\gamma_1)^*, \tag{4}$$

which will be used in the following. The coefficient $(+\,|)$ is independent of the indices γ_2, γ, and γ_1. Equation (4) trivially follows from the Racah lemma applied to the chain $SU_2\supset G$ or alternatively from the G Wigner–Eckart theorem (WEt) written in a $SU_2\supset G$ basis.

The U function: The isoscalar factor $(+\,|)$ resembles the coefficient U rediscovered (cf. Ref. 12) by Buch[6] for a chain $SO_3\supset\mathcal{G}$, where $\mathcal{G}$ is a finite multiplicity-free group. Actually, the relation

$$U\begin{Bmatrix} a_1\Gamma_1 & a_2\Gamma_2 & a\Gamma \\ l_1 & l_2 & k\end{Bmatrix}=\left(\frac{\dim\Gamma_1}{2l_1+1}\right)^{1/2}(l_2a_2\Gamma_2+ka\Gamma\,|\,l_1a_1\Gamma_1)^*$$

holds for the integer representations of the chain $SU_2\supset\mathcal{G}^*$, where $\mathcal{G}^*$ is the spinor group of $\mathcal{G}$. It should be noted that the arguments of the function U generally comprise three a's, a point which was apparently overlooked in the formalism described in Ref. 6 (cf. also Ref. 12).

Wigner–Eckart theorems: Emphasis is placed on the U function in Buch's paper. We believe that the function important for the applications (to molecular physics) is the f function. As a matter of fact, the SU_2 WEt in a $SU_2\supset$ basis reads[8]

$$(\alpha_1J_1a_1\Gamma_1\gamma_1\,|\,T^{*a\Gamma}_{\gamma}\,|\,\alpha_2J_2a_2\Gamma_2\gamma_2)$$
$$=(\alpha_1J_1\|T^*\|\alpha_2J_2)f\begin{pmatrix} J_1 & J_2 & k \\ a_1\Gamma_1\gamma_1 & a_2\Gamma_2\gamma_2 & a\Gamma\gamma\end{pmatrix}, \tag{5}$$

where the reduced matrix element $(\|\ \|)$, independent of the U^j matrices, coincides with the one defined by Racah. So that all the geometrical dependence of the right-hand side of Eq. (5) is contained within a single coefficient, viz., the f coefficient. The U coefficient, or more generally the $(+\,|)$ coefficient, makes it possible to connect the SU_2 WEt and the G WEt both expressed in a $SU_2\supset G$ basis. Indeed, the left-hand side of Eq. (5) may alternatively be written as

$$(\alpha_1J_1a_1\Gamma_1\gamma_1\,|\,T^{*a\Gamma}_{\gamma}\,|\,\alpha_2J_2a_2\Gamma_2\gamma_2)$$
$$=(\dim\Gamma_1)^{-1/2}\sum_{\beta}(\alpha_1J_1a_1\Gamma_1\|T^{*a\Gamma}\|\alpha_2J_2a_2\Gamma_2)_\beta$$
$$\times(\Gamma_2\Gamma\gamma_2\gamma\,|\,\beta\Gamma_1\gamma_1)^* \tag{6}$$

owing to the G WEt. Consequently, from Eqs. (4)–(6), we get[10]

$$(\alpha_1J_1a_1\Gamma_1\|T^{*a\Gamma}\|\alpha_2J_2a_2\Gamma_2)_\beta$$
$$=(-1)^{2k}[\dim\Gamma_1/(2J_1+1)]^{1/2}(\alpha_1J_1\|T^*\|\alpha_2J_2)$$
$$\times(J_2a_2\Gamma_2+ka\Gamma\,|\,J_1a_1\beta\Gamma_1)^*,$$

a relation which extends to an arbitrary chain $SU_2\supset G$ the relation (7) of Ref. 6 valid for the chain $SO_3\supset\mathcal{G}$.

Basis for SU_2: Before leaving this Section it is perhaps worthwhile to shortly connect the WRa of SU_2 in an $SU_2\supset G$ basis with the representation theory of SU_2. The theory of the representation of SU_2 has been revived in the last few years (for example, see Refs. 13–16). In the terminology of Patera and Winternitz,[15,17] there are two approaches to the representation theory of SU_2: (i) the "Lie subgroup type" one and (ii) the "non-Lie subgroup type" one.

(i) There exists only one, up to isomorphism, Lie subgroup type approach, namely, the standard or canonical one corresponding to the set $\{J^2, J_z\}$ of commuting operators.[15] This quantum-mechanical approach is the starting point for the WRa of SO_3 (or SU_2) in the standard $SO_3\supset SO_2$ (or $SU_2\supset U_1$) basis. We thus have the $\{jm\}$ scheme: the quantities relevant for the representation algebra and the WRa of SU_2 in the canonical basis $SU_2\supset U_1$ are labeled by j's and m's.

(ii) On the other hand, there exists only one, up to isomorphism, second-order non-Lie subgroup type approach, viz., that one corresponding to the set $\{J^2, J_x^2+rJ_y^2\}_{0<r<1}$ of commuting operators.[15] This leads to the $\{j\lambda\}$ scheme: the labels consist in that case of j's and λ's where λ denotes an eigenvalue of $J_x^2+rJ_y^2$.

To the two above schemes we can add the $\{ja\Gamma\gamma\}$ scheme which is relative to the WRa of SU_2 in a nonstandard or noncanonical $SU_2\supset G$ basis. An operator formulation of this scheme could be the following: the $\{ja\Gamma\gamma\}$ scheme corresponds to the set

$$\{J^2, P(\Gamma\gamma)=\int_G d\mu(R)D^{\Gamma}(R)_{\gamma\gamma}{}^*P_R\text{: all possible }\Gamma\gamma\text{'s}\}$$

of commuting operators, where $P(\Gamma\gamma)$ is the $\Gamma\gamma$th Wigner projection operator of G. The $\{ja\Gamma\gamma\}$ scheme covers, to some extent, the two preceding ones: obviously the $\{jm\}$ scheme corresponds to $G\equiv U_1$ and the $\{j\lambda\}$ scheme corresponds to $G\equiv D_2^*$, the covering of the dihedral group D_2. This last point allows us to qualitatively obtain the results of Secs. 3, 4, and 5 of Ref. 15.[18] From a quantitative point of view, the using of vectors adapted to the chain $SU_2\supset D_2^*$ could then simplify the calculation of the eigenvalues and eigenvectors of $J_x^2+rJ_y^2$. In addition, the consideration of the chain $SU_2\supset O^*\supset D_4^*\supset D_2^*$ makes it possible to partly fill in the gap between SU_2 and D_2^* and therefore: (i) to partly overcome the missing label problem when $\sigma(\Gamma\,|\,j)>1$, where Γ stands for an IRC of D_2^* (the problem is thus completely solved for $j=\frac{1}{2}, 1, \ldots, 4$) (ii) to possibly further simplify the calculation of the eigenstates of $J_x^2+rJ_y^2$. In the same way, the consideration of the chain $SU_2\supset D_\infty^*\supset D_2^*$ allows us to successfully handle the missing label problem. This and other ways out[19] are the subjects of future research.

4. EXTENSION OF RESULTS 1 AND 2

In view of our physical problem we now go to the introduction of Eqs. (2) and (3) into the CGc's for the chains $SO_3\supset O$ and $SU_2\supset O^*$, respectively. From Eqs. (4) and (2), we get the first master formula

$$f\begin{pmatrix} j_1 & j_2 & k \\ a_1t\gamma_1 & a_2t\gamma_2 & aT_1\gamma\end{pmatrix}=A[3/(2j_1+1)]^{1/2}$$
$$\times(j_2a_2t+kaT_1\,|\,j_1a_1t)^*f\begin{pmatrix} 1 & 1 & 1 \\ T_1\gamma_1 & T_1\gamma_2 & T_1\gamma\end{pmatrix}, \tag{7}$$

where $t\equiv T_1$ or T_2 and A is the following phase factor

$$A=(1T_1+1T_1\,|\,1T_1).$$

The other master formula

$$f\begin{pmatrix} j_1 & j_2 & k \\ a_1e\gamma_1 & a_2e\gamma_2 & aT_1\gamma\end{pmatrix}=B[2/(2j_1+1)]^{1/2}$$

$$\times(j_2 a_2 e + kaT_1 \,|\, j_1 a_1 e)^* f\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ E'\gamma_1 & E'\gamma_2 & T_1\gamma \end{pmatrix}, \tag{8}$$

where $e \equiv E'$ or E'' and the phase factor B is

$$B = (\tfrac{1}{2}E' + 1T_1 \,|\, \tfrac{1}{2}E'),$$

follows from Eqs. (4) and (3).

The combination of Eqs. (5) and (7) leads, after some manipulations, to

$$(ja_1 t\gamma_1 \,|\, J_\gamma^{1T_1} \,|\, ja_2 t\gamma_2) = \alpha(1T_1\gamma_1 \,|\, J_\gamma^{1T_1} \,|\, 1T_1\gamma_2), \tag{9}$$

where the proportionality constant α (independent of γ_1, γ, and γ_2) writes

$$\alpha = A[j(j+1)/2]^{1/2}(ja_2 t + 1T_1 \,|\, ja_1 t)^*.$$

Equation (9) shows that the matrix of J within the t ($\equiv T_1$ or T_2) components of a j state ($j = 1, 2, 3, \cdots$) is proportional to that one within the T_1 components of a p state. In the same way, from Eqs. (5) and (8) we have

$$(ja_1 e\gamma_1 \,|\, J_\gamma^{1T_1} \,|\, ja_2 e\gamma_2) = \beta(\tfrac{1}{2}E'\gamma_1 \,|\, J_\gamma^{1T_1} \,|\, \tfrac{1}{2}E'\gamma_2), \tag{10}$$

where

$$\beta = B2[j(j+1)/3]^{1/2}(ja_2 e + 1T_1 \,|\, ja_1 e)^*.$$

Equation (10) proves the proportionality of the matrices of J within the e ($\equiv E'$ or E'') components of a j state ($j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots$) and within the E' components of a $\frac{1}{2}$ state.

Results 1 and 2 appear as particular cases of Eqs. (9) and (10), respectively. As an example, the sets B_1 and B_2 are SO_3 ITS's, in a $SO_3 \supset O \supset D_4 \supset D_2$ basis, of order 1 and 2, respectively. Consequently, the proportionality constant between the subspaces B_1 and $B_{j=2}$ reads

$$\alpha(B_1, B_2) = A\sqrt{3}(2T_2 + 1T_1 \,|\, 2T_2)^*$$

an expression which makes precise the corresponding result obtained in Ref. 6.

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[1]Cf. the ficititious orbital angular momentum (for Result 1) and the fictitious spin angular momentum (for Result 2) introduced by A. Abragam and M.H.L. Pryce, Proc. Roy. Soc. A **205**, 135 (1951).
[2]J.S. Griffith, *The Theory of Transition-Metal Ions* (Cambridge U.P., London and New York, 1961).
[3]J.S. Griffith, *The Irreducible Tensor Method for Molecular Symmetry Groups* (Prentice-Hall, Englewood Cliffs, N.J., 1962); see also J.S. Griffith, Mol. Phys. **3**, 285 (1960).
[4]A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Ions* (Clarendon, Oxford, 1970).
[5]Result 1 is at the root of the so-called $(j=1)^n$ isomorphism (Ref. 2). Result 2 could be the starting point towards a $(j=1/2)^n$ isomorphism.
[6]T. Buch, J. Math. Phys. **13**, 1892 (1972).
[7]See E.P. Wigner, "On the Matrices Which Reduce the Kronecker Products of Representations of S.R. Groups," (Princeton, 1951), in *Quantum Theory of Angular Momentum*, edited by L.C. Biedenharn and H. van Dam (Academic, New York, 1965); see also W.T. Sharp, "Racah Algebra and the Contraction of Groups," Report No. AECL-1098 (Atomic Energy of Canada Ltd., Chalk River, 1960); J.-R. Derome and W.T. Sharp, J. Math. Phys. **6**, 1584 (1965). It is perhaps interesting to note that, while the WRa of a finite group has been largely investigated by Wigner, Sharp, and Derome and Sharp (cf. the three preceding works), the first textbook version of WRa for use in molecular physics has been given by Griffith (Ref. 3) on the basis of works achieved principally by Racah, Tanabe and Sugano, Koster, Tanabe and Kamimura, and Griffith (cf. Ref. 3). To enlarge this short list on WRa, let us also mention two recent papers dealing with ITS's for a finite or compact group: A.J. van Zanten and E. de Vries, J. Math. Phys. **14**, 1423 (1973); P. Kasperkovitz and R. Dirl, J. Math. Phys. **15**, 1203 (1974); the concept of ITS is discussed in these last two works within the framework of group algebra.
[8]M. Kibler, J. Mol. Spectry. **26**, 111 (1968).
[9]M. Kibler, Int. J. Quantum Chem. **3**, 795 (1969).
[10]M. Kibler, C.R. Acad. Sci. (Paris) B **268**, 1221 (1969).
[11]Extensive tables of f coefficients have been set up by M.R. Kibler and P.A.M. Guichon, "Clebsch-Gordan Coefficients Adapted to the Cubical, Tetragonal and Digonal Double Groups," Report No. LYCEN-7537 (Lyon, 1975).
[12]Tang Au-chin, Sun Chia-chung, Kiang Yuan-sun, Deng Zung-hau, Liu Jo-chuang, Chang Chian-er, Yan Go-sen, Goo Zien, and Tai Shu-shan, Sci. Sinica (Peking) **15**, 610 (1966).
[13]J.A.R. Coope and R.F. Snider, J. Math. Phys. **11**, 1003 (1970).
[14]J.A.R. Coope, J. Math. Phys. **11**, 1591 (1970).
[15]J. Patera and P. Winternitz, J. Math. Phys. **14**, 1130 (1973).
[16]A.J. Torruella, J. Math. Phys. **16**, 1637 (1975).
[17]See the introduction in the following paper: J. Patera, P. Winternitz, and H. Zassenhaus, J. Math. Phys. **16**, 1597 (1975).
[18]An essential difference between the $\{jm\}$ and $\{j\lambda\}$ schemes is as follows: for any half-odd-integer value of j, the eigenvalues λ of $J_x^2 + rJ_y^2$ are twofold degenerate (Ref. 15) whereas the eigenvalues m of J_z are nondegenerate. The twofold degeneracy is directly related to the fact that the half-integer representation of D_2^* is two-dimensional. Looked at differently, the impossibility of obtaining nondegenerate eigenvectors for $J_x^2 + rJ_y^2$ when j is half-odd-integer follows from the invariance of this operator (to be compared with the noninvariance of J_z) under time reversal. The foregoing agrees with Kramer's theorem of molecular physics.
[19]For example, the irreducible Cartesian tensors theory developed by Coope and Snider (Ref. 13) and Coope (Ref. 14) might also be related to the WRa of the chain $SU_2 \supset D_2^*$.

The Weyl transform of distributions

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The Weyl transform is defined rigorously on the twisted product algebra of c^∞ functions slowly increasing at ∞. The image set under the Weyl rule of correspondence is shown to contain linear unbounded operators. In particular, the momentum and the coordinate operators P and Q and the polynomial functions of P and Q are included.

I. INTRODUCTION

The present paper aims at giving a mathematically rigorous definition of the Weyl transform[1] on a sufficiently large class of tempered distributions, so that the image set under the Weyl correspondence contains densely defined, not necessarily bounded linear operators on a Hilbert space. In particular, the momentum and the coordinate operators P and Q and the polynomial functions in P and Q are to be included.

In Ref. 2, Kastler showed that the Weyl correspondence can be viewed as a faithful $*$-representation of the $B*$-algebra of bounded measures on a $2n$-dimensional symplectic space under the twisted convolution. Lonpias and Miracle-Sole[3] extended Kastler's result to a class of tempered distributions whose image set under the Weyl correspondence consisted of bounded operators. Other work related to this topic can also be found in Refs. 4, 5, and 6. While Refs. 4, 5 deal with bounded operators only, Ref. 6 is mainly concerned with the relationship between the phase space formulation of quantum mechanics and the theory of pseudodifferential operators.

The notations in this paper are those used in Ref. 7. The reader is also referred to Sec. III of the same paper for definitions and facts about the twisted convolution and the twisted product of distributions.

In Sec. II of this paper, some noncommutative algebra of distributions are constructed, with multiplication given by the twisted convolution and the twisted product. These are generalizations of the $*$-algebras E', O_C', and O_M of L. Schwartz.[8,9] Using these results, in Sec. III we extend the domain of definition of the Weyl transform to elements in $O_M(R^{2n})$. The properties of the Weyl transform so defined form the contents of Theorem 4.1. The Weyl correspondence is seen to be a $*$ and product preserving bijection from the $*$-algebra O_M with the twisted product to the set of closable linear operators on a common dense set in a Hilbert space.

II. SOME NONCOMMUTATIVE ALGEBRAS OF DISTRIBUTIONS

It is known in the theory of distributions that E' and O_C' form convolution algebras.[8] We generalize these results to the case where the twisted convolution and the twisted product are used. If δ_0 is the delta distribution concentrated at 0 and $O_c'(R^{2n},{}^*c)$ and $O_M(R^{2n},\circ c)$ are spaces of $O_c'(R^{2n})$ and $O_M'(R^{2n})$ equipped with the twisted convolution and the twisted product as multiplication respectively, we have the following results:

Theorem 2.1: $O_c'(R^{2n},*c)$ is a noncommutative algebra with unit element δ_0 for each $c\neq 0$.

Corollary 2.1: $E'(R^{2n},*c)$ is a subalgebra of $O_c'(R^{2n},*c)$ with unit element δ_0.

Corollary 2.2: $O_M(R^{2n},\circ c)$ is a non-commutative algebra with unit element 1.

To prove Theorem 2.1 and its corollaries, we need the following lemmas:

Lemma 2.1: Let $\Phi\in O_c$. Then $E_\eta(c)\Phi\in O_c$.

Proof: For each $\eta\in R^{2n}$ and c real, $E_\eta(c,\xi)=\exp[(ic/2)\eta\times\xi]$ is infinitely differentiable as a function of ξ. Using the Leibniz rule for differentiation, we have

$$\partial^p(E_\eta(c)\Phi)=\sum_{q\leq p}\binom{p}{q}\partial^q(E_\eta(c))\partial^{p-q}\Phi.$$

Now $\partial^q E_\eta(c)=P_q(\eta,c)E_\eta(c)$, where $P_q(\eta,c)$ is a polynomial in η and c of degree $\leq|q|$, so that

$$(1+|\xi|^2)^k\partial^p(E_\eta(c)\Phi)=\sum_{q\leq p}\binom{q}{p}P_q(\eta,c)(1+|\xi|^2)^kE_\eta(c)\partial^{p-q}\Phi.$$

It follows that

$$\left|(1+|\xi|^2)^k\partial^p(E_\eta(c)\Phi)\right|$$

$$\leq\sum_{q\leq p}\binom{p}{q}\left|P_q(\eta,c)\right|\ \left|(1+|\xi|^2)^k\partial^{p-q}\Phi\right|\to 0$$

as $|\xi|\to\infty$ if k is taken to be an integer so that $|(1+|\xi|^2)^k\partial^{p-q}\Phi|\to 0$ as $|\xi|\to\infty$. Such integer k exists since $\Phi\in 0_c$. |||

Lemma 2.2: Let $u,v\in O_c'$. Then $u^*cv\in O_c'$.

Proof: Consider v as a tempered distribution; we have

$$\langle E_\eta(c)v,\Phi\rangle=\langle v,E_\eta(c)\Phi\rangle,\quad \Phi\in S(R^{2n}).$$

Since $E_\eta(c)$ as a function of ξ is a member of O_M, so that $E_\eta(c)v\in S'(R^{2n})$. By Lemma 2.1, $E_\eta(c)\Phi\in O_c$ if $\Phi\in O_c$. From the fact that S is dense in O_c, there is a sequence $\{\Phi_n\}$ in S and $\Phi_n\to\Phi$. Also, we have $E_\eta(c)\Phi_n\to E_\eta(c)\Phi$. From the continuity of v,

$$\langle E_\eta(c)v,\Phi_n\rangle=\langle v,E_\eta(c)\Phi_n\rangle\to\langle v,E_\eta(c)\Phi\rangle=\langle E_\eta(c)v,\Phi\rangle,\quad\Phi\in O_c.$$

This shows $E_\eta(c)v\in O_c'$. Now $u*cv=u*(E_\eta(c)v)\in O_c'$ since $E_\eta(c)v\in O_c'$. This follows from the fact that O_c' is a convolution algebra of distributions. |||

Lemma 2.3: $\delta_0 * cu = u * c\delta_0 = u$ for all $u \in O_c'$.

Proof: $\delta_0 * cu = \delta_0 * (E_\eta(c)u)$ so that

$$\langle \delta_0 * E_\eta(c)u, \Phi\rangle = \langle \delta_0(\eta), \langle (E_\eta(c)u)(\xi), \Phi(\xi+\eta)\rangle\rangle$$
$$= \langle u(\xi), \Phi(\xi)\rangle = \langle u, \Phi\rangle \quad \text{for all } \Phi \in O_c.$$

A similar computation shows $u * c\delta_0 = u$. |||

Lemma 2.4: Let $u, v, w \in O_c'$. Then $u * c(v * cw) = (u * cv) * cw$.

Proof: Both sides of the above equation are well defined and are members of O_c' by Lemma 2.2. A rather lengthy but straightforward computation shows that equality holds. We omit the details.

Proof of Theorem 2.1

The results of Lemmas 2.1, 2.2, 2.3, and 2.4 together with the fact that the twisted convolution $* c$ is noncommutative for $c \neq 0$ can be used to give a proof of Theorem 2.1.

Proof of Corollary 2.1

Since $E'(R^{2n}) \subset O_c'(R^{2n})$ and $\delta_0 \in E'(R^{2n})$, it is enough to verify the closure property for $u, v \in E'(R^{2n})$. Let A, B be the supports of u, v. Now $u * cv = u * (E_\eta(c)v)$. We wish to show that $E_\eta(c)v$ has compact support and the $\operatorname{supp}[E_\eta(c)v] = B$. For each $\eta \in R^{2n}$ and c real, $E_\eta(c)v$ is a distribution since $E_\eta(c, \xi)$ is infinitely differentiable. That is,

$$\langle E_\eta(c)v, \Phi\rangle = \langle v, E_\eta(c)\Phi\rangle \quad \text{for all } \Phi \in C_c^\infty(R^{2n}).$$

Now $\operatorname{supp}(E_\eta(c)\Phi) = \operatorname{supp}\Phi$; we have $\langle E_\eta(c)v, \Phi\rangle = \langle v, E_\eta(c)\Phi\rangle = 0$ for all $\Phi \in C_c^\infty(B^c)$, and B^c is the complementary set of B in R^{2n}. It follows that $\operatorname{supp}(E_\eta(c)v) = \operatorname{supp} v = B$. Therefore, $u * cv \in E'(R^{2n})$ since $E'(R^{2n})$ is a convolution algebra. |||

Proof of Corollary 2.2

The closure property of $O_M(R^{2n})$ under the twisted product from the way it is defined, the properties of the Fourier transform F and the results of Theorem 2.1. Since the unit function $1 \in O_M(R^{2n})$ and $F1 = (2\pi)^n\delta_0$, one verifies readily that $1 \circ cg = g \circ c1 = g$ for all $g \in O_M$.

To verify that the twisted product is associative, let f, g, h be elements of $O_M(R^{2n})$. Now

$$f \circ c(g \circ ch) = (2\pi)^{-n}F^{-1}[Ff * cF(g \circ ch)]$$
$$= (2\pi)^{-2n}F^{-1}[Ff * cFF^{-1}(Fg * cFh)]$$
$$= (2\pi)^{-2n}F^{-1}[Ff * c(Fg * cFh)]$$
$$= (2\pi)^{-2n}F^{-1}[(Ff * cFg) * c(Fh)] \text{ by Theorem 2.1.}$$

On the other hand,

$$(f \circ cg) \circ ch = (2\pi)^{-n}[F^{-1}(Ff * cFg) \circ ch]$$
$$= (2\pi)^{-2n}F^{-1}[FF^{-1}(Ff * cFg) * c(Fh)]$$
$$= (2\pi)^{-2n}F^{-1}[(Ff * cFg) * c(Fh)]. \quad |||$$

III. WEYL TRANSFORM OF DISTRIBUTIONS

Let

$$P = (P_1, P_2, \ldots, P_n), \quad Q = (Q_1, Q_2, \ldots, Q_n),$$

where P_j, Q_j, $1 \leq j \leq n$ are linear unbounded self-adjoint Schrödinger operators[10] defined in dense sets D_{P_j}, D_{Q_j} in $L^2(R^n)$ respectively by

$$(P_j\varphi)(x) = -ic\frac{d\varphi}{d\chi_j}, \quad \varphi \in D_{P_j}$$

and

$$(Q_j\Psi)(x) = \chi_j\Psi(\chi), \quad \Psi \in D_{Q_j}.$$

c is a positive constant (usually denoted by $\hbar$, the Planck constant). If (s, t) is an element of R^{2n} with

$$t \cdot P = \sum_{j=1}^{n} t_jP_j,$$

$$s \cdot Q = \sum_{j=1}^{n} s_jQ_j,$$

$\{\exp(it_jP_j)\}$, $\{\exp(is_jQ_j)\}$ are the one-parameter unitary groups generated by iP_j and iQ_j.

The unitary operators $\exp(it \cdot P)$ and $\exp(is \cdot Q)$ can also be defined and their actions on an element φ of $L^2(R^n)$ is given by

$$(\exp(it \cdot P)\varphi)(x) = \varphi(x + ct),$$
$$(\exp(is \cdot Q)\varphi)(x) = \exp(is \cdot \chi)\varphi(x),$$

from which the Weyl form of CCR follows:

$$\exp(it \cdot P)\exp(is \cdot Q) = \exp(it \cdot s)\exp(is \cdot Q)\exp(it \cdot P).$$

Consequently, for each $(s, t) \in R^{2n}$, the operator

$$\pi(s, t) = \exp[(ic/2)s \cdot t]\exp(-it \cdot P)\exp(is \cdot Q)$$

is unitary and

$$(\pi(s, t)\varphi)(x) = \exp[(is \cdot (x - c/2t)]\varphi(x - ct).$$

It follows then

$$\pi(s, t)\pi(u, v) = \exp[ic(s \cdot v - t \cdot u)/2]\,\pi(s + u, t + v)$$

for each (s, t), (u, v) in R^{2n}. The map π: $(s, t) \to \pi(s, t)$ is the "Schrödinger representation" of the irreducible Weyl system on $L^2(R^n)$.[10]

Let $f \in L^2(R^{2n})$ and $\varphi, \Psi \in L^2(R^n)$. The Weyl transform of f, denoted by $w(f)$, is given by

$$(w(f)\varphi, \Psi) = (2\pi)^{-n}\iint (\pi(s, t)\varphi, \Psi)(Ff)(s, t)\,ds\,dt$$

where $(\cdot, \cdot)$ denotes the inner product in $L^2(R^n)$. $W(f)$ can be shown[5,6] to be a linear operator on $L^2(R^n)$ of Hilbert–Schmidt type. In fact the Weyl correspondence $f \to w(f)$ is an algebra isomorphism from the twisted algebra $L^2(R^{2n}, \circ c)$ to the B^*-algebra of Hilbert–Schmidt operators on $L^2(R^n)$.[6]

With the above preliminaries, we generalize the Weyl transform as a map from $O_M(R^{2n}, \circ c)$ to the set A of closable linear operators defined on the common domain $D = C_C^\infty(R^n)$, the space of infinitely differential functions with compact support, as a dense set in $L^2(R^n)$.

The following lemma is needed before we can give a precise definition of the Weyl transform of elements of $O_M(R^{2n}, \circ c)$.

Lemma 4.1: Let $\varphi \in D$, $(q, p) \in R^{2n}$, and

$$\varphi_\pi(q, p, x) = (\pi(q, p)\varphi)(x) = \exp[iq \cdot (x - cp/2)]\varphi(x - cp).$$

(1) As a function of x, $\varphi_\pi \in \mathcal{D}$.

(2) As a function of (q,p), $\varphi_\pi \in O_C(R^{2n})$.

(3) $\varphi \to \varphi_\pi$ is a bijection from $\mathcal{D}$ to itself.

(4) $(\varphi_\pi, \Psi)(q,p) \in O_C(R^{2n})$ for each φ, $\Psi \in \mathcal{D}$.

(5) Let $g \in O_M(R^{2n})$ and $Fg = \hat{g} \in O_C'(R^{2n})$.

Then

$$\langle \hat{g}, \varphi_\pi(q,p)\rangle(x) = \varphi_{\pi,g}(x) \in \mathcal{D}.$$

(6) The transformation $w(g)$ given by $(w(g)\varphi)(x) = \varphi_{\pi,g}(x) = \langle \hat{g}, \varphi_\pi\rangle$ is a linear closable operator on $\mathcal{D}$ to itself.

Proof:

(1) This follows immediately from the fact that $\varphi \in \mathcal{D}$.

(2) φ_π is infinitely differentiable in q and p. For a fixed x and c, $\partial^\alpha \varphi_\pi$ behaves like polynomials in q, p for any multi-index α. Consequently, $\varphi_\pi \in O_C(R^{2n})$.

(3) Let φ_1 and $\varphi_2 \in \mathcal{D}$ and $(\varphi_1)_\pi = (\varphi_2)_\pi$. But $\pi(q,p)$ is unitary and its inverse is $\pi(-q,-p)$; hence $\varphi_1 = \varphi_2$. To show $\varphi \to \varphi_\pi$ is a surjection, let $\varphi \in \mathcal{D}$. Then $\pi(-q,-p)\varphi \in \mathcal{D}$ and $\pi(q,p)[\pi(-q,-p)\varphi] = \varphi$.

(4) Since

$$(\varphi_\pi, \Psi)(q,p) = \int \varphi_\pi(q,p,x)\bar{\Psi}(x)\,dx$$
$$= \int \exp[iq\cdot(x - cp/2)]\varphi(x - cp)\bar{\Psi}(x)\,dx,$$

and $\partial^\alpha_{(q,p)}(\varphi_\pi, \Psi)$ behaves like a polynomial in q,p for any multi-index α.

(5) Treating x as a parameter, and α as any multi-index,

$$\partial_x^\alpha \varphi_{\pi,g}(x) = \partial_x^\alpha \langle \hat{g}, \varphi_\pi\rangle = \langle \hat{g}, \partial_x^\alpha \varphi_\pi\rangle$$

with $\partial_x^\alpha \varphi_\pi \in O_C(R^{2n})$ by (2). $\varphi_{\pi,g}$ has compact support since φ_π, as a function of x, has compact support.

(6) Let $\varphi_n \in \mathcal{D}$, $\lim_{n\to\infty} \varphi_n = \varphi$ and $\lim_{n\to\infty} w(g)\varphi_n = \Psi$. Now $\pi(q,p)\varphi_n(x) = \varphi_{\pi n}(x) \in \mathcal{D}$ for each n and $\lim_{n\to\infty}(\pi(q,p)\varphi_n)(x) = \lim_{n\to\infty}\varphi_{\pi n}(x) = \pi(q,p)(\lim_{n\to\infty}\varphi_n)(x) = \varphi_\pi$ since $\pi(q,p)$ is unitary. As a sequence in $O_C(R^{2n})$, $\varphi_{\pi n}(q,p) \to \varphi_\pi(q,p)$ for each x. Therefore, from the continuity of $\hat{g}$, $\Psi = \lim_{n\to\infty}(w(g)\varphi_n)(x) = \lim_{n\to\infty}\langle \hat{g}, \varphi_{\pi n}\rangle = \langle \hat{g}, \lim_{n\to\infty}\varphi_{\pi n}\rangle = \langle \hat{g}, \varphi_\pi\rangle = w(g)\varphi$. Linearity is obvious and $w(g)\varphi \in \mathcal{D}$ by (5). |||

The results of Lemma 4.1 justify the following definition:

Definition 4.1: Let $g \in O_M(R^{2n}, \circ c)$. The linear operator $w(g)$ on $\mathcal{D}$ is called the Weyl transform of the distribution g. The map $W: g \to w(g)$ from $O_M(R^{2n}, \circ c)$ to A is called the Weyl correspondence.

The properties of the Weyl transform and the Weyl correspondence are given in the following theorem:

Theorem 4.1: Let $g \in O_M(R^{2n}, \circ c)$.

(1) $w(g)^* = w(\bar{g})$, where $*$ is the adjoint operator of $w(g)$ and $\bar{g}$ is the complex conjugate of g.

(2) The Weyl correspondence is an injection.

(3) Let $g_1, g_2 \in O_M(R^{2n}, \circ c)$. Then $w(g_1)w(g_2) = w(g_1 \circ c g_2)$ on $\mathcal{D}$ and $w(g_1 \circ c g_2) \in A$.

Proof of Theorem 4.1

(1) Since the domain of $w(\bar{g})$ is $\mathcal{D}$, we wish to show $(w(g)\varphi, \Psi) = (\varphi, w(g)^*\Psi) = (\varphi, w(\bar{g})\Psi)$ for all $\varphi, \Psi \in \mathcal{D}$. Using the fact that $g \in O_C'(R^{2n})$ has the property that for every $k \geq 0$ there is an integer $m = m(k)$ such that

$$\hat{g} = \sum_{|\alpha| \leq m} \partial^\alpha g_\alpha,$$

where g_α is a continuous function on R^{2n} such that

$$\lim_{|\xi|\to\infty}(1 + |\xi|^2)^{k/2}|g_\alpha(\xi)| = 0,$$

we have

$$(w(g)\varphi, \Psi) = (\langle \hat{g}(\xi), \varphi_\pi(\xi)\rangle, \Psi)$$
$$= \sum_{|\alpha|\leq m}(\langle \partial^\alpha g_\alpha, \varphi_\pi\rangle, \Psi) = (-1)^{|\alpha|}\sum_{|\alpha|\leq m}(\langle g_\alpha, \partial^\alpha \varphi_\pi\rangle, \Psi)$$
$$= (-1)^{|\alpha|}\sum_{|\alpha|\leq m}\iint g_\alpha(\xi)\partial_\xi^\alpha \varphi_\pi(\xi,x)\bar{\Psi}(x)\,d\xi\,dx$$
$$= (-1)^{|\alpha|}\sum_{|\alpha|\leq m}\int g_\alpha(\xi)(\varphi_\pi, \Psi)(\xi)\,d\xi$$
$$= \langle \hat{g}, (\varphi_\pi, \Psi)\rangle.$$

On the other hand,

$$(\varphi, w(\bar{g})\Psi) = \overline{(w(\bar{g})\Psi, \varphi)} = \overline{\langle \hat{\bar{g}}, (\Psi_\pi, \varphi)\rangle}$$
$$= \overline{\langle \hat{\bar{g}}(-\xi), (\Psi_\pi, \varphi)\rangle} = \langle \hat{g}(-\xi), \overline{(\Psi_\pi, \varphi)}\rangle,$$
$$= \langle \hat{g}(-\xi), (\varphi, \Psi_\pi)\rangle = \langle \hat{g}(-\xi), (\pi(-\xi)\varphi, \Psi)\rangle$$
$$= \langle \hat{g}, (\varphi_\pi, \Psi)\rangle.$$

(2) Suppose $g_1, g_2 \in O_M(R^{2n})$ and let $w(g_1)$, $w(g_2)$ be the Weyl transforms of g_1 and g_2 and

$$(w(g_1)\varphi)(x) = (w(g_2)\varphi)(x) \quad \text{for all } \varphi \in \mathcal{D}.$$

Then by definition,

$$\langle \hat{g}_1, \varphi_\pi\rangle = \langle \hat{g}_2, \varphi_\pi\rangle$$

or

$$\langle \widehat{g_1 - g_2}, \varphi_\pi\rangle = 0 \quad \text{for all } \varphi \in \mathcal{D} \text{ and } x \in R^n.$$

Since if $\varphi \neq 0$, $\varphi_\pi \neq 0$, we have $\widehat{g_1 - g_2} = 0$. This implies that $g_1 = g_2$, since the Fourier transform is an isomorphism.

(3) Let $\varphi \in \mathcal{D}$. Since $w(g_2)\varphi \in \mathcal{D}$, therefore $w(g_1)[w(g_2)\varphi] \in \mathcal{D}$.

Now $(w(g_2)\varphi)(x) = \langle \hat{g}_2, \varphi_\pi\rangle = \varphi_{\pi,g_2}(x)$ and

$$w(g_1)[w(g_2)\varphi] = \langle \hat{g}_1(q^1,p^1), \pi(q^1,p^1)\varphi_{\pi,g_2}(q,p)\rangle.$$

But

$$\pi(q^1,p^1)\langle \hat{g}_2, (\pi(q,p)\varphi)(x)\rangle$$
$$= \langle \hat{g}_2, [\pi(q^1,p^1)\pi(q,p)\varphi](x)\rangle$$
$$= \langle \hat{g}_2, \exp[ic(q^1\cdot p - p^1\circ q)/2]\pi(q^1+q, p^1+p)\varphi\rangle$$
$$= \langle \exp[ic(q^1\circ p - p^1\circ q)/2]\hat{g}_2, \pi(q^1+q, p^1+p)\varphi\rangle$$
$$= \langle (E_{(q^1,p^1)}\hat{g}_2)(q,p), \varphi_\pi(q^1+q, p^1+p)\rangle$$

where

$$E(q^1,p^1)(q,p)=\exp[ic(q^1\cdot p-p^1\circ q)/2].$$

Hence,

$$w(g_1)[w(g_2)\varphi]$$

$$=\langle\hat{g}_1(q^1,p^1),\langle(\widehat{E_{(q^1,p^1)}}\hat{g}_2)(q,p),\varphi_\pi(q^1+q,p^1+p)\rangle\rangle$$

$$=\langle\hat{g}_1*c\hat{g}_2,\varphi_\pi\rangle=\langle\widehat{g_1\circ cg_2},\varphi_\pi\rangle$$

$$=w(g_1\circ cg_2)\varphi \text{ for all } \varphi\in\mathcal{D}.$$

This shows that $w(g_1)w(g_2)=w(g_1\circ cg_2)$ on $\mathcal{D}$ and $w(g_1\circ cg_2)\varphi\in\mathcal{D}$. |||

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[1]G. Loupias and S. Miracle-Sole, Commun. Math. Phys. **2**, 31 (1966).
[2]D. Kastler, Commun. Math. Phys. **1**, 14 (1965).
[3]G. Loupias and S. Miracle-Sole, Ann. Inst. H. Poincaré **6**, 1 (1967).
[4]C.M. Edwards and J.I. Lewis, Commun. Math. Phys. **13**, 119 (1969).
[5]J. Pool, J. Math. Phys. **7**, 66 (1966).
[6]A. Grossmann, G. Loupias, and E.M. Stein, Ann. Inst. Fourier, Univ. Grenoble, **18**, 2 (1968).
[7]K.C. Liu, J. Math. Phys. **16**, 2054 (1975).
[8]J. Horváth, *Topological Vector Spaces and Distributions, Vol. I* (Addison-Wesley, Reading, Mass. 1966).
[9]L. Schwartz, *Théorie des distributions, Vols. I, II* (Hermann, Paris, 1957), 2nd ed.
[10]C.R. Putnam, *Commutation Properties of Hilbert Space Operators* (Springer, New York, 1967), Chap. IV.

Almost singular potentials*

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Explicit solutions are constructed for the lowest bound states of the Schrödinger equation with an attractive potential that behaves typically as $r^{-2+\epsilon}$ at the origin. The energy levels and wavefunctions, which depend on the small parameter ϵ in a nonanalytic way, show some interesting properties; and some relations between this model and aspects of elementary particle physics are noted.

REVIEW OF SINGULAR POTENTIALS

In the usual study of the Schrödinger equation, in a state of orbital angular momentum l (in units with $\hbar^2/2m=1$),

$$\left(-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{l(l+1)}{r^2}+V(r)-E\right)R_l(r)=0, \tag{1}$$

we have the boundary condition at the origin

$$R_l(r)\underset{r\to 0}{\to}\text{const}\times r^l. \tag{2}$$

In order to make this selection, and to discard the solution which behaves as r^{-l-1}, it is necessary to assume that

$$r^2V(r)\underset{r\to 0}{\to}0; \tag{3}$$

that is, that the kinetic energy term dominates the potential energy term as r goes to zero. If the potential should be more singular than $1/r^2$ at the origin, then we must investigate the equation more carefully: If this singular potential is repulsive, then we conclude that the correct solution to Eq. (1) does go to zero at the origin, but in some fashion different from (2), and we can proceed to do the usual sort of bound state and scattering calculations; however, if this singular potential is attractive at the origin, we are unable to make any sensible solution to the equation. This latter situation may be described by saying that the potential has an infinite number of bound states going down to $E=-\infty$.

The borderline case, which we will study in detail, involves the potential

$$V(r)\underset{r\to 0}{\to}-g/r^2. \tag{4}$$

If we put this into Eq. (1) and postulate the behavior

$$R_l(r)\underset{r\to 0}{\to}r^s, \tag{5}$$

we get the indicial equation

$$-s(s+1)+l(l+1)-g=0 \tag{6}$$

with the solutions

$$s^{\pm}=-\tfrac{1}{2}\pm[(l+1/2)^2-g]^{1/2}. \tag{7}$$

We see that there is a critical value of the coupling strength,

$$g^*=+(l+\tfrac{1}{2})^2, \tag{8}$$

such that if $g<g^*$, the root s^+ describes the allowed solution and the root s^- describes the improper solution—and everything is normal. However, if $g>g^*$, then then the two roots s are a pair of complex conjugate numbers

$$s^{\pm}=-\tfrac{1}{2}\pm i\sigma \tag{9}$$

and there is no apparent way to select the "good" from the "bad" solutions. This situation is frequently described by saying that we now have a continuous spectrum (instead of a discrete spectrum for bound states), due to the loss of our boundary condition at the origin. Some insight into what has happened can be gained by looking at the wavefunction;

$$\begin{aligned}R_l(r)&\sim a_+r^{-1/2+i\sigma}+a_-r^{-1/2-i\sigma}\\&\sim Ar^{-1/2}\sin(\sigma\ln r+\phi).\end{aligned} \tag{10}$$

As we trace this function down to $r=0$, starting from any finite value of r, we see that it has an infinite number of nodes; and its value at $r=0$ is not defined, although this wavefunction is still normalizeable in the usual sense. The number of nodes in the solution to Schrödinger's equation at any given energy E is the number of bound states that exist at energies below E; thus we see here that there must be an infinity of bound states below any value of E (the energy level spectrum is bottomless, as well as topless).

In an attempt to make some sense out of this situation, Case[1] applied the condition that two solutions of the Schrödinger equation, belonging to different energy eigenvalues, must be orthogonal. This is equivalent to requiring that the Hamiltonian must be a Hermitian operator, acting upon the proper wavefunctions. He thus derived the condition, for any two solutions R and R',

$$\lim_{r\to 0}r^2\left(R\frac{d}{dr}R'-R'\frac{d}{dr}R\right)=0. \tag{11}$$

With solutions of the form given by Eq. (10) this condition reads

$$AA'\sigma\sin(\phi-\phi')=0, \tag{12}$$

and this is satisfied by requiring the phase angle ϕ to be the same for all states. This gives a discrete bound state spectrum, but the number of bound states is still infinite; furthermore, there is no way to determine the phase angle ϕ.

By taking the complete potential to be $-g/r^2$, the Schrödinger equation can be exactly solved in terms of Bessel functions, and Case showed that the resulting energy level formula was

$$E = E_0 \exp(-2n\pi/\sigma), \tag{13}$$

where E_0 is a negative constant—depending on the angle ϕ and thus arbitrary—and the quantum number n is any positive or negative integer or zero. $\{E_0 = -2\exp[2(\phi - \theta)/\sigma]$, where θ is the phase of the gamma function of argument $1 - i\sigma\}$.

In addition to the infinity of bound states at energies approaching minus infinity ($n \to -\infty$), the $1/r$ potential also has an infinity of bound states as the energy approaches zero, from below ($n \to +\infty$). These are really two distinct phenomena: The first arises from the singular nature of the potential at short distances; the second arises from the very long tail of the potential at large distances (reminiscent of the Coulomb potential). Only the first situation—the short distance singularity—is of interest to us here; we shall imagine that the potentials we are interested in fall off faster at large distances so that there is a discrete cutoff to the bound states as the binding energy lessens.

Other attempts have been made to handle the difficulty at $r = 0$ [2] but all these methods are artificial, and we generally conclude that the potentials, singular as $1/r^2$, cannot be sensible if the strength exceeds the critical value g^*.

The situation of a marginally singular equation, such as the $1/r^2$ potential in the Schrödinger equation, will occur in any differential equation when the number of inverse powers of coordinate in the differential operator is equalled by the number of inverse powers of the coordinate in the potential. Thus this situation can be found in the Dirac equation with a Coulomb potential, in the Klein—Gordon equation with a Coulomb potential,[1] and in several models of the Bethe—Salpeter equation.[3,4]

It is sometimes said that there is a correspondence between marginally singular equations and renormalizable field theories. It is not clear precisely what is meant by this statement, but the analogy is probably that, as was shown by Case's work, the divergence difficulties in this marginally singular case can be summarized in a single parameter.

ALMOST SINGULAR POTENTIALS

In this paper we will study a Schrödinger equation model in which the potential is mathematically rigged so as to be not singular, but with a small parameter which will allow us to approach as a limit the marginally singular situation. Two explicit forms for this are

$$\text{Model I:}\quad V = \frac{-g}{r^2}\left(\frac{r}{r_0}\right)^{\epsilon}, \tag{14}$$

$$\text{Model II:}\quad V = \frac{-g}{r^2}\left[1 + \epsilon \ln\left(\frac{r}{r_0}\right)\right], \tag{15}$$

$$\epsilon \to 0+ .$$

No standard perturbation theory (expansion in power series in ϵ) will work here because of the singular nature of the perturbing operators. Expressed another way, the resulting formulas will not be analytic functions about $\epsilon = 0$, and it is just from this nonanalytic behavior that some of the most interesting features of this model flow.

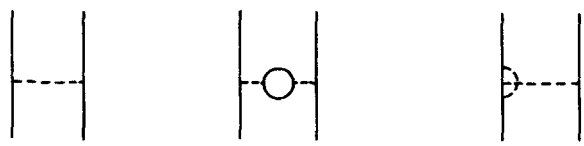
The motivation for studying these models actually is based on more than just a mathematical game. According to quantum field theory, potentials arise from the exchange of virtual quanta. Thus, the exchange of a spin zero quantum of mass μ is described by the propagator

$$1/(q^2 - \mu^2 + i\epsilon), \tag{16}$$

where q is the 4-vector momentum transfer. Making the Fourier transform to coordinate space, we get a potential which behaves like $\exp(-\mu R)$ for large R (R is the space—time distance between the two interacting particles), and behaves like $1/R^2$ for small distances.

If one performs a time average on this relativistic potential, the result is the familiar Yukawa potential $\exp(-\mu r)/r$. Letting μ become zero, one has the familiar Coulomb potential. Since we are chiefly interested in behavior at small distances in coordinate space, we want to concentrate on the large q behavior in momentum space.

The single-quantum exchange is only the lowest order field theory approximation to the complete interaction of particles. The following are two familiar diagrams from quantum electrodynamics, carried to a higher order of approximation:



The first diagram, single photon exchange, gives the momentum space potential $\sim 1/q^2$. The second diagram is a vacuum polarization correction and the third is a vertex correction. These contributions to the interaction have been calculated, and, if one looks at the high q behavior of the well known results,[5] they give correction factors to the single photon exchange of

$$\left[1 + \frac{\alpha}{3\pi}\ln\left(\frac{-q^2}{m^2}\right)\right] \quad \text{and} \quad \left[1 - \frac{\alpha}{\pi}\ln\frac{m}{\lambda}\ln\left(\frac{-q^2}{m^2}\right)\right] \text{ resp.} \tag{17}$$

Looking at the Fourier transforms of these functions, we see that the improved field theory potential behaves at small distances as

$$V \sim \frac{\text{const}}{R^2} + \text{const}' \times \frac{\ln R}{R^2}, \tag{18}$$

which is like our Model II, Eq. (15). Another convenient field theory model is fixed source meson theory. Here one calculates the time independent potential between two sources by usual Schrödinger perturbation theory methods. In second order one gets the usual Yukawa potential, behaving like $1/r$ at small r. In fourth order one finds terms which behave like $(\ln r)/r$; and in sixth order we have found terms that behave like $(\ln r)^2/r$. (If one has purely scalar coupling in this fixed source model, then all these more exotic potential terms cancel out and the pure Yukawa formula is exact. However, with inclusion of spin and/or isotropic spin couplings, then, these new potential terms do survive.)

It is an interesting question to ask what the exact small distance behavior of the complete (i.e., all orders of perturbation theory) field theoretic potential looks like, and we have no idea what the correct answer is. Our Model I potential (14) may be looked upon as a guess, taken as alternative to the perturbation theory guess of Model II, (15).

SOLUTION OF MODEL I

We will solve for the lowest bound states of Eq. (1) with the potential (14). With the change of variables,

$$r=y^{2/\epsilon}/2\sqrt{-E},\quad R_l=y^{-(1/\epsilon+1/2)}u, \tag{19}$$

the differential equation becomes

$$\left(-\frac{d^2}{dy^2}+\frac{\{[(2l+1)/\epsilon]^2-\frac{1}{4}\}}{y^2}+\frac{1}{\epsilon^2}\,y^{4/\epsilon-2}\right)u=\Lambda u, \tag{20}$$

where

$$\Lambda=(4g/\epsilon^2)(2r_0\sqrt{-E})^{-\epsilon}. \tag{21}$$

[For $\epsilon=1$ this is the transformation that reduces the hydrogen atom to a harmonic oscillator.] This looks like a normal Schrödinger equation, having a very large angular momentum; the effective potential $(1/\epsilon^2)y^{4/\epsilon-2}$ has the following behavior in the limit $\epsilon\to 0$: For $y<1$ this term vanishes, and for $y>1$ this term becomes positive infinite. Thus we interpret this like an infinite potential barrier and replace it with the familiar boundary condition

$$u(y=1)=0. \tag{22}$$

The remainder of the equation is solved in terms of Bessel functions; the boundary condition at $y=0$ is that u must vanish; and so we get the resulting eigenvalue condition:

$$J_\nu(Z_n)=0, \tag{23}$$

where

$$\nu=(2l+1)/\epsilon \quad\text{and}\quad Z_n=\Lambda^{1/2}. \tag{24}$$

From Jahnke and Emde[6] we have the following formula for the zeroes of Bessel functions of very large order:

$$Z_n=\nu+C_n\nu^{1/3}+D_n\nu^{-1/3}+O(\nu^{-1}) \tag{25}$$

n	C_n	D_n
1	1.8558	1.0332
2	3.2447	3.1584
3	4.3817	5.7598

Putting these results together, we have the energy eigenvalue formula (for $\epsilon\to 0$)

$$E_n=-\frac{1}{4r_0^{\,2}}\exp\left(\frac{2}{\epsilon}\ln\frac{g}{(l+1/2)^2}\right)\exp\left(-\frac{4C_n}{\epsilon^{1/3}(2l+1)^{2/3}}\right). \tag{26}$$

We see that this formula becomes very singular in the limit of $\epsilon=0$. The first exponential factor, which is the same for all states, establishes the very large numerical *scale* of the eigenvalues. (Note that if g were less than $g^*=(l+\frac{1}{2})^2$, then the sign in this exponent would change and the limit would be $E=0$ instead of $E=-\infty$.)

The second exponential factor gives us the *structure* of the eigenvalue spectrum. This factor also is singular in the limit of $\epsilon=0$ but not as strongly as the leading factor. The rather bizarre dependence—$\exp(1/\epsilon^{1/3})$—could hardly have been anticipated. Thus we find that not only the depth of the lowest eigenvalues, but their ratios as well are governed by very large pure numbers produced by the mathematics of this problem. Thus, for $l=0$,

$$E_2/E_1=\exp(-5.6/\epsilon^{1/3}). \tag{27}$$

SOLUTION OF MODEL II

Now we shall solve for the lowest bound states of Eq. (1) with the potential (15). Here we start with the transformations

$$R_l=r^{-1/2}u,\quad r=xr_1,\quad E=-\lambda/r_1^{\,2}, \tag{28}$$

where

$$r_1=r_0\exp\{-(1/g\epsilon)][g-(l+1/2)^2]\} \tag{29}$$

to get the equation

$$\left(\frac{d^2}{dx}+\frac{1}{x}\frac{d}{dx}+g\epsilon\frac{\ln x}{x^2}-\lambda\right)u=0. \tag{30}$$

Next we write

$$x=\exp[\eta/(g\epsilon)^{1/3}],\quad \lambda=\exp[-2\mu/(g\epsilon)^{1/3}] \tag{31}$$

to get

$$\left(\frac{d^2}{d\eta^2}+\eta-(g\epsilon)^{-2/3}\exp[2(\eta-\mu)/(g\epsilon)^{1/3}]\right)u=0. \tag{32}$$

This is looked upon similarly to Eq. (20) in that the last term behaves, in the limit of $\epsilon\to 0$, like an infinite potential barrier at $\eta=\mu$. Therefore, we need only solve the equation

$$\left(\frac{d^2}{d\eta^2}+\eta\right)v(\eta)=0 \tag{33}$$

with the boundary conditions

$$v(-\infty)=0,\quad v(\eta=\mu_n)=0, \tag{34}$$

to get our eigenvalues

$$E_n=-\frac{1}{r_0^{\,2}}\exp\left(\frac{2}{g\epsilon}[g-(l+\tfrac{1}{2})^2]-\frac{2\mu_n}{(g\epsilon)^{1/3}}\right) \tag{35}$$

Equation (33) may be solved in terms of Bessel functions; with the required boundary condition at $\eta\to-\infty$ ($r=0$), we find

$$v=A\eta^{1/2}[J_{1/3}(\tfrac{2}{3}\eta^{3/2})+J_{-1/3}(\tfrac{2}{3}\eta^{3/2})]. \tag{36}$$

Thus the values μ_n are just the zeroes of this tabulated function. Actually, if one looks at the derivation of the earlier quoted formula (25) for the zeroes of Bessel functions of large order,[7] it is found that the exponential transformation (31) is involved, leading to the same Eq. (33) that we are now studying. The resulting identification is

$$\mu_n=2^{1/3}C_n \tag{37}$$

in terms of the coefficients given earlier. The energy formulas for the two models are quite similar in structure.

SOLUTION OF A GENERALIZED MODEL

The similarity in results of these two models suggest that we try to solve the generalized almost singular potential,

$$V=-(g/r^2)f(r), \tag{38}$$

where the modifying factor f is very close to unity, except at very small distances. With the transformation $R=r^{-1/2}u$ we write

$$\left(-\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}+U-E\right)u=0, \tag{39}$$

where

$$U=[(l+1/2)^2-gf(r)]/r^2. \tag{40}$$

We assume that $g>g^*$ and also that f is such as to make the potential less attractive at very small distances. Thus U is positive at small r and negative at large r. We identify the point where U passes through zero as r_1, and then we write

$$U(r_1)=0, \quad r=r_1e^{\theta}, \quad E=-\frac{1}{r_1^2}\exp(-2\lambda), \tag{41}$$

$$\left(\frac{d^2}{d\theta^2}+W(\theta)-\exp[2(\theta-\lambda)]\right)u=0, \tag{42}$$

where

$$W=-r^2U=-(l+\tfrac{1}{2})^2+gf(r_1e^{\theta}). \tag{43}$$

Now we expand about $\theta=0$, where U, and therefore W, vanishes:

$$W=\alpha\theta+O(\alpha^2\theta^2). \tag{44}$$

The parameter α is assumed to be very small, as in our previous models it is proportional to ϵ. One more variable change

$$\theta=\eta\alpha^{-1/3}, \quad \lambda=\mu\alpha^{-1/3} \tag{45}$$

and we have

$$\left[\frac{d^2}{d\eta^2}+\eta+O(\alpha^{2/3}\eta^2)-\alpha^{-2/3}\exp\left(\frac{2(\eta-\mu)}{\alpha^{1/3}}\right)\right]u=0, \tag{46}$$

and so in the limit of $\alpha\to 0$ we have the earlier solution (33), (34).

We can actually do a little bit better by watching more closely what happens around the point $\eta=\mu$, that is, at

$$r=r_1\exp(\mu/\alpha^{1/3})\equiv r_2. \tag{47}$$

By matching solutions of the equation approaching this barrier from both sides we pick up one more correction term to the energy, and our final formula is

$$E_n=-\frac{1}{r_1^2}\exp\left(-\frac{2^{4/3}C_n}{\alpha^{1/3}}+2(\ln 2-C)\right), \tag{48}$$

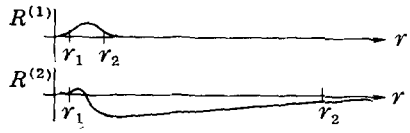
where C is Euler's constant. This formula reproduces the two earlier results as special cases—except for the last factor, which was lacking before.

DESCRIPTION OF THE WAVEFUNCTIONS

The several transformations of variables may obscure the picture of what the eigenfunctions for these deeply bound states look like. The wavefunction goes to zero at the origin and has its first turning point at the very small distance r_1. Then it may oscillate; finally it has its second turning point at r_2 – which is still a very small distance compared to the basic unit of length, r_0, but is a rather large distance compared to r_1 (see (47)). Furthermore the distance r_2 will be very strongly dependent on the quantum number n, for example

$$r_2(\text{for } n=2)/r_2(\text{for } n=1)=\exp(\mu_2-\mu_1)/\alpha^{1/3}$$

We also note that the tail of the function decays with length r_2. Pictures of the functions will look as follows:



The functions are, of course, orthogonal to one another; but there is a more interesting property contained here. If one should have some reasonably smooth operator (such as a dipole length) and calculate its matrix element between these two states, the result will be a small number—depending on the ratio of the distances r_2—due to the great disparity in the spatial extent of the two wavefunctions.

Thus a transition rate between the nth state and the mth state (m less than n) would be characterized by the small number:

$$G^2=\left[\frac{r_2^{(m)}}{r_2^{(n)}}\right]^3 \xrightarrow{m=1,n=2} \exp\left(\frac{-5.25}{\alpha^{1/3}}\right),$$

$$\alpha=10^{-1}, \quad G^2\approx 10^{-5}$$

$$\alpha=10^{-2}, \quad G^2\approx 10^{-11},$$

$$\alpha=10^{-3}, \quad G^2\approx 10^{-23}.$$

CONCLUSIONS

This study of almost singular potentials in the Schrödinger equation has led to some interesting results and suggests some interesting ideas for future study. The small parameter built into the model (called ϵ or α) allows us to construct solutions without introducing a cutoff or similar device; the answers can be expanded for small values of this parameter, although it is not a power series expansion. The resulting energy level spectrum is characterized by very large numbers—resulting from an exponentiation of the small parameter originally introduced—and the same is found for the overlap of the wavefunctions that would occur in any calculation of transition probabilities under some external interaction. These general features are characteristic of the basic properties of elementary particles: large ratios of masses (as between baryons and leptons) and severe heirarchy of interactions (strong, weak).

A next step should be to explore the behavior of almost singular potentials in the context of some relativistic equations, rather than the Schrödinger equation. One immediate problem will be the following: in the above study the energy E took on very large negative values;

in relativistic calculations (for example, in the Klein–Gordon equation) the analogous role is played by the quantity $E^2 - m^2$ and one does not know what to say about states with negative values of E^2.

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[1]K. M. Case, Phys. Rev. 80, 797 (1950).
[2]See the review article by W. F. Frank, D. J. Land, and R. M. Spector, Rev. Mod. Phys. 43, 36 (1971).
[3]J. S. Goldstein, Phys. Rev. 91, 1516 (1953).
[4]A. Bastai, *et al.*, Nuovo Cimento 30, 1512 (1963).
[5]See, for example, J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964), pp. 159 and 171.
[6]E. Jahnke and F. Emde, *Tables of Functions* (Dover, New York, 1945), 4th ed., p. 143.
[7]G. N. Watson, *Theory of Bessel Functions* (Cambridge U. P., Cambridge, 1962), 2nd ed., p. 518.

On the structure of simple pseudo Lie algebras and their invariant bilinear forms

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By definition simple pseudo Lie algebras do not contain any nontrivial ideal. We show that "graded simplicity" implies "simplicity" and discuss the uniqueness of invariant bilinear forms on a simple pseudo Lie algebra. A lot of examples of simple pseudo Lie algebras is given together with their invariant bilinear forms. Under certain general assumptions we derive that the Lie algebra $\mathfrak{g}$ contained in a simple pseudo Lie algebra $\mathfrak{a}$ is reductive. Assuming that $\mathfrak{g}$ is reductive, we prove that the "adjoint representation of $\mathfrak{g}$ in the odd subspace of $\mathfrak{a}$" is completely reducible with at most two irreducible components. Finally we show that the pseudo Lie algebras with nondegenerate "generalized Killing form" are direct products of simple pseudo Lie algebras.

1. INTRODUCTION

Recently there has been a remarkable interest in pseudo Lie algebras (or, as they are also called, graded Lie algebras,[1] both in the physical and in the mathematical literature. There is no need to establish a list of references since this has been done to a considerable extent in a recent article by Corwin, Ne'eman, and Sternberg.[2]

Despite of the interest in these algebras the literature devoted to a systematic study of the structure of pseudo Lie algebras seems to be rather limited (at least to the knowledge of the authors).

It can be shown[3] that many of the elementary constructions with Lie algebras and especially with their representations and their universal enveloping algebras (for example tensor products of representations, representations in spaces of linear mappings, representations on spaces of multilinear forms, ..., and the theorem of Poincaré, Birkhoff, and Witt) can be adapted rather directly to pseudo Lie algebras. Nevertheless there are sufficiently many examples which show that the theory of pseudo Lie algebras is not merely a transcription of the theory of Lie algebras.

To get some insight into the structure of pseudo Lie algebras we have decided to study the class of simple pseudo Lie algebras, with the hope that—as in the case of Lie algebras—the assumption of simplicity might be strong enough to enable a lucid theory.

Our paper is arranged as follows. In the next section we introduce our notational conventions and give some definitions concerning the representations of pseudo Lie algebras. Section 3 contains some elementary properties of simple pseudo Lie algebras. We show that "graded simplicity" implies "simplicity" and discuss the uniqueness of invariant bilinear forms on a simple pseudo Lie algebra over an algebraically closed field. Section 4 contains a lot of examples of simple pseudo Lie algebras and their invariant bilinear forms. These algebras are to some extent analogous to the classical simple Lie algebras. We hope that this stack of examples might be sufficiently rich to lead to realistic hypotheses concerning the general structure of simple pseudo Lie algebras.

For any pseudo Lie algebra $\mathfrak{a}$ the even subspace $\mathfrak{g}$ of $\mathfrak{a}$ (which is an ordinary Lie algebra) has a natural representation in the odd subspace $\mathfrak{u}$ of $\mathfrak{a}$. In Sec. 5 we prove (partly under certain additional assumptions) that this representation is completely reducible with at most two irreducible components. Presumably, our results constitute a reasonable starting-point for a classification of simple pseudo Lie algebras (over an algebraically closed field). This is explained in Sec. 6.

We do not try to give a definition of semisimple pseudo Lie algebras. Presumably any simple pseudo Lie algebra should be semisimple. Therefore we prefer to wait until our knowledge of simple pseudo Lie algebras has been improved. In any case the pseudo Lie algebras with nondegenerate "generalized Killing form" are to be considered as semisimple, for we prove in Sec. 7 that these algebras are direct products of simple pseudo Lie algebras.

2. PRELIMINARY REMARKS AND NOTATIONAL CONVENTIONS

Pseudo Lie algebras are a special type of graded (nonassociative) algebras, whose multiplication behaves partly as a commutator and partly as an anticommutator.

(a) In order to be able to give a precise definition (see also Ref. 2) we have to remind the reader of the concepts of graded vector spaces[4] and graded algebras.[5] In this paper we shall be concerned only with gradings with values in the additive two element group $Z_2 = Z/2Z$. Correspondingly, a vector space V will be called graded, if for each of the two elements 0 and 1 of Z_2 there is given a subspace V_0 resp. V_1 of V such that V is the direct sum of V_0 and V_1,

$$V = V_0 \oplus V_1. \tag{2.1}$$

The elements of V_0 (resp. V_1) are called even (resp. odd). An element X of V is called homogeneous if it is even or odd, i.e., if $X \in V_0 \cup V_1$.

(b) The grading of V may be described by the linear map

$$\gamma_V : V \to V \tag{2.2a}$$

defined by

$$\gamma_V(X+Y)=X-Y \text{ if } X\in V_0,\ Y\in V_1. \tag{2.2b}$$

We call γ_V the grading automorphism of V.

For any $Z\in V$ the elements $\frac{1}{2}[Z+\gamma_V(Z)]$ resp. $\frac{1}{2}[Z-\gamma_V(Z)]$ are the uniquely determined elements $Z_0\in V_0$ resp. $Z_1\in V_1$ such that $Z=Z_0+Z_1$. They are called the even resp. odd component of Z.

(c) A subspace U of V is called graded if

$$U=(U\cap V_0)+(U\cap V_1), \tag{2.3}$$

i.e., if for every element $Z\in U$ its even and odd components belong to U, i.e., if $\gamma_V(U)\subset U$.

(d) If $V=V_0\oplus V_1$ and $V'=V_0'\oplus V_1'$ are two graded vector spaces then there is a natural procedure to define a grading of the tensor product $V\otimes V'$, of the vector space $\mathcal{L}(V,V')$ of linear mappings from V into V', of the vector space $\mathcal{B}(V,V')$ of bilinear forms on $V\times V'$, $\cdots$. In fact if $\mathcal{L}_0(V,V')$ [resp. $\mathcal{L}_1(V,V')$] denotes the subspace of even (resp. odd) linear mappings, then

$$\begin{aligned}\mathcal{L}_0(V,V')&=\{g\in\mathcal{L}(V,V')\,|\,g(V_0)\subset V_0',\ g(V_1)\subset V_1'\},\\ \mathcal{L}_1(V,V')&=\{g\in\mathcal{L}(V,V')\,|\,g(V_0)\subset V_1',\ g(V_1)\subset V_0'\},\end{aligned} \tag{2.4}$$

and if $\mathcal{B}_0(V,V')$ [resp. $\mathcal{B}_1(V,V')$] denotes the subspace of even (resp. odd) bilinear forms, then

$$\begin{aligned}&\mathcal{B}_0(V,V')\\ &=\{\phi\in\mathcal{B}(V,V')\,|\,\phi(V_0\times V_1')=\phi(V_1\times V_0')=\{0\}\}\\ &\mathcal{B}_1(V,V')\\ &=\{\phi\in\mathcal{B}(V,V')\,|\,\phi(V_0\times V_0')=\phi(V_1\times V_1')=\{0\}\}.\end{aligned} \tag{2.5}$$

(e) An algebra L is called graded if it is graded as a vector space

$$L=L_0\oplus L_1 \tag{2.6}$$

and if the usual rules for the "multiplication of even and odd elements" are satisfied, i.e., if

$$L_\alpha L_\beta\subset L_{\alpha+\beta},\quad \alpha,\beta\in Z_2. \tag{2.7}$$

A homomorphism of a graded algebra L into a graded algebra L' is by convention always even (as a linear map).

It is easy to check that the grading automorphism γ $(=\gamma_L)$ of L is in fact an automorphism of the algebra L, i.e.,

$$\gamma(AB)=\gamma(A)\gamma(B) \text{ if } A,B\in L. \tag{2.8}$$

(f) To give a concise definition of a pseudo Lie algebra we need the concept of a commutation factor.[6] This is (in the present paper) the map

$$\epsilon: Z_2\times Z_2\to Z \tag{2.9a}$$

defined by

$$\epsilon(\alpha,\beta)=(-1)^{\alpha\beta},\quad \alpha,\beta\in Z_2. \tag{2.9b}$$

(g) A pseudo Lie algebra is then a graded (nonassociative) algebra $L=L_0\oplus L$, whose multiplication (denoted by a bracket $\langle\ ,\ \rangle$) obeys the following identities:

$$\langle A,B\rangle=-\epsilon(\alpha,\beta)\langle B,A\rangle, \tag{2.10}$$

$$\langle\langle A,B\rangle,C\rangle=\langle A,\langle B,C\rangle\rangle-\epsilon(\alpha,\beta)\langle B,\langle A,C\rangle\rangle \tag{2.11}$$

(generalized Jacobi identity),

if $A\in L_\alpha$, $B\in L_\beta$, $C\in L$, $\alpha,\beta\in Z_2$.

Observe that L_0 (with the multiplication inherited from L) is an ordinary Lie algebra.

We shall always assume that $L_1\neq\{0\}$.

(h) An important class of examples of pseudo Lie algebras is the following. Choose any graded vector space $V=V_0\oplus V_1$. Then the associative algebra $\mathcal{L}(V)$ of linear mappings of V into itself is also graded. Define a bracket operation on $\mathcal{L}(V)$ by

$$\langle A,B\rangle=AB-\epsilon(\alpha,\beta)BA, \tag{2.12}$$

if $A\in\mathcal{L}_\alpha(V)$, $B\in\mathcal{L}_\beta(V)$, $\alpha,\beta\in Z_2$. Then the vector space $\mathcal{L}(V)$ equipped with this multiplication is a pseudo Lie algebra which we shall denote by $\mathrm{pl}(V)$ and which plays much the same role in the theory of pseudo Lie algebras as $\mathfrak{gl}(V)$ does in the theory of ordinary Lie algebras.

(j) Suppose L is a pseudo Lie algebra and V is a graded vector space. A graded representation of L in V is by definition a homomorphism of L into $\mathrm{pl}(V)$, normally denoted by

$$A\to A_V,\quad A\in L. \tag{2.13}$$

It is obvious from (2.11) that the map

$$\mathrm{ad}_L: L\to\mathrm{pl}(L) \tag{2.14a}$$

defined by

$$\mathrm{ad}_L(A)(B)=\langle A,B\rangle \tag{2.14b}$$

is a graded representation of the pseudo Lie algebra L in the graded vector space L, called the adjoint representation of L.

(k) The restriction of ad_L to L_0 is a representation of the Lie algebra L_0 in L, therefore we can speak of L_0-invariant (L_0-irreducible, $\cdots$) subspaces of L. If V is an L_0-invariant subspace of L, then the representation of L_0 in V induced by ad_L will be called the adjoint representation of L_0 in V.

The Jacobi identity (2.11) shows that multiplication is an L_0-invariant bilinear map of $L\times L$ into L. Hence if U and V are two L_0-invariant subspaces of L, then $\langle U,V\rangle$ is L_0-invariant, too. (Recall that according to common usage, $\langle U,V\rangle$ denotes the subspace of L generated by all elements of the form $\langle A,B\rangle$, $A\in U$, $B\in V$.

(l) Suppose we are given two graded representations of L in two graded vector spaces V and V', respectively. Then there are natural definitions[3] of graded representations of L in $V\otimes V'$, $\mathcal{L}(V,V')$, $\mathcal{B}(V,V')$, $\cdots$. In the second case one defines

$$(A\mathcal{L}g)=A_{V'}\circ g-\epsilon(\alpha,\gamma)g\circ A_V \tag{2.15}$$

if $A\in L_\alpha$, $g\in\mathcal{L}_\gamma$, $\alpha,\gamma\in Z_2$, and in the third case

$$\begin{aligned}(A\mathcal{B}\phi)(X,Y)=&-\epsilon(\alpha,\psi)\phi(A_VX,Y)\\ &-\epsilon(\alpha,\psi+\xi)\phi(X,A_{V'}Y)\end{aligned} \tag{2.16}$$

if $A\in L_\alpha$, $\phi\in\mathcal{B}_\psi$, $X\in V_\xi$, $Y\in V'$, $\alpha,\psi,\xi\in Z_2$.

(m) Given a graded representation of a pseudo Lie

algebra L in a graded vector space V, an element $X \in V$ is called invariant (with respect to this representation) if

$$A_V X = 0 \quad \text{for all } A \in L. \tag{2.17}$$

If X is invariant then its even and odd component are invariant, too.

(n) It is now natural to look for invariant bilinear forms on L, and especially to ask: Suppose we are given a graded representation of a pseudo Lie algebra L in a finite dimensional graded vector space V. Can we associate with this representation an invariant bilinear form on L (just as in the case of Lie algebras)?

This can in fact be done,[3] for if γ_V is the grading automorphism of V, then the bilinear form ϕ_V on L defined by

$$\phi_V(A,B) = \mathrm{tr}(\gamma_V A_V B_V), \quad A, B \in L \tag{2.18}$$

is invariant. Note that ϕ_V is even and that

$$\phi_V(A,B) = \epsilon(\alpha,\beta)\,\phi_V(B,A) \tag{2.19}$$

if $A \in L_\alpha$, $B \in L_\beta$, $\alpha, \beta \in Z_2$.

If L is finite dimensional we can consider the adjoint representation of L and obtain an even invariant bilinear form ϕ on L which we call the Killing form of L. (This form has been found independently by Pais and Rittenberg.[7])

We remark that the procedure above also works in the case of higher multilinear forms and that it is easy to find the corresponding invariants in the universal enveloping algebra of L, provided there is an even non-degenerate invariant bilinear form on L.

(p) After these general remarks it is useful (to avoid indices) to modify the notation for pseudo Lie algebras. In the following a pseudo Lie algebra will normally be called $\mathfrak{a}$ and the even (resp. odd) subspace of $\mathfrak{a}$ will be denoted by $\mathfrak{g}$ (resp. $\breve{\mathfrak{u}}$),

$$\mathfrak{a} = \mathfrak{g} \oplus \breve{\mathfrak{u}}, \quad \breve{\mathfrak{u}} \neq \{0\}. \tag{2.20}$$

Then $\mathfrak{g}$ is an ordinary Lie algebra.

From now on all vector spaces and algebras are supposed to be finite dimensional over a field K of characteristic zero.

3. DEFINITION AND ELEMENTARY PROPERTIES OF SIMPLE PSEUDO LIE ALGEBRAS

Apart from minor modifications an algebra L is called simple if it does not contain any nontrivial (i.e., different from $\{0\}$ and L) ideal. In the case of graded algebras one can also restrict the attention to the graded ideals [see Sec. 2. (c)] of the algebra; then the concept of graded simplicity emerges. For pseudo Lie algebras there is no difference between these two standpoints, because we have the following proposition.

Proposition 1: Suppose that $\mathfrak{a} = \mathfrak{g} \oplus \breve{\mathfrak{u}}$ is a pseuso Lie algebra without nontrivial graded ideals. Then $\mathfrak{a}$ does not contain any nontrivial left or right ideal.

Proof: We remark that any graded left (or right) ideal of a pseudo Lie algebra is in fact a two sided ideal. Suppose now that $\mathfrak{f}$ is a left ideal of $\mathfrak{a}$, different from $\{0\}$ and $\mathfrak{a}$. If γ is the grading automorphism of $\mathfrak{a}$ [see Sec. 2. (b), (e)], then $\gamma(\mathfrak{f})$ is a left ideal, too; therefore $\mathfrak{f} + \gamma(\mathfrak{f})$ and $\mathfrak{f} \cap \gamma(\mathfrak{f})$ are graded left (hence two sided) ideals of $\mathfrak{a}$, and consequently

$$\mathfrak{f} + \gamma(\mathfrak{f}) = \mathfrak{a}, \quad \mathfrak{f} \cap \gamma(\mathfrak{f}) = \{0\}. \tag{3.1}$$

Then, clearly,

$$\begin{aligned} \mathfrak{g} &= \{H + \gamma(H) \,|\, H \in \mathfrak{f}\}, \\ \breve{\mathfrak{u}} &= \{H - \gamma(H) \,|\, H \in \mathfrak{f}\}. \end{aligned} \tag{3.2}$$

Now we define a linear map

$$\tau : \mathfrak{a} \to \mathfrak{a} \tag{3.3a}$$

$$\text{by } \tau(H) = H, \quad \tau(\gamma(H)) = -\gamma(H) \text{ if } H \in \mathfrak{f}. \tag{3.3b}$$

Then

$$\tau^2 = \mathrm{id} \tag{3.4}$$

(hence τ is bijective) and

$$\tau(\mathfrak{g}) = \breve{\mathfrak{u}}, \quad \tau(\breve{\mathfrak{u}}) = \mathfrak{g}. \tag{3.5}$$

Finally [since $\mathfrak{f}$ and $\gamma(\mathfrak{f})$ are left ideals] it is easy to check that τ commutes with the adjoint representation of $\mathfrak{a}$, that is

$$\tau(\langle A, B\rangle) = \langle A, \tau(B)\rangle, \quad A, B \in \mathfrak{a}. \tag{3.6}$$

But a map τ with these properties cannot exist. In fact, if $X, Y \in \mathfrak{g}$, then

$$\begin{aligned} \langle \tau(X), \tau(Y)\rangle &= \tau(\langle \tau(X), Y\rangle) = -\tau(\langle Y, \tau(X)\rangle) \\ &= -\tau^2\langle Y, X\rangle = \langle X, Y\rangle. \end{aligned} \tag{3.7}$$

This equation yields

$$\langle X, Y\rangle = 0 \tag{3.8}$$

if $X, Y \in \mathfrak{a}$ are both even or both odd. If one of the elements $X, Y \in \mathfrak{a}$ is even and the other is odd, then X and $\tau(Y)$ have the same degree and therefore

$$\tau(\langle X, Y\rangle) = \langle X, \tau(Y)\rangle = 0, \tag{3.9}$$

hence $\langle X, Y\rangle = 0$ in this case, too. This means

$$\langle \mathfrak{a}, \mathfrak{a}\rangle = \{0\}. \tag{3.10}$$

But then $\mathfrak{g}$ and $\breve{\mathfrak{u}}$ are graded ideals in $\mathfrak{a}$ and it follows at once that $\mathfrak{g} = \breve{\mathfrak{u}} = \{0\}$, contrary to the assumption that $\mathfrak{f}$ is different from $\{0\}$. The case of right ideals is treated similarly, or one can use the fact that the graded vector space $\mathfrak{a}$ equipped with the (opposed) multiplication $(A, B) \to \langle B, A\rangle$ is a pseudo Lie algebra, too. Thus we can give the following definition.

Definition: A pseudo Lie algebra $\mathfrak{a}$ is called simple if it does not contain any nontrivial ideal, and if $\langle \mathfrak{a}, \mathfrak{a}\rangle \neq \{0\}$.

The last condition serves to eliminate the trivial one-dimensional pseudo Lie algebra. The definition yields at once the following lemma.

Lemma 1: Let $\mathfrak{a} = \mathfrak{g} \oplus \breve{\mathfrak{u}}$ be a simple pseudo Lie algebra (recall that we suppose $\breve{\mathfrak{u}} \neq \{0\}$). Then:

(α) $\langle \breve{\mathfrak{u}}, \breve{\mathfrak{u}}\rangle = \mathfrak{g}$;

(β) $\langle \mathfrak{g}, \breve{\mathfrak{u}}\rangle = \breve{\mathfrak{u}}$;

(γ) the adjoint representation $\mathrm{ad}_{\mathfrak{u}}$ of $\mathfrak{g}$ in $\mathfrak{u}$ [see Sec. 2. (k)] is faithful;

(δ) if ϕ is a homogeneous (i.e., even odd) invariant bilinear form [see Sec. 2. (l),(m)] on , then either $\phi = 0$ or ϕ is nondegenerate;

(ϵ) If γ is the grading automorphism of $\mathfrak{a}$, then

$$\mathrm{tr}(\gamma\, \mathrm{ad}_{\mathfrak{a}} X) = 0 \quad \text{for all } X \in \mathfrak{g}.$$

In fact, for any pseudo Lie algebra $\mathfrak{a} = \mathfrak{g} \oplus \mathfrak{u}$ and any homogeneous invariant bilinear form ϕ on $\mathfrak{a}$, the following four sets are (graded) ideals of $\mathfrak{a}$:

$$\mathfrak{f}_\alpha = \langle \mathfrak{u}, \mathfrak{u} \rangle \oplus \mathfrak{u}, \quad \mathfrak{f}_\beta = \mathfrak{g} \oplus \langle \mathfrak{g}, \mathfrak{u} \rangle,$$
$$\mathfrak{f}_\gamma = \{A \in \mathfrak{g} \mid \langle A, B \rangle = 0 \text{ for all } B \in \mathfrak{u}\}, \tag{3.11}$$
$$\mathfrak{f}_\delta = \{A \in \mathfrak{a} \mid \phi(B, A) = 0 \text{ for all } B \in \mathfrak{a}\}.$$

Finally, if $A, B \in \mathfrak{u}$, then

$$\mathrm{tr}[\gamma\, \mathrm{ad}(\langle A, B \rangle)]$$
$$= \mathrm{tr}[\gamma(\mathrm{ad}A)(\mathrm{ad}B)] + \mathrm{tr}[\gamma(\mathrm{ad}B)(\mathrm{ad}A)] = 0 \tag{3.12}$$

since $\mathrm{ad}A$ anticommutes with γ. Therefore, (ϵ) follows from (α). Concerning the invariant bilinear forms on simple pseudo Lie algebras we prove the following proposition.

Proposition 2: Suppose that K is algebraically closed and that $\mathfrak{a} = \mathfrak{g} \oplus \mathfrak{u}$ is a simple pseudo Lie algebra (over K). Then all invariant bilinear forms on $\mathfrak{a}$ are proportional and hence homogeneous of the same degree.

Proof: Let ϕ and ϕ' be two invariant bilinear forms on $\mathfrak{a}$. Then the even and odd components of ϕ and ϕ' are also invariant. Therefore we may assume that ϕ and ϕ' are homogeneous; let ψ (resp. ψ') be the degree of ϕ (resp. ϕ').

The cases $\phi = 0$ or $\phi' = 0$ are trivial, hence (see Lemma 1(δ)] we suppose that ϕ and ϕ' are nondegenerate. Then there is a linear map $\sigma: \mathfrak{a} \to \mathfrak{a}$ such that

$$\phi'(A, B) = \phi(\sigma(A), B) \quad \text{for all } A, B \in \mathfrak{a}. \tag{3.13}$$

It is easy to prove that σ is a homogeneous linear bijective map of degree $\psi + \psi'$. From the invariance of ϕ and ϕ' it follows that [see Sec. 2. (f)]

$$\sigma(\langle A, B \rangle) = \epsilon(\alpha, \psi + \psi')\langle A, \sigma(B) \rangle \tag{3.14}$$

if $A \in \mathfrak{a}$ is homogeneous of degree α and if $B \in \mathfrak{a}$ is arbitrary.

Let us now first assume that ϕ and ϕ' have the same degree, i.e., that $\psi + \psi' = 0$. Then σ is an even linear map of $\mathfrak{a}$ into itself. Let S be an eigenvalue of σ and define

$$\mathfrak{f} = \{B \in \mathfrak{a} \mid \sigma(B) = sB\}. \tag{3.15}$$

Since σ is even, $\mathfrak{f}$ is a graded subspace of $\mathfrak{a}$, and from (3.14) it follows that

$$\sigma(\langle A, B \rangle) = \langle A, \sigma(B) \rangle = s\langle A, B \rangle \tag{3.16}$$

for all $A \in \mathfrak{a}$, $B \in \mathfrak{f}$, i.e., $\mathfrak{f}$ is a graded ideal of $\mathfrak{a}$. Therefore $\mathfrak{f} = \mathfrak{a}$ and

$$\phi'(A, B) = s\, \phi(A, B) \tag{3.17}$$

for all $A, B \in \mathfrak{a}$.

Let us now assume that ϕ and ϕ' have different degrees. We define a bilinear form ϕ'' on $\mathfrak{a}$ by

$$\phi''(A, B) = \phi(\sigma^2(A), B), \quad A, B \in \mathfrak{a}. \tag{3.18}$$

Then ϕ'' is nondegenerate and has the same degree as ϕ. Furthermore, it is easy to check that ϕ'' is invariant. According to what we have just proved there is, therefore, a constant $t \in K$, $t \neq 0$, such that

$$\sigma^2 = t\, \mathrm{id}. \tag{3.19}$$

From (3.14) we know that

$$\sigma(\langle A, B \rangle) = \epsilon(\alpha, 1)\langle A, \sigma(B) \rangle \tag{3.20}$$

if $A \in \mathfrak{a}$ is homogeneous of degree α and $B \in \mathfrak{a}$ is arbitrary. If γ is the grading automorphism of $\mathfrak{a}$ [see Sec. 2. (b),(e)], this equation is equivalent to

$$\sigma(\langle A, B \rangle) = \langle \gamma(A), \sigma(B) \rangle \tag{3.21}$$

for all $A, B \in \mathfrak{a}$. It follows that

$$(\sigma \circ \gamma)(\langle A, B \rangle) = \sigma(\langle \gamma(A), \gamma(B) \rangle)$$
$$= \langle A, (\sigma \circ \gamma)(B) \rangle. \tag{3.22}$$

Now we define

$$\tau = (1/\sqrt{-t})\sigma \circ \gamma \tag{3.23}$$

(where $\sqrt{-t}$ is one of the two square roots of $-t$). Then τ is an odd linear bijective map of $\mathfrak{a}$ onto itself such that

$$\tau(\langle A, B \rangle) = \langle A, \tau(B) \rangle \quad \text{for all } A, B \in \mathfrak{a}, \tag{3.24}$$
$$\tau^2 = \mathrm{id}. \tag{3.25}$$

But from the proof of Proposition 1 we know that this leads to a contradiction. The proposition is proved.

Remark: As we shall see in the next section, the study of invariant bilinear forms on a simple pseudo Lie algebra $\mathfrak{a}$ is more complicated than the corresponding problem for Lie algebras.

In fact, the following four situations all do occur:

(I) the Killing form [see Sec. 2. (n)] of $\mathfrak{a}$ is nondegenerate;

(II) the Killing form of $\mathfrak{a}$ is zero but there exist nondegenerate even invariant bilinear forms on $\mathfrak{a}$;

(III) the Killing form of $\mathfrak{a}$ is zero but there exist nondegenerate odd invariant bilinear forms on $\mathfrak{a}$;

(IV) there is no nonzero invariant bilinear form on $\mathfrak{a}$.

4. EXAMPLES OF SIMPLE PSEUDO LIE ALGEBRAS AND THEIR INVARIANT BILINEAR FORMS

Before we shall derive some general theorems on the structure of simple pseudo Lie algebras it will be helpful to have at our disposal a stock of examples, since on one hand they may give some advice in obtaining realistic hypotheses and on the other hand they may serve to illustrate our theorems. Most of the results of this section have been obtained by direct calculation. Since this is sometimes a bit cumbersome and does not give any further insight, we omit all the details.

Our starting point is the general pseudo Lie algebra $\mathrm{pl}(V)$ [see Sec. 2. (h)]. We choose

$$V=K^n\oplus K^m,\quad n,m\geq 1 \tag{4.1}$$

with K^n the even and K^m the odd subspace of V. It is then natural to write $\mathrm{pl}(n,m)$ instead of $\mathrm{pl}(K^n\oplus K^m)$. The elements X of $\mathrm{pl}(n,m)$ are (or rather may be identified with) $(n+m)\times(n+m)$ matrices and will be written in block form

$$X=\begin{pmatrix}A & B\\ C & D\end{pmatrix} \tag{4.2}$$

with A an arbitrary $n\times n$ matrix, B an arbitrary $n\times m$ matrix, C an arbitrary $m\times n$ matrix, and D an arbitrary $m\times m$ matrix. If $X'=\left(\begin{smallmatrix}A' & B'\\ C' & D'\end{smallmatrix}\right)$ is a second element of $\mathrm{pl}(n,m)$, then

$$\langle X,X'\rangle = \begin{pmatrix}AA'-A'A+BC'+B'C & BD'-B'D+AB'-A'B\\ CA'-C'A+DC'-D'C & DD'-D'D+CB'+C'B\end{pmatrix}. \tag{4.3}$$

It is obvious that the mapping

$$\begin{pmatrix}A & B\\ C & D\end{pmatrix}\to\begin{pmatrix}D & C\\ B & A\end{pmatrix} \tag{4.4}$$

is an isomorphism of $\mathrm{pl}(n,m)$ onto $\mathrm{pl}(m,n)$.

(a) Evidently, all elements $\langle X,X'\rangle$; $X,X'\in\mathrm{pl}(n,m)$, are of the form $\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)$ with $\mathrm{tr}(A)=\mathrm{tr}(D)$. Hence we may define a pseudo Lie algebra $\mathrm{spl}(n,m)$ by

$$\mathrm{spl}(n,m)=\left\{\begin{pmatrix}A & B\\ C & D\end{pmatrix}\in\mathrm{pl}(n,m)\,\middle|\,\mathrm{tr}(A)=\mathrm{tr}(D)\right\}. \tag{4.5}$$

We remark that the algebra $\mathrm{spl}(n,n)$ does contain the unit matrix; it generates a one-dimensional ideal of $\mathrm{spl}(n,n)$ which turns out to be the center of $\mathrm{spl}(n,n)$ and will be denoted by $\mathfrak{z}_n$.

By direct calculation we obtain the following results:

(i) the algebras $\mathrm{spl}(n,m)$ with $n\neq m$ are simple;

(ii) if $n\geq 2$, the only nontrivial (left) ideal of $\mathrm{spl}(n,n)$ is $\mathfrak{z}_n$, hence the quotient algebra $\mathrm{spl}(n,n)/\mathfrak{z}_n$ is simple;

(iii) the (left) ideals of $\mathrm{spl}(1,1)$ which are different from $\{0\}$ are the subspaces of $\mathrm{spl}(1,1)$ which contain $\mathfrak{z}_1$.

Let γ_V be the grading automorphism of $V=K^n\oplus K^m$. Then we know that

$$(X,Y)\to\mathrm{tr}(\gamma_V XY) \tag{4.6}$$

is an even invariant bilinear form on $\mathrm{pl}(n,m)$ and on $\mathrm{spl}(n,m)$.

The Killing form of $\mathrm{pl}(n,m)$ is found to be

$$(X,Y)\to 2(n-m)\,\mathrm{tr}(\gamma_V XY)-2\,\mathrm{tr}(\gamma_V X)\,\mathrm{tr}(\gamma_V Y), \tag{4.7}$$

hence the Killing form of $\mathrm{spl}(n,m)$ is

$$(X,Y)\to 2(n-m)\,\mathrm{tr}(\gamma_V XY). \tag{4.8}$$

It follows that the Killing form of $\mathrm{spl}(n,n)/\mathfrak{z}_n$ is zero. Nevertheless, by going to the quotient, the invariant bilinear form (4.6) on $\mathrm{spl}(n,n)$ furnishes a nondegenerate invariant even bilinear form on $\mathrm{spl}(n,n)/\mathfrak{z}_n$.

(b) Suppose now that we are given a bilinear form Ψ on $V=K^n\oplus K^m$ and let us consider the set of all elements of $\mathrm{pl}(n,m)$ that leave Ψ invariant [see Sec. 2. (l), (m)]. If Ψ is homogeneous then it is easy to see that this set is a subalgebra of $\mathrm{pl}(n,m)$.

In the following we write the elements of V in the form of pairs (x,y) with two column vectors $x\in K^n$ and $y\in K^m$.

(c) We consider first the case where Ψ is even.

Then Ψ has the form

$$\Psi((x_1,y_1),(x_2,y_2))={}^tx_1M^{gg}x_2+{}^ty_1M^{uu}y_2 \tag{4.9}$$

with an $n\times n$ matrix M^{gg} and an $m\times m$ matrix M^{uu}.

An element $\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)\in\mathrm{pl}(n,m)$ leaves Ψ invariant if and only if

$$\begin{aligned}&{}^tAM^{gg}+M^{gg}A=0,\quad {}^tBM^{gg}-M^{uu}C=0,\\ &{}^tCM^{uu}+M^{gg}B=0,\quad {}^tDM^{uu}+M^{uu}D=0.\end{aligned} \tag{4.10}$$

It is now appropriate to choose M^{gg} and M^{uu} nondegenerate and one of them symmetric, the other skew-symmetric.

Hence let $m,p\geq 1$ be any positive integers and let $n=2p$. Choose

$$M^{gg}=G=\begin{pmatrix}0 & I_p\\ -I_p & 0\end{pmatrix},\quad M^{uu}=I_m, \tag{4.11}$$

where I_k denotes the k-dimensional unit matrix.

Then our conditions read

$${}^tAG+GA=0,\quad {}^tD+D=0,\quad C={}^tBG. \tag{4.12}$$

Let $\mathfrak{a}(2p,m)$ be the subalgebra of $\mathrm{pl}(2p,m)$ described by these conditions. The first equation says that A is an element of the symplectic Lie algebra $\mathrm{sp}(2p)$ and the second condition demands D to be an element of the orthogonal Lie algebra $\mathrm{o}(m)$.

In a more detailed investigation it might be advantageous to distinguish between the cases where m is odd or even and to choose for M^{uu} the symmetric matrices well known from the discussion of the simple Lie algebras of types B_k or D_k. But we would like to stress that the cases $m=1$ and $m=2$ are not excluded.

With these definitions we have shown that:

(i) All pseudo Lie algebras $\mathfrak{a}(2p,m)$; $p,m\geq 1$, are simple;

(ii) The bilinear form on $\mathfrak{a}(2p,m)$,

$$(X,Y)\to\mathrm{tr}(\gamma_V XY), \tag{4.13}$$

is even, nondegenerate, and invariant.

(iii) The Killing form of $\mathfrak{a}(2p,m)$ is equal to

$$(X,Y)\to(2p-m+2)\,\mathrm{tr}(\gamma_V XY). \tag{4.14}$$

(d) Next we consider the case where Ψ is odd.

Then Ψ has the form

$$\Psi((x_1,y_1),(x_2,y_2))={}^tx_1M^{gu}y_2+{}^ty_1M^{ug}x_2 \tag{4.15}$$

with an $n\times m$ matrix $M^{\varepsilon u}$ and an $m\times n$ matrix $M^{u\varepsilon}$. An element $\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)\in \mathrm{pl}(n,m)$ leaves Ψ invariant if and only if

$$\begin{aligned} &{}^tAM^{\varepsilon u}+M^{\varepsilon u}D=0, \quad {}^tBM^{\varepsilon u}-M^{u\varepsilon}B=0,\\ &{}^tCM^{u\varepsilon}+M^{\varepsilon u}C=0, \quad {}^tDM^{u\varepsilon}+M^{u\varepsilon}A=0. \end{aligned} \tag{4.16}$$

It is then appropriate to choose

$$M^{u\varepsilon}={}^tM^{\varepsilon u}. \tag{4.17}$$

Suppose now $n=m\geq 1$ and

$$M^{\varepsilon u}=M^{u\varepsilon}=I_n. \tag{4.18}$$

Then our conditions read

$${}^tA+D=0, \quad {}^tB-B=0, \quad {}^tC+C=0. \tag{4.19}$$

Evidently an element of $\mathrm{pl}(n,n)$ satisfying these conditions lies in $\mathrm{spl}(n,n)$ if and only if $\mathrm{tr}(A)=0$, i.e., if and only if $A\in \mathrm{sl}(n)$. Hence we define a subalgebra $\mathfrak{b}(n)$ of $\mathrm{spl}(n,n)$ by

$$\mathfrak{b}(n)=\left\{\begin{pmatrix}A & B\\ C & -{}^tA\end{pmatrix}\;\middle|\;\mathrm{tr}(A)=0,\ {}^tB=B,\ {}^tC=-C\right\}, \tag{4.20}$$

where A,B,C are $n\times n$ matrices.

The case $n=1$ is trivial. For $n\geq 2$ we have shown:

(i) If $n\geq 3$, then the pseudo Lie algebra $\mathfrak{b}(n)$ is simple and there is no nonzero invariant bilinear form on $\mathfrak{b}(n)$;

(ii) the only nontrivial (left) ideal of $\mathfrak{b}(2)$ consists (in the notation introduced above) of those elements of $\mathfrak{b}(2)$ for which $C=0$;

(iii) all invariant bilinear forms on $\mathfrak{b}(2)$ are even and degenerate.

(e) Suppose finally that $m=n$ and consider the set of all matrices $\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)\in \mathrm{pl}(n,n)$ with $A=D$ and $B=C$.[8] It is easy to see that this set is a subalgebra of $\mathrm{spl}(n,n)$, namely the subalgebra of all elements of $\mathrm{pl}(n,n)$ that leave invariant [see Sec. 2. (l),(m)] the odd linear map of V into itself, described by the matrix $\left(\begin{smallmatrix}0 & I_n\\ -I_n & 0\end{smallmatrix}\right)$. If X,X' are two elements of this subalgebra, then $\langle X,X'\rangle$ has the form $\left(\begin{smallmatrix}A & B\\ B & A\end{smallmatrix}\right)$ with $\mathrm{tr}(B)=0$.

Hence we define a subalgebra $\mathfrak{b}_n$ of $\mathrm{spl}(n,n)$ by

$$\mathfrak{b}_n=\left\{\begin{pmatrix}A & B\\ B & A\end{pmatrix}\;\middle|\;A\in \mathfrak{g}l(n),\ B\in \mathrm{sl}(n)\right\}. \tag{4.21}$$

Evidently $\mathfrak{d}_n$[as defined in (a)] is contained in $\mathfrak{b}_n$. To simplify the notation we write (A,B) instead of $\left(\begin{smallmatrix}A & B\\ B & A\end{smallmatrix}\right)$.

The case $n=1$ is trivial. For $n\geq 2$ we have shown:

(i) If $n\geq 3$ then $\mathfrak{d}_n$ is the only nontrivial (left) ideal of $\mathfrak{b}_n$. The nonzero invariant bilinear forms on $\mathfrak{b}_n$ are odd and proportional to

$$((A,B),(A',B'))\to \mathrm{tr}(AB'+BA'). \tag{4.22}$$

(ii) The algebra $\mathfrak{b}_2$ contains a second nontrivial (left) ideal besides $\mathfrak{d}_2$ namely

$$\{(\lambda I_2,B)\,|\,\lambda\in K,\ B\in \mathrm{sl}(2)\}. \tag{4.23}$$

(iii) The even (resp. odd) invariant bilinear forms on $\mathfrak{b}_2$ are proportional to

$$\begin{aligned} &((A,B),(A',B'))\to \mathrm{tr}(AA')-\tfrac{1}{2}\mathrm{tr}(A)\mathrm{tr}(A')\\ &[\text{resp. } ((A,B),(A',B'))\to \mathrm{tr}(AB'+BA')]. \end{aligned} \tag{4.24}$$

From this we conclude: Suppose $n\geq 3$. Then the quotient algebra $\mathfrak{b}_n/\mathfrak{d}_n$ is simple. Going to the quotient the odd invariant bilinear form (4.22) yields a nondegenerate odd invariant bilinear form on $\mathfrak{b}_n/\mathfrak{d}_n$. Consequently, there cannot exist any nonzero even invariant bilinear form on $\mathfrak{b}_n/\mathfrak{d}_n$, especially the Killing form of $\mathfrak{b}_n/\mathfrak{d}_n$ is equal to zero.

The algebras $\mathfrak{b}_n/\mathfrak{d}_n$ are the (f,d) algebras of Gell-mann, Michel, and Radicati.[8]

5. ON THE COMPLETE REDUCIBILITY OF THE ADJOINT REPRESENTATION OF $\mathfrak{g}$ IN $\breve{\mathfrak{u}}$

The examples of the preceding section have the following property in common: The adjoint representation of $\mathfrak{g}$ in $\breve{\mathfrak{u}}$ [see Sec. 2.(k)] is either irreducible or it is the direct sum of two irreducible representations. In this section we shall show (partly under additional assumptions on $\mathfrak{g}$ and K) that this is a general property of simple pseudo Lie algebras. We begin with the following theorem.

Theorem 1: Let $\mathfrak{a}=\mathfrak{g}\oplus\breve{\mathfrak{u}}$ be a simple pseudo Lie algebra. Suppose that $\breve{\mathfrak{u}}$ is the sum

$$\breve{\mathfrak{u}}=\breve{\mathfrak{u}}_1+\breve{\mathfrak{u}}_2 \tag{5.1}$$

of two $\mathfrak{g}$-invariant subspaces $\breve{\mathfrak{u}}_1$ and $\breve{\mathfrak{u}}_2$, both different from $\breve{\mathfrak{u}}$. Then the sum is direct, i.e.,

$$\breve{\mathfrak{u}}_1\cap\breve{\mathfrak{u}}_2=\{0\}, \tag{5.2}$$

and the adjoint representations of $\mathfrak{g}$ in $\breve{\mathfrak{u}}_1$ and $\mathfrak{u}_2$ are irreducible. Furthermore we have

$$\langle\breve{\mathfrak{u}}_1,\breve{\mathfrak{u}}_1\rangle=\langle\breve{\mathfrak{u}}_2,\breve{\mathfrak{u}}_2\rangle=\{0\}, \quad \langle\breve{\mathfrak{u}}_1,\breve{\mathfrak{u}}_2\rangle=\mathfrak{g}. \tag{5.3}$$

Proof: We start with a lemma.

Lemma 2: Let $\mathfrak{a}=\mathfrak{g}\oplus\breve{\mathfrak{u}}$ be a simple pseudo Lie algebra. Suppose that $\breve{\mathfrak{u}}$ is the direct sum

$$\breve{\mathfrak{u}}=\breve{\mathfrak{u}}_1\oplus\cdots\oplus\breve{\mathfrak{u}}_r \tag{5.4}$$

of $\mathfrak{g}$-invariant subspaces $\breve{\mathfrak{u}}_1,\cdots,\breve{\mathfrak{u}}_r$, all different from $\{0\}$. Then $r=1$ or $r=2$, and in the case $r=2$ we have (5.3).

Proof of Lemma 2: The case $r=1$ is trivial. Let us consider the case $r=2$; once this case has been settled the rest will follow immediately. We shall prove that

$$\mathfrak{f}=\langle\breve{\mathfrak{u}}_1,\breve{\mathfrak{u}}_1\rangle\oplus\langle\breve{\mathfrak{u}}_1,\langle\breve{\mathfrak{u}}_1,\breve{\mathfrak{u}}_1\rangle\rangle \tag{5.5}$$

is an ideal of $\mathfrak{a}$.

Evidently $\mathfrak{f}$ is $\mathfrak{g}$-invariant [see Sec. 2.(k)]; furthermore

$$\langle\breve{\mathfrak{u}}_1,\langle\breve{\mathfrak{u}}_1,\breve{\mathfrak{u}}_1\rangle\rangle\subset\langle\breve{\mathfrak{u}}_1,\mathfrak{g}\rangle\subset\breve{\mathfrak{u}}_1, \tag{5.6}$$

hence $\mathfrak{f}$ is invariant under $\mathrm{ad}\,\breve{\mathfrak{u}}_1$.

Finally

$$\langle\breve{\mathfrak{u}}_2,\langle\breve{\mathfrak{u}}_1,\breve{\mathfrak{u}}_1\rangle\rangle\subset\langle\breve{\mathfrak{u}}_2,\mathfrak{g}\rangle\subset\breve{\mathfrak{u}}_2, \tag{5.7}$$

and on the other hand

$$\langle \breve{u}_2, \langle \breve{u}_1, \breve{u}_1 \rangle \rangle \subset \langle \langle \breve{u}_2, \breve{u}_1 \rangle, \breve{u}_1 \rangle + \langle \breve{u}_1, \langle \breve{u}_2, \breve{u}_1 \rangle \rangle \subset \langle \mathfrak{g}, \breve{u}_1 \rangle + \langle \breve{u}_1, \mathfrak{g} \rangle \subset \breve{u}_1, \tag{5.8}$$

hence

$$\langle \breve{u}_2, \langle \breve{u}_1, \breve{u}_1 \rangle \rangle = \{0\} \tag{5.9}$$

and therefore

$$\langle \breve{u}_2, \langle \breve{u}_1, \langle \breve{u}_1, \breve{u}_1 \rangle \rangle \rangle \subset \langle \langle \breve{u}_2, \breve{u}_1 \rangle, \langle \breve{u}_1, \breve{u}_1 \rangle \rangle \subset \langle \mathfrak{g}, \langle \breve{u}_1, \breve{u}_1 \rangle \rangle \subset \langle \breve{u}_1, \breve{u}_1 \rangle, \tag{5.10}$$

i.e., $\mathfrak{f}$ is invariant under $\mathrm{ad}\,\breve{u}_2$.

Since evidently $\mathfrak{f} \neq \mathfrak{a}$ we conclude that

$$\langle \breve{u}_1, \breve{u}_1 \rangle = \{0\}$$

and similarly $\langle \breve{u}_2, \breve{u}_2 \rangle = \{0\}$, (5.11)

hence [see Lemma 1(α)]

$$\langle \breve{u}_1, \breve{u}_2 \rangle = \langle \breve{u}, \breve{u} \rangle = \mathfrak{g}. \tag{5.12}$$

If now $r \geq 3$ and if $k \in \{1, \ldots, r\}$, then

$$\breve{u} = \breve{u}_k \oplus \bigoplus_{j \neq k} \breve{u}_j \tag{5.13}$$

and the case $r = 2$ yields

$$\Big\langle \bigoplus_{i \neq k} \breve{u}_i, \bigoplus_{j \neq k} \breve{u}_j \Big\rangle = \{0\}. \tag{5.14}$$

It follows that

$$\langle \breve{u}_i, \breve{u}_j \rangle = \{0\} \text{ for all } i, j \in \{1, \ldots, r\}, \tag{5.15}$$

that is

$$\langle \breve{u}, \breve{u} \rangle = \{0\}, \tag{5.16}$$

contrary to the assumption that $\mathfrak{a}$ is simple [see Lemma 1(α)].

Let us now come to the main proof. If $\breve{u}_i$, $i = 1, 2$, are the $\mathfrak{g}$-invariant subspaces of $\breve{u}$ mentioned in the theorem, then we define

$$\breve{u}_i^{-1} = \breve{u}, \quad \breve{u}_i^0 = \mathfrak{g}, \quad \breve{u}_i^1 = \breve{u}_i, \qquad \breve{u}_i^n = \langle \breve{u}_i, \breve{u}_i^{n-1} \rangle \text{ if } n \geq 2. \tag{5.17}$$

It is easy to see that for all $n \geq -1$

$$\breve{u}_i^n \text{ is } \mathfrak{g}\text{-invariant}, \tag{5.18}$$

$$\langle \breve{u}, \breve{u}_i^{n+1} \rangle \subset \breve{u}_i^n, \tag{5.19}$$

$$\breve{u}_i^{n+2} \subset \breve{u}_i^n. \tag{5.20}$$

From (5.20) we deduce that there is an integer $k \geq 1$ such that

$$\breve{u}_i^{2k} = \breve{u}_i^{2k+2}. \tag{5.21}$$

Using (5.18) and (5.19) it is then obvious that $\breve{u}_i^{2k} \oplus \breve{u}_i^{2k+1}$ is an ideal of $\mathfrak{a}$, hence equal to zero. We conclude that

$$\breve{u}_i^n = \{0\} \tag{5.22}$$

if the positive integer n is sufficiently large.

Now we define for each integer $l \geq 0$

$$\mathfrak{f}_l^{\mathfrak{g}} = \sum_{k=0}^{l} (\breve{u}_1^{2(l-k)} \cap \breve{u}_2^{2k}),$$
$$\mathfrak{f}_l^{u} = \sum_{k=0}^{l+1} (\breve{u}_1^{2(l-k)+1} \cap \breve{u}_2^{2k-1}), \tag{5.23}$$
$$\mathfrak{f}_l = \mathfrak{f}_l^{\mathfrak{g}} \oplus \mathfrak{f}_l^{u}.$$

It is easy to see [using (5.18), (5.19) and (5.1)] that $\mathfrak{f}_l$ is an ideal of $\mathfrak{a}$, for every $l \geq 0$. We remark that

$$\mathfrak{f}_0^{\mathfrak{g}} = \mathfrak{g}, \quad \mathfrak{f}_0^{u} = \breve{u}_1 + \breve{u}_2 = \breve{u}. \tag{5.24}$$

Evidently

$$\mathfrak{f}_l^{u} \subset (\breve{u}_1^{2l+1} + \breve{u}_2) \cap (\breve{u}_1 + \breve{u}_2^{2l+1}). \tag{5.25}$$

Therefore if $\breve{u}_1^{2l+1} = \{0\}$ or $\breve{u}_2^{2l+1} = \{0\}$ (and this will happen for sufficiently large l), then $\mathfrak{f}_l^{u} \neq \breve{u}$ and consequently $\mathfrak{f}_l = \{0\}$. Now let L be the smallest of the integers $l \geq 1$ such that

$$\breve{u}_1^{2(l-k)+1} \cap \breve{u}_2^{2k-1} = \{0\} \text{ if } 1 \leq k \leq l. \tag{5.26}$$

Then on the one hand $\breve{u}_1^{2L-1}$ and $\breve{u}_2^{2L-1}$ are different from $\{0\}$, since otherwise $\mathfrak{f}_{L-1} = \{0\}$ and therefore L would not be minimal. In particular we conclude that $\mathfrak{f}_{L-1}^{\mathfrak{g}} = \mathfrak{a}$, hence $\mathfrak{f}_{L-1}^{u} = \breve{u}$. But on the other hand it follows from (5.26) that the sum defining $\mathfrak{f}_{L-1}^{u}$ is direct. Since we already known that the two terms $\breve{u}_1^{2L-1}$ and $\breve{u}_2^{2L-1}$ of this sum are not equal to $\{0\}$, Lemma 2 shows that all the remaining terms be equal to $\{0\}$. It follows that $L = 1$, for otherwise L would not be minimal.

Thus we have shown that $\mathfrak{f}_0^{u} = \breve{u}$ is the direct sum of $\breve{u}_1$ and $\breve{u}_2$. It is now evident that $\breve{u}_1$ and $\breve{u}_2$ are $\mathfrak{g}$-irreducible. For suppose for instance that $\breve{u}_1'$ is a $\mathfrak{g}$-invariant subspace of $\breve{u}_1$ different from $\breve{u}_1$. Then we can apply the result just proved to $\breve{u}_1$ and $\breve{u}_2 + \breve{u}_1'$ and see that the sum of these two subspaces of $\breve{u}$ must be direct, that is $\breve{u}_1' = \{0\}$.

The theorem is completely proved.

Corollary: Under the conditions of Theorem 1 the Lie algebra $\mathfrak{g}$ is reductive (i.e., $\mathfrak{g}$ is the direct product of a semisimple with an abelian Lie algebra).

Proof: In fact, $\mathfrak{g}$ has a faithful completely reducible representation.[9]

It is instructive to state Theorem 1 in the following equivalent form:

Let $\mathfrak{a} = \mathfrak{g} \oplus \breve{u}$ be a simple pseudo Lie algebra. Then either $\breve{u}$ is the direct sum of two $\mathfrak{g}$-irreducible subspaces $\breve{u}_1$ and $\breve{u}_2$ which satisfy the equations (5.1) or else there exists a unique maximal $\mathfrak{g}$-invariant proper subspace $\breve{u}_0$ of $\breve{u}$.

Of course in the second case one would like to know whether in fact $\breve{u}_0 = \{0\}$, i.e., whether $\breve{u}$ must be $\mathfrak{g}$-irreducible. If this would be true, then we could conclude that generally the Lie algebra contained in a simple pseudo Lie algebra must be reductive.

Up to now we have been unable to answer these two questions. The following proposition gives another hint that the "reductiveness conjecture" might be true.

Proposition 3: Let $\mathfrak{a} = \mathfrak{g} \oplus \breve{u}$ be an arbitrary pseudo Lie algebra. Suppose that $\mathfrak{a}$ has a graded representation

such that the corresponding invariant bilinear form on $\mathfrak{a}$ [see Sec. 2(n)] is nondegenerate. Then $\mathfrak{g}$ is reductive.

Proof: This proposition follows easily from Ref. 10.

To proceed it is now reasonable to assume that $\mathfrak{g}$ is reductive. If in addition K is algebraically closed, then we can prove even more than our conjecture above.

Theorem 2: Let K be algebraically closed and let $\mathfrak{a}=\mathfrak{g}\oplus\breve{\mathfrak{u}}$ be a simple pseudo Lie algebra. Suppose that $\mathfrak{g}$ is reductive and that the adjoint representation of $\mathfrak{g}$ in $\breve{\mathfrak{u}}$ is undecomposable. Then $\mathfrak{g}$ is semisimple and the adjoint representation of $\mathfrak{g}$ in $\breve{\mathfrak{u}}$ is irreducible.

Proof: The proof of this theorem is rather lengthy. We begin with two lemmas which bring the adjoint representation of $\mathfrak{g}$ in $\breve{\mathfrak{u}}$ (denoted by $\mathrm{ad}\,\breve{\mathfrak{u}}$) to some normal form. (As in the theorem we shall assume here and in the following that K is algebraically closed.)

Lemma 3: Let $\mathfrak{g}$ be a reductive Lie algebra, i.e., $\mathfrak{g}=\mathfrak{g}^s\times\mathfrak{g}^a$ is the direct product of a semisimple Lie algebra $\mathfrak{g}^s$ with an Abelian Lie algebra $\mathfrak{g}^a$. Then any undecomposable representation of $\mathfrak{g}$ is isomorphic to the tensor product of an irreducible representation of $\mathfrak{g}^s$ with an undecomposable representation of $\mathfrak{g}^a$.

Lemma 4: Suppose ρ is an undecomposable representation of an Abelian Lie algebra $\mathfrak{g}^a$ in a vector space V. Then there exists a basis $(e_i)_{1\leq i\leq n}$ of V such that for all $A\in\mathfrak{g}^a$ and all $i\in\{1,\ldots,n\}$,

$$\rho(A)e_i=\lambda(A)e_i+\sum_{j<i}\lambda_{ji}(A)\,e_j \tag{5.27}$$

with suitable linear forms λ and λ_{ji}, $1\leq j<i\leq n$, on $\mathfrak{g}^a$ (i.e., the matrices of the representation are upper triangular and the elements on the diagonal coincide).

Both lemmas are well known; Lemma 3 follows for example from Ref. 11 and Schur's lemma, and Lemma 4 is a special case of Ref. 12.

We apply these lemmas to $\mathrm{ad}_{\breve{\mathfrak{u}}}$. From Lemma 1($\epsilon$) we know that

$$\mathrm{tr}(\mathrm{ad}_{\breve{\mathfrak{u}}}A)=0 \quad \text{for all } A\in\mathfrak{g}^a, \tag{5.28}$$

hence the linear form λ in (5.27) must vanish in the present case. Since $\mathrm{ad}_{\breve{\mathfrak{u}}}$ is faithful we conclude: There exist $\mathfrak{g}^s$-irreducible subspaces $\breve{\mathfrak{u}}^i$, $1\leq i\leq n$, of $\breve{\mathfrak{u}}$ such that

(α) $\breve{\mathfrak{u}}$ is the direct sum of the $\breve{\mathfrak{u}}^i$, $1\leq i\leq n$,

(β) the representations of $\mathfrak{g}^s$ in the subspaces $\breve{\mathfrak{u}}^i$ (induced by $\mathrm{ad}_{\breve{\mathfrak{u}}}$ and denoted by $\mathrm{ad}_{\breve{\mathfrak{u}}^i}$) are all isomorphic and faithful,

(γ) $\langle\mathfrak{g}^a,\breve{\mathfrak{u}}^i\rangle\subset\oplus_{j<i}\breve{\mathfrak{u}}^j$ especially $\langle\mathfrak{g}^a,\breve{\mathfrak{u}}^1\rangle=\{0\}$.

If $n=1$, then we have the situation which according to the theorem must hold: In fact, $\langle\mathfrak{g}^a,\breve{\mathfrak{u}}\rangle=\{0\}$ and hence $\mathfrak{g}^a=\{0\}$ since $\mathrm{ad}_{\breve{\mathfrak{u}}}$ is faithful.

Let us now assume $n\geq 2$. We shall show that $\mathfrak{g}^a\oplus\langle\mathfrak{g}^a,\breve{\mathfrak{u}}\rangle$ is an ideal of $\mathfrak{a}$. Once that this has been established the theorem is proved: According to (γ) this ideal is different from $\mathfrak{a}$, hence equal to $\{0\}$; but $\mathfrak{g}^a=\{0\}$ is in contradiction with $n\geq 2$.

To begin with we remark that

$$\langle\mathfrak{g}^a,\breve{\mathfrak{u}}\rangle=\bigoplus_{j<n}\breve{\mathfrak{u}}^j. \tag{5.29}$$

By (γ) we know that

$$\langle\mathfrak{g}^a,\breve{\mathfrak{u}}\rangle\subset\bigoplus_{j<n}\breve{\mathfrak{u}}^j. \tag{5.30}$$

If equality would not hold, then we could write

$$\breve{\mathfrak{u}}=(\breve{\mathfrak{u}}^n+\langle\mathfrak{g}^a,\breve{\mathfrak{u}}\rangle)+\bigoplus_{j<n}\breve{\mathfrak{u}}^j, \tag{5.31}$$

which according to Theorem 1 is in contradiction to our assumption that $\breve{\mathfrak{u}}$ is undecomposable.

Now let $\mathcal{A}$ be the association subalgebra (without unit) of $\mathcal{L}(\breve{\mathfrak{u}})$ generated by the linear mappings $\mathrm{ad}_{\breve{\mathfrak{u}}}A$, $A\in\mathfrak{g}^a$. It is then easy to see that every element of $\mathcal{A}$ commutes with every linear map $\mathrm{ad}_{\breve{\mathfrak{u}}}X$, $X\in\mathfrak{g}$, and that the product of n arbitrary elements of $\mathcal{A}$ is zero. Furthermore, we obtain from (5.29)

$$\bigoplus_{j<n}\breve{\mathfrak{u}}^j=\mathcal{A}(\breve{\mathfrak{u}}^n). \tag{5.32}$$

Next we choose a Cartan subalgebra $\mathfrak{f}$ of $\mathfrak{g}^s$. For any linear form λ on $\mathfrak{f}$ we define

$$\mathfrak{g}_\lambda=\{X\in\mathfrak{g}\mid\langle H,X\rangle=\lambda(H)X \text{ for all } H\in\mathfrak{f}\}, \tag{5.33}$$

$$\breve{\mathfrak{u}}^j_\lambda=\{Y\in\breve{\mathfrak{u}}^j\mid\langle H,Y\rangle=\lambda(H)Y \text{ for all } H\in\mathfrak{f}\}. \tag{5.34}$$

Then

$$\mathfrak{g}_0=\mathfrak{f}+\mathfrak{g}^a, \tag{5.35}$$

the linear forms $\lambda\neq 0$ with $\mathfrak{g}_\lambda\neq\{0\}$ are the roots of $\mathfrak{g}^s$ (with respect to $\mathfrak{f}$) and the linear forms λ with $\breve{\mathfrak{u}}^j_\lambda\neq\{0\}$ are the weights of $\mathrm{ad}_{\breve{\mathfrak{u}}^j}$. Since all representations $\mathrm{ad}_{\breve{\mathfrak{u}}^j}$, $1\leq j\leq n$, are isomorphic, all these representations have the same weights. As is well known,

$$\mathfrak{g}^s=\mathfrak{f}\oplus\bigoplus_{\lambda\neq 0}\mathfrak{g}_\lambda, \tag{5.36}$$

$$\breve{\mathfrak{u}}^j=\bigoplus_\lambda\breve{\mathfrak{u}}^j_\lambda. \tag{5.37}$$

For all linear forms α, β on $\mathfrak{f}$ and all i, $j\in\{1,\ldots,n\}$ we have

$$\langle\breve{\mathfrak{u}}^i_\alpha,\breve{\mathfrak{u}}^j_\beta\rangle\subset\mathfrak{g}_{\alpha+\beta}, \tag{5.38}$$

hence

$$\begin{aligned}&\langle\breve{\mathfrak{u}}^i_\alpha,\breve{\mathfrak{u}}^j_\beta\rangle=\{0\} \text{ if } \alpha+\beta\neq 0 \text{ is not a root},\\ &\langle\breve{\mathfrak{u}}^i_\alpha,\breve{\mathfrak{u}}^j_\beta\rangle\subset\mathfrak{g}_{\alpha+\beta} \text{ if } \alpha+\beta\neq 0 \text{ is a root},\\ &\langle\breve{\mathfrak{u}}_\alpha,\breve{\mathfrak{u}}^j_{-\alpha}\rangle\subset\mathfrak{f}+\mathfrak{g}^a.\end{aligned} \tag{5.39}$$

On the other hand, if we suppose $\alpha\neq 0$, then

$$\langle\mathfrak{g}_\alpha,\breve{\mathfrak{u}}^i_\beta\rangle\subset\breve{\mathfrak{u}}^i_{\alpha+\beta}. \tag{5.40}$$

We can now prove a more precise version of (5.32). In fact, suppose $j\in\{1,\ldots,n-1\}$ is given and let $Z\neq 0$ be some element of $\breve{\mathfrak{u}}^j$. Then (5.32) shows that there exist elements $Q_r\in\mathcal{A}$ and $\tilde{Z}_r\in\breve{\mathfrak{u}}^n$, $1\leq r\leq s$, such that

$$Z=\sum_{r=1}^{s}Q_r(\tilde{Z}_r). \tag{5.41}$$

But if we choose a weight λ such that $\breve{\mathfrak{u}}^n_\lambda$ is one-dimensional (such weights do exist) and if $Z\in\breve{\mathfrak{u}}^n_\lambda$, then it is easy to see (since $\mathcal{A}$ and $\mathrm{ad}_{\breve{\mathfrak{u}}}$ commute) that we can find one element $P_j\in\mathcal{A}$ and one element $\tilde{Z}\in\breve{\mathfrak{u}}^n_\lambda$ such that

$$Z=P_j(\tilde{Z}), \tag{5.42}$$

and consequently

$$\breve{u}^j_\alpha = P_j(\breve{u}^n_\alpha) \quad \text{for all weights } \alpha. \tag{5.43}$$

After these preliminaries we are ready to prove that $\mathfrak{g}^a \oplus \langle \mathfrak{g}^a, u \rangle$ is an ideal of $\mathfrak{a}$ (at least if $n \geq 3$).

The Jacobi identity shows that

$$\langle\langle \langle \mathfrak{g}^a, \breve{u} \rangle, \langle \mathfrak{g}^a, \breve{u} \rangle\rangle, \breve{u}^n \rangle \subset \langle \mathfrak{g}^a, \breve{u} \rangle. \tag{5.44}$$

Since $\mathrm{ad}_{\breve{u}_n}$ is faithful we conclude that

$$\langle\langle \mathfrak{g}^a, \breve{u} \rangle, \langle \mathfrak{g}^a, \breve{u} \rangle\rangle \subset \mathfrak{g}^a, \tag{5.45}$$

i.e., that

$$\langle \breve{u}^i, \breve{u}^j \rangle \subset \mathfrak{g}^a \text{ if } 1 \leq i, j \leq n-1. \tag{5.46}$$

If $i = 1$, then we can even prove that

$$\langle u^1, u^j \rangle = \{0\} \text{ if } 1 \leq j \leq n-1, \tag{5.47}$$

for we know that $\langle \mathfrak{g}^a, u^1 \rangle = \{0\}$ and therefore

$$\langle \breve{u}^1, \langle \mathfrak{g}^a, \breve{u} \rangle\rangle = \langle \mathfrak{g}^a, \langle \breve{u}^1, \breve{u} \rangle\rangle = \{0\}. \tag{5.48}$$

As a consequence of (5.45) we derive that

$$\langle\langle P(U), V\rangle, W\rangle = -\langle\langle U, P(V)\rangle, W\rangle \tag{5.49}$$

for all $P \in \mathcal{A}$; U, $V \in \breve{u}$, and $W \in \breve{u}^1$.

To prove (5.49), we distinguish two cases. If $P = \mathrm{ad}\ A$, $A \in \mathfrak{g}^a$, then

$$\langle\langle A, U\rangle, V\rangle + \langle U, \langle A, V\rangle\rangle = \langle A, \langle U, V\rangle\rangle = 0. \tag{5.50}$$

If on the other hand

$$P = (\mathrm{ad}_{\breve{u}} A_1)(\mathrm{ad}_{\breve{u}} A_2) Q \tag{5.51}$$

with A_1, $A_2 \in \mathfrak{g}^a$ and some $Q \in \mathcal{L}(\breve{u})$, then with $Q(U) = \tilde{U}$,

$$\begin{aligned} \langle P(U), V\rangle &= \langle\langle A_1, \langle A_2, \tilde{U}\rangle\rangle, V\rangle \\ &= \langle A_1, \langle\langle A_2, \tilde{U}\rangle, V\rangle\rangle - \langle\langle A_2, \tilde{U}\rangle, \langle A_1, V\rangle\rangle \\ &\in \langle \mathfrak{g}^a, \langle \breve{u}, \breve{u}\rangle\rangle + \langle\langle \mathfrak{g}^a, \breve{u} \rangle, \langle \mathfrak{g}^a, \breve{u} \rangle\rangle \end{aligned} \tag{5.52}$$

and therefore [see (5.45)]

$$\langle P(U), V\rangle \in \mathfrak{g}^a, \tag{5.53}$$

Hence $\langle\langle P(U), V\rangle, W\rangle = 0$ and similarly $\langle\langle U, P(V)\rangle, W\rangle = 0$.

Next we shall show that

$$\langle \breve{u}^n, \breve{u}^j \rangle \subset \mathfrak{g}^a \text{ if } 1 \leq j \leq n-1, \tag{5.54}$$

provided that $n \geq 3$. Suppose first that $2 \leq j \leq n-1$. Then we have for all weights α, β, γ

$$\begin{aligned} &\langle\langle \breve{u}^n_\alpha, \breve{u}^j_\beta\rangle, \breve{u}^1_\gamma\rangle \\ &\subset \langle \breve{u}^n_\alpha, \langle \breve{u}^j_\beta, \breve{u}^1_\gamma\rangle\rangle = \langle \breve{u}^j_\beta, \langle \breve{u}^n_\alpha, \breve{u}^1_\gamma\rangle\rangle \end{aligned} \tag{5.55}$$

and because $\langle \breve{u}^j, \breve{u}^1 \rangle = \{0\}$ [see (5.47)]

$$\langle\langle \breve{u}^n_\alpha, \breve{u}^j_\beta\rangle, \breve{u}^1_\gamma\rangle \subset \langle \breve{u}^j_\beta, \langle \breve{u}^n_\alpha, \breve{u}^1_\beta\rangle\rangle. \tag{5.56}$$

The left-hand side is contained in $\breve{u}^1$, the right-hand side lies in $\breve{u}^j$ provided $\alpha + \gamma \neq 0$. Hence

$$\langle\langle \breve{u}^n_\alpha, \breve{u}^j_\beta\rangle, \breve{u}^1_\gamma\rangle = \{0\} \text{ if } \alpha + \gamma \neq 0. \tag{5.57}$$

But we know that [see (5.43) and (5.49)]

$$\begin{aligned} \langle\langle \breve{u}^n_\alpha, \breve{u}^j_\beta\rangle, \breve{u}^1_\gamma\rangle &= \langle\langle \breve{u}^n_\alpha, P_j(\breve{u}^n_\beta)\rangle, \breve{u}^1_\gamma\rangle \\ &= \langle\langle P_j(\breve{u}^n_\alpha), \breve{u}^n_\beta\rangle, \breve{u}^1_\gamma\rangle \\ &= \langle\langle \breve{u}^j_\alpha, \breve{u}^n_\beta\rangle, \breve{u}^1_\gamma\rangle \\ &= \langle\langle \breve{u}^n_\beta, \breve{u}^j_\alpha\rangle, \breve{u}^1_\gamma\rangle, \end{aligned} \tag{5.58}$$

which together with (5.57) yields

$$\langle\langle \breve{u}^n_\alpha, \breve{u}^j_\beta\rangle, \breve{v}^1_\gamma\rangle = \{0\} \text{ if } \alpha + \gamma \neq 0 \text{ or } \beta + \gamma \neq 0 \tag{5.59}$$

and consequently

$$\langle\langle \breve{u}^n, \breve{u}^j\rangle, \breve{u}^1_\gamma\rangle = \langle\langle \breve{u}^n_{-\gamma}, \breve{u}^j_{-\gamma}\rangle, \breve{u}^1_\gamma\rangle \subset \breve{u}^1_{-\gamma} \tag{5.60}$$

for all weights γ.

Now $\langle \breve{u}^n, \breve{u}^j \rangle$ is a $\mathfrak{g}^s$-invariant subspace of $\mathfrak{g}$, hence the direct sum of an ideal $\mathfrak{b}$ of $\mathfrak{g}^s$ with some subspace of $\mathfrak{g}^a$. Let $H \in \mathfrak{b} \cap \mathfrak{f}$. Then by (5.60)

$$\langle H, \breve{u}^1_\gamma\rangle \subset \breve{u}^1_{-\gamma} \tag{5.61}$$

whereas trivially

$$\langle H, \breve{u}^1_\gamma\rangle \subset \breve{u}^1_\gamma. \tag{5.62}$$

Therefore,

$$\langle H, \breve{u}^1_\gamma\rangle = \{0\} \tag{5.63}$$

for all weights $\gamma \neq 0$. Since this equation is trivial if $\gamma = 0$, we conclude that

$$\langle H, \breve{u}^1\rangle = \{0\}. \tag{5.64}$$

But we know that $\mathrm{ad}\breve{u}_1$ is faithful. Therefore $H = 0$, i.e., $\mathfrak{b} \cap \mathfrak{f} = \{0\}$. This implies $\mathfrak{b} = \{0\}$, hence

$$\langle \breve{u}^n, \breve{u}^j\rangle \subset \mathfrak{g}^a \text{ if } 2 \leq j \leq n-1. \tag{5.65}$$

It is now easy to prove the same relation for $j = 1$. In fact, because

$$\langle \breve{u}^2, \breve{u}^n\rangle \subset \mathfrak{g}^a, \quad \langle \breve{u}^2, \breve{u}^1\rangle = \{0\} \tag{5.66}$$

[see (5.65) and (5.47)] we have

$$\begin{aligned} \langle \breve{u}^2, \langle \breve{u}^n, \breve{u}^1\rangle\rangle &\subset \langle\langle \breve{u}^2, \breve{u}^n\rangle, \breve{u}^1\rangle + \langle \breve{u}^n, \langle \breve{u}^2, \breve{u}^1\rangle\rangle \\ &= \{0\}, \end{aligned} \tag{5.67}$$

and since $\mathrm{ad}\breve{u}_2$ is faithful we conclude that

$$\langle \breve{u}^n, \breve{u}^1\rangle \subset \mathfrak{g}^a. \tag{5.68}$$

Collecting our results we have shown that for $n \geq 3$

$$\langle \breve{u}, \langle \mathfrak{g}^a, \breve{u}\rangle\rangle \subset \mathfrak{g}^a. \tag{5.69}$$

But then $\mathfrak{g}^a \oplus \langle \mathfrak{g}^a, \breve{u} \rangle$ is an ideal of $\mathfrak{a}$, as desired.

Hence we are left with the case $n = 2$. This case will be dealt with by an examination of the most general ansatz for the product $\breve{u} \times \breve{u} \to \mathfrak{g}$. Since $\mathrm{ad}\breve{u}$ is faithful we conclude that

$$\dim \mathfrak{g}^a = 1. \tag{5.70}$$

For the following discussion it will be adequate to modify our notation. From Lemmas 3 and 4 we know that there exists an irreducible representation of $\mathfrak{g}^s$ in some vector space $\breve{u}^0$ such that $\breve{u}$ (equipped with the adjoint representation of $\mathfrak{g}^s$ in $\breve{u}$) is isomorphic to the direct sum of two copies of $\breve{u}^0$. Therefore, we shall write the elements of $\breve{u}$ in the form of pairs $\binom{u_1}{u_2}$ with u_1, $u_2 \in \breve{u}^0$. The subspace $\breve{u}^1$ (resp. $\breve{u}^2$) consists of the vectors of the form $\binom{u}{0}$ [resp. $\binom{0}{u}$] with $u \in \breve{u}^0$. Furthermore, there is an element $E \in \mathfrak{g}^a$ such that

$$\left\langle E, \binom{u_1}{u_2} \right\rangle = \binom{u_2}{0}, \quad u_1, u_2 \in \mathfrak{u}^0. \tag{5.71}$$

The Jacobi identity for E and two elements of $\breve{\mathfrak{u}}$ yields

$$\left\langle \begin{pmatrix} u \\ 0 \end{pmatrix}, \begin{pmatrix} v \\ 0 \end{pmatrix} \right\rangle = 0, \tag{5.72}$$

$$\left\langle \begin{pmatrix} u \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ v \end{pmatrix} \right\rangle = -\left\langle \begin{pmatrix} v \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ u \end{pmatrix} \right\rangle \tag{5.73}$$

for all $u,\ v \in \breve{\mathfrak{u}}^0$. [The first equation is of course a special case of (5.47)].

Let us now define two bilinear maps ($i=1,2$)

$$\beta_i : \breve{\mathfrak{u}}^0 \times \breve{\mathfrak{u}}^0 \to \mathfrak{g}^s \tag{5.74a}$$

and two bilinear forms

$$\phi_i : \breve{\mathfrak{u}}^0 \times \breve{\mathfrak{u}}^0 \to K \tag{5.74b}$$

by

$$\begin{aligned} \left\langle \begin{pmatrix} u \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ v \end{pmatrix} \right\rangle &= \beta_1(u,v) + \phi_1(u,v)E, \\ \left\langle \begin{pmatrix} 0 \\ u \end{pmatrix}, \begin{pmatrix} 0 \\ v \end{pmatrix} \right\rangle &= \beta_2(u,v) + \phi_2(u,v)E \end{aligned} \tag{5.75}$$

Then β_1 and ϕ_1 are skew-symmetric [see (5.73)] whereas β_2 and ϕ_2 are symmetric [by (2.10)]. Furthermore, the β_i and ϕ_i are $\mathfrak{g}^s$ invariant. In order to prove that $\mathfrak{g}^a \oplus \langle \mathfrak{g}^a, \breve{\mathfrak{u}} \rangle = \mathfrak{g}^a \oplus \breve{\mathfrak{u}}^1$ is an ideal of $\mathfrak{a}$ we have to show that $\beta_1 = 0$.

The Jacobi identity (with all three elements taken from $\breve{\mathfrak{u}}$) yields the following conditions on the β_i and ϕ_i (the representation of $\mathfrak{g}^s$ in $\breve{\mathfrak{u}}^0$ will be denoted by $X \to \tilde{X}$):

$$\tilde{\beta}_2(u,v)w + \tilde{\beta}_2(v,w)u + \tilde{\beta}_2(w,u)v = 0, \tag{5.76}$$

$$\phi_2(u,v)w + \phi_2(v,w)u + \phi_2(w,u)v = 0, \tag{5.77}$$

$$\tilde{\beta}_1(u,v)w + \tilde{\beta}_1(u,w)v = 0, \tag{5.78}$$

$$\tilde{\beta}_2(v,w)u + \phi_1(u,v)w + \phi_1(u,w)v = 0, \tag{5.79}$$

$$\tilde{\beta}_1(u,w)v + \tilde{\beta}_1(v,w)u = 0, \tag{5.80}$$

for all $u,\ v,\ w \in \breve{\mathfrak{u}}^0$.

Evidently, now,

$$\tilde{\beta}_1(u,v)w \text{ is totally skew-symmetric in } u,\ v,\ w \tag{5.81}$$

hence we may suppose

$$\dim \breve{\mathfrak{u}}_0 \geq 3, \tag{5.82}$$

for otherwise $\beta_1 = 0$. From (5.77) we conclude that

$$\phi_2 = 0. \tag{5.83}$$

Note that as a consequence of (5.79) $\tilde{\beta}_2$ is completely determined by ϕ_1. Equation (5.76) then says that ϕ_1 is skew-symmetric (as we already know).

As we have seen, $\phi_2 = 0$. But then $\phi_1 \neq 0$, for otherwise we would conclude that $\langle \breve{\mathfrak{u}}, \breve{\mathfrak{u}} \rangle \neq \mathfrak{g}$. Now the representation of $\mathfrak{g}^s$ in $\breve{\mathfrak{u}}^0$ is irreducible, and the bilinear form ϕ_1 is $\mathfrak{g}^s$-invariant. Therefore

$$\begin{aligned} &\phi_1 \text{ is skew-symmetric and nondegenerate; in particular } \breve{\mathfrak{u}}^0 \\ &\text{has even dimension.} \end{aligned} \tag{5.84}$$

Now let $\mathrm{sp}(\phi_1)$ denote the symplectic Lie algebra of all linear maps of $\breve{\mathfrak{u}}^0$ into itself that leave ϕ_1 invariant. Since ϕ_1 is $\mathfrak{g}^s$-invariant we know that

$$\tilde{\beta}_i(u,v) \in \mathrm{sp}(\phi_1) \text{ for all } u,\ v \in \breve{\mathfrak{u}}^0,\quad i=1,2. \tag{5.85}$$

For $\tilde{\beta}_2(u,v)$ this condition is automatically satisfied as a consequence of (5.79).

It is now easy to show that the linear mappings $\tilde{\beta}_2(u,v)$, $u,\ v \in \breve{\mathfrak{u}}^0$, generate the vector space $\mathrm{sp}(\phi_1)$. In fact, consider the linear map

$$\begin{aligned} &\hat{\beta}_2 : \breve{\mathfrak{u}}^0 \otimes \breve{\mathfrak{u}}^0 \to \mathrm{sp}(\phi_1) \\ &u \otimes v \to \tilde{\beta}_2(u,v) \end{aligned} \tag{5.86}$$

defined by $\tilde{\beta}_2$. We have to show that $\hat{\beta}_2$ is surjective.

Using (5.79) and the fact that ϕ_1 is nondegenerate it is easy to see that the kernel of $\hat{\beta}_2$ is equal to the subspace of skew-symmetric tensors. Our assertion then follows by considering the dimensions.

We consider next the linear map

$$\begin{aligned} &\hat{\beta}_1 : \breve{\mathfrak{u}}^0 \otimes \breve{\mathfrak{u}}^0 \to \mathrm{sp}(\phi_1), \\ &u \otimes v \to \tilde{\beta}_1(u,v), \end{aligned} \tag{5.87}$$

defines by $\tilde{\beta}_1$. As we have seen, every element of $\mathrm{sp}(\phi_1)$ is the representative of some element of $\mathfrak{g}^s$. Since β_1 is $\mathfrak{g}^s$-invariant, we conclude that β_1 is $\mathrm{sp}(\phi_1)$-invariant. Now β_1 is skew-symmetric; hence all symmetric tensors are in the kernel of $\hat{\beta}_1$. Considering the dimensions we see that $\hat{\beta}_1$ is certainly not surjective. But then $\hat{\beta}_1 = 0$ since $\hat{\beta}_1$ is $\mathrm{sp}(\phi_1)$-invariant and since the Lie algebra $\mathrm{sp}(\phi_1)$ is simple. We conclude that $\tilde{\beta}_1 = 0$ and hence $\beta_1 = 0$, as desired.

The theorem is proved. There should exist a simpler proof which in particular avoids the ugly separation of the cases $n=2$ and $n \geq 3$.

Remark: Let us suppose further on that K is algebraically closed and that $\mathfrak{a} = \mathfrak{g} \oplus \breve{\mathfrak{u}}$ is a simple pseudo Lie algebra. We assume that $\mathfrak{g}$ is reductive with nontrivial center, i.e., $\mathfrak{g}$ is the direct product of a semisimple Lie algebra $\mathfrak{g}^s$ with an Abelian Lie algebra $\mathfrak{g}^a \neq \{0\}$. Then $\breve{\mathfrak{u}}$ is the direct sum of two $\mathfrak{g}$ irreducible subspaces $\breve{\mathfrak{u}}_1$ and $\breve{\mathfrak{u}}_2$ such that

$$\langle \breve{\mathfrak{u}}_1, \breve{\mathfrak{u}}_1 \rangle = \langle \breve{\mathfrak{u}}_2, \breve{\mathfrak{u}}_2 \rangle = \{0\},\quad \langle \breve{\mathfrak{u}}_1, \breve{\mathfrak{u}}_2 \rangle = \mathfrak{g}. \tag{5.88}$$

Call $\mathrm{ad}_{\breve{\mathfrak{u}}_i}$ the representation of $\mathfrak{g}$ in $\breve{\mathfrak{u}}_i$ induced by the adjoint representation. As Lemma 3 shows, $\breve{\mathfrak{u}}_1$ and $\breve{\mathfrak{u}}_2$ are even $\mathfrak{g}^s$-irreducible; hence $\mathrm{ad}_{\breve{\mathfrak{u}}_i} A$ is, for any $A \in \mathfrak{g}^a$, a scalar multiple of the identity, i.e.,

$$\mathrm{ad}_{\breve{\mathfrak{u}}_i} A = \alpha_i \mathrm{id}_{\breve{\mathfrak{u}}_i},\quad \alpha_i \in K.1 \tag{5.89}$$

Define $\dim \breve{\mathfrak{u}}_i = m_i$ and let ϕ denote the Killing form of $\mathfrak{a}$. Then [see Lemma 1, (ϵ)]

$$\begin{aligned} &m_1\alpha_1 + m_2\alpha_2 = \mathrm{tr}(\mathrm{ad}_{\breve{\mathfrak{u}}} A) = 0, \\ &m_1\alpha_1^2 + m_2\alpha_2^2 = -\phi(A,A). \end{aligned} \tag{5.90}$$

since $\mathrm{ad}_{\breve{\mathfrak{u}}}$ is faithful we conclude that

$$\dim \mathfrak{g}^a = 1 \tag{5.91}$$

and, furthermore, that $\phi \neq 0$, hence that ϕ is nondegenerate. From Eqs. (5.88) and the definition of the Killing form one can easily deduce that the restrictions of ϕ to $\breve{\mathfrak{u}}_1$ and to $\breve{\mathfrak{u}}_2$ are zero. Therefore, the restriction of

ϕ to $\breve{u}_1 \times \breve{u}_2$ is nondegenerate, which implies that the representations $\mathrm{ad}_{\breve{u}_1}$ and $\mathrm{ad}_{\breve{u}_2}$ of $\mathfrak{g}^s$ are contragredient with respect to each other (and in particular that $m_1 = m_2$).

6. DISCUSSION OF OUR RESULTS CONCERNING SIMPLE PSEUDO LIE ALGEBRAS

Let K be algebraically closed and let $\mathfrak{a} = \mathfrak{g} \oplus \breve{u}$ be a simple pseudo Lie algebra. Suppose that $\mathfrak{g}$ is reductive: $\mathfrak{g} = \mathfrak{g}^s \times \mathfrak{g}^a$ with $\mathfrak{g}^s$ semisimple and $\mathfrak{g}^a$ Abelian. Then $\mathfrak{a}$ belongs to one of the following four classes.

(I) $\mathfrak{g}$ has a nontrivial center $\mathfrak{g}^a$. Then $\mathfrak{g}^a$ is one-dimensional, the Killing form of $\mathfrak{a}$ is nondegenerate and $\breve{u}$ decomposes into the direct sum of two $\mathfrak{g}$-irreducible (hence $\mathfrak{g}^s$-irreducible) subspaces $\breve{u}_1, \breve{u}_2$. The representations of $\mathfrak{g}^s$ in $\breve{u}_1$ and $\breve{u}_2$ are contragredient with respect to each other. Examples of this class are the algebras $\mathrm{spl}(n,m)$, $n > m \geq 1$, of Sec. 4($\mathfrak{g}$) and the algebras $\mathfrak{a}(2p,2)$, $p \geq 1$, of Sec. 4(c). Note that $\mathrm{spl}(2,1)$ and $\mathfrak{a}(2,2)$ are isomorphic.

(II) $\mathfrak{g}$ is semisimple and there exists a nondegenerate even invariant bilinear form on $\mathfrak{a}$. Perhaps one should distinguish between two cases:

(1) the Killing form of $\mathfrak{a}$ is nondegenerate;

(2) the Killing form of $\mathfrak{a}$ is zero.

Members of the class (II.1) are the algebras $\mathfrak{a}(2p,m)$ with p, $m \geq 1$ but $m \neq 2$ and $2p \neq m-2$, of Sec. 4(c).[13] Algebras of the class (II.2) are $\mathrm{spl}(n,n)/\mathfrak{z}_n$, $n \geq 2$, and $\mathfrak{a}(2p, 2p+2)$, $p \geq 1$; see Sec. 4(a),(c).

(III) $\mathfrak{g}$ is semisimple and there exists a nondegenerate odd invariant bilinear form on $\mathfrak{a}$ (in particular the Killing form is zero). One can prove[14] that the algebras of this class are precisely those for which the adjoint representation of $\mathfrak{g}$ in $\breve{u}$ is isomorphic to the adjoint representation of $\mathfrak{g}$ (in $\mathfrak{g}$) and that the members of this class are just the algebras $\mathfrak{b}_n/\mathfrak{z}_n$, $n \geq 3$, of Sec. 4(e).

(IV) $\mathfrak{g}$ is semisimple and there is no nonzero invariant bilinear form on $\mathfrak{a}$. Examples of this type are the algebras $\mathfrak{b}_n$, $n \geq 3$, of Sec. 4(d).

Presumably, with this classification we have reached a position where a detailed inspection of the representations of semisimple Lie algebras could lead to the construction of all simple pseudo Lie algebras whose appertaining Lie algebra is reductive.

As we have mentioned case (III) has already been settled. For the classes (I) and (II) the methods of Pais and Rittenberg will be useful. One should note, furthermore, that the vanishing of the Killing form of $\mathfrak{a}$ implies in particular that the Killing form of the (semisimple) Lie algebra $\mathfrak{g}$ is equal to the invariant bilinear form on $\mathfrak{g}$ associated with the adjoint representation of $\mathfrak{g}$ in $\breve{u}$. Work along these lines is in progress.

7. SOME RESULTS ON SEMISIMPLE PSEUDO LIE ALGEBRAS

In this section we do not try to give a general definition of semisimple pseudo Lie algebras. Presumably any simple pseudo Lie algebra should be semisimple. Therefore we prefer to wait until our knowledge of simple pseudo Lie algebras has been improved. Nevertheless the pseudo Lie algebras with nondegenerate Killing form should be semisimple according to every reasonable definition of semisimplicity, for we can prove that these algebras are direct products of simple pseudo Lie algebras. In fact, we have the more general following theorem.

Theorem 3: Suppose that a pseudo Lie algebra $\mathfrak{a}$ has the following properties:

(1) there exists a nondegenerate homogeneous invariant bilinear form ϕ on $\mathfrak{g}$,

(2) $\mathfrak{a}$ does not contain any nonzero graded Abelian ideal. Then $\mathfrak{a}$ has only a finite number of minimal graded ideals $\mathfrak{b}_1, \ldots, \mathfrak{b}_r$ and $\mathfrak{g}$ is their direct product. The ideals $\mathfrak{b}_j$ are simple pseudo Lie algebras and they are orthogonal with respect to ϕ. Any left or right ideal of $\mathfrak{a}$ is graded and is equal to $\bigoplus_{j \in J} \mathfrak{b}_j$ with a suitable subset J of $\{1, \ldots, r\}$.

Proof: The first part of this proof is a trivial modification of a proof originally due to Dieudonné (see Ref. 15). We repeat it here for the convenience of the reader.

If $\mathfrak{b}$ is any graded ideal of $\mathfrak{a}$, then

$$\mathfrak{b}^\perp = \{X \in \mathfrak{a} \mid \phi(X, Y) = 0 \text{ for all } Y \in \mathfrak{b}\} \tag{7.1}$$

is also a graded ideal of $\mathfrak{a}$.

Now suppose that $\mathfrak{b}$ is a minimal graded ideal of $\mathfrak{a}$ (of course we assume that $\mathfrak{b} \neq \{0\}$). Then $\mathfrak{b} \cap \mathfrak{b}^\perp$ is a graded ideal of $\mathfrak{a}$, hence equal to $\mathfrak{b}$ or to $\{0\}$. In the first case we conclude that

$$\phi(\mathfrak{a}, \langle \mathfrak{b}, \mathfrak{b} \rangle) = \phi(\langle \mathfrak{b}, \mathfrak{a} \rangle, \mathfrak{b}) \subset \phi(\mathfrak{b}^\perp, \mathfrak{b}) = \{0\}. \tag{7.2}$$

But ϕ is nondegenerate, hence $\langle \mathfrak{b}, \mathfrak{b} \rangle = \{0\}$ and therefore [because of property (2)] $\mathfrak{b} = \{0\}$, contrary to our assumption. It follows that $\mathfrak{a} = \mathfrak{b} \oplus \mathfrak{b}^\perp$ and furthermore (since $\mathfrak{b}$ and $\mathfrak{b}^\perp$ are ideals) that

$$\langle \mathfrak{b}, \mathfrak{b}^\perp \rangle \subset \mathfrak{b} \cap \mathfrak{b}^\perp = \{0\} \quad . \tag{7.3}$$

Therefore $\mathfrak{a}$ is the direct product of its graded ideals $\mathfrak{b}$ and $\mathfrak{b}^\perp$. Consequently any graded ideal of $\mathfrak{b}$ or $\mathfrak{b}^\perp$ is a graded ideal of $\mathfrak{a}$. This shows on the one hand that $\mathfrak{b}$ is a simple pseudo Lie algebra. On the other hand, using in addition the obvious fact that the restriction of ϕ to $\mathfrak{b}^\perp \times \mathfrak{b}^\perp$ is nondegenerate, we see that $\mathfrak{b}^\perp$ satisfies the conditions (1) and (2), too. Induction on $\dim \mathfrak{a}$ then implies that

$$\mathfrak{a} = \mathfrak{b}_1 \times \cdots \times \mathfrak{b}_r, \tag{7.4}$$

where $\mathfrak{b}_j$, $1 \leq j \leq r$, are minimal graded (and hence simple) ideals of $\mathfrak{a}$ which are orthogonal with respect to ϕ.

Now let $\mathfrak{f}$ be any left ideal of $\mathfrak{a}$. If $j \in \{1, \ldots, r\}$, then $\mathfrak{b}_j \cap \mathfrak{f}$ is a left ideal of $\mathfrak{b}_j$, hence (see Sec. 3, Proposition 1) equal to $\{0\}$ or to $\mathfrak{b}_j$. In the first case

$$\langle \mathfrak{b}_j, \mathfrak{f} \rangle \subset \mathfrak{b}_j \cap \mathfrak{f} = \{0\}, \tag{7.5}$$

in the second case $\mathfrak{b}_j \subset \mathfrak{f}$. Define

$$J = \{j \mid 1 \leq j \leq r, \ \mathfrak{b}_j \subset \mathfrak{f}\}. \tag{7.6}$$

If $H \in \mathfrak{f}$ and if

$$H = \sum_{j=1}^{r} H_j, \quad H_j \in \mathfrak{f}_j, \quad 1 \leq j \leq r, \tag{7.7}$$

then $i \in \{1, \ldots, r\}$, $i \notin J$, implies that

$$\langle B, H_i \rangle = \langle B, H \rangle = 0 \text{ for all } B \in \mathfrak{b}_i. \tag{7.8}$$

This means that H_i is an element of the center of $\mathfrak{b}_i$, hence it is equal to zero (since $\mathfrak{b}_i$ is simple). Consequently

$$\mathfrak{f} = \bigoplus_{j \in J} \mathfrak{b}_j \tag{7.9}$$

as desired. In particular, every minimal graded ideal of $\mathfrak{a}$ is equal to some $\mathfrak{b}_j$.

The case of a right ideal $\mathfrak{f}$ is treated similarly, hence our theorem is proved.

If the Killing form ϕ of a pseudo Lie algebra $\mathfrak{a}$ is nondegenerate, then Theorem 3 is applicable. In fact, we have to show that assumption (2) is satisfied. Let γ be the grading automorphism of $\mathfrak{a}$ [see Sec. 2(b), (e)]. If $\mathfrak{b}$ is a graded ideal of $\mathfrak{a}$ such that $\langle \mathfrak{b}, \mathfrak{b} \rangle = \{0\}$ and if $A \in \mathfrak{a}$, $B \in \mathfrak{b}$, then

$$\gamma\langle A, \langle B, \mathfrak{a} \rangle\rangle \subset \mathfrak{b}, \quad \gamma\langle A, \langle B, \mathfrak{b} \rangle\rangle = \{0\}, \tag{7.10}$$

and therefore

$$\phi(A, B) = \mathrm{tr}(\gamma(\mathrm{ad}A)(\mathrm{ad}B)) = 0. \tag{7.11}$$

Since ϕ is nondegenerate, we conclude that $\mathfrak{b} = \{0\}$, as desired.

With the notations of Theorem 3, the $\mathfrak{b}_j$ are orthogonal with respect to ϕ and it is easy to see that the restriction of ϕ to $\mathfrak{b}_j \times \mathfrak{b}_j$ is the Killing form of $\mathfrak{b}_j$. Consequently, the Killing form of $\mathfrak{b}_j$ is nondegenerate. Thus we have proved the following corollary.

Corollary 1: If the Killing form of a pseudo Lie algebra $\mathfrak{a}$ is nondegenerate, then $\mathfrak{a}$ is the direct product of simple pseudo Lie algebras whose Killing forms are nondegenerate.

Theorem 3 and Corollary 1 are useful if one wants to change the base field K. For example, using Corollary 1 as well as Theorem 1, 2, and Proposition 3 of Sec. 5, we deduce Corollary 2.

Corollary 2: If the Killing form of a pseudo Lie algebra $\mathfrak{a} = \mathfrak{g} \oplus \mathfrak{u}$ is nondegenerate, then the adjoint representation of $\mathfrak{g}$ in $\mathfrak{u}$ is completely reducible.

In particular, for simple pseudo Lie algebras with nondegenerate Killing form the two conjectures of Sec. 5 are true. Note that we do not assume that K is algebraically closed.

[1]We prefer to call them "pseudo Lie algebras" since the name "graded Lie algebras" might lead to confusion with Lie algebras (in the ordinary sense) which are graded (such objects occur in the mathematical literature, too).
[2]L. Corwin, Y. Ne'eman, and S. Sternberg, Rev. Mod. Phys. 47, 573 (1975).
[3]M. Scheunert, to be published.
[4]Bourbaki, *Algèbre* (Hermann, Paris, 1962), 3rd ed., Chap. Chap. II, Sec. 11.
[5]Bourbaki, *Algèbre* (Hermann, Paris, 1971), Chap. III.
[6]Ref. 5, Sec. 4, *n*°7.
[7]A. Pais and V. Rittenberg, Preprint Rockefeller University, New York, C00-2232B-74.
[8]See also Ref. 2.
[9]Bourbaki, *Groups et algèbres de Lie* (Hermann, Paris, 1960), Chap. I, Sec. 6, Proposition 5.
[10]See Ref. 9, Sec. 6, Proposition 6.
[11]See Ref. 9, Sec. 3, Proposition 1.
[12]Bourbaki, *Algèbre* (Hermann, Paris, 1958), Chap. VIII, Sec. 9, Propostion 10.
[13]Note that the algebras of class (II, 1) are of the type studied by A. Pais and V. Rittenberg in Ref. 7, but the authors seem to have assumed that $\mathfrak{g}$ is simple [otherwise $\alpha^i \alpha_i$ in their formula (3.39) may be zero], and hence they have found (essentially) only the algebras $\mathfrak{a}(2p, 1)$, $p \geq 1$.
[14]M. Scheunert, to be published.
[15]N. Jacobson, *Lie algèbras* (Interscience, New York, 1962), Chap. III, *n*°5, Theorem 3.

Phase integral approximations for calculating energy bands*

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The phase integral approximation is modified to incorporate an energy-dependent effective potential that manifests the energy band character of lattice potentials. The resultant phase integral approximation because of its inherent renormalization demonstrates superior validity. Numerical examples which compare this approximation with other methods substantiate the superior convergence of this modified phase integral approximation.

I. INTRODUCTION

In application to the one-dimensional periodic potential, neither the ordinary WKB approximation, nor its progeny, the phase integral approximation (we use N. Fröman's definition of phase integral approximation[1]; regrettably this terminology is not universal), predict in general the existence of band gaps in energy when applied to the nearly free electron (NFE) (i.e., an electron with sufficient energy to preclude the existence of classical turning points). This deficiency manifests that both of these approximations ignore the effects of continuous reflections of a wave in a slowly varying medium which accumulates coherently for a periodic medium under conditions of Bragg reflection.

In order to correct the aforementioned deficiency, the phase integral approximation is modified to develop a new method herein by introducing an energy-dependent effective potential in the phase integral. This effective potential, which is developed from first principles to first order in potential, has innate renormalization which renders a most robust approximation with superior validity. We emphasize fidelity of the approximate eigenfunctions as well as the accuracy of the associated eigenvalue estimate.

In Sec. II we develop an energy-dependent effective potential which is substituted into the phase integral approximation. This effective potential manifests band gaps for periodic potentials that are consistent with first-order degenerate perturbation theory. The high-wavenumber spectral components of the original potential are shown to be attenuated in the effective potential. In Sec. III, we investigate the innate renormalization of the effective potential phase integral approximation. We make a comparison among the spectral analyses of a Matheiu function and both its WKB and its effective potential phase integral approximations. Leading order error terms are deduced, and these establish the superiority of the effective potential. In Sec. IV, numerical examples are adduced to substantiate the improvement in performance of the approximation that is rendered by using the effective potential.

II. THE EFFECTIVE POTENTIAL

The time-independent Schrödinger equation in the one-dimensional case may be expressed as

$$\frac{d^2\psi(x)}{dx^2} + Q^2(x)\psi(x) = 0,$$

where

$$Q(x) = \{(2\mu/\hbar^2)[E - V(x)]\}^{1/2},$$

E is the energy, and V is the potential. The lattice periodicity is assumed to be "a", i.e., $V(x+a) = V(x)$. For application of the ordinary WKB approximation, the first-order (in $\hbar$) prerequisities of Fröman and Fröman[2] are

$$\frac{1}{4Q^2}\left|(\Upsilon;\ x)\right| \ll \frac{1}{2}\left|\frac{d}{dx}(Q^{-1})\right| \ll 1 \tag{1}$$

and

$$\tfrac{1}{4}\left|\int_0^a (\Upsilon;\ x)Q^{-1}\,dx\right| \ll 1, \tag{2}$$

where $(\Upsilon; x)$ is the Schwarzian derivative of Υ and is defined by

$$(\Upsilon; x) = -2Q^{1/2}\frac{d^2}{dx^2}(Q^{-1/2})$$

and where

$$\Upsilon = \int^x Q(x')\,dx'.$$

Let us substitute into the time-independent Schrödinger equation that

$$\psi(x) = \phi[z(x)]/[z_1(x)]^{1/2},$$

where $z_1 = dz/dx$ and in general $z_n = (d^n z/dx^n)$. The Schrödinger equation is then mapped into

$$\frac{d^2\phi(z)}{dz^2} + R(z)\phi(z) = 0, \tag{3}$$

where

$$R(z) = z_1^{-2}\{Q^2 - \tfrac{1}{2}(z; x)\} \tag{4}$$

and where the Schwarzian derivative of z is defined by

$$(z; x) = -2z_1^{1/2}\frac{d^2}{dx^2}(z_1^{-1/2}).$$

With $R(z)$ appropriately assigned, the solution to Eq. (3) will be in closed form: for $R(z) = 1$, $\phi = \exp(\pm iz)$; for $R(z) = bz^n$,

$$\phi = z^{1/2}J_{1/(n+2)}\left(\frac{2b^{1/2}}{n+2}z^{(n/2)+1}\right),$$

etc. Equation (4) must be solved for z to develop an explicit expression for $\psi(x)$.

If $R(z)$ is chosen to mimic $Q^2(x)$ throughout the domain of interest, z_1 will then be nearly constant, and $(z; x)$ in Eq. (4) may be neglected. Then

$$z_1 \approx [Q^2(x)/R(z)]^{1/2}. \tag{5}$$

If $R(z)=1$, then $\psi(x)$ becomes the phase integral approximation to first order in $\hbar$. Consistent with well-known results, the approximation of Eq. (5) improves as $E \to -\infty$.

In the case of $R(z)=1$, contemporary workers have used an asymptotic expansion in powers of $\hbar$ when solving for z_1 where the right side of Eq. (5) represents the first term. (The asymptotic expansions for the phase integral and WKB approximations begin to differ with the $\hbar^3$ order term.[1]) N. Fröman[1] has shown that those points at which the asymptotic expansion for z_1 diverges without limit and the zeroes of z_1 are singular branch points of $\psi(x)$. The form of the higher order phase integral approximations is convenient for choosing branch cuts that allow a reasonable contour path close to the real axis in order to satisfy the conditions of Eq. (2). As in the WKB case, the domain of applicability of this phase integral expansion is limited by its asymptotic nature.

Hecht and Mayer[3] offer an alternative approach for solving the time-independent Schrödinger equation based upon iterative approximate solutions to Eq. (4). Their results are modified herein with $R(z)$ carried explicitly. Let $z^{(m)}$ represent the mth iteration for the approximation of z. If $z^{(m)}$ is a close approximation, then $dz/dz^{(m)} \approx 1$ and $(z; z^{(m)})$ may be neglected. Under these circumstances, Hecht and Mayer have shown that[4]

$$[R(z^{(m+1)})]^{1/2}\frac{dz^{(m+1)}}{dz^{(m)}} = \left(\frac{dz^{(m)}}{dx}\right)^{-1}[Q^2(x) - \tfrac{1}{2}(z^{(m)}; x)]^{1/2}, \tag{6}$$

where $z^{(m)}$ must be a function such that the quantity inside the brackets on the right side of Eq. (6) remains positive nonzero.

Let us now return to the lattice potential case with periodicity "a" where the potential may be expanded into a Fourier series as

$$V = \sum_{q=-\infty}^{\infty} \gamma_q \exp(i2q\pi x/a).$$

In the nondegenerate case (i.e., E is interior to an energy band) for $E \gg V(x)$, a solution for z_1 may be represented by an effective potential, $W(E,x)$, such that for given E

$$z_1 = \left(\frac{2\mu}{\hbar^2}\right)^{1/2}[E-W]^{1/2} \approx \left(\frac{2\mu}{\hbar^2}\right)^{1/2}\left[E^{1/2} - \frac{W}{2E^{1/2}}\cdots\right]. \tag{7}$$

(The following analysis may be generalized for nonperiodic potentials.) Consistent with Eq. (6), the behavior of $W(E,x)$ is such that $[E-W]$ is always positive nonzero. We therefore have to first order in V by Eqs. (4) and (7) that

$$W = V - \frac{\hbar^2}{8\mu}\frac{d^2W/dx^2}{E}.$$

The effective potential W is then the solution to the inhomogeneous wave equation

$$W'' + \frac{8\mu}{\hbar^2}EW = \frac{8\mu}{\hbar^2}EV \tag{8}$$

or

$$W = \frac{8\mu}{\hbar^2}E\int_0^a G_{4E}(x,x')V(x')\,dx', \tag{9}$$

where the Green's function for the wave equation for $E=\hbar^2k^2/(2\mu)$ is of the form

$$G_{4E}(x,x') = \frac{1}{2k\sin 2ka} \times \begin{cases} \cos[2k(x'-a)]\cos(2kx), & 0 \le x < x', \\ \cos(2kx')\cos[2k(x-a)], & x' < x \le a, \end{cases}$$

for unstable equilibrium points of $V(x')$ located at $x' = 0, \pm a, \cdots$. A tacit nonlocal character of the effective potential is manifested in Eq. (9). By Eq. (8), the effective potential may be represented by

$$W(E,x) = \sum_q \gamma_q \frac{\exp(ik_q x)}{1 - E_q/4E}, \tag{10}$$

where

$$E_q = (\hbar k_q)^2/2\mu, \quad k_q = 2q\pi/a.$$

By Eq. (10) for $E_q > 8E$, the high-wavenumber components of the potential, which are so deleterious to the WKB approximation in accordance with Eqs. (1) and (2), are filtered out from the effective potential progressively with increasing wavenumber.

In accordance with Eq. (7), the previous assumption that $V \ll E$ should now be altered and substituted with the requirement that $W \ll E$. If a large potential, V, is nearly orthogonal over the unit cell to the Green's function for a particular E, such that $E < V_{\max}$ but $E \gg W$, then the domain of validity of the iterative approximation can be extended to include bands of lower energy.

For completeness and mathematical rigor, the exact effective potential W can be described without approximation by the nonlinear differential equation

$$W = V + \frac{\hbar^2}{4\mu}(z;x) = V - \frac{\hbar^2}{8\mu}\frac{d^2W/dx^2}{(E-W)} - \frac{5\hbar^2}{32\mu}\frac{(dW/dx)^2}{(E-W)^2}. \tag{11}$$

In general Eq. (11) is simpler and more tractable to approximation than either Eq. (6) with $R(z)=1$ or Eq. (4).

The Bloch wavenumber k may be deduced from the effective potential by applying the periodic boundary conditions to the modified phase integral, that is,

$$\frac{(2\mu)^{1/2}}{\hbar}\int_0^a [E - W(E,x)]^{1/2}dx = k'a + n\pi, \quad n = 0 \pm 1, \pm 2, \cdots, = ka, \tag{12}$$

where $|k'| < \pi/a$ and $k = k' + (n\pi/a)$. Hence E may be expressed as an explicit function of k. Also as the integration limits in Eq. (12) represent a complete rotation period, $z(a)$ represents an effective action variable [where $z(0)=0$].

Any small but finite effective potential W has an explicit energy dependence [Eq. (10)] with singular points that consist of first-order poles in accordance with the associated Green's function. These singular points in the small potential limit locate the centers of the band

gaps that exist in the allowed energy values for stable solutions to the Schrödinger equation with periodic potential. In order to deduce the width of these band gaps, let $E(k)$ at $k = k_q/2$ for nonzero γ_q be given as

$$E(k_q/2) = \tfrac{1}{8}\hbar^2 k_q^2 + C\gamma_q \tag{13}$$

where C is a constant to be determined. From Eqs. (7), (10), and (13) we have at the qth band gap that

$$z_1 = \left(\frac{k_q^2}{4} + \frac{2\mu C\gamma_q}{\hbar^2}\right)^{1/2}\left(1 - \frac{\exp(ik_q x)}{C} - \sum_{n\neq q}\frac{\gamma_n \exp(ik_n x)}{\hbar^2 k_q^2/8\mu + C\gamma_q - \hbar^2 k_n^2/8\mu}\right)^{1/2}. \tag{14}$$

For z_1 to be positive nonzero in Eq. (14) in accordance with Eq. (6), then $|C| > 1$. Thus, the values $C = +1, -1$ are the limit points for allowed values of E in the vicinity of the band gap [albeit nonstable solutions for $W(E, x)$ may be generated from Eq. 8 for $|C| < 1$ by relaxing the requirement for periodicity in $W(E, x)$], and to first order in γ_q the width of the qth band gap for periodic solutions for $W(E, x)$ is $2\gamma_q$ consistent with first-order degenerate perturbation theory.

For three dimensions, we may now guess the effective potential that is inserted into the phase integral solution, $\psi(\mathbf{r})$, for a lattice potential, $V(\mathbf{r})$ with a lattice cell described by the spatial triad $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$. We assert that

$$\psi(\mathbf{r}) = q^{-1/2}\exp\left(i\int^{\mathbf{r}}\mathbf{q}\cdot d\mathbf{r}'\right),$$

where

$$q = |\mathbf{q}|$$

and

$$\mathbf{q} = \mathbf{K}\left[1 - \sum_{l,m,n}\alpha_{l,m,n}\exp(i\mathbf{k}_{l,m,n}\cdot\mathbf{r})\right]^{1/2},$$

where K is a constant vector such that

$$\int_0^{\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3}\mathbf{q}\cdot d\mathbf{r} = (s+t+u)\pi + \sum_{i+1}^{3}\mathbf{k}\cdot\hat{\mathbf{b}}_i a_i, \quad s,t,u = 0, \pm 1, \pm 2, \cdots,$$

where k has the magnitude of the reduced Bloch wave number and the $\mathbf{b}_i$'s are the unit vectors for the reciprocal space triad. The Fourier coefficients α_{lmn} are given by

$$\alpha_{lmn} = \alpha'_{lmn}/[1 - (k_{lmn}/2K)^2],$$

where α'_{lmn} is the lmnth Fourier coefficient for $V(\mathbf{r})$. Hence the wavefronts of constant phase for $\psi(\mathbf{r})$ may be described as a series of parallel planes that are corrugated along the two dimensions of the planes themselves to produce wafflelike wavefronts. The degree of undulation of the corrugations along the ray normal to the wavefront is dependent upon the running value of the phase integral.

III. RENORMALIZATION

As the effective potential phase integral approximation,

$$[E - W(E,x)]^{-1/4}\exp\left(i\frac{(2\mu)^{1/2}}{\hbar}\int^x [E - W(E,x')]^{1/2}dx'\right),$$

may be represented as a compoundly modulated carrier wave, it is innately a renormalization of the spectral resolution of the solution to the Schrödinger equation. This renormalization offers the prospects of a more uniformly valid approximation than the approximation formed by a perturbation expansion of similar order over the plane-wave set.[5-7]

We shall investigate the ramifications of renormalization by considering the effective potential phase integral approximation for Matheiu functions. Mathieu's equation, when it is represented with periodic coefficients as

$$\frac{d^2\Phi}{dz^2} + (\alpha - 2\gamma\cos 2z)\Phi = 0, \tag{15}$$

has often been used[8,9] as a didactic example with a known exact solution for the study of energy bands of one-dimensional crystals. In Eq. (15) the eigenvalues, α, and the normalized potential, $2\gamma\cos 2z$, correspond respectively to $2\mu E/\hbar^2$ and $2\mu V/\hbar^2$ of the time-independent Schrödinger equation. The solution to Eq. (15), a Mathieu function, is well known to obey Floquet's theorem, and may be expressed as

$$\Phi(z) = \exp(i\nu z)\phi(z) = \exp(i\nu z)\sum_{n=-\infty}^{\infty}c_{2n}\exp(i2nz),$$

where $\phi(z)$ is periodic with period π and ν, the characteristic exponent, is a function of α and γ. For certain ranges of α and γ, ν is entirely real. These ranges form regions (bands) in the α—γ plane where $\exp(i\nu z)$ is the Bloch factor and $\phi(z)$ is stable. For $\gamma \neq 0$ these bands are separated by gaps where $\nu(\alpha, \gamma \neq 0)$ has a nonzero imaginary component which generates unstable solutions, $\Phi(z)$, as $z \to \pm\infty$. For the nth band in the limit $\gamma \to 0$, $(n-1)^2 \leq |\nu^2| = \alpha^2 \leq n^2$ and the bands oscillate in consonance with the order of α. Thus, the qualitative behavior of Mathieu functions, resembles the observed features of electron band theory.

Let us assume that $\alpha \gg \gamma$. We now expand the effective potential phase integral approximation in a power series in γ and rearrange terms as a spectral analysis in order to compare this power series to a higher order perturbation expansion for a plane wave set (i.e., an expansion of Floquet's solution). It is noted that for consistency α must be deduced from the effective action variable, i.e., $z(\pi) = \nu\pi$. This leads to

$$\alpha = \nu^2 + [\gamma^2/2(\nu - \nu^{-1})^2]\cdots \tag{16}$$

vis-a-vis the actual value[10] of

$$\alpha = \nu^2 + [\gamma^2/2(\nu^2 - 1)\cdots. \tag{17}$$

Had α been established by Eq. (17), one would observe a higher order (in γ) wavenumber shift in the characteristic exponent. After a tedious, but straightforward expansion, we have derived the ratio of

$$\frac{c_2}{c_0} = \frac{-\gamma}{4(\nu+1)} - \frac{\gamma^3(\nu^5 - \nu^4 + 39\nu^3 + 4\nu^2 - 56\nu - 5)}{128(\nu+1)^4(\nu-1)^4}\cdots, \quad |\nu| \neq 1, \tag{18}$$

which compares to the tabled value[11] of

$$\frac{c_2}{c_0} = \frac{-\gamma}{4(\nu+1)} - \frac{\gamma^3(\nu^2 + 4\nu + 7)}{128(\nu+1)^3(\nu+2)(\nu-1)}\cdots, \quad |\nu| \neq 1, 2, 3, \cdots. \tag{19}$$

Hence, the relative error in Eq. (18) is $O(\gamma^3/\nu^4)$. Likewise, this approximation gives

$$\frac{c_4}{c_0}=\frac{\gamma^2(\nu^2-3\nu+5)}{32(\nu+1)^2(\nu-1)^2}\cdots, \quad |\nu|\neq 1, 2, \tag{20}$$

vis-a-vis the tabled value[11] for Floquet solutions of

$$\frac{c_4}{c_0}=\frac{\gamma^2}{32(\nu+1)(\nu+2)}\cdots, \quad |\nu|\neq 1, 2, \cdots.$$

The relative error in Eq. (20) is $O(\gamma^2/\nu^4)$. In turn, for large α, our approximation to leading orders in γ and ν for the general term gives

$$\frac{c_{2N}}{c_0}\approx\frac{(-)^N\gamma^N\Gamma(\nu+1)}{2^{2N}\nu^{N-1}N!\,\Gamma(\nu+2)}, \quad \nu\neq 1, 2, \cdots, N, \tag{21}$$

vis-a-vis the correct value[11] of

$$\frac{c_{2N}}{c_0}=\frac{(-)^N\gamma^N\Gamma(\nu+1)}{2^{2N}N!\,\Gamma(\nu+N+1)}\cdots, \quad \nu\neq 1, 2, \cdots N,$$

which indicates an error in Eq. (21) of $O(\gamma^N/\nu^{N+1})$ for $N\neq -2, -1, 0, 1, 2$. Thus, the leading ν dependence in the error terms (located in both the γ^2 and γ^3 terms) is $O(\nu^{-4})$. Hence, as a result of renormalization, the effective potential phase integral approximation is expected to approach the accuracy of a second order perturbation solution. These error terms also manifest the limits where validity breaks down.

The set of WKB approximations has been identified as nonorthogonal.[12] However, here we observe that the orthogonality of the set of effective potential phase integral approximations is consistent to almost second order perturbation theory; again the deviation from orthogonality is of $O(\gamma^2/\nu^4)$.

Had we analyzed the WKB approximation, then the corresponding ratio for the WKB representation is

$$\frac{c_{\pm 2}}{c_0}=\frac{\mp\gamma}{4\nu}(1\mp\nu^{-1})+O(\gamma^2). \tag{22}$$

By Eqs. (19) and (22), the leading relative error for the WKB approximation is in the term $O(\gamma/\nu^3)$. Consequently, one expects the WKB approximation to approach the accuracy of only a first order perturbation solution and to have limits of validity inferior to those of the effective potential phase integral approximation. For completeness, Furry[13] described the error in the WKB approximation as $x\to\infty$ as $O(E^{-1})$, i.e., $O(\nu^{-2})$. However, Furry applied the WKB approximation to the harmonic oscillator where the Schwarzian derivative $(z; x)$ does not remain small over the entire range. Here we have applied the WKB approximation to a unit cell of a periodic potential with α sufficiently great to preclude the existence of any classical turning points, and consequently the Schwarzian derivative remains small throughout the unit cell.

IV. NUMERICAL EXAMPLES

Let us make some energy calculations for the normalized (i.e., $\hbar^2/2\mu=1$) lattice potential of Mathieu, $V=2\gamma\cos 2x$. Exact energies are the eigenvalues, α's, for Mathieu's equation. For the effective potential phase integral approximation, a first approximation for the eigenvalue, $\alpha_{(1)}$, is deduced from the effective action variable consistent with Eq. (16) and for a Mathieu potential may be derived in closed form for a given characteristic exponent ν (i.e., Bloch wavenumber) as

$$\int_0^\pi[\alpha_{(1)}-W(\alpha_{(1)},x)]^{1/2}dx$$
$$=2\left[\alpha_{(1)}+\frac{2\gamma}{1-\alpha_{(1)}^{-1}}\right]^{1/2}\mathrm{E}\left(\frac{4\gamma}{\alpha_{(1)}-1+2\gamma}\right)$$
$$=\nu\pi,$$

where $\mathrm{E}(x)$ is the complete elliptic function of the second kind and

$$W(\alpha_{(1)},x)=\frac{2\gamma}{1-\alpha_{(1)}^{-1}}\cos 2x.$$

$\alpha_{(1)}$ is equivalent to a first principles quantum defect method for the calculation of α. A more sophisticated calculation for the eigenvalue, $\alpha_{(2)}$, is given by evaluating the expected value of the Hamiltonian, i.e.,

$$\alpha_{(2)}=\langle\alpha_{(1)}|H|\alpha_{(1)}\rangle/\langle\alpha_{(1)}|\alpha_{(1)}\rangle$$
$$=\alpha_{(1)}-\frac{\gamma^2\Omega^2}{2\alpha_{(1)}^{5/2}}\frac{[\alpha_{(1)}+2\gamma\Omega]^{1/2}}{(2/\pi)\mathrm{K}(4\gamma\Omega/(\alpha_{(1)}+2\gamma\Omega))}$$
$$\times\left[1-\frac{5}{8}\frac{\gamma^2\Omega^2}{\alpha_{(1)}^2}\right]\cdots, \tag{23}$$

TABLE I. Calculated eigenvalues, α's, of Mathieu's equation, $\psi''+(\alpha-2\gamma\cos 2x)\psi=0$ for selected γ and selected values of the characteristic exponent ν.

Characteristic exponent, ν	0.3	1.9	3.5	4.5	5.5
γ	0.03	1.0	1.0	1.0	1.0
α, Rounded-off Exact	.089 505 558 48	3.710	12.294 632	20.276 003 36	30.267 101 56
$\alpha_{(2)}$, Phase Integral[a]	.089 506 323 82	3.714	12.294 607	20.276 002 09	30.267 101 41
$\alpha_{(1)}$, Phase Integral[b]	.090 048 982 32	3.676	12.298 481	20.277 342 59	30.267 684 18
$\alpha_{(2)}$, WKB[a]	.1649[d]	3.780	12.294 290	20.275 937 27	30.267 082 55
$\alpha_{(1)}$, WKB[c]	.095 194[d]	3.752	12.290 901	20.274 710 22	30.266 534 58
α, second order perturbation	.089 505 494 50	3.802	12.294 444	20.275 974 02	30.267 094 01
α, fourth order perturbation	.089 505 558 50	3.689	12.294 626	20.276 003 20	30.267 101 55

[a] $\alpha_{(2)}=\langle\alpha_{(1)}|H|\alpha_{(1)}\rangle/\langle\alpha_{(1)}|\alpha_{(1)}\rangle$.

[b] $\int_0^\pi(\alpha_{(1)}-W)^{1/2}dx=\nu\pi$.

[c] $\int_0^\pi(\alpha_{(1)}-V)^{1/2}dx=\nu\pi$.

[d] The poor convergence manifests that the WKB method is a short-wavelength approximation.

where $\Omega = (1 - \alpha_{(1)}^{-1})^{-1}$ and $K(x)$ is the complete elliptic integral of the first kind. Had we used the WKB approximation for band calculation, then for $\alpha_{(1)}$ we would have

$$\int_0^\pi [\alpha_{(1)} - V(x)]^{1/2} dx = 2[\alpha_{(1)} + 2\gamma]^{1/2} E\left(\frac{4\gamma}{\alpha_{(1)} + 2\gamma}\right) = \nu\pi$$

and the analogy to Eq. (23) would be

$$\alpha_{(2)} = \alpha_{(1)} + \frac{\gamma^2}{2\alpha_{(1)}^{5/2}} \frac{[\alpha_{(1)} + 2\gamma]^{1/2}}{(2/\pi)K(4\gamma/(\alpha_{(1)} + 2\gamma))} \times \left[1 + \frac{35}{8}\frac{\gamma^2}{\alpha_{(1)}^2}\right] \cdots .$$

Table I exhibits the computations of energy levels (i.e., eigenvalues) for a normalized Mathieu lattice potential, $V = 2\gamma \cos 2x$, by various methods for both the characteristic exponential values of $\nu = 3.5, 4.5, 5.5$ and $\gamma = 1$. For these, $\alpha_{(1)}$ and $\alpha_{(2)}$ are computed for both the effective potential phase integral approximation and the WKB approximation; for comparison α is computed by second and fourth order plane-wave perturbation theory as well as given for rounded-off exact values. Although the effective potential phase integral approximation is computed to only first order in V, it renders the $\alpha_{(2)}$'s through the power of renormalization that approaches the accuracy of a fourth order perturbation calculation. For the WKB approximation, by contrast, $\alpha_{(2)}$ approaches the accuracy of only a second order perturbation calculation in consonance with Eq. (23).

The observed error in $\alpha_{(2)}$ of the effective potential phase integral approximation for $\nu = 3.5, 4.5, 5.5$ is observed to fall off almost as $O(\nu^{-12})$. This is consistent with variational methods for perturbation computations. As a variational trial function, the effective potential phase integral approximation deviates from the Floquet solution by an error of $O(\nu^{-4})$ in accordance with Eqs. (18), (20), and (21). Thus, one naively might suppose that the eigenvalue calculation is in error of $O(\nu^{-8})$; however, the situation is more complex since the eigenvalues of α are dependent upon the variational parameter ν. As the effective potential approximation renders correctly the γ^0 and γ^2 term of a power series expansion[10] for α and as the γ^4 term of this expansion is also of $O(\nu^{-4})$, the correct expected error is of $O(\nu^{-12})$.

Since the observed accuracy for calculating eigenvalues is consistent for the various levels of eigenvalues with the predictions for variational methods with a trial function consisting of the effective potential phase integral approximation, the trial functions must be innately orthogonal to a degree consistent with the error of the trial function as predicted in Sec. III.

Table I exhibits a comparison among various methods for calculating the eigenvalue α for a normalized Mathieu potential, $V = 2\gamma \cos 2x$, with $\gamma = 0.03$ and $\nu = 0.3$. Since the lattice period of this potential is shorter than the carrier wave's period, the WKB method is not justified as confirmed by the poor performance manifested by the WKB calculations for either $\alpha_{(1)}$ or $\alpha_{(2)}$. Concurrently, the accuracy of $\alpha_{(2)}$ for the effective potential phase integral approximation is consistent with the anticipated accuracy of the variational method using this approximation as a trial function.

Also Table I exhibits this same comparison for another normalized Mathieu potential, $V = 2\gamma \cos 2x$, with $\gamma = 1$ and $\nu = 1.9$. Since we are in the neighborhood of the associated effective potential's resonance at $\nu = 2$, the effective potential phase integral approximation is degraded.

For completeness, it is noted that the excellent results in Table I for $\alpha_{(1)}$ reckoned by the WKB method are expected because the associated isolated ionic potential is the potential for the harmonic oscillator[8,9] for which $\alpha_{(1)}$ is by coincidence exact.

The eigenvalue calculations were made for a given Bloch wavenumber (characteristic exponent) in order to facilitate a comparison among various methods. For conventional methods, the convenient method of calculation is from the Bloch wavenumber to the eigenvalue. In contrast, for the effective potential phase integral approximation, the convenient direction of computation is from $\alpha_{(1)}$ to the Bloch wavenumber and $\alpha_{(2)}$. The effective potential phase integral method computes the Bloch wavenumber and $\alpha_{(2)}$ by a finite real space integration.

Note added in manuscript: We make use of the new Physics Auxiliary Publication Service (PAPS) to deposit ancillary material.[14]

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[1]N. Fröman, Ann. Phys. 61, 451 (1970).
[2]N. Fröman and P.O. Fröman, *JWKB-Aprproximation, Contributions to the Theory* (North-Holland, Amsterdam, 1965), p. 14.
[3]C.E. Hecht and J.E. Mayer, Phys. Rev. 106, 1156 (1957).
[4]Ref. 3. Hecht and Mayer also offer a more elaborate iterative scheme which neglects only $(\ln z;\ \ln z^{(m)})/2$. However, for a periodic potential, the periodic solutions have a z that increases without bound, and this other iterative scheme may be reduced to Eq. (6) in the large z limit.
[5]A. Nayfeh, *Perturbation Methods* (Wiley, New York, 1973), pp. 367—73.
[6]M.I. Sancer and A.D. Varvatsis, Proc. IEEE 58, 140 (1970).
[7]J.B. Keller, J. Opt. Soc. Am. 59, 1003 (1969).
[8]J.R. Reitz, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1955), Vol. 1, p. 38.
[9]J.C. Slater, Phys. Rev. 87, 807 (1952).
[10]M. Abramowitz and Irene A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964), Paragraph 20.3.15.
[11]Ref. 10, Paragraph 20.3.16.
[12]L.D. Landau and E.M. Lifshitz, *Quantum Mechanics, Non-Relativistic Theory* (Addison-Wesley, Reading, Mass., 1958), pp. 178—83.
[13]W.H. Furry, Phys. Rev. 71, 360 (1947).
[14]See AIP document No. PAPS 760128-01 for 18 pages of ancillary material on the NFE WKB analogy, relationship to the pseudopotential and QDM, reductions for Mathieu and generalized mappings, validity, and higher order effective potentials. Order by PAPS number and journal reference from American Institute of Physics, Physics Auxiliary Publication Service, 335 East 45th Street, New York, N.Y. 10017. The price is $1.50 for each microfiche (98 pages), or $5 for photocopies of up to 30 pages with $0.15 for each additional page over 30 pages. Airmail additional. Make checks payable to the American Institute of Physics. This material also appears in *Current Physics Microfilm*, the monthly microfilm edition of the complete set of journals published by AIP, on the frames immediately following this journal article.

Linear boson transformation coefficients

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A simple expression for the coefficients which connect a Fock state containing an arbitrary number of quasiparticles with its tranformed state under a boson Bogoliubov transformation is obtained.

I. INTRODUCTION

The coefficients which connect a Fock state containing an arbitrary number of quasiparticles with its transformed state under a boson Bogoliubov transformation[1,2] have been calculated by several authors.[3–5] Tanabe[3] has obtained a result using eigenfunctions of the linear harmonic oscillator. The result, however, is extremely complicated. Rashid[4] has calculated these coefficients using recursion relations the coefficients satisfy and constructing the generating function for them. Aronson, Malkin, and Man'ko[5] have obtained the coefficients using coherent states.

In this note we present a calculation of these coefficients utilizing a Baker–Campbell–Hausdorff (BCH) formula for the generators of the SU(1,1) group, previously noted by Gilmore.[6] In our opinion our calculation is much simpler than the previous ones.

II. A BAKER-CAMPBELL-HAUSDORFF FORMULA

We first derive the Baker–Campbell–Hausdorff formula which plays an important role in our calculation. It has been noted by Gilmore[6] that BCH formulas giving $e^X e^Y$ in the form $e^{Z(X,Y)}$ can be obtained by matrix multiplication if X, Y are operators in a finite-dimensional Lie algebra.

Consider the Lie algebra of the noncompact SU(1,1) group which is spanned by the three operators $K_\pm$, K_3 which satisfy the commutation relations

$$[K_3, K_\pm] = \pm K_\pm, \tag{1}$$

$$[K_+, K_-] = -2K_3. \tag{2}$$

We consider the disentanglement of the operator $\exp[x(K_- - K_+)]$ in the form

$$\exp[x(K_- - K_+)] = \exp(\alpha K_+)\exp(\beta K_3)\exp(\gamma K_-). \tag{3}$$

Consistent with Gilmore's observation we note that $K_\pm$, K_3 have the finite-dimensional faithful matrix representation

$$K_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{4}$$

$$K_- = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}, \tag{5}$$

$$K_3 = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{6}$$

which yields the form of Eq. (3) in this representation as

$$\begin{pmatrix} \cosh x & -\sinh x \\ -\sinh x & \cosh x \end{pmatrix} = \begin{pmatrix} \exp(\beta/2) - \alpha\gamma\exp(-\beta/2) & \alpha\exp(-\beta/2) \\ -\gamma\exp(-\beta/2) & \exp(-\beta/2) \end{pmatrix}. \tag{7}$$

Solving for α, β, γ, we get

$$\exp[x(K_- - K_+)] = \exp(-\tanh x\, K_+)\exp(2\ln\cosh x\, K_3) \times \exp(\tanh x\, K_-). \tag{8}$$

Although the result has been derived in the 2×2 matrix representation, it is valid for all faithful representations.[6] In the following sections we consider the representations of $K_\pm$, K_3 in terms of harmonic oscillator creation and annihilation operators and apply Eq. (8) to calculate linear boson transformation coefficients.

III. DETERMINATION OF THE COEFFICIENTS FOR ZERO MOMENTUM BOSONS

In this case the Bogoliubov transformation is

$$b = e^S a e^{-S} \tag{9}$$

$$b^\dagger = e^S a^\dagger e^{-S}, \tag{10}$$

where the annihilation and creation operators a and $a^\dagger$ satisfy

$$[a, a^\dagger] = 1. \tag{11}$$

The operator S is given by

$$S = \tfrac{1}{2}x(aa - a^\dagger a^\dagger) = -S^\dagger. \tag{12}$$

We must compute

$$G_{k;l}(x) = {}_a\langle k | e^S | l\rangle_a \tag{13}$$

$$= \sqrt{k!\,l!}\, H_{k;l}(x). \tag{14}$$

We note now that the operators $K_\pm$, K_3 of Sec. II have the following representation:

$$K_+ = \tfrac{1}{2}a^\dagger a^\dagger, \tag{15}$$

$$K_- = \tfrac{1}{2}aa, \tag{16}$$

$$K_3 = \tfrac{1}{4}(a^\dagger a + aa^\dagger). \tag{17}$$

Equation (8) is valid for this representation too.

Next, by using Eq. (11) and the representation of $K_\pm$, K_3 above, we get the following results:

$$\exp(\tanh x\, K_+)a\exp(-\tanh x\, K_+) = a - \tanh x\, a^\dagger, \tag{18}$$

$$\exp(\tanh x\, K_-)a^\dagger\exp(-\tanh x\, K_-) = a^\dagger + \tanh x\, a, \tag{19}$$

$$\exp(-2\ln\cosh x K_3)(a^\dagger+\tanh x\, a)\exp(2\ln\cosh x K_3)$$
$$=\operatorname{sech}x\, a^\dagger+\sinh x\, a, \tag{20}$$
$$\exp(-2\ln\cosh x K_3)\,|0\rangle_a=(\operatorname{sech}x)^{1/2}\,|0\rangle_a. \tag{21}$$

Noting that

$$\exp S=\exp[x(K_- - K_+)] \tag{22}$$

and

$$|k\rangle_a=(a^{\dagger k}/\sqrt{k!})\,|0\rangle_a, \tag{23}$$
$$a\,|0\rangle_a=0 \tag{24}$$

and using the results mentioned above, we get

$$H_{k;l}(x)=\frac{(\operatorname{sech}x)^{1/2}}{k!\,l!}\;{}_a\langle 0|(a-\tanh x a^\dagger)^k \times(a^\dagger\operatorname{sech}x+a\sinh x)^l\,|0\rangle_a. \tag{25}$$

Next for two operators P,Q such that $[P,Q]$ is a c-number we have the normal ordering formula of Wilcox[7]

$$(P+Q)^n=\sum_{k=0}^{[n/2]}\sum_{s=0}^{n-2k}\frac{[P,Q]^k n!}{k!\,s!\,(n-2k-s)!\,2^k}\circ Q^s P^{n-2k-s}, \tag{26}$$

where

$$[n/2]=n/2 \text{ for } n=\text{even integer}$$
$$=(n-1)/2 \text{ for } n=\text{odd integer}. \tag{27}$$

From Eq. (26) we get

$$\frac{1}{k!}\;{}_a\langle 0|(a-\tanh x\, a^\dagger)^k =\sum_{n=0}^{[k/2]}\frac{(-\frac{1}{2}\tanh x)^n}{n!\,(k-2n)!}\;{}_a\langle 0|a^{k-2n} \tag{28}$$

and

$$\frac{1}{l!}(a^\dagger\operatorname{sech}x+a\sinh x)^l\,|0\rangle_a =\sum_{m=0}^{[l/2]}\frac{(\frac{1}{2}\tanh x)^m}{m!\,(l-2m)!}(a^\dagger\operatorname{sech}x)^{l-2m}\,|0\rangle_a. \tag{29}$$

Thus from Eqs. (25), (28), (29) we get

$H_{k;l}(x)=0$ unless k,l are both even or both odd integers

and the nonvanishing values of $H_{k;l}(x)$ are

$$H_{k;l}(x)=(\tfrac{1}{2}\tanh x)^{(l-k)/2}(\operatorname{sech}x)^{k+1/2}\times\sum_{n=0}^{[k/2]}\frac{(-\frac{1}{4}\sinh^2 x)^n}{n!\,(k-2n)!\,[n+(l-k)/2]!}$$
$$\text{for } l\geq k$$
$$=(-\tfrac{1}{2}\tanh x)^{(k-l)/2}(\operatorname{sech}x)^{l+1/2}\times\sum_{n=0}^{[l/2]}\frac{(-\frac{1}{4}\sinh^2 x)^n}{n!\,(l-2n)!\,[n+(k-l)/2]!}\quad\text{for } k\geq l \tag{30}$$

Defining $[k,l]=\min(k,l)$, we get a single formula for $G_{k;l}(x)$:

$$G_{k;l}(x)=(k!\,l!)^{1/2}(-1)^{(|l-k|-l+k)/4}\times\tfrac{1}{2}\tanh x)^{[l-k|/2}(\operatorname{sech}x)^{[k,l]+1/2}\times\sum_{n=0}^{[k/2,l/2]}\frac{(-\frac{1}{4}\sinh^2 x)^n}{n!\,([k,l]-2n)!\,(n+|l-k|/2)!}$$
$$\text{for } k,l \text{ both odd or both even integers}$$
$$=0 \text{ otherwise}. \tag{31}$$

The appearance of our result is different from that obtained by Rashid.[4] However, we have checked that by using the technique outlined one can easily derive the generating function of $H_{k;l}(x)$,

$$H(\alpha,\beta;x)=\sum_{kl}H_{k;l}(x)\alpha^k\beta^l, \tag{32}$$

in the form

$$H(\alpha,\beta;x)=(\operatorname{sech}x)^{1/2}\exp[(\alpha\beta/\cosh x)-\tfrac{1}{2}(\alpha^2-\beta^2)\tanh x], \tag{33}$$

which is identical with Rashid's result.

IV. DETERMINATION OF COEFFICIENTS FOR NONZERO MOMENTUM BOSONS

In this case the Bogoliubov transformation is

$$b_{\mathbf{k}}=e^T a_{\mathbf{k}}\bar{e}^T, \tag{34}$$
$$b_{\mathbf{k}}^\dagger=e^T a_{\mathbf{k}}^\dagger\bar{e}^T, \tag{35}$$

where

$$[a_{\mathbf{k}},a_{\mathbf{k}'}^\dagger]=\delta_{\mathbf{k},\mathbf{k}'} \tag{36}$$

and

$$T=-x_{\mathbf{k}}(a_{\mathbf{k}}a_{-\mathbf{k}}^\dagger-a_{\mathbf{k}}a_{-\mathbf{k}})=-T^\dagger \tag{37}$$

We have to compute

$$G_{p,q;r,s}(x_{\mathbf{k}})=(1/\sqrt{p!\,q!\,r!\,s!}) \times{}_a\langle 0|(a_{\mathbf{k}})^p(a_{-\mathbf{k}})^q e^T(a_{\mathbf{k}}^\dagger)^2(a_{-\mathbf{k}}^\dagger)^s\,|0\rangle_a \tag{38}$$
$$=\sqrt{p!\,q!\,r!\,s!}\,H_{p,q;r,s}(x_{\mathbf{k}}). \tag{39}$$

In this case the operators

$$K_+=a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger, \tag{40}$$
$$K_-=a_{\mathbf{k}}a_{-\mathbf{k}}, \tag{41}$$
$$K_3=\tfrac{1}{2}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger+1) \tag{42}$$

generate the algebra of the SU(1, 1) group.

It is easy to see that

$$K_+|r,s\rangle=[(r+1)(s+1]^{1/2}|r+1,s+1\rangle, \tag{43}$$
$$K_-|r,s\rangle=(rs)^{1/2}|r-1,s-1\rangle, \tag{44}$$
$$K_3|r,s\rangle=\tfrac{1}{2}(r+s+1)|r,s\rangle. \tag{45}$$

Thus

$$G_{p,q;r,s}(x_{\mathbf{k}})=\langle p,q|\exp(-\tanh x_{\mathbf{k}}K_+)\exp(-2\ln\cosh x_{\mathbf{k}}K_3)\times\exp(\tanh x_{\mathbf{k}}K_-)|r,s\rangle\times\sum_{\lambda\mu}\frac{(-1)^\lambda(\tanh x_{\mathbf{k}})^{\lambda+\mu}}{\lambda!\,\mu!}\times\langle p,q|K_+^\lambda\exp(-2\ln\cosh x_{\mathbf{k}}K_3)K_-^\dagger|r,s\rangle. \tag{46}$$

Using the recursion relations (43)–(45), we get finally

$$G_{p,q;r,s}(x_k) = \delta_{p-q,r-s}(\mathrm{sech}x_k)^{r+s+1}(-\tanh x_k)^{p-r} \times \sum_{\mu} [(-\sinh^2 x_k)^{\mu}/(p-r+\mu)!\,\mu!] \times [(r-\mu+1)!\,(s-\mu+1)!\,|\times(p-1)!\,(q-1)!\,(r-1)!\,(s-1)!\,|^{1/2}]. \quad (47)$$

In this case also the expression for $G_{p,q;r,s}$ differs in appearance from that of Rashid[4] but again the generating function

$$H(\alpha,\beta;\gamma,\delta;x_k) = \sum_{pqrs} \alpha^p \beta^q \gamma^r \delta^s H_{p,q;r,s}(x_k) \quad (48)$$

can be shown to be

$$H(\alpha,\beta;\gamma,\delta;x_k) = \exp[(\alpha\gamma+\beta\delta)\,\mathrm{sech}x_k + (\gamma\delta-\alpha\beta)\tanh x_k] \quad (49)$$

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[1]N. N. Bogoliubov, Nuovo Cimento 7, 794 (1958).
[2]J. G. Valatin, Nuovo Cimento 7, 843 (1958).
[3]K. Tanabe, J. Math. Phys. 14, 618 (1973).
[4]M. A. Rashid, J. Math. Phys. 16, 378 (1975).
[5]E. B. Aronson, I. A. Malkin, and V. I. Man'ko Lett. Nuovo Cimento 11, 44 (1974).
[6]R. Gilmore, J. Math. Phys. 15, 2090 (1974).
[7]R. M. Wilcox, J. Math. Phys. 8, 962 (1967).

The Riemann solution and the inverse quantum mechanical problem

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Systematic use is made of the Riemann function to find the conditions for the existence of the kernel of the inverse problem at fixed value of the angular momentum. When the reference potential is the centrifugal one, only an l-dependent condition on the potential must be required in the Marchenko case; in the Gel'fand–Levitan case, the condition is l-independent. When the Coulomb potential is included in the reference potential, an exponential decrease of the potential is needed in both instances.

1. INTRODUCTION

By inverse problem, we mean the derivation of the forces from experimental data. A well-known solution of an inverse problem was the discovery of the law of gravitation by Newton from the observations of Kepler.[1] The present inquiry is limited to nuclear physics, and it is assumed that the Schrödinger equation can be expanded into uncoupled differential (not integro–differential) equations. Two different approaches are possible. They separate inverse problems at fixed energy[2] from inverse problems at fixed angular momentum.[3] Only the latter types are discussed in this paper.

Consequently, exclusively differential equations of the form

$$[D(x)]u(x,k,l) \equiv \left(\frac{d^2}{dx^2} + k^2 - W(l,x)\right) u(x,k,l) = 0 \tag{1}$$

are considered.

The function $W(l,x)$ of Eq. (1) is called the *potential*.

If a part $W_0(l,x)$ of W is known, one defines $D_0(x)$ by replacing W by W_0; the solution is then u_0. In addition, one writes

$$W(l,x) = W_0(l,x) + V(l,x). \tag{2}$$

$W_0(l,x)$ is called the reference potential, and V the perturbation potential. In most instances

$$W_0(l,x) = -[l(l+1)/x^2] + 2\alpha/x, \tag{3}$$

that is, the centrifugal + Coulomb potential. $V(l,x)$ is then the nuclear potential.

To solve the inverse problem is to find the nuclear potential from the scattering data. However, an important question has to be answered: What conditions must be satisfied by the nuclear potential for the inverse problem to have a solution? The present paper is essentially concerned with this subject and relies on Refs. 3(c) and 3(d), which are shown here to be complementary studies.

The possibility of a solution for the inverse problem depends upon the existence of an integral representation for the solution of the equation

$$D(r)u(r) = 0$$

in terms of the solution of the equation

$$D_0(r)u_0(r) = 0.$$

Two integral representations for u are considered, namely that of the regular solution and that of the Jost solution: They correspond to two different sets of boundary conditions imposed on the solution.

Regular solution:

$$u(0) = u_0(0) = 0,$$

$$u(x) = u_0(x) + \int_0^x K_G(x,y)u_0(y)\,dy, \tag{4}$$

$$x > y.$$

The kernel K_G is the solution of a partial differential equation

$$D(x)K_M(x,y) = D_0(y)K_G(x,y),$$

$$K_G(x,x) = \tfrac{1}{2}\int_0^x V(s)\,ds, \tag{5}$$

$$K_G(x,0) = 0,$$

$$x > y.$$

Jost solution:

$$u(x) = u_0(x) \underset{x\to\infty}{\sim} \exp(ikx + \alpha \ln 2kx),$$

$$u(x) = u_0(x) + \int_x^\infty K_M(x,y)u_0(y)\,dy, \tag{6}$$

$$y > x.$$

Now one has

$$D(x)K_M(x,y) = D_0(y)K_M(x,y),$$

$$K_M(x,x) = \tfrac{1}{2}\int_x^\infty V(s)\,ds, \tag{7}$$

$$\lim_{x+y\to\infty} K_M(x,y) = \lim_{x+y\to\infty} \frac{\partial}{\partial y} K_M(x,y) = 0,$$

$$y > x.$$

The Gel'fand–Levitan kernel K_G is obviously different from the Marchenko kernel K_M, because the boundary conditions are different.

In order to proceed further, we transform Eqs. (5) and (7) into integral equations which incorporate their boundary conditions.

Afterwards we determine the conditions on the nuclear potential V for Eqs. (5) and (7) to have a solution K, in the sense of function theory (not in the enlarged sense of distributions[4]).

Results of this paper are the following:

If the reference potential is the centrifugal one alone, in the Gel'fand—Levitan case the condition on the behavior of the potential is independent of the value of the angular momentum; but an l-dependence appears in the Marchenko case.

In both cases the presence of the Coulomb potential requires an exponential decrease in the nuclear potential.

This agrees with Refs. 3(c) and 3(d) for the Jost solution but extends the study to regular solutions.

2. MATHEMATICAL PREREQUISITES

A. Riemann solution

The Darboux hyperbolic partial differential equation[5]

$$D(x)R(x,y;s,u)=D(y)R(x,y;s,u) \tag{9}$$

with the conditions

$$\begin{aligned} &R(x,y;x,y)=1,\\ &\frac{\partial R}{\partial x}=\frac{\partial R}{\partial y} \quad \text{when } x+y=u+s,\\ &\frac{\partial R}{\partial x}=-\frac{\partial R}{\partial y} \quad \text{when } x-y=u-s, \end{aligned} \tag{10}$$

is considered. The solution R is the Riemann solution[6] for Eq. (9), which plays the same role for hyperbolic equations as the Green solution does for elliptic equations.

Coordinates (x,y) are called physical variables. Instead of the physical variables it is often convenient to use canonical (characteristic) variables. If $y>x$, one defines[5]

$$\begin{aligned} &2\xi=y-x, \quad 2\eta=y+x,\\ &2\xi_0=u-s, \quad 2\eta_0=u+s. \end{aligned} \tag{11}$$

(If $x>y$, one sets $2\xi=x-y$, $2\xi_0=s-u$; η and η_0 are unchanged.)

The following notations are used from now on: Let $F(x,y)$ be a function defined in physical coordinates and $x(\xi,\eta)$, $y(\xi,\eta)$ the transformation from physical to characteristic variables, we abbreviate systematically the notation:

$$F(\xi,\eta)\equiv F(x(\xi,\eta),y(\xi,\eta)),$$

even though the formal dependence of F on its variables changes.

Equation (9) takes the standard form in characteristic variables. $R(\xi,\eta;\xi_0,\eta_0)$ is now the solution of

$$\frac{\partial^2 R}{\partial\xi\partial\eta}-[\Delta(\xi,\eta)]R=0 \tag{12}$$

with

$$\Delta(\xi,\eta)=[W(\xi+\eta)-W(\xi-\eta)],$$

while conditions (10) become

$$\begin{aligned} &R(\xi,\eta;\xi,\eta)=1,\\ &\frac{\partial R}{\partial\xi}=0 \quad \text{if } \eta=\eta_0,\\ &\frac{\partial R}{\partial\eta}=0 \quad \text{if } \xi=\xi_0. \end{aligned} \tag{13}$$

B. Integral equations for the kernels K_G, K_M

With the use of the Riemann function R_0 defined by

$$D_0(x)R_0=D_0(y)R_0 \tag{14}$$

Eqs. (5), (7) are replaced by Eqs. (15), (17), below; the equation for K_G is

$$\begin{aligned} K_G(x,y)=&\tfrac{1}{2}\int_{(x-y)/2}^{(x+y)/2} ds\, V(s)R_0(x,y;s,s)\\ &+\tfrac{1}{2}\int_{x-y}^{x} ds\, V(s)\int_{y-x+s}^{s} du\, K_G(s,u)R_0(x,y;s,u)\\ &+\tfrac{1}{2}\int_{(x-y)/2}^{x-y} ds\, V(s)\int_{-y+x-s}^{s} du\, K_G(s,u)R_0(x,y;s,u)\\ &-\tfrac{1}{2}\int_{(x+y)/2}^{x} ds\, V(s)\int_{y+x-s}^{s} du\, K_G(s,u)R_0(x,y;s,u) \end{aligned} \tag{15}$$

$$\begin{aligned} K_G(x,y)=&\tfrac{1}{2}\int_{(x-y)/2}^{(x+y)/2} ds\, V(s)R_0(x,y;s,s)\\ &+\tfrac{1}{2}\int\int_{D_G} du\, ds\, V(s)K_G(s,u)R_0(x,y;s,u). \end{aligned} \tag{16}$$

The domain D_G is given in Eq. (15) and shown in Fig. 1. The equation for K_M is

$$\begin{aligned} K_M(x,y)=&\tfrac{1}{2}\int_{(x+y)/2}^{\infty} ds\, V(s)R_0(x,y;s,s)\\ &+\tfrac{1}{2}\int_{x}^{(x+y)/2} ds\, V(s)\int_{y-s+x}^{y+s-x} ds\, K_M(s,u)\\ &\times R_0(s,y;s,u)+\tfrac{1}{2}\int_{(x+y)/2}^{\infty} ds\, V(s)\\ &\times\int_{s}^{y+s-x} du\, K_M(s,u)R_0(s,y;s,u) \end{aligned} \tag{17}$$

or

$$\begin{aligned} K_M(x,y)=&\tfrac{1}{2}\int_{(x+y)/2}^{\infty} ds\, V(s)R_0(x,y;s,s)\\ &+\tfrac{1}{2}\int\int_{D_M} du\, ds\, V(s)K_M(s,u)R_0(x,y;s,u). \end{aligned} \tag{18}$$

The domain D_M is shown in Fig. 2 and comes originally from Ref. 3(b). Proof of Eqs. (15) and (17) depends on application of $[D_0(y)-D_0(x)]K(x,y)=V(y)K(x,y)$ to the

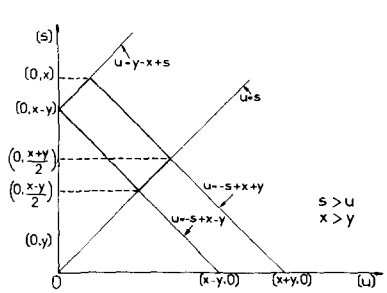

FIG. 1. Gel'fand—Levitan domain.

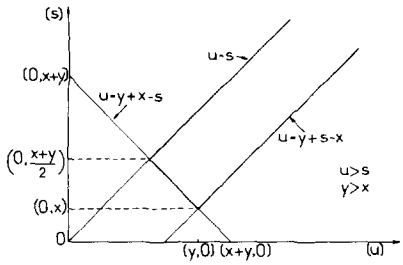

FIG. 2. Marchenko domain.

rhs and the lhs of Eq. (18), together with the dependence of R_0 on its boundary conditions. Equations similar to Eqs. (16) and (18) are also found in Ref. 7, where one-dimensional Schrödinger equations are investigated.

C. Composition of Riemann functions

Canonical variables are used. One has, as an analogy with Green solutions,

$$R(\xi,\eta;\xi_0,\eta_0) = R_0(\xi,\eta;\xi_0,\eta_0) + \int_\xi^{\xi_0} d\xi' \int_{\eta_0}^{\eta} d\eta' \Delta(\xi',\eta') \times R_0(\xi,\eta;\xi_0,\eta_0) R(\xi',\eta';\xi_0,\eta_0), \tag{19}$$

that is, $R = R_0 + R_0 \Delta R$.

D. Reduction theorems

(a) A Riemann function R is defined to possess a reduction of *type* 1 if one has

$$|R(\xi,\eta;\xi_0,\eta_0)| \le g(\xi,\eta)/g(\xi_0,\eta_0). \tag{20}$$

(b) A Riemann function R is defined to possess a reduction of *type* 2 if one has either

$$|R(\xi,\eta;\xi_0,\eta_0)| \le f(\xi,\eta) \quad \text{(case a)} \tag{21}$$

or

$$|R(\xi,\eta;\xi_0,\eta_0)| \le f(\xi_0,\eta_0) \quad \text{(case b)}. \tag{22}$$

(c) A Riemann function R possesses a reduction of type 3a or b if one has

$$|R(\xi,\eta;\xi_0,\eta_0)| \le \frac{g(\xi,\eta)}{g(\xi_0,\eta_0)} f(\xi,\eta) \quad \text{(case a)}, \tag{23a}$$

$$|R(\xi,\eta;\xi_0,\eta_0)| \le \frac{g(\xi,\eta)}{g(\xi_0,\eta_0)} f(\xi_0,\eta_0) \quad \text{(case b)}. \tag{23b}$$

Theorem 1: If R_0 possesses a reduction of type 1, the solution of Eq. (19) exists if

$$\tilde{R}(\xi,\eta;\xi_0,\eta_0) = 1 + \left| \int_\xi^{\xi_0} d\xi' \int_{\eta_0}^{\eta} d\eta' \Delta(\xi',\eta') \tilde{R}(\xi',\eta';\xi_0,\eta_0) \right| \tag{24}$$

exists.

Proof: Write

$$R = \tilde{R} g(\xi,\eta)/g(\xi_0,\eta_0)$$

$$R_0 = \tilde{R}_0 g(\xi,\eta)/g(\xi_0,\eta_0),$$

where $|\tilde{R}_0| < 1$.

Theorem 2: If R_0 possesses a reduction of type 1, Eqs. (15) and (17) have a solution if the modified potential $\tilde{V}(s) = V(s)/g(s,s)$ has its moment of order zero finite and if the potential $V(s)$ also has its moment of order one finite.

Consider first D_G and Ref. 3(c). When $|R_0| \le 1$, the bound for K_G, which we have developed in the Appendix, is

$$|K_G(x,y)| \le \tfrac{1}{2}\sigma_0\left(\frac{x+y}{2}\right) \exp\sigma_1(x). \tag{25}$$

Now assume for R_0 a reduction of type 1 and define $K(x,y) = \tilde{K}(x,y) g(x,y)$, where $K = K_G$ or K_M and

$$R_0(x,y;s,u) = \tilde{R}_0(x,y;s,u) g(x,y)/g(s,u). \tag{26}$$

The methods of Ref. 3(b) and the Appendix are used to get the bound:

$$|K(x,y)| \le \tfrac{1}{2} g(x,y) \tilde{\sigma}_0((x+y)/2) \exp[\sigma_1(x)]. \tag{27}$$

The moments of order i defined were

$$K_G: \quad \tilde{\sigma}_i(t) = \int_0^t s^i |\tilde{V}(s)| ds \tag{28}$$

and

$$K_M: \quad \tilde{\sigma}_i(t) = \int_1^\infty s^i |\tilde{V}(s)| ds. \tag{29}$$

Theorem 3: If R_0 possesses a reduction of type 2a and if $1 \le f(s,u) \le f(s,s)$, then Eqs. (15) and (17) have a solution provided that the potential $V(s)$ and the modified potential $\tilde{V}(s) = V(s) f(s,s)$ have respectively zeroth order and first order moments σ_0 and $\tilde{\sigma}_1$ finite.

Using again the methods of Ref. 3(b) and the Appendix, one obtains

$$|K(x,y)| \le \tfrac{1}{2}\sigma_0((x+y)/2) \exp[\tilde{\sigma}_1(x)] f(x,y). \tag{30}$$

Theorem 4: If R_0 possesses a reduction of type 2b and if $f(s,s) > f(s,u)$, one obtains

$$|K(x,y)| \le \tfrac{1}{2}\tilde{\sigma}_0((x+y)/2) \exp\tilde{\sigma}_1(x). \tag{31}$$

Therefore, a zeroth order and a first order moments for $\tilde{V}$ are needed.

Theorems 2, 3, 4 can be combined to obtain the bounds and the conditions corresponding to the reductions (3a) and (3b).

3. APPLICATION TO THE KERNELS OF THE INVERSE PROBLEM AT l FIXED (NON-COULOMBIAN CASE)

By defining

$$1 - 2z = 1 + \frac{1}{8xyus}(u+s-x-y)(s-u+y-x) \times [(u+y)^2 - (s+x)^2] = 1 - \frac{1}{8xyus}[(u-s)^2 - (y-x)^2] \times [(u+s)^2 - (y+x)^2] = 1 - 2\frac{(\xi_0^2-\xi^2)(\eta_0^2-\eta^2)}{(\eta^2-\xi^2)(\eta_0^2-\xi_0^2)}, \tag{32}$$

the Riemann function for the hyperbolic equation (9) with the centrifugal potential as found by Chaundy[8] is

$$R_0^l(x,y;s,u) = P_l(1-2z), \tag{33}$$

where P_l denotes the lth-Legendre polynomial.

In the Gel'fand—Levitan case:

$$x > y, \quad 0 \le \xi_0 \le \xi \le \eta_0 \le \eta < \infty.$$

So z is positive and less than one. Hence

$$-1 \leq 1-2z \leq +1.$$

And following Ref. 9, p. 303, one has, for l real,

$$|P_l(1-2z)| \leq 1, \tag{34}$$

$$|R_0^l(x,y;\ s,u)| \leq 1. \tag{35}$$

The bound given in Eq. (25) exists. The Gel'fand–Levitan kernel exists. In addition, from Eq. (A6) it follows that if V is continuous, $|K_G^{(0)}(x,y)| - 0$ with y.

In conclusion, no l dependence has appeared in the bound nor therefore in the condition for K_G.

In the Marchenko case, one uses the integral representation for P_l:

$$P_l(z) = \frac{1}{\pi}\int_0^\pi [z+(z^2-1)^{1/2}\cos\phi]^l\, d\phi$$

with $z > 0$. Consequently,

$$|P_l(z)| \leq (2z)^l. \tag{36}$$

In Ref. 3(d) it was shown that for $0 \leq \xi_0 \leq \xi < \eta \leq \eta_0 < \infty$

$$1-2z \leq 2(\eta+\xi)(\eta_0-\xi_0)/(\eta-\xi)(\eta_0+\xi_0),$$

which implies, in the Marchenko domain, where $y = x$, $1-2z \leq 2(y/x)s/u$.

Therefore, the Riemann function possesses a reduction of type 1 modulo a multiplicative constant

$$|R_0^l(x,y;\ s,u)| \leq 2^l[2(y/x)s/u]^l = 4^l g(x,y)/g(s,u) \tag{37}$$

with $g(s,s) = 1$. We write

$$K_M(x,y) = \tfrac{1}{2}\int ds[V(s)4^l][4^{-l}R_0^l(x,y;\ s,s] + \int\int_{D_M} du\, ds[V(s)4^l]K_M(s,u)(4^{-l}R_0^l(x,y;\ s,u)). \tag{38}$$

Theorem 2 shows that if the first two moments of the potential $\overline{V(s)} = 4^l V(s)$ exist, one has

$$|K_M(x,y)| \leq \tfrac{1}{2}(y/x)^l \sigma_0((x+y)/2)\exp[\sigma_1(x)]. \tag{39}$$

From now on, as in Eq. (39), whenever K_M is concerned, σ_0 and σ_1 will refer to $\overline{V}$ not to V; this definition is followed consistently until the end of this paper. Accordingly, one defines

$$\sigma_0 = \int_{(x+y)/2}^\infty \overline{V}(s)\, ds.$$

In the last equation, the integration variable s is such that

$$2s \geq x+y; \quad \text{then } |2s|^l \geq (x+y)^l \geq y^l,$$

$$y^l\sigma_0((x+y)/2) \leq 2^l\sigma_l((x+y)/2),$$

where σ_l is the moment of order l of $\overline{V}$. So

$$|K_M(x,y)| \leq \tfrac{1}{2}(2/x)^l\sigma_l((x+y)/2)\exp[\sigma_1(x)]. \tag{40}$$

If σ_l exists, K_M exists, and condition (7.3) is obviously realized.

If the moments may be extended from zero to infinity, the regular solution is finite everywhere, and the Jost solution behaves like $(1/x)^l$ at the origin.

4. INCLUSION OF COULOMB POTENTIAL IN THE REFERENCE POTENTIAL

A. Study of the Riemann function

Although the Riemann function corresponding to the Coulomb potential is not known, some limitations can be expressed for it.

Let R_c^l be the Riemann function for the reference potential of Eq. (3) (Coulomb + centrifugal). Then Eq. (19) is valid with

$$\Delta(\xi',\eta') = -4\alpha\xi'/(\eta'^2-\xi'^2)$$
$$R = R_c^l, \quad R_0 = R_0^l. \tag{41}$$

According to Theorem 1 the problem reduces to studying the equation

$$\tilde{R}_c^l(\xi,\eta;\ \xi_0,\eta_0) = 1 + |\beta|\int_{\xi_0}^{\xi} d\xi' \int_a^b d\eta' \times[\xi'/(\eta'^2-\xi'^2)]\tilde{R}_c^l(\xi',\eta';\ \xi_0,\eta_0). \tag{42}$$

In Eq. (42) (a,b) is the couple (η_0,η) or (η,η_0) according to whether η_0 is smaller or greater than η (the smaller regularly preceding). Since $\eta' > \xi'$, all quantities involved in Eq. (42) are positive. We define with G, M indices

$$\beta_G = 4\alpha, \quad \beta_M = 4\times 4^l\alpha,$$
$$R_{CG}^l(\xi,\eta;\ \xi_0,\eta_0) \equiv R_{CG}^l(\xi,\eta;\ \xi_0,\eta_0),$$
$$R_{CM}^l(\xi,\eta;\ \xi_0,\eta_0) = 4l[(\eta+\xi)(\eta_0-\xi_0)^l/(\eta-\xi)(\eta_0+\xi_0)] \times\tilde{R}_{CM}^l(\xi,\eta;\ \xi_0,\eta_0), \quad |\tilde{R}_{CM}^l| < 1.$$

Suppose now a separable function $\phi(\xi')\psi(\eta')$ such as

$$\xi'/(\eta'^2-\xi'^2) \leq \phi(\xi')\psi(\eta') \text{ exists.} \tag{43}$$

Then each term $\tilde{R}_C^{l(n)}$ of the series obtained in solving Eq. (42) by successive approximations is dominated by the series $\rho_C^{l(n)}$, which is the solution of an equation analogous to Eq. (42), where $\xi'/(\eta'^2-\xi'^2)$ is replaced by $\phi(\xi')\psi(\eta')$.

On the other hand $\rho_C^{(l)} = \sum_{n=0}^\infty \rho_C^{(l)n}$ is the solution of the second order partial differential equation:

$$\frac{\partial^2 z}{\partial\xi\partial\eta} \mp |\beta|\phi(\xi)\psi(\eta) = 0. \tag{44}$$

The minus sign corresponds to the Gel'fand–Levitan and the plus sign to the Marchenko cases. Equation (44) can be solved exactly. Following Valiron,[10] we define

$$v = \int_{\xi_0}^{\xi}\phi(\xi')\, d\xi' \int_{\eta_0}^{\eta}\psi(\eta')\, d\eta' \tag{45}$$

and look for a solution $z \equiv \Phi(v)$. Such a solution fulfills the conditions of a Riemann function if $\Phi(0) = 1$. In fact

$$\xi = \xi_0 \text{ or } \eta = \eta_0 \text{ implies } v = 0$$

and either $\dfrac{\partial z}{\partial\eta} = 0$ or $\dfrac{\partial z}{\partial\xi} = 0$.

The function $\Phi(v)$ satisfies the Bessel equation

$$v\Phi''(v) + \Phi'(v) \mp |\beta|\Phi(v) = 0. \tag{46}$$

Therefore, one has

$$z=\Phi(v)=J_0(\sqrt{\mp 4|\beta|v})=1\pm|\beta|v+|\beta|^2v^2/2^2 + \cdots + (\pm)^n|\beta|^n v^n/(n')^2+\cdots.$$

Therefore,

$$z(\xi,\eta;\ \xi_0,\eta_0)\equiv\rho_C^l(\xi,\eta;\ \xi_0,\eta_0). \tag{47}$$

This shows that the series ρ_C^l converges uniformly for every set $(\xi,\eta;\ \xi_0,\eta_0)$ and moreover that the series R_C^l converges uniformly and absolutely.

The bound for z (and for $\tilde{R}_C^l$) is independent of the sign of v

$v>0$ (Gel'fand—Levitan domain):

$$J_0(\sqrt{-4|\beta|v})=I_0(2\sqrt{|\beta|v})\leq\exp(2\sqrt{|\beta|v}), \tag{48a}$$

$v<0$ (Marchenko domain):

$$J_0(\sqrt{4|\beta|v})=I_0(2\sqrt{|\beta v|})\leq\exp(2\sqrt{|\beta v|}). \tag{48b}$$

To use the preceding, we look for a separable function Φ which satisfies Eq. (43).

For the Marchenko domain, Gugushvili and Mentkovsky wrote

$$v=\int_\xi^{\xi_0}\frac{d\xi'}{\sqrt{\eta-\xi'}}\int_{\eta_0}^{\eta}\frac{d\eta'}{\sqrt{\eta'-\xi}} \tag{49}$$

$$|v|\leq 4(\eta_0-\xi_0). \tag{50}$$

So

$$|\tilde{R}_{CM}^l(\xi,\eta;\ \xi_0,\eta_0)|\leq\exp(4\sqrt{|\beta|(\eta_0-\xi_0)}.$$

In the Gel'fand—Levitan case one has

$$\frac{\xi'}{\eta'^2-\xi'^2}<\frac{1}{\eta'-\xi'}<\frac{1}{\sqrt{\eta'-\xi}}\frac{1}{\sqrt{\eta_0-\xi'}},$$

$$v=\int_{\xi_0}^{\xi}\frac{d\xi'}{\sqrt{\eta_0-\xi}}\int_{\eta_0}^{\eta}\frac{d\eta'}{\sqrt{\eta'-\xi}}$$

$$=4[\sqrt{\eta_0-\xi_0}-\sqrt{\eta_0-\xi}\,][\sqrt{\eta-\xi}-\sqrt{\eta_0-\xi}\,] \tag{51}$$

$$v\leq 4\sqrt{\eta_0-\xi_0}\,\sqrt{\eta-\xi}\leq 4\eta. \tag{52}$$

The function ϕ therefore provides

$$|\tilde{R}_{CG}^l(\xi,\eta;\ \xi_0,\eta_0)|\leq\exp(4\sqrt{|\beta|\eta}). \tag{53}$$

B. Consequences for the kernels K

In the Marchenko case one has

$$|R_{CM}^l(\xi,\eta;\ \xi_0,\eta_0)|\leq 4^l\left(\frac{(\eta+\xi)(\eta_0-\xi_0)}{(\eta-\xi)(\eta_0+\xi_0)}\right)^l \times\exp[8(2)^l\sqrt{|\alpha|(\eta_0-\xi_0)}\,]. \tag{54}$$

If $l=0$, R_{CM}^l possesses a reduction of type 2b, with

$$f(\xi_0,\eta_0)=\exp[8\sqrt{|\alpha|(\eta_0-\xi_0)}\,] \tag{55}$$

so

$$f(s,u)=\exp(8\sqrt{|\alpha|s})=f(s,s),$$

$$f(x,y)=\exp(8\sqrt{|\alpha|x})>1.$$

Then one defines $\tilde{V}(s)=\exp(8\sqrt{|\alpha|s})\bar{V}(s)$, and obtains

$$|K_M(x,y)|\leq\tfrac{1}{2}\tilde{\sigma}_0((x+y)/2)\exp[\tilde{\sigma}_1(x)]. \tag{56}$$

If $l\neq 0$, $4^{-l}R_{CM}^l$ possesses a reduction of type 3b. According to Eq. (38) we define

$$\tilde{V}(s)=\bar{V}(s)\exp[8(2)^l\sqrt{|\alpha|s}\,]. \tag{57}$$

Equations (15) and (17) have a solution if both $\tilde{\sigma}_0(x)$ and $\tilde{\sigma}_1(x)$ exist. We have

$$|K_M(x,y)|\leq\tfrac{1}{2}(y/x)^l\,\tilde{\sigma}_0((x+y)/2)\exp[\tilde{\sigma}_1(x)]. \tag{58}$$

To conclude the Marchenko case, one may write a bound for K_M including the moment of order l of $\bar{V}(s)$:

$$|K_M(x,y)|\leq\tfrac{1}{2}(2/x)^l\tilde{\sigma}_l((x+y)/2)\exp[\tilde{\sigma}_1(x)] \tag{59}$$

so the existence of the kernel corresponding to the lth partial wave is tied to an lth moment of $\bar{V}(s)$.

In the Gel'fand—Levitan case, one has

$$|R_{CG}^l(\xi,\eta;\ \xi_0,\eta_0)|\leq\exp(4\sqrt{|\beta|\eta}). \tag{60}$$

Equation (60) is l independent. For all l, R_{CG} possesses a reduction of type 2a with

$$f(x,y)=\exp[4\sqrt{|\beta|(x+y)/2}\,],$$

$$f(s,u)=\exp[4\sqrt{|\beta|(s+u)/2}\,]\leq\exp(4\sqrt{|\beta|s}).$$

Theorem 3 applies and requires the existence of $\sigma_0(x)$ and of $\tilde{\sigma}_1(x)$ with $\tilde{\sigma}_1$ defined in terms of $\tilde{V}(s)=V(s)\times\exp(4\sqrt{|\beta|s})$. Then

$$|K_G(x,y)|\leq\tfrac{1}{2}\exp[4\sqrt{|\beta|(x+y)/2}\,]\sigma_0((x+y)/2)\exp[\tilde{\sigma}_1(x)].$$

The existence of K is again independent of the value of l.

5. CONCLUSION

Three remarks may conclude this short study.

—In the Marchenko case, and for the two reference potentials studied, our results concord with those of Gugushvili and Mentkovsky [Ref. 3(d)] and with Ref. 3(c), that is, the necessity of the existence of the lth order moment for the nuclear potential.

—In the Gel'fand—Levitan case we have improved the bound of Ref. 3(c), and found a bound independence of l.

—In the Coulomb case, in both instances, it might be possible to improve the bounds given here. However, to do this, it would be necessary to obtain the Riemann function itself.

APPENDIX

The bound of Ref. 3(c) for K_G is improved. The solution of Eq. (15) is found by successive approximations and we make the assumption that $|R_0(x,y;\ s,u)|<1$. So

$$K_G^{(0)}(x,y)=\tfrac{1}{2}\int_{(x-y)/2}^{(x+y)/2}ds\ V(s)R_0(x,y;s,s). \tag{A1}$$

$$K_G^{(n)}(x,y)=\tfrac{1}{2}\int\int_{D_G}du\,ds\ V(s)R_0(s,y;\ s,u)K_G^{(n-1)}(s,u) \tag{A2}$$

$$|K_G^{(0)}(x,y)|\leq\tfrac{1}{2}[\sigma_0((x+y)/2)-\sigma_0((x-y)/2)].$$

And we obtain the following estimates

$$|K_G^{(0)}(x,y)| \leq \tfrac{1}{2}\sigma_0((x+y)/2),$$

$$\begin{aligned}
|K_G^{(1)}(x,y)| &\leq \tfrac{1}{2}\int_{x-y}^{x} ds\,|V(s)| \int_{y-x+s}^{s} du[\tfrac{1}{2}\sigma_0((s+u)/2)] \\
&\quad + \tfrac{1}{2}\int_{(x-y)/2}^{x-y} ds\,|V(s)| \int_{-y+x-s}^{s} du[\tfrac{1}{2}\sigma_0((s+u)/2)] \\
&\quad + \tfrac{1}{2}\int_{(x+y)/2}^{x} ds\,|V(s)| \int_{y+x-s}^{s} du[\tfrac{1}{2}\sigma_0((s+u)/2)] \\
&\leq \tfrac{1}{2}\sigma_0((x+y)/2)[\tfrac{1}{2}(x-y)\int_{x-y}^{x} ds\,|V(s)| \\
&\quad + \tfrac{1}{2}[2s-(x-y)]\int_{(x-y)/2}^{x-y} ds\,|V(s)| \\
&\quad + \tfrac{1}{2}[2s-(x+y)]\int_{(x+y)/2}^{x} ds\,|V(s)|] \\
&\leq \tfrac{1}{2}\sigma_0((x+y)/2)[\tfrac{1}{2}\int_{x-y}^{x} s\,|V(s)|\,ds \\
&\quad + \int_{(x-y)/2}^{x-y} s\,|V(s)|\,ds + \int_{(x+y)/2}^{x} s\,|V(s)|\,ds \\
&\quad - \tfrac{1}{2}(x-y)\int_{(x-y)/2}^{x-y} |V(s)|\,ds - \tfrac{1}{2}(x+y)\int_{(x+y)/2}^{x} |V(s)|\,ds],
\end{aligned} \tag{A3}$$

$$\begin{aligned}
|K_G^{(1)}(x,y)| &\leq \tfrac{1}{2}\sigma_0((x+y)/2)[\tfrac{1}{2}\int_{(x-y)/2}^{x} s\,|V(s)|\,ds \\
&\quad + \tfrac{1}{2}\int_{(x-y)/2}^{x-y} s\,|V(s)|\,ds + \int_{(x+y)/2}^{x} s\,|V(s)| \\
&\quad - \tfrac{1}{2}(x-y)\int_{(x-y)/2}^{x-y} |V(s)|\,ds - \tfrac{1}{2}(x+y)\int_{(x+y)/2}^{x} |V(s)|\,ds],
\end{aligned}$$

$$\tfrac{1}{2}[\int_{(x-y)/2}^{x-y} s\,|V(s)|\,ds - (x-y)\int_{(x-y)/2}^{x-y} |V(s)|\,ds] \leq 0,$$

$$\tfrac{1}{2}[\int_{(x+y)/2}^{x} s\,|V(s)|\,ds - (x+y)\int_{(x+y)/2}^{x} ds\,|V(s)|] \leq 0$$

for $x+y>x$,

$$\begin{aligned}
|K_G^{(1)}(x,y)| &\leq \tfrac{1}{2}\sigma_0((x+y)/2)[\int_{(x+y)/2}^{x} s\,|V(s)|\,ds + \int_{(x-y)/2}^{(x+y)/2} s\,|V(s)|\,ds].
\end{aligned}$$

Therefore,

$$|K_G^{(1)}(x,y)| \leq \tfrac{1}{2}\sigma_0((x+y)/2)[\sigma_1(x) - \sigma_1((x-y)/2)]. \tag{A4}$$

A fortiori

$$|K_G^{(1)}(x,y)| \leq \tfrac{1}{2}\sigma_0((x+y)/2)\sigma_1(x). \tag{A5}$$

In the same way

$$\begin{aligned}
|K^{(n)}(x,y)| &\leq \tfrac{1}{2}\sigma_0((x+y)/2)(1/n!)\sigma_1^{(n-1)}(x) \\
&\quad \times[\sigma_1(x) - \sigma_1((x-y)/2)].
\end{aligned} \tag{A6}$$

So we can conclude, *a fortiori* again,

$$|K_G^{(n)}(x,y)| \leq \tfrac{1}{2}\sigma_0((x+y)/2)\sigma_1^{(n)}(x)/n!\,. \tag{A7}$$

The series $K_G(x,y) = \sum_{n=0}^{\infty} K_G^{(n)}(x,y)$ converges uniformly in the interval $0 \leq y \leq x$, and the inequality

$$|K_G(x,y)| \leq \tfrac{1}{2}\sigma_0((x+y)/2)\exp[\sigma_1(x)] \tag{A8}$$

holds, which can be compared with Eq. (1.3.3) of Agranovitch and Marchenko [Ref. 3(b)].

In addition by (A2), (A4), and (A6) each term of the series goes to zero with y. It follows from (A7) that $K_G(x,y)$ vanishes when y approaches zero.

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[1] J. Chazy, *Cours de mécanique rationnelle* (Gauthier-Villars, Paris, 1933, t.1.)

[2] (a) T. Regge, Nuovo Cimento 14, 1251 (1950); (b) R.G. Newton, J. Math. Phys. 3, 75 (1962); (c) P.C. Sabatier, J. Math. Phys. 7, 1515 (1966); (d) C. Coudray and M. Coz, Ann. Phys. (N.Y.) **61**, 488 (1970).

[3] (a) I.M. Gel'fand and B.M. Levitan, Am. Math. Soc. Transl. 2, 1960); (b) L.S. Agranovitch and V.A. Marchenko, *The Inverse Problem in Scattering Theory* (Gordon and Breach, New York, 1963); (c) M. Coz and C. Coudray, J. Math. Phys. 14, 1574 (1973); (d) H.I. Gugushvili and Y.L. Mentkovski, Nuovo Cimento A 10, 277 (1972).

[4] L. Schwartz, *Théorie des distributions* (Herman, Paris, 1966).

[5] G. Darboux, *Théorie des surfaces t.* 2 (Gauthier-Villars, Paris, 1915), p. 71; E.T. Copson, Arch. Ratl. Mech. Anal. **1**, 324 (1958).

[6] B. Riemann, Abhandl. Kön. Ges. Wiss. Göttingen **8**, (1960), in *Collected works of Bernard Riemann* (Dover, New York, 1953), p. 156.

[7] L.D. Faddeyev, AMS Transl. Ser. **2**, **65** (1965); H.E. Moses, J. Math. Phys. **16**, 1044 (1975).

[8] T.W. Chaundy, Quart. J. Math. Oxford **10**, 310 (1939).

[9] E.T. Whittaker and G.W. Watson, *A Course of Modern Analysis* (Cambridge U.P., Cambridge, 1952).

[10] G. Valiron, *Equations fonctionnelles, Applications* (Masson, Paris, 1950), p. 569.

Partial differential matrix equations for the inverse problem of scattering theory

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Sufficient conditions for the existence of a continuous translation operator are found in the case of a system of differential equations in which the matrix potential has the singularity of the centripetal term. The sufficient conditions are found in terms of moments of the nuclear potential. The method used employs the Riemann Green's function. Threshold energies introduce a threshold energy dependence into the translation kernel and lead to a requirement of an exponential decrease for terms of the matrix potential.

1. INTRODUCTION

The partial differential equations for the inverse problem of scattering have received considerable attention since Agranovitch and Marchenko's excellent monograph[1] (A and M) appeared. Leaving aside the one-dimensional problem,[2] authors who have followed A and M have limited their concern to scalar potentials.[3-6] By so doing they lost the purpose of Ref. 1, where explicitly matrix differential equations were studied. However, the primary concern of Ref. 1 was not differential equations as such; after the results for the nonsingular case were obtained, they considered an indirect approach to the singular case via the transformation techniques of Crum and Krein.[7,8]

Since the work of Gugushvili and Mentkovsky[5] and Coz and Coudray,[6] it is possible to study directly systems of differential equations where the singularity comes from an explicit dependence on the angular momentum. In the present paper, we consider finite systems of n differential equations:

$$[L(x)+\Lambda^2]u(\Lambda,x)=Vu(\Lambda,x), \tag{1}$$

where L, Λ, V, u are $(n\times n)$ matrices. The columns of $u(\Lambda,x)$ are solutions of Eq. (1) which differ from each other by their boundary conditions. Λ is the diagonal matrix of the channel wavenumbers $\lambda_1,\ldots,\lambda_n$:

$$\Lambda_{ij}\equiv\lambda_i\delta_{ij}, \tag{2}$$

V is an Hermitian matrix potential which is called the nuclear potential; finally, the elements of the differential operator $L(x)$ are

$$L(x)=D(x)-l(x),$$
$$D_{ij}(x)\equiv\frac{d^2}{dx^2}\delta_{ij},\quad l_{ij}(x)\equiv\frac{l_i(l_i+1)}{x^2}\delta_{ij}. \tag{3}$$

The solution we are concerned with is the solution which is singular at the origin and defined by its behavior at infinity. Our choice of solution, that of Ref. 1, is dictated by the relationship of this solution to the S matrix. The matrix solution $H(\Lambda,x)$ for the homogeneous system is the Riccati Hankel function:

$$H_{ij}(\Lambda,x)=-ixh_i^{(2)}(\lambda_ix)\delta_{ij}=-i\sqrt{\pi x/2}\,H^{(2)}_{i+1/2}(\lambda_ix)\delta_{ij}$$
$$=(-)^{l_i}H_{ij}(-\Lambda,x). \tag{4}$$

The Green's function for the homogeneous system is the diagonal G function matrix:

$$G_{ij}(\Lambda;x,y)=0\quad\text{for } y\leq x$$
$$G_{ij}(\Lambda;x,y)=i(-)^{l_i}(2\lambda_i)^{-1}[h_{l_i}^{(2)}(\lambda_ix)h_{l_i}^{(2)}(-\lambda_iy)$$
$$-h_{l_i}^{(2)}(-\lambda_ix)h_{l_i}^{(2)}(\lambda_iy)]\delta_{ij}\quad\text{for } x\leq y. \tag{5}$$

The irregular matrix solution $F(\Lambda,x)$ is then defined by

$$F(\Lambda,x)=H(\Lambda,x)-\int_x^\infty G(\Lambda,x,y)V(y)F(\Lambda,y)\,dy, \tag{6}$$

where its boundary conditions have been incorporated. We consider the possible integral representation for $F(\Lambda,x)$:

$$F(\Lambda,x)=H(\Lambda,x)+\int_x^\infty K(x,y)H(\Lambda,y)\,dy. \tag{7}$$

The case where all λ_i are equal is studied first. Then no dependence on the threshold energies appears in the translation kernel $K(x,y)$ of Eq. (7). The general case is investigated in Sec. 4. Sufficient conditions for the matrix K to exist are the goal of this paper.

The kernel K is connected with the solution of the inverse problem as is seen from Eq. (9) below. It satisfies the matrix partial differential equation

$$[D(x)-D(y)]K(x,y)-[l(x)K(x,y)-K(x,y)l(y)]$$
$$=V(x)K(x,y). \tag{8}$$

The boundary conditions for Eq. (8) are

$$K(x,x)=\tfrac{1}{2}\int_x^\infty V(s)\,ds, \tag{9}$$

$$\lim_{y\to\infty}K(x,y)=\lim_{y\to\infty}\frac{\partial}{\partial y}K(x,y)=0. \tag{10}$$

The development of Eq. (8) with its conditions (9) and (10) is sketched in Appendix A. The same type of equation is found in Ref. 9. The kernel K is therefore connected with the resolvent of Eq. (6). The equation defining K belongs to the hyperbolic type and our work is dependent upon results for these equations in Refs. 10 and 11, which we extend here beyond scalar interactions.

2. THE RIEMANN'S SOLUTION AND NOTATIONS

Equation (8) is rewritten explicitly

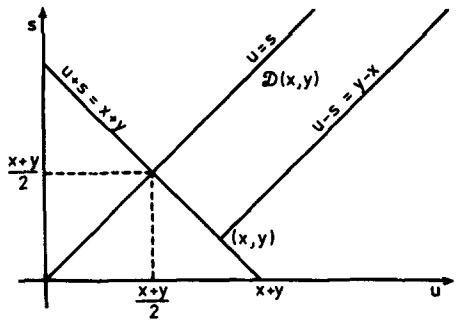

FIG. 1.

$$\left(\frac{d^2}{dx^2}-\frac{l_i(l_i+1)}{x^2}\right)K_{ij}(x,y)=\left(\frac{d^2}{dy^2}-\frac{l_j(l_j+1)}{y^2}\right)K_{ij}(x,y)+\sum_k V_{ik}(x)K_{kj}(x,y). \quad (11)$$

It is solved using Riemann's method, which is recalled now.[12] A Riemann solution $R(x,y;s,u)$ is defined. It satisfies

$$\left(\frac{d^2}{dx^2}-\frac{l_i(l_i+1)}{x^2}\right)R_{ij}(x,y;s,u)=\left(\frac{d^2}{dy^2}-\frac{l_j(l_j+1)}{y^2}\right)R_{ij}(x,y;s,u), \quad (12)$$

$$R_{ij}(x,y;x,y)=1, \quad (13)$$

$$\frac{\partial}{\partial x}R+\frac{\partial}{\partial y}R=0 \quad \text{if } y-x=u-s, \quad (14)$$

$$\frac{\partial}{\partial x}R-\frac{\partial}{\partial y}R=0 \quad \text{if } y+x=u+s. \quad (15)$$

With the use of characteristic curves, Eq. (11) with its boundary conditions is solved by the Riemann's method, and one has

$$\begin{aligned}K_{ij}(x,y)=&\tfrac{1}{2}\int_{(x+y)/2}^{\infty}R_{ij}(x,y;s,s)V_{ij}(s)\,ds\\&+\tfrac{1}{2}\int_x^{(x+y)/2}ds\int_{y+x-s}^{y+s-x}R_{ij}(x,y;s,u)\\&\times\sum_k V_{ik}(s)K_{kj}(s,u)\,du\\&+\tfrac{1}{2}\int_{(x+y)/2}^{\infty}ds\int_s^{y+s-x}R_{ij}(x,y;s,u)\\&\times\sum_k V_{ik}(s)K_{kj}(s,u)\,du,\quad 0<x\leq y.\end{aligned} \quad (16)$$

We will shorten our notations by writing

$$\begin{aligned}K_{ij}(x,y)=&\tfrac{1}{2}\int_{(x+y)/2}^{\infty}R_{ij}(x,y;s,s)V_{ij}(s)\,ds\\&+\tfrac{1}{2}\iint_{\mathcal{D}(x,y)}R_{ij}(x,y;s,u)\\&\times\sum_k V_{ik}(s)K_{kj}(s,u)\,du\,ds,\end{aligned} \quad (17)$$

with du preceding ds in the double integral. $\mathcal{D}(x,y)$ is the integration domain of Fig. 1.

Together with Riemann's solution, we shall introduce, for each matrix A, the matrix of its absolute values $|A|$ whose elements are

$$|A|_{ij}=|A_{ij}|. \quad (18)$$

If A and B are matrices, we will write $A\leq B$ if

$$|A_{ij}|\leq|B_{ij}| \quad \text{for all } i,j\leq n.$$

Clearly, Eq. (18) implies

$$|ABC|\leq|A|\,|B|\,|C|. \quad (19)$$

For each matrix A, we will also define a norm $\|A\|$ by

$$\|A\|=\max_j\sum_k|A_{jk}|, \quad (20)$$

Clearly, $\|A\|$ introduced by Eq. (20) has the usual properties of a norm.[13]

3. A PARTICULAR CASE

A special case is studied now since it allows us to use standard matrix methods and to indicate how results can be obtained. It contains an extension of Marchenko's results.

This special case is obtained by writing

$$[D(x)-l(x)]K(x,y)=[D(y)-l(y)]K(x,y)=V(x)K(x,y).$$

To be more specific, Eq. (11) is replaced by Eq. (20):

$$\left(\frac{d^2}{dx^2}-\frac{l_i(l_i+1)}{x^2}\right)K_{ij}(x,y)=\left(\frac{d^2}{dy^2}-\frac{l_i(l_i+1)}{y^2}\right)K_{ij}(x,y)+\sum_k V_{ik}(x)K_{kj}(x,y).$$

However, the boundary conditions which K should satisfy, i.e., Eqs. (9) and (10), are retained.

The Riemann functions to be used are the solutions of

$$\left(\frac{d^2}{dx^2}-\frac{l_i(l_i+1)}{x^2}\right)R_{ii}(x,y;s,u)=\left(\frac{d^2}{dy^2}-\frac{l_i(l_i+1)}{y^2}\right)R_{ii}(x,y;s,u). \quad (21)$$

We can define a Riemann matrix by

$$[D(x)-l(x)]R(x,y;s,u)=[D(y)-l(y)]R(x,y;s,u).$$

Using Chaundy's results, Ref. 9, one can write

$$R(x,y;s,u)=\{P_{l_i}(1-2z)\}\delta_{ij} \quad (22)$$

with

$$z=(1/16usxy)(x+y-u-s)(s-u+y-x)(u+y+s+x)\times(u+y-s-x), \quad (23)$$

as illustrated in Ref. 6. Instead of z we use Chaundy's variables x_1 and x_2 defined as follows

$$x_1=\frac{(u+s-x-y)(x-z-s+u)}{4xs},$$

$$x_2=\frac{(x+y-u-s)(x-y+u-s)}{4uy},$$

$$1-2z=1-2x_1-2x_2+2x_1x_2,$$

and write

$$R(x,y;u,s)=\{P_{l_i}(1-2x_1-2x_2+2x_1x_2)\delta_{ij}\}.$$

In the Domain $\mathcal{D}(x,y)$, in Fig. 1, the following inequalities are satisfied:

$$u-s\leq y-x, \quad (24)$$

$$u+s \geq y+x, \tag{25}$$

$$u \geq s, \tag{26}$$

$$s \geq x, \tag{27}$$

$$y \geq x. \tag{28}$$

From these inequalities the following estimates can be derived:

$$u+s-x-y \leq 2(s-x) \leq 2s \quad \text{by (24)},$$

$$s-u+y-x \leq 2(s-x) \leq 2s \quad \text{by (24)},$$

$$u+y+s+x \leq 2(u+s) \leq 4u \quad \text{by (25) and (26)},$$

$$u+y-s-x \leq 2(y-x) \leq 2y \quad \text{by (24)}. \tag{29}$$

While x_1 is negative and

$$-x_1 \leq s/x,$$

x_2 is positive

$$x_2 = \frac{(u+s-x-y)(y-x+s-u)}{4uy} \leq \frac{(u+s)(u+y-s-x)}{4uy},$$

since one has

$$(u+y-s-x)-(y-x-s-u) = 2(u-s) \geq 0.$$

Therefore, one obtains

$$0 \leq x_2 \leq 1. \tag{30}$$

We rewrite the argument

$$z = (1-2x_1) - 2x_2(1-x_1) \tag{31}$$

with the two parentheses positive. Equations (29) and (30) imply

$$1 \leq x \leq 1-2x_1 \leq 3s/x. \tag{32}$$

The argument X of the Legendre functions being greater than unity, one has

$$|P_l(X)| \leq (2X)^l \leq (6s/x)^l. \tag{33}$$

Consequently,

$$|R(x,y;s,u)| \leq D^{-1}(x)CD(s) \tag{34}$$

where the diagonal matrices D and C have the following elements:

$$C_{ij} = 6^{l_i}\delta_{ij}, \tag{35}$$

$$D_{ij}(s) = s^{l_i}\delta_{ij}. \tag{36}$$

The integral equation for the matrix K can be written in a matrix form:

$$K(x,y) = \tfrac{1}{2}\int_{(x+y)/2}^{\infty} R(x,y,;s,s)V(s)\,ds + \tfrac{1}{2}\int\int_{D(x,y)} R(x,y;s,u)V(s)K(s,u)\,du\,ds. \tag{37}$$

We use now the reduction method of Ref. 6b and define

$$K(x,y) = D^{-1}(x)\tilde{K}(x,y), \tag{38}$$

$$R(x,y;s,u) = D^{-1}(x)\tilde{R}(x,y;s,u)D(s)C \tag{39}$$

with

$$|R| \leq I \quad \text{(matrix unity)}.$$

With these reductions Eq. (37) becomes

$$\tilde{K}(x,y) = \tfrac{1}{2}\int_{(x+y)/2}^{\infty} \tilde{R}(x,y;s,s)D(s)CV(s)\,ds + \tfrac{1}{2}\int\int_{D(x,y)} \tilde{R}(x,y;s,u)D(s) \times CV(s)D^{-1}(s)\tilde{K}(s,u)\,du\,ds. \tag{40}$$

We are led to define the two interactions

$$\tilde{V}(s) = D(s)CV(s),$$

$$W(s) = D(s)CV(s)D^{-1}(s), \tag{41}$$

which should allow us to use the estimates of Appendix B. We decide here to proceed otherwise for a better interpretation of the conditions we obtain.

Equation (41) is rewritten as

$$\tilde{K}(x,y) = \tfrac{1}{2}\int_{(x+y)/2}^{\infty} \tilde{R}(x,y;s,s)\tilde{V}(s)\,ds + \int\int_{D(x,y)} \tilde{R}(x,y;s,u)W(s)\tilde{K}(s,u)\,du\,ds \tag{42}$$

and solved by the method of successive approximations:

$$\tilde{K}(x,y) = \sum_{n=0}^{\infty} \tilde{K}^{(n)}(x,y), \tag{43}$$

where

$$\tilde{K}^{(0)}(x,y) = \tfrac{1}{2}\int_{(x+y)/2}^{\infty} \tilde{R}(x,y;s,s)\tilde{V}(s)\,ds \tag{44}$$

and

$$\tilde{K}^{(n)}(x,y) = \tfrac{1}{2}\int\int_{D(x,y)} \tilde{R}(x,y;s,u)W(s) \times \tilde{K}^{(n-1)}(s,u)\,du\,ds. \tag{45}$$

The following bounds are found for the different terms of the series defined in Eq. (43):

$$|\tilde{K}^{(0)}(x,y)| \leq \tfrac{1}{2}\int_{(x+y)/2}^{\infty} |\tilde{V}(s)|\,ds \equiv \tfrac{1}{2}\sigma((x+y)/2), \tag{46}$$

$$|\tilde{K}^{(1)}(x,y)| \leq \tfrac{1}{2}\int\int_{D(x,y)} |\tilde{R}(x,y;s,u)|\,|W(s)| \times |\tilde{K}^{(0)}(s,u)|\,du\,ds \leq \tfrac{1}{2}\int_x^{\infty} |W(s)|\,s\,ds\,\sigma((x+y)/2). \tag{47}$$

More generally one has

$$|\tilde{K}^{(n)}(x,y)| \leq \tfrac{1}{2}\int_x^{\infty} dx_{n-1}x_{n-1}|W(x_{n-1})| \int_{x_{n-1}}^{\infty} dx_{n-2}x_{n-2}|W(x_{n-2})| \times \cdots \int_{x_1}^{\infty} dx_0 x_0 |W(x_0)|\,\sigma((x+y)/2). \tag{48}$$

We determine now necessary and sufficient conditions for a convergence of the series (43) which is both uniform and absolute. These conditions, however, are simply *sufficient* conditions for the existence of $\tilde{K}$. For the series (43) to converge uniformly and absolutely it is necessary to impose

$$\int_x^{\infty} |\tilde{V}(s)|\,ds < \infty, \tag{49}$$

$$\int_x^{\infty} |W(s)|\,s\,ds < \infty. \tag{50}$$

The potential V_{ij} should have a moment of order l_i from Eq. (49) and a moment of order $(l_i - l_j + 1)$ from Eq. (50).

To prove the sufficiency of these conditions, norms are used as in Appendix B. With Eqs. (49) and (50) one can write

$$\|\tilde{K}(x,y)\| \leq \tfrac{1}{2}\eta((x+y)/2)\exp[\xi(x)], \tag{51}$$

with

$$\eta((x+y)/2) = \int_{(x+y)/2}^{\infty} \|V(s)\|\, ds \tag{52}$$

$$\xi(x) = \int_x^{\infty} \|W(s)\|\, ds. \tag{53}$$

Equation (51) defines an estimate for the norm of $K(x,y)$

$$\|K(x,y)\| = D^{-1}(x)\|\tilde{K}(x,y)\|. \tag{54}$$

From Eq. (54) it can be seen that the matrix $K(x,y)$ when $\tilde{K}$ satisfies Eq. (51) is a matrix of absolutely integrable functions with respect to y.

A physical application of this section is that when all the l_i are equal

$$l_i = l. \tag{55}$$

Equation (55) contains as a particular case Marchenko's study where all the $l_i = 0$. From what precedes, moments of order l and one should be required from the elements of the matrix potential. So we state:

Theorem: If

$$\sigma_1(x) = \int_x^{\infty} t\,|V(t)|\, dt < \infty,$$

$$\sigma_l(x) = \int_x^{\infty} t^l\,|V(t)|\, dt < \infty,$$

then an integral representation[7] exists for the solution of a partial differential matrix equation with all l equal, and one has

$$(1/x)^l\|K(x,y)\| \leq \tfrac{1}{2}\sigma_l((x+y)/2)\exp[\sigma_1(x)].$$

4. THE GENERAL CASE EQ. (11)

To follow the same method, we need to use the Riemann's solutions of Eq. (12). These two can be found in Refs. 10 and 11:

$$R_{ij}(x,y;s,u) = \varkappa\begin{bmatrix} l_i, l_j \\ x_1, x_2 \end{bmatrix}$$

$$\varkappa\begin{bmatrix} l_i, l_j \\ x_1, x_2 \end{bmatrix} = P_{l_i}(1-2x_1) - 2x_2\int_0^1 P_{l_i}(1-2x_1+2x_1t)P'_{l_j}(1-2x_2t)\, dt, \tag{56}$$

where $\varkappa$ is a Chinese letter, to be pronounced "pa," introduced by Chaundy (Ref. 10).

Equation (56) is integrated by parts to get

$$R_{ij} = P_{l_j}(1-2x_2) - 2x_1\int_0^1 P_{l_j}(1-2x_2t)P'_{l_i}(1-2x_1+2x_1t)\, dt.$$

Now we consider

$$I = \left|(-1)\int_0^1 P_{l_j}(1-2x_2t)2x_1P'_{l_i}(1-2x_1+2x_1t)\, dt\right|$$

$$\leq \int_0^1 \left|[-2x_1P'_{l_1}(1-2x_1+2x_1t)\right| dt. \tag{57}$$

To get Eq. (57), we used the fact that $|1-2x_2t| \leq 1$ implied

$$|P_{l_j}(1-2x_2t)| \leq 1.$$

The integrand in Eq. (57) has a constant sign since P_{l_1} is an increasing function of its argument whenever the latter is greater than unity.

Consequently,

$$I \leq \left|\int_0^1 (-2x_1)P'_{l_1}(1-2x_1+2x_1t)\right|$$

$$\leq P_{l_i}(1-2x_1).$$

The estimate for R_{ij} follows:

$$|R_{ij}| \leq (6s/x)^{l_i} + 1 \leq (7s/x)^{l_i}. \tag{58}$$

Back to Eq. (17), we use again reductions

$$\begin{cases} (1/x^{l_i})K_{ij} = \tilde{K}_{ij}, \\ R_{ij} = (1/x^{l_i})\tilde{R}_{ij}(7s)^{l_i}, \quad |\tilde{R}_{ij}| < 1, \\ \tilde{V}_{ij} = (7s^{l_i})V_{ij}, \\ W_{ij} = (7s^{l_i})V_{ij}/x^{l_j}. \end{cases} \tag{59}$$

Thus we write Eq. (17) as

$$\tilde{K}_{ij}(x,y) = \tfrac{1}{2}\int_{(x+y)/2}^{\infty}\tilde{R}_{ij}(x,y;s,s)\tilde{V}_{ij}(s)\, ds + \tfrac{1}{2}\int\int_{D(x,y)}\tilde{R}_{ij}(x,y;s,u) \times\sum_k W_{ik}(s)\tilde{K}_{kj}(s,u)\, ds\, du. \tag{60}$$

So we will get

$$|\tilde{K}^{(0)}_{ij}(x,y)| \leq \tfrac{1}{2}\int_{(x+y)/2}^{\infty}|\tilde{V}_{ij}(s)|\, ds,$$

$$|\tilde{K}^{(1)}_{ij}(x,y)| \leq \tfrac{1}{2}\int_x^{\infty}|s|\sum_k|W_{ik}(s)|\,|\tilde{K}^{(0)}_{kj}(x,y)|\, ds. \tag{61}$$

Equations (61) are similar in form to Eqs. (46) and (47) when the latter are made explicit in i and j. The analysis of the previous section applies therefore, and we can state the theorem.

Theorem: If

$$\sigma^{(1)}_{ij}(x) = \int_x^{\infty} t\,|V_{ij}(t)|\,t^{(l_i-l_j)}\, dt < \infty,$$

$$\sigma^{(0)}_{ij}(x) = \int_x^{\infty} t^{l_i}\,|V_{ij}(t)|\, dt < \infty,$$

then an integral representation[7] for the solution of the partial differential matrix equation exists, and one has

$$D^{-1}(x)\|K(x,y)\| \leq \tfrac{1}{2}\eta((x+y)/2)\exp[\xi(x)]. \tag{62}$$

In Eq. (62) the definitions

$$\eta((x+y)/2) = \int_{(x+y)/2}^{\infty}\|V(s)\|\, ds \quad \eta(x) = \int_x^{\infty}\|W(s)\|s\, ds$$

were used with $\tilde{V}$ and W taken from Eq. (59).

We proceed now to remove the restriction that all the λ_i's should be equal. If they are not equal, the K_{ij} elements of the K matrix are the solutions of the equation

$$\left(\frac{\partial^2}{\partial x^2}+\lambda_i^2-\frac{l_i(l_i+1)}{x^2}\right)K_{ij}(x,y) =\left(\frac{\partial^2}{\partial y^2}+\lambda_j^2-\frac{l_j(l_j+1)}{y^2}\right)K_{ij}(x,y) +\sum_k V_{ik}(x)K_{kj}(x,y), \tag{63}$$

which introduces a λ dependence in the K matrix.

We need now the Riemann solution X_{ij} for the partial differential equation:

$$\left(\frac{\partial^2}{\partial x^2}+\lambda_i^2-\frac{l_i(l_i+1)}{x^2}\right)X_{ij} =\left(\frac{\partial^2}{\partial y^2}+\lambda_j^2-\frac{l_j(l_j+1)}{y^2}\right)X_{ij}. \tag{64}$$

To obtain an estimate for these X_{ij}, Theorem 1 of Ref. 6b is used. Using characteristic variables $(\xi, \eta, \xi_0, \eta_0)$ instead of the physical variables $(x, y; s, u)$ and denoting

$$\mathcal{X}(\xi,\eta;\xi_0,\eta_0)\equiv X(x,y;s,u),$$
$$\mathcal{R}(\xi,\eta;\xi_0,\eta_0)\equiv R(x,y;s,u),$$

we have

$$\mathcal{X}_{ij}(\eta,\eta;\xi_0,\eta_0)=\mathcal{R}_{ij}(\xi,\eta;\xi_0,\eta_0)+\int_\xi^{\xi_0}d\xi' \times\int_\eta^{\eta_0}d\eta'\mathcal{R}_{ij}(\xi,\eta;\xi',\eta')(\lambda_i^2-\lambda_j^2) \times\mathcal{X}_{ij}(\xi',\eta',\xi_0,\eta_0). \tag{65}$$

Since $|R_{ij}|\leq(7s/x)^{l_i}$, we have

$$|\mathcal{R}_{ij}|\leq[7(\xi_0-\eta_0)/(\xi-\eta)]^{l_i}.$$

We set

$$\mathcal{R}_{ij}=\tilde{\mathcal{R}}_{ij}[7(\xi_0-\eta_0)/(\xi-\eta)]^{l_i},$$
$$\mathcal{X}_{ij}=\tilde{\mathcal{X}}_{ij}[7(\xi_0-\eta_0)/(\xi-\eta)]^{l_i},$$

and obtain the reduced equation for $\tilde{\mathcal{X}}_{ij}$:

$$\tilde{\mathcal{X}}_{ij}(\xi,\eta;\xi_0,\eta_0) =\tilde{\mathcal{R}}_{ij}(\xi,\eta;\xi_0,\eta_0)+\int_\xi^{\xi_0}d\xi'\int_\eta^{\eta_0}d\eta' \times\tilde{\mathcal{R}}_{ij}(\xi,\eta;\xi',\eta')(\lambda_i^2-\lambda_j^2)\tilde{\mathcal{X}}_{ij}(\xi',\eta';\xi_0,\eta_0). \tag{66}$$

From this Eq. (66) we get[14]

$$|\tilde{\mathcal{X}}_{ij}(\xi,\eta;\xi_0,\eta_0)| \leq\exp[2(|\lambda_i^2-\lambda_j^2|\,|\xi_0-\xi|\,|\eta_0-\eta|)^{1/2}]$$
$$|\tilde{\mathcal{X}}_{ij}(x,y;s,u)| \leq\exp[2(|\lambda_i^2-\lambda_j^2|\,|u-s-y+x|\,|u+s-y-x|)^{1/2}].$$

Now we have from Eq. (29)

$$u+s-x-y\geq 0,\quad u+s-y-x\leq 2s,$$
$$u-s+x-y\leq 0,\quad s-u+y-x\leq 2s. \tag{67}$$

Setting

$$\beta^2=\sup_{i,j}|\lambda_i^2-\lambda_j^2|, \tag{68}$$

we obtain the estimate

$$|\mathcal{X}_{ij}(x,y;s,u)|\leq(7s/x)^{l_i}\exp(4\beta s),$$

valid for all i and all j.

Now we define

$$\tilde{V}_{ij}(s)=(7s)^{l_i}V_{ij}(s)\exp(4\beta s),$$
$$W_{ij}(s)=(7)^{l_i}s^{(l_i-l_j)}V_{ij}(s)\exp(4\beta s). \tag{69}$$

The equation for $\tilde{K}_{ij}$ follows:

$$\tilde{K}_{ij}(x,y)=\tfrac{1}{2}\int_{(x+y)/2}^{\infty}\tilde{\mathcal{X}}_{ij}(x,y;s,s)\tilde{V}_{ij}(s)\,ds +\tfrac{1}{2}\int\int_{\Box(x,y)}\tilde{\mathcal{X}}_{ij}(x,y;s,u)\sum_k W_{ik}(s) \times K_{kj}(s,u)\,du\,ds. \tag{70}$$

Equation (70) yields

$$\|K^{(0)}(x,y)\|\leq\tfrac{1}{2}\int_{(x+y)/2}^{\infty}\|\tilde{V}(s)\|\,ds=\tfrac{1}{2}\eta((x+y)/2), \tag{71}$$

and

$$\|K^{(1)}(x,y)\|\leq\tfrac{1}{2}\sigma((x+y)/2)\xi(x),$$

where we defined

$$\xi(x)=\int_x^{\infty}\|W(s)\|s\,ds.$$

By mathematical induction we obtain again

$$\|K(x,y)\|\leq\tfrac{1}{2}\eta((x+y)/2)\exp[\xi(x)],$$

which provides the estimate

$$D^{-1}(x)\|K(x,y)\leq\tfrac{1}{2}\exp(2\beta|x|)\eta((x+y)/2)\exp[\xi(x)]. \tag{72}$$

Equations (72) and (62) are very similar; the main differences are the definitions of the involved nuclear potentials and the presence of the $\exp(2\beta|x|)$ factor.

From Eqs. (63) and (72) it is seen that threshold energies have two consequences:

(a) The threshold energies appear explicitly in the translation kernel;

(b) An exponential decrease is required from the nuclear potentials, the measure of this decrease being expressed by

$$4\sup_{i,j}(|\lambda_i^2-\lambda_j^2|)^{1/2}.$$

Introduction of Coulomb forces in the scheme does not modify the method of solution, the Coulomb interaction being a scalar operator. Conditions similar to those of Ref. 6b should be superimposed on the ones formulated in the present paper.

APPENDIX A

Let A_0 and A be two partial differential matrix operators

$$A\equiv\frac{d^2}{dx^2}-W_0(x)-V(x)\equiv\frac{d^2}{dx^2}-W(x),$$
$$A_0\equiv\frac{d^2}{dx^2}-W_0(x). \tag{A1}$$

Let now a transformation X be defined by

$$Xf = If + \int_x^\infty K(x,y) f(y)\, dy. \tag{A2}$$

In Eq. (A2) I is the identity matrix and f and twice differential matrix satisfying

$$\begin{cases} \lim_{y\to\infty} f(y) \sim \exp(ikx) \\ k \text{ real.} \end{cases}$$

The transformation X is said to be a translation from A_0 to A if for all f's one has

$$AXf \equiv XA_0 f. \tag{A3}$$

By integrations and derivations under the integral sign the kernel $K(x,y)$ of Eq. (A2) must satisfy the following Eq. (A4) for X to exist. Equation (A4) is

$$\begin{aligned} &\left(\frac{d^2}{dx^2} - W_0(x) - V(x)\right) K(x,y) = \frac{d^2}{dy^2} K(x,y) - K(x,y) W_0(y), \\ &\lim_{y\to\infty} K(x,y) = \lim_{y\to\infty} \frac{\partial}{\partial y} K(x,y) = 0, \\ &K(x,x) = \tfrac{1}{2} \int_x^\infty V(s)\, ds. \end{aligned} \tag{A4}$$

APPENDIX B

We consider the partial differential matrix equation

$$\begin{aligned} &\left(\frac{d^2}{dx^2} - \frac{d^2}{dy^2}\right) L(x,y) = V(s) L(x,y), \\ &L(x,x) = \tfrac{1}{2} \int_x^\infty W(s)\, ds \\ &\lim_{y\to\infty} L(x,y) = \lim_{y\to\infty} \frac{\partial}{\partial x} L(x,y) = 0. \end{aligned} \tag{B1}$$

By the Riemann method Eq. (B1) is transformed into an integral equation:

$$L(x,y) = \tfrac{1}{2} \int_{(x+y)/2}^\infty V(s)\, ds + \tfrac{1}{2} \int\int_{\Omega} W(s) L(s,u)\, du\, ds. \tag{B2}$$

Equation (B2) is a matrix equation similar to Eq. (1.3.6) of Ref. 1. Ω is the domain of Fig. (1). Therefore, one defines

$$\begin{aligned} \eta(x) &= \int_x^\infty \|V(s)\|\, ds, \\ \xi(x) &= \int_x^\infty \|W(s)\|\, ds, \end{aligned} \tag{B3}$$

and obtains the estimate for the norm of $L(x,y)$,

$$\|L(x,y)\| \leq \tfrac{1}{2} \eta((x+y)/2) \exp[\xi(x)]. \tag{B4}$$

Equation (B4) gives sufficient conditions for the existence of a solution $L(x,y)$ for Eq. (B1).

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[1]Z.S. Agranovitch and V.A. Marchenko, *The Inverse Problem of Scattering Theory*, translated by B.D. Seckler (Gordon and Breach, New York, 1963).
[2]For references for the one-dimensional problem: H.E. Moses, J. Math. Phys. **16**, 1044 (1975).
[3]J.J. Loeffel, Ann. Inst. Henri Poincaré **8**, (4), 339 (1968).
[4]P.J. Kelemen, J. Math. Phys. **12**, 1142 (1971).
[5]H.I. Gugusvili and Y.L. Mentovski, Nuovo Cimento A **10**, 277 (1972).
[6](a) M. Coz and C. Coudray, J. Math. Phys. **14**, 1574 (1973); (b) J. Math. Phys. (1976) to be published.
[7]M.M. Crum, Quart. J. Math. **6**, (2), 121 (1955).
[8]M.G. Krein, Dokl. Akad. Nauk SSSR **113** (5), 970 (1957).
[9]R.G. Newton and R. Jost, Nuovo Cimento **1**, 505 (1955).
[10]T.W. Chaundy, Quart. J. Math. Oxford **10**, 310 (1939).
[11]E.T. Copson, Arch. Ratl. Mech. Anal. **1**, 324 (1958).
[12]R. Courant and Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1943), TII, p. 450.
[13]H.G. Garnir, M. de Wilde, and J. Schmets, *Analyse fonctionnelle*. 1 (Birkhauser Verlag, Bassel and Stuttgart, 1968).
[14]G. Valiron, *Equations fonctionnelles, Applications* (Masson, Paris, 1950), p. 569; see also Ref. 6b.

Some new identities of Clebsch–Gordan coefficients and representation functions of SO(2,1) and SO(4)

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A systematic derivation of various relations and identities among the Clebsch–Gordan coefficients and for the representation functions of SO(4) and SO(2,1), is given. These relations are essential in work involving the matrix elements of arbitrary group elements in higher noncompact groups such as O(4,2).

I. INTRODUCTION

During the past years the concept of internal dynamical groups has been widely adopted, in the solution to various problems of quantum dynamics, both relativistic and nonrelativistic. Especially noteworthy is the infinite component wave equation using the most degenerate unitary irreducible representation of the noncompact orthogonal group O(4, 2) which has found many applications. Although many more physical results are yet to be computed, this theory seems to be particularly adopted to the composite nature of not only the H-atom but also hadrons, in particular the proton. On the mathematical side the group O(4, 2) contains most of the physical groups like the Lorentz Group O(3, 1), O(2, 1), E(3), etc., and consequently many already known physical concepts are built into the theory. Recently we have succeeded in expressing the "Universal" inelastic form factors and structure functions of the proton and spin-0 particles in such a way that a better and closer study of these functions is now possible. This has been achieved by explicitly expressing the O(4, 2)-transition amplitudes in terms of O(4)- and O(2, 1)-representation functions and this further demands a number of new identities and relations in these representation functions and in O(3)-Clebsch—Gordan coefficients. The purpose of this paper is to offer these relations separately and derive them explicitly. The representation functions themselves are assumed to be known. We have tried to adopt throughout a unified approach of using the symmetry and recursion properties of generalized hypergeometric polynomials, although here and there we have deviated from this approach for simplicity.

In Sec. II, we deal with the well-known O(3)-Clebsch—Gordan coefficients. Smorodinskiĭ and Shelepin suggest that because of the three "nontrivial" Regge symmetries, there can be three nontrivial forms (due to Racah, Majumdar and van der Waerden) of CG coefficient other than the original expression due to Wigner. We are able to obtain these expressions through Thomae—Whipple symmetries of the generalized hypergeometric polynomial ${}_3F_2$ of unit argument. Also we derive some important recursion relations of the CG coefficients using the recurrence relations satisfied by ${}_3F_2$. These recursion relations are extremely useful when one wants to study the action of the O(4, 2) generators on canonical basis. We have also derived two identities involving negative angular momenta and discussed different asymptotic expressions of the CG-coefficients. Although some of the results in this section are familiar, we have derived them mainly using the properties of hypergeometric functions.

In Sec. III we give some important properties of the O(2, 1)-representation function (D_k^+-series) due to Bargmann. Using various recurrence relations of the ${}_2F_1$ hypergeometric function we have derived many recursion relations of this representation function and they are being used elsewhere to compute the O(4, 2)-transition amplitudes. Finally we use the famous Burchnall—Chaundy multiplication formula to obtain the O(2, 1) CG-coefficient and to derive explicitly a decomposition rule for the product of two O(2, 1)-functions. This rule is extremely useful and enables one to express the O(4, 2)-transition amplitudes in closed form.

The last section deals with the O(4)-representation function. There we have derived two new formulas for the representation function and have expressed them in terms of Gegenbauer polynomials. For this we have used the simple differential operator method due to Ström. We have also given some asymptotic expressions for the O(4)-functions as we find them very useful for the discussion of the asymptotic behavior of form factors. Using various results of this paper, we have explicitly evaluated the matrix elements of finite Lorentz transformations between the so-called tilted O(4, 2)-states and have expressed them in terms of two O(4)- and one O(2, 1)-representation functions. These results, we believe, are very important and useful for explicit calculations in the O(4, 2)-theory.

II. THE CLEBSCH-GORDAN COEFFICIENTS FOR O(3)

1. Definition and general expressions

The Clebsch—Gordan coefficients[1] $C(l_1l_2m_1m_2|lm)$ (or in Dirac's notation $\langle l_1l_2m_1m_2|lm\rangle$) are generally defined as the coefficients in the expansion

$$g_m^l = \sum_{\substack{l_1l_2m_1m_2 \\ (m_1+m_2=m)}} \langle l_1l_2m_1m_2|lm\rangle e_{m_1}^{l_1} f_{m_2}^{l_2}, \qquad \text{(II. 1. 1)}$$

where $g_m^l (|l_1 - l_2| \leq l \leq l_1 + l_2)$ are the vectors of canonical bases in the Kronecker product space of two irreducible unitary representations of weights l_1 and l_2 of the three-dimensional rotation group, and the canonical bases of the Kronecker "factors" are given by $e_{m_1}^{l_1}$ and $f_{m_2}^{l_2}$, $(-l_i \leq m_i \leq l_i; i = 1, 2)$. The weight l is an integer or a semi-integer simultaneously with $l_1 + l_2$. These coefficients are physically interpreted as the probability amplitude for obtaining the total angular momentum

(l, m) in the addition of the angular momenta (l_1, m_1) and (l_2, m_2). In order to investigate the underlying symmetries and invariants of these coefficients under certain transformations one conveniently makes use of Wigner's[2] 3-j symbol, defined as

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} = (-1)^{l_2-l_1-m}(2l+1)^{-1/2}\langle l_1 l_2 m_1 m_2 | l m\rangle$$
$$= (-1)^{l_2-l_1-m}(2l+1)^{-1/2}\begin{bmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{bmatrix}. \quad \text{(II. 1. 2)}$$

This 3-j symbol possesses the so-called "classical symmetries"—12 symmetries under the 3! permutations and the reversal ($m_i \to -m_i$ and $m \to -m$) of the three angular momenta (l_1, l_2 and l) as well as Regge symmetries. All these symmetries may be made more apparent if one considers the so-called Regge symbol,[3]

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix} \equiv \boxed{\begin{matrix} -l_1+l_2+l & l_1-l_2+l & l_1+l_2-l \\ l_1-m_1 & l_2-m_2 & l-m \\ l_1+m_1 & l_2+m_2 & l+m \end{matrix}}. \quad \text{(II. 1. 3)}$$

This symbol is symmetric under (i) permutation of the columns, (ii) permutation of the rows, and (iii) transposition about the major diagonal [also transposition about the "opposite" diagonal—this symmetry is not new since this can be obtained by the products of (i) and (ii), but it is convenient]. The classical symmetries are built into (i) and (ii). If one allows also the negative values of the angular momenta through the substitutions $l_1 \to l_1 - 1$, $l_2 \to -l_2 - 1$, and $l \to -l - 1$ (with the triangle condition $|l_1 - l_2| \le l \le l_1 + l_2$), then one obtains $3! \times 3! \times 2 \times 4 = 288$ symmetries (3! for permutation of columns, 3! for permutation of rows, 2 for transposition, and 4 for negative values of l). This means that there are 288 identical Clebsch–Gordan coefficients with positive or negative values of the angular momenta. The physical origin of the classical symmetries is well understood, but that of the remaining Regge symmetries is not at all clear. Bincer[4] interprets the third Regge symmetry (symmetry under transposition) in the classical limit (l_1 and l_2 large but fixed l) as the symmetry under the interchange of "body-fixed" and "space-fixed" frames of reference and this conclusion is based on the Brussard–Tolhock asymptotic condition[5] that in the classical limit CG coefficients approach the representation functions (the matrix element of a finite rotation) of the group SO(3).

A general expression for CG coefficients was first derived by Wigner. If one imposes the three symmetries (under permutations, transposition, and the product of the two) into Wigner's expression then three more nontrivial expressions may be obtained and one may select them as the ones[6] due to van der Waerden, Racah and Majumdar. All these expressions involve a finite sum with the summand containing five factorial terms besides the term which is just the factorial of summation variable. This leads to the possibility that the CG-coefficient may be expressed in terms of a generalized hypergeometric function ${}_pF_q$ with $p+q=5$. Rose[6] succeeded in expressing Wigner's relation in terms of the generalized hypergeometric function ${}_3F_2$ with unit argument, i. e.,

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}_W = (-1)^{l_2-l_1-m}\Delta \frac{(l_1+l_2+m_1)!}{(l_1-l_2-m)!}$$
$$\times {}_3F_2\begin{bmatrix} -l-m, & -l+l_1-l_2, & l_1-m_1+1; \\ l_1-l_2-m+1, & -l-l_2-m_1; & 1 \end{bmatrix},$$

where

$$\Delta = (-1)^{l_2+m_2} \times \left(\frac{(l+l_1-l_2)!(-l+l_1+l_2)!}{(l-l_1+l_2)!(l+l_1+l_2+1)!(l+m)!} \times \frac{(l-m)!(l_1-m_1)!}{(l_1+m_1)!(l_2+m_2)!(l_2-m_2)!} \right)^{1/2}. \quad \text{(II. 1. 4)}$$

Here the hypergeometric function ${}_3F_2$ is a terminating series since it has two upper parameters which are negative integers. For such cases, it can be easily seen[7] that there are 24 such terminating series (in comparison with 18 when only one upper parameter is negative) which are simply related one to one. Since each hypergeometric function is invariant under the permutations of upper and lower parameters, one obtains the total number of different forms of ${}_3F_2$ (with two negative upper parameters) to be $24 \times 3! \times 2! = 288$ which is exactly the total number of symmetries of the CG coefficients. All the different symmetries of such ${}_3F_2$ may be obtained from Thomae–Whipple formalism,[7] and many of them are already used. For example the symmetry derived by Hardy (in Whipple's notation[7]) is

$$\Gamma[\alpha_{123}, \alpha_{124}, \alpha_{125}]F_p[0; 4, 5] = (-1)^m \Gamma[\alpha_{124}, \alpha_{024}, \alpha_{014}]F_n[4; 0, 1],$$

or

$${}_3F_2\begin{bmatrix} a, & b, & c; \\ d, & e; & 1 \end{bmatrix} = \frac{\Gamma(d)\Gamma(d-a-b)}{\Gamma(d-a)\Gamma(d-b)} {}_3F_2\begin{bmatrix} a, & b, & e-c; \\ 1+a+b-d, & e; & 1 \end{bmatrix}. \quad \text{(II. 1. 5)}$$

Using this twice in Eq. (II. 1. 4) we get the Majumdar form of CG-coefficients,

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}_M = (-1)^{l_2-l_1-m}\Delta \frac{(l_1+m_1)!(l_2-m_2)!(2l)!}{(l-m)!(l+l_1-l_2)!(-l+l_1-m_2)!}$$
$$\times {}_3F_2\begin{bmatrix} -l-m, & -l+l_1-l_2, & -l+l_1+l_2+1; \\ -2l, & -l+l_1-m_2+1; & 1 \end{bmatrix}. \quad \text{(II. 1. 6)}$$

Furthermore, the Thomae–Dixon symmetry gives

$$F_p[0; 4, 5] = F_p[0; 2, 3],$$

or

$${}_3F_2\begin{bmatrix} a, & b, & c; \\ d, & e; & 1 \end{bmatrix} = \frac{\Gamma(d)\Gamma(e)\Gamma(s)}{\Gamma(a)\Gamma(s+b)\Gamma(s+c)} \times {}_3F_2\begin{bmatrix} d-a, & e-a, & s; \\ s+b, & s+c; & 1 \end{bmatrix},$$
$$s = d+e-a-b-c. \quad \text{(II. 1. 7)}$$

Using this in Eq. (II. 1. 6) we get the Racah form

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}_R$$
$$= (-1)^{2(l_2-l_1)}\Delta\frac{(l+m)!\,(l_2-m_2)!\,(l+l_2-m_1)!}{(l-m)!\,(l+l_1-l_2)!\,(-l+l_2+m_1)!}$$
$$\times {}_3F_2\begin{bmatrix} -l+m, & -l_1+m_1, & l_1+m_1+1; \\ -l-l_2+m_1, & -l+l_2+m_1+1; & 1 \end{bmatrix}. \qquad \text{(II. 1. 8)}$$

Also if we use the symmetry

$$\Gamma[\alpha_{123}, \alpha_{124}, \alpha_{125}]F_p[0; 4, 5]$$
$$= (-1)^m\Gamma[\alpha_{124}, \alpha_{024}, \alpha_{014}]F_n[4; 1, 5],$$

or

$${}_3F_2\begin{bmatrix} a, & b, & c; \\ d, & e; & 1 \end{bmatrix} = (-1)^a\frac{\Gamma(1-e+c)\Gamma(1-e+b)\Gamma(d)\Gamma(e)}{\Gamma(e-a)\Gamma(1+a+c-e)\Gamma(1+d-e)\Gamma(b)}$$
$$\times {}_3F_2\begin{bmatrix} d-b, & 1-e+c, & 1-e+a; \\ 1+a+c-e, & 1+d-e; & 1 \end{bmatrix}, \qquad \text{(II. 1. 9)}$$

substitute in Eq. (II. 1. 8), and then use the symmetry due to Hardy [Eq. (II. 1. 5)], then we get the van der Waerden form of CG coefficients

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}_V = (-1)^{2(l_2-l_1)}$$
$$\times\Delta\frac{(l-l_1+l_2)!\,(l+m)!\,(l_2-m_2)!}{(-l+l_1+l_2)!\,(l-l_2+m_1)!\,(l-l_1-m_2)!}$$
$$\times {}_3F_2\begin{bmatrix} -l_2-m_2, & -l_1+m_1, & l-l_1-l_2; \\ l-l_1-m_2+1, & l-l_2+m_1+1; & 1 \end{bmatrix}. \qquad \text{(II. 1. 10)}$$

All the above four forms of CG coefficients are extremely useful for practical purposes, especially in deriving recursion relations. There is also the Rodrigues form due to Akim and Levin, [8]

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$= (-1)^{l-m-2l_1}\left(\frac{(l+l_1-l_2)!\,(l-l_1+l_2)!\,(l+m)!}{(-l+l_1+l_2)!\,(l+l_1+l_2+1)!}\right)$$
$$\times\left(\frac{(l_1+m_1)!\,(l_1-m_1)!\,(l_2+m_2)!}{(l-m)!\,(l_2-m_2)!}\right)^{1/2}$$
$$\times[(l-l_1+l_2)!\,(l_1-l_2+m)!\,]^{-1}$$
$$\times\left\{\frac{d^{l_2-m_2}}{dz^{l_2-m_2}}(1-z)_2F_1\begin{bmatrix} -l+m, & -l+l_1-l_2; \\ l_1-l_2+m+1; & z \end{bmatrix}\right\}_{z=0}. \qquad \text{(II. 1. 11)}$$

This expression is particularly helpful since the properties of ${}_2F_1$ are well understood and widely used.

2. Recursion relations

In this subsection we proceed to derive some very useful recursion relations of CG coefficients. For this we conveniently make use of Rainville's[9] contiguous function relations for generalized hypergeometric functions. For ${}_3F_2$ with unit argument we have the following contiguous relations:

(a) $$(a-b)\,{}_3F_2 = a\,{}_3F_2[a+1] - b\,{}_3F_2[b+1], \qquad \text{(II. 2. 1a)}$$

(b) $$(a-d+1)\,{}_3F_2 = a\,{}_3F_2[a+1] - (d-1)\,{}_3F_2[d-1], \qquad \text{(II. 2. 1b)}$$

(c) $$sed(e-d)\,{}_3F_2 = e(a-d)(b-d)(c-d)\,{}_3F_2[d+1] - d(a-e)(b-e)(c-e)\,{}_3F_2[e+1], \qquad \text{(II. 2. 1c)}$$

(d) $$-ed(e-d)\,{}_3F_2[a-1] = e(b-d)(c-d)\,{}_3F_2[d+1] - d(a-e)(c-e)_3F_2[e+1], \qquad \text{(II. 2. 1d)}$$

where $s = d+e-a-b-c$. When we substitute Eq. (II. 1. 4) into Eq. (II. 2. 1b) we get

$$[(l+l_1+l_2+2)(-l+l_1+l_2+1)]^{1/2}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$= [(l_1+m_1+1)(l_2-m_2+1)]^{1/2}\begin{pmatrix} l_1+\frac{1}{2} & l_2+\frac{1}{2} & l \\ m_1+\frac{1}{2} & m_2-\frac{1}{2} & -m \end{pmatrix}$$
$$- [(l_1-m_1+1)(l_2+m_2+1)]^{1/2}\begin{pmatrix} l_1+\frac{1}{2} & l_2+\frac{1}{2} & l \\ m_1-\frac{1}{2} & m_2+\frac{1}{2} & -m \end{pmatrix}. \qquad \text{(II. 2. 2)}$$

If we use the symmetry given by Eq. (II. 1. 5) in Eq. (II. 1. 4) and substitute the resulting expression in Eq. (II. 2. 1b), we get

$$[(l+l_1+l_2+1)(-l+l_1+l_2)]^{1/2}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$= [(l_1+m_1)(l_2-m_2)]^{1/2}\begin{pmatrix} l_1-\frac{1}{2} & l_2-\frac{1}{2} & l \\ m_1-\frac{1}{2} & m_2+\frac{1}{2} & -m \end{pmatrix}$$
$$- [(l_1-m_1)(l_2+m_2)]^{1/2}\begin{pmatrix} l_1-\frac{1}{2} & l_2-\frac{1}{2} & l \\ m_1+\frac{1}{2} & m_2-\frac{1}{2} & -m \end{pmatrix}. \qquad \text{(II. 2. 3)}$$

If we again take the resulting expression after substituting Eq. (II. 1. 5) into Eq. (II. 1. 4) and use the symmetry due to Bailey, i. e.,

$$\Gamma[\alpha_{123}, \alpha_{124}, \alpha_{125}]F_p[0; 4, 5] = \Gamma[\alpha_{023}, \alpha_{024}, \alpha_{025}]F_p[1; 4, 5]$$

or

$${}_3F_2\begin{bmatrix} a, & b, & c; \\ d, & e; & 1 \end{bmatrix} = \frac{\Gamma(e-a-c)\Gamma(d-a-c)\Gamma(e)\Gamma(d)}{\Gamma(e-a)\Gamma(d-a)\Gamma(e-c)\Gamma(d-c)}$$
$$\times {}_3F_2\begin{bmatrix} 1-s, & a, & c; \\ 1+a-e+c, & 1+a-d+c; & 1 \end{bmatrix},$$
$$c \text{ is a negative integer,} \qquad \text{(II. 2. 4)}$$

and then substitute the final expression in Eq. (II. 2. 1b), we obtain

$$[(l+l_1-l_2+1)(l+l_2-l_1)]^{1/2}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$= [(l_1-m_1+1)(l_2-m_2)]^{1/2}\begin{pmatrix} l_1+\frac{1}{2} & l_2-\frac{1}{2} & l \\ m_1-\frac{1}{2} & m_2+\frac{1}{2} & -m \end{pmatrix}$$
$$+ [(l_1+m_1+1)(l_2+m_2)]^{1/2}\begin{pmatrix} l_1+\frac{1}{2} & l_2-\frac{1}{2} & l \\ m_1+\frac{1}{2} & m_2-\frac{1}{2} & -m \end{pmatrix}. \qquad \text{(II. 2. 5)}$$

Furthermore, if we combine Eqs. (II. 2. 1c) and (II. 2. 1d) then we obtain

$$sd(e-d)\,{}_3F_2 + d(b-e)(e-d)\,{}_3F_2[a-1] - (b-d)(c-d)(a+e-b-d)\,{}_3F_2[d+1] = 0. \qquad \text{(II. 2. 1e)}$$

We then substitute into the above relation Wigner's expression [Eq. (II. 1. 4)] to get

$$[(l+m+1)(l-m)]^{1/2}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$=[(l_1+m_1+1)(l_1-m_1)]^{1/2}\begin{pmatrix} l_1-\frac{1}{2} & l_2 & l+\frac{1}{2} \\ m_1-\frac{1}{2} & m_2 & -(m-\frac{1}{2}) \end{pmatrix}$$
$$-[(l_2+m_2+1)(l_2-m_2)]^{1/2}\begin{pmatrix} l_1 & l_2-\frac{1}{2} & l+\frac{1}{2} \\ m_1 & m_2-\frac{1}{2} & -(m-\frac{1}{2}) \end{pmatrix}. \quad \text{(II. 2. 6)}$$

Many more recursion relations of CG coefficients may be similarly derived.

One can also note that the Rodrigues form of the GG coefficient is very handy. If we substitute Eq. (II. 1. 11) into the recurrence relation[7]

$$(a-1)\,{}_2F_1\left[\begin{matrix} a, & b; \\ c; & z \end{matrix}\right]+(c-a)\,{}_2F_1\left[\begin{matrix} a-1, & b; \\ c; & z \end{matrix}\right]$$
$$-(c-1)\,{}_2F_1\left[\begin{matrix} a-1, & b-1; \\ c-1; & z \end{matrix}\right]=0,$$

we can reproduce Eq. (II. 2. 6). Also, if we use the relation

$$(c-a-1)\,{}_2F_1\left[\begin{matrix} a, & b; \\ c; & z \end{matrix}\right]+a\,{}_2F_1\left[\begin{matrix} a+1, & b; \\ c; & z \end{matrix}\right]$$
$$-(c-1)\,{}_2F_1\left[\begin{matrix} a, & b; \\ c-1; & z \end{matrix}\right]=0,$$

we obtain

$$[(l+l_1-l_2)(l+l_1+l_2+1)]^{1/2}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$=-[(l+m)(l_1+m_1)]^{1/2}\begin{pmatrix} l_1-\frac{1}{2} & l_2 & l-\frac{1}{2} \\ m_1-\frac{1}{2} & m_2 & -(m-\frac{1}{2}) \end{pmatrix}$$
$$+[(l-m)(l_1-m_1)]^{1/2}\begin{pmatrix} l_1-\frac{1}{2} & l_2 & l-\frac{1}{2} \\ m_1+\frac{1}{2} & m_2 & -(m+\frac{1}{2}) \end{pmatrix}. \quad \text{(II. 2. 7)}$$

Finally we show one more relation which we will use later. This can be easily obtained through the symmetry of the Regge symbol upon the transposition about the so-called "opposite" diagonal, i. e.,

$$\begin{vmatrix} -l_1+l_2+l & l_1-l_2+l & l_1+l_2-l \\ l_1-m_1 & l_2-m_2 & l-m \\ l_1+m_1 & l_2+m_2 & l+m \end{vmatrix}$$
$$=\begin{vmatrix} l+m & l-m & l_1+l_2-l \\ l_2+m_2 & l_2-m_2 & l_1-l_2+l \\ l_1+m_1 & l_1-m_1 & -l_1+l_2+l \end{vmatrix},$$

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}$$
$$=\begin{pmatrix} \frac{1}{2}(l_1+l_2+m) & \frac{1}{2}(l_1+l_2-m) & l \\ \frac{1}{2}(l_1-l_2+m_1-m_2) & \frac{1}{2}(l_1-l_2-m_1+m_2) & -(l_1-l_2) \end{pmatrix}. \quad \text{(II. 2. 8)}$$

Some of the above relations have been derived by Vilenkin[10,11] using group theoretical arguments.

3. CG coefficients with negative angular momenta

We derive two relations of CG-coefficients involving negative angular momenta through the substitutions $l_1 \to -l_1-1$, $l_2 \to -l_2-1$, $l \to -l-1$. Our procedure uses the symmetrics of the hypergeometric functions and the final results agree (up to a phase) with Bandzaitis *et al.*[12] First we apply the Thomae–Dixon symmetry [Eq. (II. 1. 7)] to the Wigner–Rose expression [Eq. (II. 1. 4)] and then carefully recast the hypergeometric function into the 3-j symbol. We obtain

$$\begin{pmatrix} -l_1-1 & l_2 & -l-1 \\ m_1 & m_2 & -m \end{pmatrix}$$
$$=\exp(-i\pi/2)(-1)^{l_2+m_2}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}. \quad \text{(II. 3. 1)}$$

Next, we use the Thomae–Whipple relation

$$\Gamma[\alpha_{123},\alpha_{124},\alpha_{125}]F_p[0;4,5]=\Gamma[\alpha_{013},\alpha_{014},\alpha_{015}]F_p[2;1,3],$$

or

$${}_3F_2\left[\begin{matrix} a, & b, & c; \\ d, & e; & 1 \end{matrix}\right]$$
$$=\frac{\Gamma(1-b)\Gamma(1-e+a)\Gamma(1-d+a)\Gamma(d)\Gamma(e)}{\Gamma(d-c)\Gamma(e-c)\Gamma(1-s)\Gamma(1+a-b)\Gamma(1+c-b)}$$
$$\times\,{}_3F_2\left[\begin{matrix} 1-b, & d-b, & e-b; \\ 1+a-b, & 1+c-b; & 1 \end{matrix}\right]. \quad \text{(II. 3. 2)}$$

We use this symmetry in the Wigner–Rose expression and obtain

$$\begin{pmatrix} -l_1-1 & -l_2-1 & -l-1 \\ m_1 & m_2 & -m \end{pmatrix}$$
$$=\exp(i\pi/2)(-1)^{l_1+l_2-l}\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}. \quad \text{(II. 3. 3)}$$

Between these two relations the first one is particularly very useful and physical and we will find in Sec. III that this relation clearly enables us to express the O(2, 1)-CG coefficients in a very convenient way.

4. Special cases

Various special cases of CG coefficients may be evaluated using Saalschutz's[7] and Minton's[13] theorems. Saalschutz's theorem states that if the parameters of ${}_3F_2$ satisfy the condition $1+a+b+c=d+e$ (or $s=1$) then the terminating series can be summed as

$${}_3F_2\left[\begin{matrix} a, & b, & c; \\ d, & e; & 1 \end{matrix}\right]=\frac{\Gamma(d)\Gamma(1+a-e)\Gamma(1+b-e)\Gamma(1+c-e)}{\Gamma(1-e)\Gamma(d-a)\Gamma(d-b)\Gamma(d-c)}. \quad \text{(II. 4. 1)}$$

Thus the Wigner, Racah, and Majumdar forms of CG coefficients, respectively, satisfy the above condition (Saalschutzian) when $l=l_1+l_2-l$, $m_1=-l+1$, and $m_1=l_1-1$. Minton's theorem states that if the parameters of the generalized hypergeometric function ${}_{p+1}F_p$ satisfy the condition $\alpha_0+\alpha_1+\cdots+\alpha_p=\beta_1+\cdots+\beta_p$ (or $s=0$) then,

$${}_{p+1}F_p\left[\begin{matrix} \alpha_0, & \alpha_1, & \ldots, & \alpha_p; \\ \beta_1, & \beta_2, & \ldots, & \beta_p; & 1 \end{matrix}\right]$$
$$=\frac{\Gamma(1-\alpha_0)\Gamma(1-\alpha_1)\cdots\Gamma(1-\alpha_p)}{\Gamma(1-\beta_1)\Gamma(1-\beta_2)\cdots\Gamma(1-\beta_p)}. \quad \text{(II. 4. 2)}$$

This condition is satisfied by Wigner, Racah, and Majumdar forms when $l=l_1+l_2$, $m=-l$, and $m_1=l_1$, respectively. Some of these special cases are already computed through different methods and some of them are new. We do not give the final results here since they can be obtained by trivial substitutions.

5. Asymptotic expressions

There are three important asymptotic expressions. The one due to Edmonds[3] and Brussard and Tolhock[5] is for large l_1 and l_2 but fixed l and in this case the CG-coefficient approaches Wigner's O(3)-representation function. In order to demonstrate this we apply the symmetry due to Bailey [Eq. (II. 2. 4)] to Racah's expression [Eq. (II. 1. 8)]. We then obtain

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix}_R = (-1)^{2(l_2-l_1)} \times \Delta \frac{(l+m)!\,(l_2+m_2)!\,(l_2-l_1+l)!\,(l_1+l_2-m)!}{(l-m)!\,(l_1-l_2+l)!\,(l_1+l_2-l)!\,(l_2-l_1+m)!} \times {}_3F_2\left[\begin{matrix} -l+m,\ l+m+1,\ -l_1+m_1; \\ -l_1+l_2+m+1,\ -l_1-l_2+m; \end{matrix}\ 1\right]. \tag{II. 5. 1}$$

In the limit, $l_1, l_2 \to \infty$ we use Stirling's formula $x! \approx \sqrt{2\pi}x^{x+1/2}e^{-x}$ and the hypergeometric function ${}_3F_2$ becomes ${}_2F_1$ apart from some obvious coefficients, i. e.,

$${}_3F_2\left[\begin{matrix} -l+m,\ l+m+1,\ -l_1+m_1; \\ l_2-l_1+m+1,\ -l_1-l_2+m; \end{matrix}\ 1\right] \to {}_2F_1\left[\begin{matrix} -l+m,\ l+m+1; \\ l_2-l_1+m+1; \end{matrix}\ \sin^2\tfrac{1}{2}\beta\right],$$

where $\cos\beta = m_1[l_1(l_1+1)]^{-1/2}$. We then make use of Wigner's O(3)-representation function[14]

$$D^l_{m,m'}(\alpha,\beta,\gamma) = \exp(im\alpha)d^l_{m,m'}(\beta)\exp(-im'\gamma),$$

where

$$d^l_{m,m'}(\beta) = \frac{(l+m)!\,(l-m)!}{(l+m')!\,(l-m')!}(\cos\tfrac{1}{2}\beta)^{m+m'} \times (\sin\tfrac{1}{2}\beta)^{m-m'}P_{l-m}^{m-m',\,m+m'}(\cos\beta) = (-1)^{m-m'}\frac{1}{(m-m')!}\left(\frac{(l+m)!\,(l-m')!}{(l-m)!\,(l+m')!}\right)^{1/2} \times (\cos\tfrac{1}{2}\beta)^{m+m'}(\sin\tfrac{1}{2}\beta)^{m-m'}\,{}_2F_1\left[\begin{matrix} -l+m,\ l+m+1; \\ m-m'+1; \end{matrix}\ \sin^2\tfrac{1}{2}\beta\right], \tag{II. 5. 2}$$

and get the well-known asymptotic expression

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \approx (-1)^{l_2-l-m_1}(2l+1)^{-1/2}d^l_{m_1,\,l_1-l_2}(\beta). \tag{II. 5. 3}$$

When all the angular momenta are large one gets Wigner's formula (modified by Ponzano and Regge[15] and, in the extreme limit $l_1, l_2, l \to \infty$, by Vilenkin[10]). In order to show this, we conveniently use the identity[14]

$$\begin{pmatrix} nl_1 & nl_2 & nl \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} nl_1 & nl_2 & nl \\ m_1' & m_2' & -m' \end{pmatrix} = (1/8\pi^2)\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} D^{nl_1}_{m_1,m_1'}(\alpha,\beta,\gamma)D^{nl_2}_{m_2,m_2'}(\alpha,\beta,\gamma) \times D^{nl}_{m,m'}(\alpha,\beta,\gamma)\,d\alpha\sin\beta\,d\beta\,d\gamma.$$

The asymptotic condition of the Jacobi polynomial[16]

$$\lim_{n\to\infty} n^{-\alpha}P_n^{\alpha,\beta}(\cos(z/n)) = (z/2)^{-\alpha}J_\alpha(z),$$

where $J_\alpha(z)$ is the Bessel function, and the identity[17]

$$\int_0^\infty J_\nu(l_1z)J_\nu(l_2z)J_\nu(lz)z^{1-\nu}\,dz = \begin{cases} 2^{\nu-1}A^{2\nu-1}(l_1l_2l)^{-\nu}[\Gamma(\nu+\tfrac{1}{2})\Gamma(\tfrac{1}{2})]^{-1}, \\ \qquad \text{if } |l_1-l_2| \le l \le l_1+l_2, \\ 0, \qquad \text{otherwise,} \end{cases}$$

where A is the area of the triangle of sides l_1, l_2, and l, and is given by

$$A^2 = -\frac{1}{16}\begin{vmatrix} 0 & l_1^2 & l_2^2 & 1 \\ l_1^2 & 0 & l^2 & 1 \\ l_2^2 & l^2 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{vmatrix}.$$

After a short calculation, we obtain

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \approx (-1)^{(l_2-l_1-l)/2+l_2-m} \times (\pi)^{-1/2}[4l_1^2l_2^2-(l^2-l_1^2-l_2^2)^2]^{-1/4}. \tag{II. 5. 4}$$

Finally, the asymptotic expression for $l_1, l_2, l, m \gg l_1+l_2-m$ is given by Akim and Levin.[8] We quote their result which may be easily seen from Eq. (II. 1. 11).

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} \approx (-1)^{2l_2-l-m}(l+m+1)^{l_2-m_2}\frac{1}{(l-l_2-m_1)!} \times \left(\frac{(l+l_1-l_2)!\,(l+m)!\,(l-m)!}{(l-l_1+l_2)!\,(-l+l_1+l_2)!} \times \frac{(l_1-m_1)!\,(l_2+m_2)!}{(l+l_1+l_2+1)!\,(l_1+m_1)!\,(l_2-m_2)!}\right)^{1/2}. \tag{II. 5. 5}$$

6. An application

Most of the identities and recursion relations of CG coefficients given above have been much used[18] to study the action of O(4, 2)-operators on canonical basis. On the most degenerate unitary irreducible representation space of O(4, 2) one can construct[19] the simplest fermion basis $|nj^{\pm}k\rangle$ by coupling a spin $\frac{1}{2}$ with the canonical basis $|nlm\rangle$, n being the principal quantum number, and k and m are the magnetic quantum numbers. One gets with appropriate normalization,

$$|nj^{\pm}k\rangle = (-1)^{j-k-1}\left(\frac{2j+1}{n+j+\frac{1}{2}}\right)^{1/2}\sum_{\sigma=\pm1/2}\begin{pmatrix} \frac{1}{2} & j-\frac{1}{2} & j \\ \sigma & k-\sigma & -k \end{pmatrix}[a_\sigma^\dagger \pm i(-1)^{j-1/2}b_\sigma^\dagger]\,|n\ \ j-\tfrac{1}{2}\ \ k-\sigma\rangle, \tag{II. 6. 1}$$

where $a^\dagger_{1/2} = a_1^\dagger$, $a^\dagger_{-1/2} = a_2^\dagger$, etc. are the usual creation and annihilation operators. The 3-j symbol above can be very easily computed using Eq. (II. 6. 2). Then, for convenience, one introduces the parabolic basis $|n_1n_2m\rangle$ and expands the canonical basis as

$$|nlm\rangle = (-1)^m(2l+1)^{1/2} \sum_{\substack{n_1,n_2 \\ (n_1+n_2=n-|m|-1)}} \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & l \\ \frac{1}{2}(n_2-n_1+m) & \frac{1}{2}(n_1-n_2+m) & -m \end{pmatrix} |n_1 n_2 m\rangle,$$

where, in the representation space,

$$|n_1 n_2 m\rangle = \begin{cases} |n_2+m,\ n_1,\ n_1+m,\ n_2\rangle, & m \geq 0, \\ |n_2,\ n_1-m,\ n_1,\ n_2-m\rangle, & m<0. \end{cases} \tag{II. 6. 2}$$

After substituting Eq. (II. 6. 2) into Eq. (II. 6. 1) we get, for example $m \geq 0$ with $k_\pm = k \pm \frac{1}{2}$ (this $\pm$, associated with k should not be confused with parity $\pm$),

$$\begin{aligned} |nj^\pm k\rangle = & \sum_{n_1,n_2} \left\{ (-1)^{k_-} \left[\frac{(j+k)(n_2+k_-+1)}{(n+j+\frac{1}{2})} \right]^{1/2} \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & j-\frac{1}{2} \\ \frac{1}{2}(n_2-n_1+k_-) & \frac{1}{2}(n_1-n_2+k_-) & -k_- \end{pmatrix} + (-1)^{k_+} \left[\frac{(j-k)n_1}{(n+j+\frac{1}{2})} \right]^{1/2} \right. \\ & \times \left. \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & j-\frac{1}{2} \\ \frac{1}{2}(n_2-n_1+k_-)+1 & \frac{1}{2}(n_1-n_2+k_-) & -(k_-+1) \end{pmatrix} |n_2+k_-+1,\ n_1,\ n_1+k_-,\ n_2\rangle \pm i(-1)^{j-1/2} \right. \\ & \times \sum_{n_1,n_2} \left\{ (-1)^{k_-} \left[\frac{(j+k)(n_1+k_-+1)}{n+j+\frac{1}{2}} \right]^{1/2} \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & j-\frac{1}{2} \\ \frac{1}{2}(n_2-n_1+k_-) & \frac{1}{2}(n_1-n_2+k_-) & -k_- \end{pmatrix} + (-1)^{k_+} \left[\frac{(j-k)n_2}{(n+j+\frac{1}{2})} \right]^{1/2} \right. \\ & \times \left. \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & j-\frac{1}{2} \\ \frac{1}{2}(n_2-n_1+k_-) & \frac{1}{2}(n_1-n_2+k_-)+1 & -(k_-+1) \end{pmatrix} |n_2+k_-,\ n_1,\ n_1+k_-+1,\ n_2\rangle. \end{aligned} \tag{II. 6. 3}$$

We then make use of the Regge symmetry,

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} = (-1)^{l_1+l_2+l} \begin{pmatrix} l_2 & l_1 & l \\ m_2 & m_1 & -m \end{pmatrix} \tag{II. 6. 4}$$

and the recursion relation given by Eq. (II. 2. 7) to obtain,

$$\begin{aligned} |nj^\pm k\rangle = & (-1)^{k_-} \left[\frac{2j+1}{2} \right]^{-1/2} \sum_{n_1,n_2} \left[\begin{pmatrix} \frac{1}{2}(n-1)+\frac{1}{2} & \frac{1}{2}(n-1) & j \\ \frac{1}{2}(n_2-n_1+k_-)+\frac{1}{2} & \frac{1}{2}(n_1-n_2+k_-) & -(k_-+\frac{1}{2}) \end{pmatrix} \left| \begin{matrix} n_2+k_-+1,\ n_1,\ n_1+k_-,\ n_2 \\ n_2+1,\ n_1-k_-,\ n_1,\ n_2-k_- \end{matrix} \right\rangle \right. \\ & \left. \pm i(-1)^{n-1} \begin{pmatrix} \frac{1}{2}(n-1)+\frac{1}{2} & \frac{1}{2}(n-1) & j \\ \frac{1}{2}(n_1-n_2+k_-)+\frac{1}{2} & \frac{1}{2}(n_2-n_1+k_-) & -(k_-+\frac{1}{2}) \end{pmatrix} \left| \begin{matrix} n_2+k_-,\ n_1,\ n_1+k_-+1,\ n_2 \\ n_2,\ n_1-k_-,\ n_1+1,\ n_2-k_- \end{matrix} \right\rangle \right]. \end{aligned} \tag{II. 6. 5}$$

The upper state is for $k_- \geq 0$ and the lower one for $k_- < 0$. The basis $|nj^\pm k\rangle$ as given by Eq. (II. 6. 5) is extremely useful in practice, especially in evaluating form factors and structure functions.[20]

III. O(2, 1)-REPRESENTATION FUNCTIONS

1. General expressions

Bargmann[21] was first to study in detail the single-valued, nontrivial, infinite dimensional, unitary, irreducible representations of the pseudounitary group SU(1,1) [two-to-one-homomorphic to the noncompact orthogonal semisimple group SO(2,1)] and the corresponding representation functions in the basis in which the compact subgroup SO(2) of SO(2,1) with its discrete spectrum was diagonal. After nearly twenty years different authors[22] worked out the representation functions in the basis in which the noncompact generator of the SO(1,1) subgroup of SO(2,1) with its continuous spectrum was diagonal. In this section we plan to study some of the important properties of these representation functions.

The representation function for the discrete D_k^+-representation of SO(2,1) due to Bargmann is

$$V^k_{m,n}(\alpha,\beta,\gamma) = \exp(-im\alpha) V^k_{m,n}(\beta) \exp(-in\gamma),$$

where, for $m \geq n$

$$V^k_{m,n}(\beta) = \frac{1}{(m-n)!} \left(\frac{(m-k)!\,(m+k-1)!}{(n-k)!\,(n+k-1)!} \right)^{1/2} (\tanh\tfrac{1}{2}\beta)^{m-n} \times (\cosh\tfrac{1}{2}\beta)^{-2n} {}_2F_1\left[\begin{matrix} k-n,\ 1-n-k; \\ 1+m-n; \end{matrix} -\sinh^2\tfrac{1}{2}\beta \right]. \tag{III. 1. 1}$$

Taking

$$x = 1 - 2\tanh^2\tfrac{1}{2}\beta, \quad \tfrac{1}{2}(x-1) = -\tanh^2\tfrac{1}{2}\beta,$$
$$\tfrac{1}{2}(x+1) = 1/\cosh^2\tfrac{1}{2}\beta,$$

and introducing the Jacobi polynomial[16]

$$P_\rho^{\mu,\nu}(x) = \binom{\rho+\mu}{\rho} \left(\frac{x+1}{2} \right)^\rho {}_2F_1\left[\begin{matrix} -\rho,\ -\rho-\nu; \\ 1+\mu; \end{matrix} (x-1)/(x+1) \right],$$

we get,

$$V^k_{m,n}(\beta) = \left(\frac{(n-k)!\,(m+k-1)!}{(m-k)!\,(n+k-1)!} \right)^{1/2} (\tanh\tfrac{1}{2}\beta)^{m-n} \times (\cosh\tfrac{1}{2}\beta)^{-2k} P^{m-n,\,2k-1}_{n-k}(1-2\tanh^2\tfrac{1}{2}\beta), \tag{III. 1. 2}$$

where

$$P_\rho^{\mu,\nu}(x) = \sum_{\delta=0}^{\rho} \binom{\rho+\mu}{\rho-\delta} \binom{\rho+\nu}{\delta} \left(\frac{x-1}{2} \right)^\delta \left(\frac{x+1}{2} \right)^{\rho-\delta},$$

with $P_0^{\mu,\nu}(x) = 1$. Since $(n-k)$ is always a positive integer we can use the identity[7]

$${}_2F_1\left[\begin{matrix} -a,\ b; \\ c; \end{matrix} z \right] = \frac{(a+b-1)!\,(c-1)!}{(a+c-1)!\,(b-1)!} (-z)^a {}_2F_1\left[\begin{matrix} -a,\ 1-a-c; \\ 1-a-b; \end{matrix} 1/z \right],$$

and obtain from Eq. (III. 1. 1), a more symmetric form $(m \geq n)$,

$$V^k_{m,n}(\beta)=(-1)^{n-k}\frac{1}{(2k-1)!}\left[\frac{(m+k-1)!\,(n+k-1)!}{(m-k)!\,(n-k)!}\right]$$
$$\times(\tanh\tfrac{1}{2}\beta)^{m+n}(\cosh\tfrac{1}{2}\beta)^{-2k}\,{}_2F_1\left[\begin{matrix}k-n,\ k-m;\\ 2k;\end{matrix}-1/\sinh^2\tfrac{1}{2}\beta\right]. \tag{III. 1. 3}$$

One can easily see from the above equation, and because $(n-m)$ is an integer, that

$$V^k_{m,n}(\beta)=(-1)^{n-m}V^k_{n,m}(\beta)=(-1)^{n-m}V^k_{m,n}(-\beta). \tag{III. 1. 4}$$

The latter condition may be used to compute $V^k_{m,n}(\beta)$ for $m<n$ and furthermore from Eq. (III. 1. 1) we have immediately

$$V^k_{m,n}(\beta)=V^{1-k}_{m,n}(\beta).$$

Equation (III. 1. 4) is in fact, the property of Jacobi polynomials, viz., $P^{\mu,\nu}_\rho(x)=(-1)^\rho P^{\nu,\mu}_\rho(-x)$. Also from Eq. (III. 1. 3) one can easily conclude that for large values of β the O(2, 1)-function behaves as,

$$V^k_{m,n}(\beta)\sim(\cosh\tfrac{1}{2}\beta)^{-2k}. \tag{III. 1. 5}$$

2. Special values and identities

In order to compute special values of O(2, 1)-representation functions, we conveniently use Eq. (III. 1. 2). Below we give those which are much used[20]:

$$\begin{aligned}
&V^1_{n+1,1}(\beta)=\sqrt{n+1}\,(\tanh\tfrac{1}{2}\beta)^n(\cosh\tfrac{1}{2}\beta)^{-2},\\
&V^1_{n+1,2}(\beta)=(\sqrt{n+1}/\sqrt{2}\,)(n-2\sinh^2\tfrac{1}{2}\beta)(\tanh\tfrac{1}{2}\beta)^{n-1}(\cosh\tfrac{1}{2}\beta)^{-4},\\
&V^1_{n+1,3}(\beta)=(\sqrt{n+1}/\sqrt{3}\,)[\tfrac{1}{2}n(n-1)-3n\sinh^2\tfrac{1}{2}\beta+3\sinh^4\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-2}(\cosh\tfrac{1}{2}\beta)^{-6},\\
&V^1_{n+1,4}(\beta)=(\sqrt{n+1}/2)[\tfrac{1}{6}n(n-1)(n-2)-2n(n-1)\sinh^2\tfrac{1}{2}\beta+6n\sinh^4\tfrac{1}{2}\beta-4\sinh^6\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-3}(\cosh\tfrac{1}{2}\beta)^{-8},\\
&V^1_{n+1,5}(\beta)=(\sqrt{n+1}/\sqrt{5}\,)[\tfrac{1}{24}n(n-1)(n-2)(n-3)-\tfrac{5}{6}n(n-1)(n-2)\sinh^2\tfrac{1}{2}\beta+5n(n-1)\sinh^4\tfrac{1}{2}\beta\\
&\qquad-10n\sinh^6\tfrac{1}{2}\beta+5\sinh^8\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-4}(\cosh\tfrac{1}{2}\beta)^{-10},\\
&V^2_{n+1,2}(\beta)=(1/\sqrt{6}\,)[n(n+1)(n+2)]^{1/2}(\tanh\tfrac{1}{2}\beta)^{n-1}(\cosh\tfrac{1}{2}\beta)^{-4},\\
&V^2_{n+1,3}(\beta)=(1/\sqrt{24}\,)[n(n+1)(n+2)]^{1/2}[(n-1)-4\sinh^2\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-2}(\cosh\tfrac{1}{2}\beta)^{-6},\\
&V^2_{n+1,4}(\beta)=(1/\sqrt{60}\,)[n(n+1)(n+2)]^{1/2}[\tfrac{1}{2}(n-1)(n-2)-5(n-1)\sinh^2\tfrac{1}{2}\beta+10\sinh^4\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-3}(\cosh\tfrac{1}{2}\beta)^{-8},\\
&V^3_{n+3,3}(\beta)=(1/\sqrt{120}\,)[(n+1)(n+2)(n+3)(n+4)(n+5)]^{1/2}(\tanh\tfrac{1}{2}\beta)^n(\cosh\tfrac{1}{2}\beta)^{-6},\\
&V^{1/2}_{n+1/2,1/2}(\beta)=(\tanh\tfrac{1}{2}\beta)^n(\cosh\tfrac{1}{2}\beta)^{-1},\\
&V^{1/2}_{n+1/2,3/2}(\beta)=(n-\sinh^2\tfrac{1}{2}\beta)(\tanh\tfrac{1}{2}\beta)^{n-1}(\cosh\tfrac{1}{2}\beta)^{-3},\\
&V^{1/2}_{n+1/2,5/2}(\beta)=[\tfrac{1}{2}n(n-1)-2n\sinh^2\tfrac{1}{2}\beta+\sinh^4\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-2}(\cosh\tfrac{1}{2}\beta)^{-5},\\
&V^{3/2}_{n+1/2,3/2}(\beta)=(1/\sqrt{2}\,)[n(n+1)]^{1/2}(\tanh\tfrac{1}{2}\beta)^{n-1}(\cosh\tfrac{1}{2}\beta)^{-3},\\
&V^{3/2}_{n+1/2,5/2}(\beta)=(1/\sqrt{6}\,)[n(n+1)]^{1/2}[(n-1)-3\sinh^2\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-2}(\cosh\tfrac{1}{2}\beta)^{-5},\\
&V^{3/2}_{n+1/2,7/2}(\beta)=(1/\sqrt{12}\,)[n(n+1)]^{1/2}[\tfrac{1}{2}(n-1)(n-2)-4(n-1)\sinh^2\tfrac{1}{2}\beta+6\sinh^4\tfrac{1}{2}\beta](\tanh\tfrac{1}{2}\beta)^{n-3}(\cosh\tfrac{1}{2}\beta)^{-7}.
\end{aligned} \tag{III. 2. 1}$$

Furthermore, from the recurrence relations[7]

$$\begin{aligned}
&(a-c+1)\,{}_2F_1+(c-1)\,{}_2F_1[b-1;\ c-1]-a(1-z)\,{}_2F_1[a+1]=0,\\
&(b-c+1)\,{}_2F_1+(c-1)\,{}_2F_1[a-1;c-1]-b(1-z)\,{}_2F_1[b+1]=0,\\
&c\,{}_2F_1-az\,{}_2F_1[a+1;c+1]-c\,{}_2F_1[b-1]=0,\\
&c\,{}_2F_1-(c-b)z\,{}_2F_1[a+1;c+1]-c(1-z)\,{}_2F_1[a+1]=0,\\
&(1-b)\,{}_2F_1+(b-c)\,{}_2F_1[b-1]+(c-1)\,{}_2F_1[b-1;c-1]=0,\\
&c\,{}_2F_1-bz\,{}_2F_1[b+1;c+1]-c\,{}_2F_1[a-1]=0,\\
&c(c-1)\,{}_2F_1-c(c-1)\,{}_2F_1[c-1]+abz\,{}_2F_1[a+1,b+1;c+1]=0
\end{aligned}$$

and Eq. (III. 1. 1) we obtain the identities

$$\begin{aligned}
&(m-k)^{1/2}V^k_{m,n}(\beta)=(n+k)^{1/2}\sinh\tfrac{1}{2}\beta V^{k+1/2}_{m-1/2,n+1/2}(\beta)+(n-k)^{1/2}\cosh\tfrac{1}{2}\beta V^{k+1/2}_{m-1/2,n-1/2}(\beta),\\
&(m+k-1)^{1/2}V^k_{m,n}(\beta)=(n-k+1)^{1/2}\sinh\tfrac{1}{2}\beta V^{k-1/2}_{m-1/2,n+1/2}(\beta)+(n+k-1)^{1/2}\cosh\tfrac{1}{2}\beta V^{k-1/2}_{m-1/2,n-1/2}(\beta),\\
&(m+k)^{1/2}V^k_{m,n}(\beta)=(n-k)^{1/2}\sinh\tfrac{1}{2}\beta V^{k+1/2}_{m+1/2,n-1/2}(\beta)+(n+k)^{1/2}\cosh\tfrac{1}{2}\beta V^{k+1/2}_{m+1/2,n+1/2}(\beta),\\
&(n-k)^{1/2}V^k_{m,n}(\beta)=-(m+k)^{1/2}\sinh\tfrac{1}{2}\beta V^{k+1/2}_{m+1/2,n-1/2}(\beta)+(m-k)^{1/2}\cosh\tfrac{1}{2}\beta V^{k+1/2}_{m-1/2,n-1/2}(\beta),\\
&(n+k)^{1/2}V^k_{m,n}(\beta)=-(m-k)^{1/2}\sinh\tfrac{1}{2}\beta V^{k+1/2}_{m-1/2,n+1/2}(\beta)+(m+k)^{1/2}\cosh\tfrac{1}{2}\beta V^{k+1/2}_{m+1/2,n+1/2}(\beta),\\
&(m-k+1)^{1/2}V^k_{m,n}(\beta)=(n+k-1)(n+k)^{1/2}\sinh\tfrac{1}{2}\beta V^{k-1/2}_{m+1/2,n-1/2}(\beta)+(n-k+1)^{1/2}\cosh\tfrac{1}{2}\beta V^{k-1/2}_{m+1/2,n+1/2}(\beta),\\
&(m-n)V^k_{m,n}(\beta)=[(m-k)(m+k-1)]^{1/2}\tanh\tfrac{1}{2}\beta V^k_{m-1,n}(\beta)+[(n-k)(n+k-1)]^{1/2}\tanh\tfrac{1}{2}\beta V^k_{m,n-1}(\beta).
\end{aligned} \tag{III. 2. 3}$$

These identities are very useful to express the O(4, 2) amplitudes[20] in a much simpler form.

We then use the famous Burchnall–Chaundy multiplication formula,[23]

$$ {}_2F_1\begin{bmatrix} a, & b; \\ c; & x \end{bmatrix} {}_2F_1\begin{bmatrix} a', & b'; \\ c'; & x \end{bmatrix} = \sum_{t=0}^{\infty} \frac{(a)_t (b)_t (c')_t}{t!\,(c)_t (c+c'+t-1)_t}\, x^t $$
$$ \times {}_3F_2\begin{bmatrix} a', & 1-c-t, & -t; \\ c', & 1-a-t; & 1 \end{bmatrix} {}_3F_2\begin{bmatrix} b', & 1-c-t, & -t; \\ c', & 1-b-t; & 1 \end{bmatrix} {}_2F_1\begin{bmatrix} a+a'+t, & b+b'+t; \\ c+c'+2t; & x \end{bmatrix}. \tag{III. 2. 4} $$

Substituting Eq. (III. 1. 3) in the above, we get [note that we have used square brackets as in Eq. (II. 1. 2)]

$$ V^{\rho_1}_{\mu_1,\nu_1}(\beta) V^{\rho_2}_{\mu_2,\nu_2}(\beta) = \sum_{\tau=0}^{\infty} \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau \\ \nu_1 & \nu_2 & \nu_1+\nu_2 \end{bmatrix} V^{\rho_1+\rho_2+\tau}_{\mu_1+\mu_2,\nu_1+\nu_2}(\beta), \tag{III. 2. 5} $$

where the SO(2, 1)-CG-coefficient[24] is

$$ \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} = \frac{(\rho_1-\mu_1+\tau-1)!}{(\rho_1-\mu_1-1)!\,(2\rho_2-1)!}\, {}_3F_2\begin{bmatrix} \rho_2-\mu_2, & 1-2\rho_1-\tau, & -\tau; \\ 2\rho_2, & 1-\rho_1+\mu_1-\tau; & 1 \end{bmatrix} $$
$$ \times \left(\frac{(2\rho_1+2\rho_2+2\tau-1)!\,(2\rho_2+\tau-1)!\,(2\rho_1+2\rho_2+\tau-2)!\,(\mu_1+\rho_1-1)!}{\tau!\,(2\rho_1+\tau-1)!\,(2\rho_1+2\rho_2+2\tau-2)!\,(\mu_1-\rho_1)!\,(\mu_2-\rho_2)!} \right. $$
$$ \left. \times \frac{(\mu_2+\rho_2-1)!\,(\mu_1+\mu_2-\rho_1-\rho_2-\tau)!}{(\mu_1+\mu_2+\rho_1+\rho_2+\tau-1)!} \right)^{1/2}. \tag{III. 2. 6} $$

If we define, as in Eq. (II. 1. 2), that

$$ \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} = (-1)^{\rho_2-\rho_1+\mu_1+\mu_2} [-(2\rho_1+2\rho_2+2\tau-1)]^{1/2} \begin{pmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau \\ \mu_1 & \mu_2 & -(\mu_1+\mu_2) \end{pmatrix}, \tag{III. 2. 7} $$

then the 3-j symbol

$$ \begin{pmatrix} \rho_1 & \rho_2 & \rho_1+\rho_2+\tau \\ \mu_1 & \mu_2 & -(\mu_1+\mu_2) \end{pmatrix}, $$

upon substitution of Eq. (II. 1. 9) into Eq. (III. 2. 6), reduce to the Wigner form [Eq. (II. 1. 4)] since the parameters of ${}_3F_2$ in Eq. (III. 2. 6) are integers. Also, the SO(2, 1)-CG-coefficients satisfy the usual orthogonality relation, for example,

$$ \sum_{\mu_1,\mu_2} \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau' \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} = \delta_{\tau\tau'}. \tag{III. 2. 8} $$

Furthermore, for the evaluation of the O(4, 2)-transition amplitude between the ground state and an arbitrary state, one needs only three special values of the SO(2, 1)-CG coefficients. These can be computed by using Eq. (II. 4. 2). We give here the results:

$$ \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2) \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} = \left(\frac{(2\rho_1+2\rho_2-1)(2\rho_1+2\rho_2-2)!\,(\mu_1+\rho_1-1)!\,(\mu_2+\rho_2-1)!\,(\mu_1+\mu_2-\rho_1-\rho_2)!}{(2\rho_1-1)!\,(2\rho_2-1)!\,(\mu_1-\rho_1)!\,(\mu_2-\rho_2)!\,(\mu_1+\mu_2+\rho_1+\rho_2-1)!} \right)^{1/2}, $$

$$ \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2+1) \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} = \left(\frac{(2\rho_1+2\rho_2+1)(2\rho_1+2\rho_2-1)!\,(\mu_1+\rho_1-1)!\,(\mu_2+\rho_2-1)!\,(\mu_1+\mu_2-\rho_1-\rho_2-1)!}{(2\rho_1)!\,(2\rho_2)!\,(\mu_1-\rho_1)!\,(\mu_2-\rho_2)!\,(\mu_1+\mu_2+\rho_1+\rho_2)!} \right) 2(\rho_1\mu_2-\rho_2\mu_1), $$

and

$$ \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2+2) \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \left(\frac{(2\rho_1+2\rho_2+3)(2\rho_1+2\rho_2)!\,(\mu_1+\rho_1-1)!\,(\mu_2+\rho_2-1)!\,(\mu_1+\mu_2-\rho_1-\rho_2-2)!}{(2\rho_1+1)!\,(2\rho_2+1)!\,(\mu_1-\rho_1)!\,(\mu_2-\rho_2)!\,(\mu_1+\mu_2+\rho_1+\rho_2+1)!} \right)^{1/2} $$
$$ \times [(\mu_1-\rho_1)(\mu_1-\rho_1-1)2\rho_2(2\rho_2+1) + (\mu_2-\rho_2)(\mu_2-\rho_2-1)2\rho_1(2\rho_1+1) $$
$$ - 2(\mu_1-\rho_1)(\mu_2-\rho_2)(2\rho_1+1)(2\rho_2+1)]. \tag{III. 2. 9} $$

Finally we give an important result derived by using successively the symmetries given by Eqs. (II. 2. 8), (II. 4. 4), (II. 3. 1), and again (II. 2. 8) in Eq. (III. 2. 7):

$$ \begin{bmatrix} -\rho_1 & -\rho_2 & -(\rho_1+\rho_2)-\tau \\ \mu_1 & \mu_2 & \mu_1+\mu_2 \end{bmatrix} = (-1)^{2\mu_1+\mu_2-3\rho_1+1-\tau} \begin{bmatrix} \frac{1}{2}(\mu_1+\mu_2-\rho_1+\rho_2-1) & \frac{1}{2}(\mu_1+\mu_2+\rho_1-\rho_2-1) & \rho_1+\rho_2-1+\tau \\ \frac{1}{2}(\mu_1-\mu_2+\rho_1+\rho_2-1) & \frac{1}{2}(\mu_1-\mu_2+\rho_1+\rho_2-1) & \rho_1+\rho_2-1 \end{bmatrix}. \tag{III. 2. 10} $$

This relation is very crucial because it shows that the O(2, 1)-CG coefficients are proportional to the coefficients in the expansion in Eq. (II. 4. 2).

3. A simple application

Explicit evaluation of matrix elements of O(4, 2) group generators[19,25] between the so-called titled physical states involves the computation of matrix elements of finite Lorentz transformations between those states (see Sec. IV, Part 3). In the latter case one frequently encounters a product of two SO(2, 1)-representation functions such as

$$V^{(|\lambda|+1)/2}_{n_1'+(|\lambda|+1)/2,\, n_1+(|\lambda|+1)/2}(\beta)\, V^{(|\lambda|+1)/2+\delta}_{n_2'+(|\lambda|+1)/2+|\delta|,\, n_2+(|\lambda|+1)/2+|\delta|}(-\beta),$$

and another one with the replacements $\beta \to -\beta$, $n_1' \leftrightarrow n_2'$, and $n_1 \leftrightarrow n_2$. Here n_1 and n_2 are parabolic quantum numbers and are restricted by the condition $n_1+n_2=n-|\lambda|-1$ $(0 \le n_1 \le n-|\lambda|-1)$. For the spin-0 case $\lambda=m$ and $\delta=0$ and for spin $\frac{1}{2}$, $\lambda=k_-=k-\frac{1}{2}$ (k is the spin $\frac{1}{2}$ magnetic quantum number) and $\delta=+\frac{1}{2}$ when $k_- \ge 0$ and $\delta=-\frac{1}{2}$ when $k_-<0$. This δ is in fact one of the two numbers[18] that characterize the Casimir invariants of the subgroup SO(4) of SO(4, 2) and specifies the particular representation. From Eqs. (III. 1. 4) and (III. 2. 5) we obtain,

$$V^{(|\lambda|+1)/2}_{n_1'+(|\lambda|+1)/2,\, n_1+(|\lambda|+1)/2}(\beta)\, V^{(|\lambda|+1)/2+\delta}_{n_2'+(|\lambda|+1)/2+|\delta|,\, n_2+(|\lambda|+1)/2+|\delta|}(-\beta)$$

$$= (-1)^{n_2'-n_2} \sum_{\tau=0} \begin{bmatrix} -\frac{1}{2}(|\lambda|+1) & -\frac{1}{2}(|\lambda|+1)-\delta & -(|\lambda|+1+\delta+\tau) \\ n_1'+\frac{1}{2}(|\lambda|+1) & n_2'+\frac{1}{2}(|\lambda|+1)+|\delta| & n'+|\delta| \end{bmatrix} V^{|\lambda|+1+\delta+\tau}_{n'+|\delta|,\, n+|\delta|}(\beta)$$

$$\times \begin{bmatrix} -\frac{1}{2}(|\lambda|+1) & -\frac{1}{2}(|\lambda|+1)-\delta & -(|\lambda|+1+\delta+\tau) \\ n_1+\frac{1}{2}(|\lambda|+1) & n_2+\frac{1}{2}(|\lambda|+1)+|\delta| & n+|\delta| \end{bmatrix}. \tag{III. 4. 1}$$

With Eq. (III. 2. 10), the above equation becomes,

$$V^{(|\lambda|+1)/2}_{n_1'+(|\lambda|+1)/2,\, n_1+(|\lambda|+1)/2}(\beta)\, V^{(|\lambda|+1)/2+\delta}_{n_2'+(|\lambda|+1)/2+|\delta|,\, n_2+(|\lambda|+1)/2+|\delta|}(-\beta)$$

$$= \sum_{\tau=0} V^{|\lambda|+1+\delta+\tau}_{n'+|\delta|,\, n+|\delta|}(\beta) \begin{bmatrix} \frac{1}{2}(n'-1)+\frac{1}{2}(\delta+|\delta|) & \frac{1}{2}(n'-1)+\frac{1}{2}(|\delta|-\delta) & |\lambda|+\delta+\tau \\ \frac{1}{2}(n_2'-n_1'+|\lambda|)+\frac{1}{2}(\delta+|\delta|) & \frac{1}{2}(n_1'-n_2'+|\lambda|+\frac{1}{2}(\delta-|\delta|) & (|\lambda|+\delta) \end{bmatrix}$$

$$\times \begin{bmatrix} \frac{1}{2}(n-1)+\frac{1}{2}(\delta+|\delta|) & \frac{1}{2}(n-1)+\frac{1}{2}(|\delta|-\delta) & |\lambda|+\delta+\tau \\ \frac{1}{2}(n_2-n_1+|\lambda|)+\frac{1}{2}(\delta+|\delta|) & \frac{1}{2}(n_1-n_2+|\lambda|)+\frac{1}{2}(\delta-|\delta|) & (|\lambda|+\delta) \end{bmatrix}. \tag{III. 4. 2}$$

Similarly,

$$V^{(|\lambda|+1)/2+\delta}_{n_1'+(|\lambda|+1)/2+|\delta|,\, n_1+(|\lambda|+1)/2+|\delta|}(\beta)\, V^{(|\lambda|+1)/2}_{n_2'+(|\lambda|+1)/2,\, n_2+(|\lambda|+1)/2}(-\beta)$$

$$= \sum_{\tau=0} V^{|\lambda|+1+\delta+\tau}_{n'+|\delta|,\, n+|\delta|}(\beta) \begin{bmatrix} \frac{1}{2}(n'-1)+\frac{1}{2}(|\delta|-\delta) & \frac{1}{2}(n'-1)+\frac{1}{2}(|\delta|+\delta) & |\lambda|+\delta+\tau \\ \frac{1}{2}(n_2'-n_1'+|\lambda|)+\frac{1}{2}(\delta-|\delta|) & \frac{1}{2}(n_1'-n_2'+|\lambda|)+\frac{1}{2}(\delta+|\delta|) & (|\lambda|+\delta) \end{bmatrix}$$

$$\times \begin{bmatrix} \frac{1}{2}(n-1)+\frac{1}{2}(|\delta|-\delta) & \frac{1}{2}(n-1)+\frac{1}{2}(|\delta|+\delta) & |\lambda|+\delta+\tau \\ \frac{1}{2}(n_2-n_1+|\lambda|)+\frac{1}{2}(\delta-|\delta|) & \frac{1}{2}(n_1-n_2+|\lambda|+\frac{1}{2}(\delta+|\delta|) & (|\lambda|+\delta) \end{bmatrix}, \tag{III. 4. 3}$$

with

$$0 \le \tau \le Min \begin{Bmatrix} n'-|\lambda|-1+|\delta|-\delta \\ n-|\lambda|-1+|\delta|-\delta \end{Bmatrix}.$$

If we square the above and sum over (n_1, n_2) and (n_1', n_2') then, because of the orthogonality relation Eq. (III. 2. 8) we get [from Eq. (III. 4. 2)], i. e.,

$$\sum_{n_1, n_2} \sum_{n_1', n_2'} \left| V^{(|\lambda|+1)/2}_{n_1'+(|\lambda|+1)/2,\, n_1+(|\lambda|+1)/2}(\beta)\, V^{(|\lambda|+1)/2+\delta}_{n_2'+(|\lambda|+1)/2+|\delta|,\, n_2+(|\lambda|+1)/2+|\delta|}(-\beta) \right|^2$$

$$= \sum_{\tau=0} V^{|\lambda|+1+\delta+\tau}_{n'+|\delta|,\, n+|\delta|}(\beta)\, V^{|\lambda|+1+\delta+\tau}_{n'+|\delta|,\, n+|\delta|}(\beta), \tag{III. 4. 4}$$

and a similar expression from Eq. (III. 4. 3).

IV. THE O(4)-REPRESENTATION FUNCTION

1. Definition and general expressions

The O(4)-representation functions were first studied by Dolginov and Biedenharn[26] and later by many authors.[27] The well-known fact that the group O(4) is locally isomorphic to O(3)⊗ O(3) enables one to define the representation function in the simple form

$$D^{[j_1\, j_2\, j]}_{j_1', j_2', m'}(\alpha) = \sum_{m_1} \begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} \begin{bmatrix} j_1 & j_2 & j' \\ m_1 & m_2 & m \end{bmatrix} \exp[-i\alpha(m_1-m_2)], \tag{IV. 1. 1}$$

where j and j' correspond to the angular momenta belonging to the two rotation groups and $j_+=j_1+j_2$, $j_-=j_1-j_2$. When j_+ (and j_-) is an integer and $j_-=0$, one gets self-conjugate (spin-0) representations and when j_+ (and j_-) is half-integer and $j_-=\pm\frac{1}{2}$, one gets two-valued (spin-$\frac{1}{2}$) conjugate representations. Following Ström's elegant method of differential operators in the group parameters, one obtains the following four ladder operators:

$$K_+(j')D^{[j\, j_-]}_{j_1', j_2', m'}(\alpha) = \kappa(j')D^{[j\, j_-]}_{j_1', j_2'+1, m}(\alpha), \tag{IV. 1. 2}$$

$$[K_-(j') = K_+(-j'-1)]D^{[j\, j_-]}_{j_1', j_2', m'}(\alpha) = \kappa(-j'-1)D^{[j\, j_-]}_{j_1', j_2'-1, m}(\alpha), \tag{IV. 1. 3}$$

$$L_+(m)D^{[j\, j_-]}_{j_1', j_2', m'}(\alpha) = \lambda(m)D^{[j\, j_-]}_{j_1', j_2', m+1}(\alpha), \tag{IV. 1. 4}$$

$$[L_-(m)=L_+(-m)]D^{[j_+ j_-]}_{j',j'_+,m}(\alpha)=\lambda(-m)D^{[j_+ j_-]}_{j',j'_+,m-1}(\alpha), \tag{IV.1.5}$$

where

$$K_+(j')=\left(\frac{d^2}{d\alpha^2}-2j'\cot\alpha\frac{d}{d\alpha}-\frac{2im(j_++1)j_-}{(j'+1)}\cot\alpha+\frac{1}{\sin^2\alpha}[j'(j'+1)-j(j+1)]+[j_+(j_++2)-2j'(j'+1)+j_-^2+m^2]\right),$$

$$L_+(m)=\left(\frac{d^2}{d\alpha^2}+2(m+1)\cot\alpha\frac{d}{d\alpha}+2m\cot^2\alpha+2i(j_++1)j_-\cot\alpha+\frac{1}{\sin^2\alpha}[2m^2-j'(j'+1)-j(j+1)]+[j_+(j_++2)+j_-^2-m^2]\right),$$

$$\kappa(j')=-2i\cot\alpha[1/(j'+1)][(2j'+1)/(2j'+3)]^{1/2}[(j'+m+1)(j'-m+1)(j'+j_-+1)(j'-j_-+1)(j_++j'+2)(j_+-j')]^{1/2}$$

$$\lambda(m)=-2\cot\alpha(1/\sin\alpha)[(j-m)(j+m+1)(j'-m)(j'+m+1)]^{1/2}.$$

If we redefine the ladder operators as,

$$K'_+(j')=\kappa^{-1}(j')K_+(j');\quad L'_+(m)=\lambda^{-1}(m)L_+(m),$$

$$K'_-(j')=\kappa^{-1}(-j'-1)K_-(j');\quad L'_-(m)=\lambda^{-1}(-m)L_-(m),$$

then, the function $D^{[j_+ j_-]}_{j',j'_+,m}(\alpha)$ will satisfy the following two fourth-order differential equations,

$$[K'_-(j'+1)K'_+(j')-]D^{[j_+ j_-]}_{j',j'_+,m}(\alpha)=0,\quad [L'_-(m+1)L'_+(m)-1]D^{[j_+ j_-]}_{j',j'_+,m}(\alpha)=0. \tag{IV.1.6}$$

The solutions of these equations will give the general expression for $D^{[j_+ j_-]}_{j',j'_+,m}(\alpha)$.

From Eqs. (IV.1.2)–(IV.1.5), we get,

$$\left[-i\frac{d}{d\alpha}+\frac{m(j_++1)j_-}{j'(j'+1)}\right]D^{[j_+ j_-]}_{j',j'_+,m}(\alpha)=a(j')D^{[j_+ j_-]}_{j',j'_+,m+1}(\alpha)+a(-j'-1)D^{[j_+ j_-]}_{j',j'_+,m-1}(\alpha), \tag{IV.1.7}$$

$$\left[\sin\alpha\frac{d}{d\alpha}+\cos\alpha+\frac{i}{m}(j_++1)j_-\sin\alpha\right]D^{[j_+ j_-]}_{j',j'_+,m}(\alpha)=b(m)D^{[j_+ j_-]}_{j',j'_+,m+1}(\alpha)+b(-m)D^{[j_+ j_-]}_{j',j'_+,m-1}(\alpha), \tag{IV.1.8}$$

where

$$a(j')=\{[(j'+1)^2(2j'+1)(2j'+3)]^{-1}(j'+m+1)(j'-m+1)(j'+j_-+1)(j'-j_-+1)(j_++j'+2)(j_+-j')\}^{1/2},$$

$$b(m)=-(1/2m)[(j-m)(j+m+1)(j'-m)(j'+m+1)]^{1/2}.$$

When $j'=m$, Eq. (IV.1.7) becomes

$$\left[-i\frac{d}{d\alpha}+\frac{(j_++1)j_-}{(m+1)}\right]D^{[j_+ j_-]}_{j',m,m}(\alpha)=a(m)D^{[j_+ j_-]}_{j',m+1,m}(\alpha). \tag{IV.1.9}$$

Furthermore, from Eqs. (IV.1.3), (IV.1.7), and (IV.1.8), and taking $m\to m+1$ and then $j'=m$, we obtain

$$D^{[j_+ j_-]}_{j',m+1,m+1}(\alpha)=-\frac{i}{2\sin\alpha}\left(\frac{(j+m+1)(j-m)(2m+2)(2m+3)}{(m-j_-+1)(m+j_-+1)(j_+-m)(j_++m+2)}\right)^{1/2}D^{[j_+ j_-]}_{j',m,m}(\alpha). \tag{IV.1.10}$$

The Eq. (IV.1.6) is in general very hard to solve. But for the case $j'=m$, the fourth order equation becomes a second order differential equation,

$$\left(\frac{d^2}{d\alpha^2}+2(m+1)\cot\alpha\frac{d}{d\alpha}+2i(j_++1)j_-\cot\alpha+\frac{1}{\sin^2\alpha}[m(m+1)-j(j+1)]+[j_+(j_++2)+j_-^2-m(m+2)]\right)D^{[j_+ j_-]}_{j',m,m}(\alpha)=0.$$

To solve this equation we substitute $t=\exp(-2i\alpha)$ and

$$D^{[j_+ j_-]}_{j',m,m}(\alpha)=t^\rho(1-t)^\sigma B^{[j_+ j_-]}_{j',m,m}(t).$$

After some trivial steps we obtain,

$$\left(t(1-t)\frac{d^2}{dt^2}+[\gamma'-(1+\alpha'+\beta')t]\frac{d}{dt}-\alpha'\beta'\right)B^{[j_+ j_-]}_{j',m,m}(t)=0. \tag{IV.1.11}$$

where,

$$\gamma'=2\rho-m,\quad \rho=\{\rho_1,\rho_2\},\quad \sigma=\{\sigma_1,\sigma_2\},\quad \alpha'=\rho+\sigma+\tfrac{1}{2}(m+j_++j_-+2),$$

$$\beta'=\rho+\sigma+\tfrac{1}{2}(m-j_+-j_-),\quad \rho_1=\tfrac{1}{2}(m+j_+-j_-+2),\quad \rho_2=\tfrac{1}{2}(m-j_++j_-),$$

$$\sigma_1=j-m,\quad \sigma_2=-j-m-1.$$

Eq. (IV.1.11) is the well-known hypergeometric equation and its solution bounded for $t=1$ is

$$D^{[j_+ j_-]}_{j',m,m}(\alpha)=t^\rho(1-t)^\sigma\,{}_2F_1\left[\begin{matrix}\alpha',\ \beta';\\ 1+\alpha'+\beta'-\gamma';\ 1-t\end{matrix}\right].$$

According to the values of ρ and σ, there are four such solutions:

$$(\rho_1,\sigma_1)\to u_{11}=t^{(m+j_+-j_-+2)/2}(1-t)^{j-m}\,{}_2F_1\begin{bmatrix}j_++j+2,\ -j_-+j+1;\\ 2j+2;\ (1-t)\end{bmatrix},$$

$$(\rho_1,\sigma_2)\to u_{12}=t^{(m+j_+-j_-+2)/2}(1-t)^{-j-m-1}\,{}_2F_1\begin{bmatrix}j_+-j+1,\ -j_--j;\\ -2j;\ (1-t)\end{bmatrix},$$

$$(\rho_2,\sigma_1)\to u_{21}=t^{(m-j_++j_-)/2}(1-t)^{j-m}\,{}_2F_1\begin{bmatrix}-j_++j,\ j_-+j+1;\\ 2j+2;\ (1-t)\end{bmatrix},$$

$$(\rho_2,\sigma_2)\to u_{22}=t^{(m-j_++j_-)/2}(1-t)^{-j-m-1}\,{}_2F_1\begin{bmatrix}-j_+-j-1,\ j_--j;\\ -2j;\ (1-t)\end{bmatrix}.$$

Among these four only two solutions are linearly independent, since Euler's identity,[7]

$${}_2F_1\begin{bmatrix}a,\ b;\\ c;\ z\end{bmatrix}=(1-z)^{c-a-b}\,{}_2F_1\begin{bmatrix}c-a,\ c-b;\\ c;\ z\end{bmatrix},$$

implies that $u_{21}=u_{11}$ and $u_{12}=u_{22}$. Therefore the general solution may be written as

$$D^{[j_+\,j_-]}_{j,m,m}(\alpha)=A_1t^{(m+j_+-j_-+2)/2}(1-t)^{j-m}\,{}_2F_1\begin{bmatrix}j_++j+2,\ -j_-+j+1;\\ 2j+2;\ (1-t)\end{bmatrix}+A_2t^{(m+j_+-j_-+2)/2}\ (1-t)^{-j-m-1}\,{}_2F_1\begin{bmatrix}j_+-j+1,\ -j_--j;\\ -2j;\ (1-t)\end{bmatrix}.$$

But if all the parameters of the above hypergeometric polynomials are integers [this is certainly the case for O(4)] then one can use the identity[7]

$$\frac{\Gamma(a)\Gamma(b)}{\Gamma(c)}\,{}_2F_1\begin{bmatrix}a,\ b;\\ c;\ z\end{bmatrix}=\frac{\Gamma(a-c+1)\Gamma(b-c+1)}{\Gamma(2-c)}\,{}_2F_1\begin{bmatrix}a-c+1,\ b-c+1;\\ 2-z;\ z\end{bmatrix},$$

to obtain

$$D^{[j_+\,j_-]}_{j,m,m}(\alpha)=N^j_m(j_+,j_-)t^{(m+j_+-j_-+2)/2}(1-t)^{j-m}\,{}_2F_1\begin{bmatrix}j_++j+2,\ -j_-+j+1;\\ 2j+2;\ (1-t)\end{bmatrix}. \tag{IV.1.12}$$

In order to evaluate the overall normalization $N^j_m(j_+,j_-)$ we, for convenience, first transform the above equation using Euler's identity and then use the relation[7] (a is negative integer)

$${}_2F_1\begin{bmatrix}a,\ b;\\ c;\ z\end{bmatrix}=\frac{\Gamma(c-b-a)\Gamma(c)}{\Gamma(c-b)\Gamma(c-a)}\,{}_2F_1\begin{bmatrix}a,\ b;\\ b-c+a+1;\ 1-z\end{bmatrix}, \tag{IV.1.12'}$$

and get

$$D^{[j_+\,j_-]}_{j,m,m}(\alpha)=N^j_m(j_+,j_-)t^{(m-j_++j_-)/2}(1-t)^{j-m}\left\{\frac{\Gamma(2j+2)\Gamma(j_+-j_-+1)}{\Gamma(j-j_-+1)\Gamma(j_++j+2)}\,{}_2F_1\begin{bmatrix}-j_++j,\ j+j_-+1;\\ -j_++j_-;\ t\end{bmatrix}\right\}.$$

Then we use the fact that at $t=1$ ($\alpha=0$) the O(4)-function, by definition, satisfies the condition $D^{[j_+\,j_-]}_{j,m,m}(0)=\delta_{jm}$. With this condition and the Gauss's identity[7]

$${}_2F_1\begin{bmatrix}a,\ b;\\ c;\ 1\end{bmatrix}=\frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)},$$

we compute $N^m_m(j_+,j_-)$. Then we repeatedly use Eq. (IV.1.10) to get the general normalization $N^j_m(j_+,j_-)$. With this normalization finally Eq. (IV.1.12) becomes,

$$D^{[j_+\,j_-]}_{j,m,m}(\alpha)=(2i)^{j-m}\exp[-i(j+j_+-j_-+2)\alpha](\sin\alpha)^{j-m}\,{}_2F_1\begin{bmatrix}j_++j+2,\ -j_-+j+1;\\ 2j+2;\ (1-\exp(-2i\alpha))\end{bmatrix}$$
$$\times\left(\frac{\Gamma(j-j_-+1)\Gamma(j+j_-+1)\Gamma(j_+-m+1)\Gamma(j_++j+2)\Gamma(j+m+1)\Gamma(2m+2)(2j+1)}{\Gamma(m-j_-+1)\Gamma(m+j_-+1)\Gamma(j_+-j+1)\Gamma(j_++m+2)\Gamma(j-m+1)\Gamma(2j+2)\Gamma(2j+2)}\right)^{1/2}, \tag{IV.1.13}$$

or

$$D^{[j_+\,j_-]}_{j,m,m}(\alpha)=\left(\frac{\Gamma(j_+-m+1)\Gamma(j+m+1)\Gamma(2m+2)\Gamma(1+j_-)\Gamma(1-j_-)(j_++1)}{\Gamma(m-j_-+1)\Gamma(m+j_-+1)\Gamma(j_++m+2)\Gamma(j-m+1)}\right)^{1/2}(2i)^{-m}(\sin\alpha)^{-m}D^{[j_+\,j_-]}_{j,0,0}(\alpha). \tag{IV.1.14}$$

The above formulas may also be derived directly from the definition of O(4)-functions [Eq. (IV.1.1)]. In this case, for the CG-coefficients, one uses conveniently Racah's expression [Eq. (II.1.8)] since the ${}_3F_2$ of this expression becomes a bilateral series for $j'=m$ and can be summed using[7]

$${}_2F_2\begin{bmatrix}a,\ b;\\ c,\ d;\ 1\end{bmatrix}=\frac{\Gamma(c)\Gamma(d)\Gamma(1-a)\Gamma(1-b)\Gamma(c+d-a-b-1)}{\Gamma(c-a)\Gamma(d-a)\Gamma(c-b)\Gamma(d-b)}.$$

Then one has to manipulate[28] carefully the many gamma functions (including the ones from the other CG-coefficient), recast the summation into a hypergeometric function ${}_2F_1$, and use the Euler's identity and Eq. (IV.1.12') to arrive at the desired result. The simplicity of the method we have used (due to Ström) enables one to obtain easily the above results [Eqs. (IV.1.2)—(IV.1.14)] which are not immediately seen from Eq. (IV.1.1). Furthermore, in order to obtain a general expression for $D^{[j_+\,j_-]}_{j,m,m}(\alpha)$ one may try to solve the fourth-order differential equation given

by Eq. (IV.1.6) or iterate Eq. (IV.1.13) using the recursion relation given by Eq. (IV.1.7). In either case it is necessary to introduce new higher order polynomials which, in principle, should be reduced to the product of two ${}_3F_2$ hypergeometric functions. The later can be easily obtained by substituting, say, Eq. (II.1.4) in Eq. (IV.1.1).

$$D^{[j\ j'\ j_-]}_{j_+,m}(\alpha)=\Delta'\sum_{m_1}\frac{(j_1-m_1)!\,(j+j_2+m_1)!\,(j'-j_2+m_1)!}{(j_1+m_1)!\,(j_2+m_2)!\,(j_2-m_2)!}\exp[-i(m_1-m_2)\alpha]$$
$$\times{}_3F_2\left[\begin{matrix}-j-m,\ -j+j_1-j_2,\ j_1-m_1+1;\\ j_1-j_2-m+1,\ -j-j_2-m_1;\ 1\end{matrix}\right]{}_3F_2\left[\begin{matrix}-j'-m,\ -j'+j_1-j_2,\ j_1-m_1+1;\\ j_1-j_2-m+1,\ -j'-j_2-m_1;1\end{matrix}\right],\qquad\text{(IV.1.15)}$$

where $2j_1=j_++j_-$, $2j_2=j_+-j_-$, $m_1+m_2=m$, and

$$\Delta'=(j_1-j_2-m)!\left(\frac{(j+j_1-j_2)!\,(j'+j_1-j_2)!\,(-j+j_1+j_2)!\,(-j'+j_1+j_2)!\,(j-m)!\,(j'-m)!\,(2j+1)(2j'+1)}{(j-j_1+j_2)!\,(j'-j_1+j_2)!\,(j+j_1+j_2+1)!\,(j'+j_1+j_2+1)!\,(j+m)!\,(j'+m)!}\right)^{1/2}.$$

However, for $j_-=0$ Vilenkin[27] (beware of his notations) has given an integral form for $D^{[j\ j'\ 0]}_{j_+,m}(\alpha)$.

Next we quote two expansion formulas of Ström.[27] Using them and Eqs. (IV.1.2)–(IV.1.5) one can derive many other recursion relations, i.e.,

$$(j_++j_-+1)(j_+-j_-+1)(2\cos\alpha)D^{[j\ j'\ j_-]}_{j_+,m}(\alpha)$$
$$=a'(j_+)D^{[j\ j'+1\ j_-]}_{j_+,m}(\alpha)+a'(j_+-1)D^{[j\ j'-1\ j_-]}_{j_+,m}(\alpha)+b'(j_-)D^{[j\ j'\ j_-+1]}_{j_+,m}(\alpha)+b'(j_--1)D^{[j\ j'\ j_--1]}_{j_+,m}(\alpha),$$
$$(j_++j_-+1)(j_+-j_-+1)(-2i\sin\alpha)D^{[j\ j'\ j_-]}_{j_+,m}(\alpha)\qquad\text{(IV.1.16)}$$
$$=j_-[a'(j_+)D^{[j\ j'+1\ j_-]}_{j_+,m}(\alpha)-a'(j_+-1)D^{[j\ j'-1\ j_-]}_{j_+,m}(\alpha)]+(j_++1)[b'(j_-)D^{[j\ j'\ j_-+1]}_{j_+,m}(\alpha)-b'(j_--1)D^{[j\ j'\ j_--1]}_{j_+,m}(\alpha)],$$

$$(j_++j_-+1)(j_+-j_-+1)(2i\sin\alpha)D^{[j\ j'\ j_-]}_{j_+,m}(\alpha)$$
$$=c'(j_+,j')D^{[j\ j'+1\ j_-]}_{j_+,m}(\alpha)-c'(-j_+-2,j')D^{[j\ j'-1\ j_-]}_{j_+,m}(\alpha)-d'(j_-,j')D^{[j\ j'\ j_-+1]}_{j_+,m}(\alpha)-d'(-j_-,j')D^{[j\ j'\ j_--1]}_{j_+,m}(\alpha),$$
$$(j_++j_-+1)(j_+-j_-+1)(-2i\sin\alpha)D^{[j\ j'\ j_-]}_{j_+,m}(\alpha)\qquad\text{(IV.1.16')}$$
$$=-c'(j_+,-j'-1)D^{[j\ j'+1\ j_-]}_{j_+,m}(\alpha)+c'(-j_+-2,-j'-1)D^{[j\ j'-1\ j_-]}_{j_+,m}(\alpha)$$
$$-d'(j_-,-j'-1)D^{[j\ j'\ j_-+1]}_{j_+,m}(\alpha)-d'(-j_-,-j'-1)D^{[j\ j'\ j_--1]}_{j_+,m}(\alpha),$$

where

$$a'(j_+)=[(j_++j+2)(j_+-j+1)(j_++j'+2)(j_+-j'+1)]^{1/2},\quad b'(j_-)=[(j+j_-+1)(j-j_-)(j'+j_-+1)(j'-j_-)]^{1/2},$$
$$c'(j_+,j')=\left(\frac{(2j'+1)}{(2j'+3)(j'-m+1)(j'+m+1)}(j_++j+2)(j_+-j+1)(j_++j'+2)(j_++j'+3)(j'+j_-+1)(j'-j_-+1)\right)^{1/2},$$
$$d'(j_-,j')=\left(\frac{(2j'+1)}{(2j'+3)(j'-m+1)(j'+m+1)}(j_-+j+1)(j-j_-)(j_++j'+2)(j_+-j')(j'+j_-+1)(j'+j_-+2)\right)^{1/2}.$$

Using the first of Eq. (IV.1.16) and Eqs. (IV.1.16'), we can derive the following two very useful recursion relations:

$$[(j_+-j)(j_++j+1)]^{1/2}D^{[j\ j'\ 0]}_{j_+,m}(\alpha)$$
$$=[(j_+-j')(j_++j'+1)]^{1/2}\cos\alpha D^{[j\ j'-1\ 0]}_{j_+,m}(\alpha)+i\left(\frac{(j'+m+1)(j'-m+1)(j_+-j')(j_+-j'+1)}{(2j'+1)(2j'+3)}\right)^{1/2}$$
$$\times\sin\alpha D^{[j\ j'-1\ 0]}_{j_+,m}(\alpha)+i\left(\frac{(j'-m)(j'+m)(j_++j')(j_++j'+1)}{(2j'+1)(2j'-1)}\right)^{1/2}\sin\alpha D^{[j\ j'-1\ 0]}_{j_+,m}(\alpha),$$
$$[(j_++j+2)(j_+-j+1)]^{1/2}D^{[j\ j'\ 0]}_{j_+,m}(\alpha)=[(j_++j'+2)(j_+-j'+1)]^{1/2}\cos\alpha D^{[j\ j'+1\ 0]}_{j_+,m}(\alpha)\qquad\text{(IV.1.16'')}$$
$$-i\left(\frac{(j'-m+1)(j'+m+1)(j_++j'+3)(j_++j'+2)}{(2j'+1)(2j'+3)}\right)^{1/2}\sin\alpha D^{[j\ j'+1\ 0]}_{j_+,m}(\alpha)$$
$$-i\left(\frac{(j'-m)(j'+m)(j_+-j'+1)(j_+-j'+2)}{(2j'+1)(2j'-1)}\right)^{1/2}\sin\alpha D^{[j\ j'-1\ 0]}_{j_+,m}(\alpha).$$

The first relation has been derived by Vilenkin[27] using a recurrence relation of the Gegenbauer polynomial.

Finally we derive an important and new recursion relation for the CG-coefficients, by substituting Eq. (IV.1.1) into Eq. (IV.1.7) and simplifying

$$\left[(m_1-m_2)+\frac{m(j_++1)j_-}{j(j+1)}\right]\begin{bmatrix}j_1 & j_2 & j\\ m_1 & m_2 & m\end{bmatrix}+[(j+m+1)(j-m+1)]^{1/2}\gamma'(j+1)\begin{bmatrix}j_1 & j_2 & j+1\\ m_1 & m_2 & m\end{bmatrix}$$
$$+[(j+m)(j-m)]^{1/2}\gamma'(j)\begin{bmatrix}j_1 & j_2 & j-1\\ m_1 & m_2 & m\end{bmatrix}=0,\qquad\text{(IV.1.17)}$$

where,

$$\gamma'(j)=\frac{1}{j}\left(\frac{(j^2-j_-^2)[(j_++1)^2-j^2]}{(2j+1)(2j-1)}\right)^{1/2}.$$

When $j_-=0$ ($j_1=j_2$), we obtain,

$$(m_1-m_2)\sqrt{2j+1}\begin{pmatrix} j_1 & j_1 & j \\ m_1 & m_2 & -m\end{pmatrix}+\delta'(j)\begin{pmatrix} j_1 & j_1 & j+1 \\ m_1 & m_2 & -m\end{pmatrix}+\delta'(j-1)\begin{pmatrix} j_1 & j_1 & j-1 \\ m_1 & m_2 & -m\end{pmatrix}=0, \tag{IV.1.18}$$

where

$$\delta'(j)=[(j+m+1)(j-m+1)(2j_1+j+2)(2j_1-j)]^{1/2}.$$

2. Special cases

When $j_-=0$ (j_+, j, m are all integers), we use the quadratic transformation,[7]

$${}_2F_1\left[\begin{matrix}a,\ b;\\ 2b;\end{matrix}\ z\right]=(1-z)^{-a/2}\,{}_2F_1\left[\begin{matrix}a,\ 2b-a;\\ b+\frac{1}{2};\end{matrix}\ -\tfrac{1}{4}(1-z)^{-1/2}[1-(1-z)^{1/2}]^2\right], \tag{IV.2.1}$$

the definition of the Gegenbauer (ultra spherical) polynomial[17] in terms of the hypergeometric polynomial,

$$C_n^{\nu}(z)=\frac{\Gamma(n+2\nu)}{\Gamma(n+1)\Gamma(2\nu)}\,{}_2F_1\left[\begin{matrix}-n,\ n+2\nu;\\ \nu+\frac{1}{2};\end{matrix}\ \tfrac{1}{2}(1-z)\right], \tag{IV.2.2}$$

and the Legendre's duplication formula

$$\Gamma(\tfrac{3}{2})\Gamma(2n+2)=2^{2n}\Gamma(n+\tfrac{3}{2})\Gamma(n+1),$$

in Eq. (IV.1.13) to obtain,

$$D^{[j_+\ 0]}_{j,m,m}(\alpha)=i^{j-m}2^j\sqrt{2j+1}\,\Gamma(j+1)\left(\frac{\Gamma(m+\frac{3}{2})\Gamma(j_+-m+1)\Gamma(j_+-j+1)\Gamma(j+m+1)}{\Gamma(\frac{3}{2})\Gamma(j_++m+2)\Gamma(j_++j+2)\Gamma(j-m+1)\Gamma(m+1)}\right)^{1/2}(\sin\alpha)^{j-m}C^{j+1}_{j_+-j}(\cos\alpha). \tag{IV.2.3}$$

This expression exactly agrees with the one derived by Vilenkin[27] by a different method. Furthermore, from Eq. (IV.1.9) we get

$$D^{[j_+\ 0]}_{j,m+1,m}(\alpha)=-i\left(\frac{(2m+3)}{(j_++m+2)(j_+-m)}\right)^{1/2}\frac{d}{d\alpha}D^{[j_+\ 0]}_{j,m,m}(\alpha), \tag{IV.2.4}$$

where the identity

$$\frac{d}{d\alpha}C_n^{\nu}(\cos\alpha)=-2\nu\sin\alpha\,C_{n-1}^{\nu+1}(\cos\alpha)$$

has been used.

When $j_-=+\frac{1}{2}$ and $-\frac{1}{2}$ (j_+, j, m are all semi-integers), we adopt the same procedure as in the previous case except that before we apply the quadratic transformation we use the following two recurrence relations[7]:

$$z(1+b-c)\,{}_2F_1-(c-1)(1-z)\,{}_2F_1[c-1]+(c-1)\,{}_2F_1[a-1;\ c-1]=0,$$

$$z(b-1)\,{}_2F_1-(c-1)\,{}_2F_1[b-1;\ c-1]+(c-1)\,{}_2F_1[a-1,b-1;\ c-1]=0.$$

The final results are

$$D^{[j_+\ 1/2]}_{j,m,m}(\alpha)=i^{j-m-1}a(j_+,j,m)(\sin\alpha)^{j-m-1}\ [(j_++j+1)\exp(i\alpha/2)C^{j+1/2}_{j_+-j}(\cos\alpha)-(j_+-j+1)\exp(-i\alpha/2)C^{j+1/2}_{j_+-j+1}(\cos\alpha)],$$

$$D^{[j_+\ -1/2]}_{j,m,m}(\alpha)=i^{j-m-1}a(j_+,j,m)(\sin\alpha)^{j-m-1}\ [(j_+-j+1)\exp(i\alpha/2)C^{j+1/2}_{j_+-j+1}(\cos\alpha)-(j_++j+1)\exp(-i\alpha/2)C^{j+1/2}_{j_+-j}(\cos\alpha)]. \tag{IV.2.5}$$

where,

$$a(j_+,j,m)=2^{j-1/2}\Gamma(j+\tfrac{1}{2})\left(\frac{\Gamma(m+1)\Gamma(j_+-m+1)\Gamma(j_+-j+1)\Gamma(j+m+1)}{\Gamma(\frac{3}{2})\Gamma(m+\frac{1}{2})\Gamma(j_++j+2)\Gamma(j-m+1)\Gamma(j_++m+2)}\right)^{1/2}.$$

One can easily see that

$$D^{*[j_+\ 1/2]}_{j,m,m}(\alpha)=(-1)^{j-m}D^{[j_+\ -1/2]}_{j,m,m}(\alpha),\qquad D^{*[j_+\ 1/2]}_{j,m,m}(\alpha)=D^{[j_+\ 1/2]}_{j,m,m}(-\alpha). \tag{IV.2.6}$$

Furthermore, from Eq. (IV.1.9) we obtain

$$D^{[j_+\ \pm1/2]}_{j,m+1,m}(\alpha)=\left[\frac{2(m+1)^2}{(m+\frac{1}{2})(j_++m+2)(j_+-m)}\right]^{1/2}\left[-i\frac{d}{d\alpha}\pm\frac{1}{2}\frac{(j_++1)}{(m+1)}\right]D^{[j_+\ \pm1/2]}_{j,m,m}(\alpha). \tag{IV.2.7}$$

Finally we give some special values of this function which frequently occur in the calculations.[20]

$$D^{[j,0]}_{j,m,m}(\alpha)=i^{j-m}2^j\sqrt{2j+1}\,\Gamma(j+1)\left[\frac{\Gamma(3m+\frac{3}{2})}{\Gamma(\frac{3}{2})\Gamma(2j+2)\Gamma(m+1)(j+m+1)}\right]^{1/2}(\sin\alpha)^{j-m},$$

$$D^{[m,0]}_{m,m,m}(\alpha)=1,\quad D^{[2,0]}_{1,0,0}(\alpha)=i\sqrt{\tfrac{2}{3}}\sin(2\alpha),\quad D^{[2,0]}_{1,1,1}(\alpha)=\sqrt{\tfrac{2}{3}}\cos\alpha,\quad D^{[1,0]}_{0,0,0}(\alpha)=\cos\alpha,$$

$$D^{[j,1/2]}_{j,m,m}(\alpha)=i^{j-m}2^{j-1/2}(2j+1)\Gamma(j+\tfrac{1}{2})\left[\frac{\Gamma(m+1)}{\Gamma(\frac{3}{2})\Gamma(m+\frac{1}{2})\Gamma(2j+2)(j+m+1)}\right]^{1/2}\exp(-i\alpha/2)(\sin\alpha)^{j-m},\tag{IV.2.8}$$

$$D^{[m,1/2]}_{m,m,m}(\alpha)=\exp(-i\alpha/2),\quad D^{[3/2,1/2]}_{3/2,1/2,1/2}(\alpha)=(\sqrt{2}/3)[\exp(i\tfrac{3}{2}\alpha)-\exp(+i\alpha/2)],$$
$$D^{[3/2,1/2]}_{1/2,1/2,1/2}(\alpha)=\tfrac{2}{3}[\exp(-i\tfrac{3}{2}\alpha)+\tfrac{1}{2}\exp(+i\alpha/2)].$$

In the above we have generously used the following values of Gegenhauer polynomials, i. e.,

$$C^{\nu}_0(z)=1,\quad C^{\nu}_1(z)=2\nu z,\quad C^{\nu}_2(z)=2\nu(\nu+1)[z^2-1/(2\nu+2)].$$

Also, using $C^1_n(\cos\alpha)=\sin[(n+1)\alpha]/\sin\alpha$ we obtain

$$D^{[j_+,0]}_{0,0,0}(\alpha)=\frac{1}{(j_++1)}\,\frac{\sin[(j_++1)\alpha]}{\sin\alpha},$$

$$D^{[j_+,1/2]}_{1/2,1/2,1/2}(\alpha)=\frac{\exp(-i\pi/2)}{\sin\alpha}\left[\frac{1}{(j_++\frac{1}{2})}\exp(i\alpha/2)\,\frac{\sin[(j_++\frac{1}{2})\alpha]}{\sin\alpha}-\frac{1}{(j_++\frac{3}{2})}\exp(-i\alpha/2)\,\frac{\sin[(j_++\frac{3}{2})\alpha]}{\sin\alpha}\right].\tag{IV.2.9}$$

Next we make use of the asymptotic formula of Gegenbauer polynomials,[16]

$$C^{\lambda}_n(\cos\alpha)\underset{n\to\infty}{\longrightarrow}2^{1-\lambda}\frac{n^{\lambda-1}}{\Gamma(\lambda)}(\sin\alpha)^{-\lambda}\cos[(n+\lambda)\alpha-\tfrac{1}{2}\lambda\pi],$$

and the Barnes expansion formula,[17]

$$[\Gamma(z+\beta_1)\Gamma(z+\beta_2)]^{-1}\Gamma(z+\alpha_1)\Gamma(z+\alpha_2)\underset{z\to\infty}{\longrightarrow}z^{\alpha_1+\alpha_2-\beta_1-\beta_2},$$

to obtain the following asymptotic relations of O(4) functions:

$$D^{[j_+,0]}_{j,m,m}(\alpha)\underset{j_+\to\infty}{\longrightarrow}i^{j-m}\sqrt{2j+1}\left[\frac{\Gamma(m+\frac{3}{2})\Gamma(j+m+1)}{\Gamma(\frac{3}{2})\Gamma(j-m+1)\Gamma(m+1)}\right]^{1/2}(j_+-j)^{-m-1}\frac{\cos[(j_++1)\alpha-\frac{1}{2}(j+1)\pi]}{(\sin\alpha)^{m+1}}$$

$$\longrightarrow\frac{i^{j-m}}{j_+^{m+1}}\,\frac{\cos[(j_++1)\alpha-\frac{1}{2}(j+1)\pi]}{(\sin\alpha)^{m+1}},$$

$$D^{[j_+,1/2]}_{j,m,m}(\alpha)\underset{j_+\to\infty}{\longrightarrow}i^{j-m-1}\left[\frac{\Gamma(m+1)\Gamma(j+m+1)}{\Gamma(\frac{3}{2})\Gamma(m+\frac{1}{2})\Gamma(j-m+1)}\right]^{1/2}\left\{\frac{(j_++j+1)}{(j_+-j)^{m+3/2}}\exp(i\alpha/2)\,\frac{\cos[(j_++\frac{1}{2})\alpha-\frac{1}{2}(j+\frac{1}{2})\pi]}{(\sin\alpha)^{m+3/2}}\right.$$

$$\left.-\frac{(j_+-j-1)}{(j_+-j-1)^{m+3/2}}\exp(-i\alpha/2)\frac{\cos[(j_++\frac{3}{2})\alpha-\frac{1}{2}(j+\frac{1}{2})\pi]}{(\sin\alpha)^{m+3/2}}\right\}$$

$$\longrightarrow\frac{i^{j-m}}{j_+^{m+1/2}}\,\frac{\exp\{-i[(j_++1)\alpha-\frac{1}{2}(j+\frac{1}{2})\pi]\}}{(\sin\alpha)^{m+1/2}}.\tag{IV.2.10}$$

Furthermore, we also have the asymptotic expression[29]

$$C^{\lambda+n}_{\nu-n}(\cos\alpha)\underset{n\to\infty}{\longrightarrow}(1/\sqrt{n\pi})\sin[(n-\nu)\pi]\,[4\cos^2\tfrac{1}{2}\alpha]^{-(\lambda+n-1/2)}.$$

Therefore,

$$D^{[j_+,0]}_{j,m,m}(\alpha)\underset{j_+,j\to\infty}{\longrightarrow}i^{j-m+2}\frac{\exp[\frac{1}{2}(j_+-j)]}{2^j(2\pi)^{1/4}}\,j^{j+m+1/2}j_+^{-m-1/2}\,(j_++j)^{-(j_++j+3/2)}\left[\frac{\Gamma(m+\frac{3}{2})\Gamma(j_+-j+1)}{\Gamma(\frac{3}{2})\Gamma(m+1)}\right]^{1/2}\frac{(\sin\alpha)^{j-m}\sin[(j_+-j)\pi]}{(\cos\frac{1}{2}\alpha)^{2j}},$$

$$D^{[j_+,1/2]}_{j,m,m}(\alpha)\underset{j_+,j\to\infty}{\longrightarrow}i^{j-m+1}\frac{\exp[\frac{1}{2}(j_+-j+1)]}{2^j(2\pi)^{1/4}}\,j^{j+m-1/2}j_+^{-m-1/2}\,(j_++j)^{-(j_++j+3/2)}\left[\frac{\Gamma(m+1)\Gamma(j_+-j+1)}{\Gamma(\frac{3}{2})\Gamma(m+\frac{1}{2})}\right]^{1/2}\frac{(\sin\alpha)^{j-m-1}}{(\cos\frac{1}{2}\alpha)^{2j}}$$

$$\times\{(j_++j-1)\exp(i\alpha/2)\,\sin[(j_+-j)\pi]-(j_+-j+1)\exp(-i\alpha/2)\,\sin[(j_+-j+1)\pi]\}.\tag{IV.2.11}$$

Also, it is quite clear from Eq. (IV.1.1) that $\lim_{\alpha\to\infty}D^{[j_+,j_-]}_{j,j_+,m}(\alpha)=0$. Finally, we give two relations which are obvious from Eq. (IV.1.1):

$$\sum_j D^{[j_+,j_-]}_{j,j_+,m}(\alpha)D^{[j_+,j_-]}_{j,j_+,m}(-\alpha)=\delta_{j'j''},\qquad\sum_{j=m}^{j_+}D^{[j_+,j_-]}_{j,j_+,m}(\alpha_1)D^{[j_+,j_-]}_{j,j_+,m}(\alpha_2)=D^{[j_+,j_-]}_{j,j_+,m}(\alpha_1+\alpha_2).\tag{IV.2.12}$$

3. An application

As pointed out earlier in the evaluation of transition amplitudes using O(4, 2) states[19,25] one usually faces the following two matrix elements corresponding to the boost η and tilts (θ', θ):

$$G^{n'l'm}_{nlm} = \langle n'l'm \,|\, G \,|\, nlm\rangle, \tag{IV.3.1}$$

$$G^{n'j'^{\pm}k}_{nj^{\pm}k} = \langle n'j'^{\pm}k \,|\, G \,|\, nj^{\pm}k\rangle, \tag{IV.3.2}$$

where $G = \exp(i\theta' L_{45}) \exp(i\eta L_{35}) \exp(-i\theta L_{45})$; L_{45}, L_{35}, L_{34} are generators of an O(2, 1) subgroup of O(4, 2). In order to evaluate these matrix elements one conveniently uses parabolic basis $|n_1 n_2 m\rangle$ as given in Eq. (II. 6. 2) and Eq. (II. 4. 5). Since in this basis the operator L_{34} is diagonal, one parametrizes G in terms of Euler angles α, β, γ as $G = \exp(-i\alpha L_{34}) \exp(-i\beta L_{45}) \exp(-i\gamma L_{34})$ where,

$$\begin{aligned}
&\sin\alpha \sinh\beta = \cosh\theta \sinh\eta, \quad \cos\alpha \sinh\beta = \sinh\theta \cosh\theta' - \cosh\theta \sinh\theta' \cosh\eta,\\
&\sin\gamma \sinh\beta = -\cosh\theta' \sinh\eta, \quad \cos\gamma \sinh\beta = \sinh\theta \cosh\theta' \cosh\eta - \cosh\theta \sinh\theta',\\
&\cosh\beta = \cosh\theta' \cosh\theta \cosh\eta - \sinh\theta' \sinh\theta.
\end{aligned} \tag{IV.3.3}$$

If we represent the basis states given in Eq. (II. 6. 2) as $|\phi_1\phi_2\phi_3\phi_4\rangle$, then we obtain from previous works[19,25]

$$\begin{aligned}
\langle \phi_1'\phi_2'\phi_3'\phi_4' \,|\, G \,|\, \phi_1\phi_2\phi_3\phi_4\rangle = {} & \exp[-i\alpha\tfrac{1}{2}(\phi_2' + \phi_3' + 1)]\, V^{(|\phi_2'-\phi_3'|+1)/2}_{(\phi_2'+\phi_3'+1)/2,\,(\phi_2+\phi_3+1)/2}(\beta) \exp[-i\gamma\tfrac{1}{2}(\phi_2+\phi_3+1)]\\
& \times \exp[i\alpha\tfrac{1}{2}(\phi_1' + \phi_4' + 1)]\, V^{(|\phi_1'-\phi_4'|+1)/2}_{(\phi_1'+\phi_4'+1)/2,\,(\phi_1+\phi_4+1)/2}(-\beta) \exp[i\gamma\tfrac{1}{2}(\phi_1+\phi_4+1)].
\end{aligned} \tag{IV.3.4}$$

The above matrix element vanishes unless $|\phi_2' - \phi_3'| = |\phi_2 - \phi_3|$ and $|\phi_1' - \phi_4'| = |\phi_1 - \phi_4|$. Using this matrix element and Eq. (II. 6. 2) we get

$$\begin{aligned}
G^{n'l'm}_{nlm} = {} & \sum_{n_1', n_1} \begin{bmatrix} \frac{1}{2}(n'-1) & \frac{1}{2}(n'-1) & l' \\ \frac{1}{2}(n_2'-n_1'+m) & \frac{1}{2}(n_1'-n_2'+m) & m \end{bmatrix} \begin{bmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & l \\ \frac{1}{2}(n_2-n_1+m) & \frac{1}{2}(n_1-n_2+m) & m \end{bmatrix}\\
& \times \exp[-i\alpha(n_1'-n_2')] \exp[-i\gamma(n_1-n_2)]\, V^{(|m|+1)/2}_{n_1'+(|m|+1)/2,\,n_1+(|m|+1)/2}(\beta)\, V^{(|m|+1)/2}_{n_2'+(|m|+1)/2,\,n_2+(|m|+1)/2}(-\beta).
\end{aligned}$$

By making use of Eq. (IV. 4. 2) (with $(\delta = 0)$ and the definition of the O(4)-representation function [Eq. (IV. 1. 1)] we get

$$G^{n'l'm}_{nlm} = \sum_{\tau} D^{[n'-1,\,0]}_{l',\,|m|+\tau,\,|m|}(-\alpha)\, V^{|m|+1+\tau}_{n',n}(\beta)\, D^{[n-1,\,0]}_{l,\,|m|+\tau,\,|m|}(-\gamma), \qquad 0 \le \tau \le \mathrm{Min}\begin{Bmatrix} n-|m|-1 \\ n'-|m|-1 \end{Bmatrix}. \tag{IV.3.5}$$

If we square this matrix element and sum over l and l', then by Eq. (IV. 3. 12) we obtain,

$$\sum_{l,\,l'} |G^{n'l'm}_{nlm}|^2 = \sum_{\tau} V^{|m|+1+\tau}_{n',n}(\beta)\, V^{|m|+1+\tau}_{n',n}(\beta), \tag{IV.3.6}$$

which is the same as Eq. (III. 4. 4). Similarly, using Eq. (II. 6. 5) and Eq. (IV. 3. 4) we get

$$\begin{aligned}
G^{n'j'^{\pm}k}_{nj^{\pm}k} = {} & \frac{1}{2} \sum_{n_1', n_1} \Bigg\{ \begin{bmatrix} \frac{1}{2}(n'-1)+\frac{1}{2} & \frac{1}{2}(n'-1) & j' \\ \frac{1}{2}(n_2'-n_1'+k_-)+\frac{1}{2} & \frac{1}{2}(n_1'-n_2'+k_-) & k_-+\frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2}(n-1)+\frac{1}{2} & \frac{1}{2}(n-1) & j \\ \frac{1}{2}(n_2-n_1+k_-)+\frac{1}{2} & \frac{1}{2}(n_1-n_2+k_-) & k_-+\frac{1}{2} \end{bmatrix}\\
& \times \exp\{-i\alpha[n_1' + \tfrac{1}{2}(|k_-|+1)]\}\, V^{(|k_-|+1)/2}_{n_1'+(|k_-|+1)/2,\,n_2+(|k_-|+1)/2}(\beta) \exp\{-i\gamma[n_1 + \tfrac{1}{2}(|k_-|+1)]\} \exp\{i\alpha[n_2' + \tfrac{1}{2}(|k_-|+1) + |\delta|]\}\\
& \times V^{(|k_-|+1)/2+6}_{n_2'+(|k_-|+1)/2+6|,\,n_2+(|k_-|+1)/2+|6|}(-\beta) \exp\{i\gamma[n_2 + \tfrac{1}{2}(|k_-|+1) + |\delta|]\}\\
& \pm/\mp (-1)^{n'+n} \begin{bmatrix} \frac{1}{2}(n'-1)+\frac{1}{2} & \frac{1}{2}(n'-1) & j' \\ \frac{1}{2}(n_1'-n_2'+k_-)+\frac{1}{2} & \frac{1}{2}(n_2'-n_1'+k_-) & k+\frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2}(n-1)+\frac{1}{2} & \frac{1}{2}(n-1) & j \\ \frac{1}{2}(n_1-n_2+k_-)+\frac{1}{2} & \frac{1}{2}(n_2-n_1+k\,) & k_-+\frac{1}{2} \end{bmatrix}\\
& \times \exp\{-i\alpha[n_1' + \tfrac{1}{2}(|k_-|+1) + |\delta|]\}\, V^{(|k_-|+1)/2+6}_{n_1'(|k_-|+1)/2+|6|,\,n_1+(|k_-|+1)/2+|6|}(\beta) \exp\{-i\gamma[n_1 + \tfrac{1}{2}(|k_-|+1) + |\delta|]\}\\
& \times \exp\{i\alpha[n_2' + \tfrac{1}{2}(|k_-|+1)]\}\, V^{(|k_-|+1)/2}_{n_2'+(|k_-|+1)/2,\,n_2+(|k_-|+1)/2}(-\beta) \exp\{i\gamma[n_2 + \tfrac{1}{2}(|k_-|+1)]\} \Bigg\},
\end{aligned} \tag{IV.3.7}$$

where we take $(\pm)$ if the right state has positive parity and $(\mp)$ if negative parity. Again, using Eqs. (III. 4. 2)–(III. 4. 3) (with $\delta = \pm\frac{1}{2}$), the definition of the O(4) function, and the Regge symmetries,

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} = (-1)^{l_1+l_2+l} \begin{pmatrix} l_2 & l_1 & l \\ m_2 & m_1 & -m \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} l_1 & l_2 & l \\ -m_1 & -m_2 & m \end{pmatrix} = (-1)^{l_1+l_2+l} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix},$$

we obtain

$$\begin{aligned}
G^{n'j'^{\pm}k}_{n,\,j^{\pm},\,k} = {} & \tfrac{1}{2} \sum_{\tau} (D^{[n'-1+|\delta|,\,\delta]}_{j',\,|k_-|+6+\tau,\,|k_-|+6}(-\alpha)\, V^{|k_-|+1+6+\tau}_{n'+|6|,\,n+|6|}(\beta) D^{[n-1+|6|,\,\delta]}_{j,\,|k_-|+6+\tau,\,|k_-|+6}(-\gamma) \pm/\mp \text{complex conjugate}),\\
& 0 \le \tau \le \mathrm{Min}\begin{Bmatrix} n-|k_-|-1+|\delta|-\delta \\ n'-|k_-|-1+|\delta|-\delta \end{Bmatrix}.
\end{aligned} \tag{IV.3.8}$$

Equations (IV. 3. 5) and (IV. 3. 8) play major roles in the evaluation of transition form factors and structure functions.[20]

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[1]Ya. A. Smorodinskiĭ and L. A. Shelepin, Usp. Fiz. Nauk **106**, 3 (1972) [Sov. Phys. Usp. **15**, 1 (1972)].

[2]E. P. Wigner, SIAM J. Appl. Math. **25**, 169 (1973).

[3]T. Regge, *Proceedings of the International School of Physics-"Enrico Fermi" Course* LIV, Page III, edited by R. Gatto (Academic, New York, 1972).

[4]A. M. Bincer, J. Math. Phys. **11**, 1835 (1970).

[5]P. J. Brussard and H. A. Tolhock, Physica **23**, 955 (1957).

[6]A. P. Yutsis, I. B. Levinson, and V. V. Vanagas, *Mathematical Apparatus of the Theory of Angular Momentum* (Israel Program for Scientific Translation, Jerusalem, 1962), p. 8.

[7]L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge U. P., 1966).

[8]E. L. Akim and A. A. Levin, Sov. Math. Dokl. **2**, 629 (1961).

[9]E. D. Rainville, Bull. Am. Math. Soc. **51**, 714 (1945).

[10]N. Ja. Vilenkin, *Special Functions and the theory of Group Representations*, American Math. Soc. Monograph Vol. 22 (Am. Math. Soc., Providence, R. I., 1968).

[11]See also Ronald Shaw, "Wigner 3*j*-symbols and the Lorentz Group," University of Hull Preprint (1975).

[12]A. A. Bandzaitis, A. V. Karosene, A. Yu. Savukinas, and A. P. Yutsis, Dokl. Akad. Nauk SSSR **154**, 812 (1964) [Sov. Phys. Dokl. **9**, 139 (1964)].

[13]Barry Minton, J. Math. Phys. **11**, 1375 (1970).

[14]A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U. P., Princeton, N. J., 1960).

[15]G. Ponzano and T. Regge, *Spectroscopic and Group Theoretical Methods in Physics*, Racah Memorial Volume, edited by F. Bloch, S. G. Cohen, A. De-Shalit, S. Sambursky, and I. Talmi (Wiley, New York, 1968).

[16]G. Szegö, *Orthogonal Polynomials*, American Math. Soc. Colloquium Publications Vol. 23 (Am. Math. Soc., Providence, R. I., 1959).

[17]I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965), p. 696.

[18]A. O. Barut, C. K. E. Schneider, and Raj Wilson, to be published.

[19]A. O. Barut, *Dynamical Groups and Generalized Symmetries in Quantum Theory* (University of Canterbury Publication, Christchurch, New Zealand, 1972).

[20]A. O. Barut, Rapporteur talk at the Fifteenth International Conference on High Energy Physics, Kiev, Naukova Dumka (1972). H. Kleinert, Springer Tracts Mod. Phys. **49**, 90 (1969). A. O. Barut and Raj Wilson, "Infinite Component Fields I and II," Phys. Rev. D (to be published).

[21]V. Bargmann, Ann. Math. **48**, 568 (1947).

[22]A. O. Barut and E. C. Phillips, Commun. Math. Phys. **8**, 52 (1968); N. Mukunda, J. Math. Phys. **10**, 2086, 2092 (1969); G. Lindblad and B. Nagel, Ann. Inst. Henri Poincaré **A13**, 27 (1970).

[23]J. L. Burchnall and T. W. Chaundy, Proc. London Math. Soc. Ser. 2, **50**, 56 (1944).

[24]M. Andrews and J. Gunson, J. Math. Phys. **5**, 1391 (1964); S. S. Sannikov, Dokl. Akad. Nauk SSSR **171**, 1058 (1966) [Sov. Phys. Dokl. **11**, 1045 (1967)]; Kuo-Hsiang Wang, J. Math. Phys. **11**, 2077 (1970); Y. A. Verdiev, G. A. Kerimov, and Ya. A. Smorodinskiĭ, Yad. Fiz. **20**, 827 (1974) [Sov. J. Nucl. Phys. **20**, 441 (1975)].

[25]D. Corrigan and B. Hamprecht, Boulder Lect. Theor. Phys. **11A**, 299 (1969); R. F. Peierls and Raj Wilson, Ann. Phys. (N. Y.) **81**, 15 (1973).

[26]A. Z. Dolginov and I. N. Toptygin, Zh. Eksp. Teor. Fiz. **35**, 794 (1958) [Sov. Phys. JETP **8**, 550 (1959)]; L. C. Biedenharn, J. Math. Phys. **2**, 433 (1961).

[27]N. Ja. Vilenkin, Trans. Moscow Math. Soc. **12**, 209 (1963); Staffan Ström, Ark. Fys. **29**, 467 (1965); **40**, 1 (1969); A. Sciarrino and M. Toller, J. Math. Phys. **8**, 1252 (1967).

[28]Ya. A. Smorodinskiĭ and G. I. Shepelev, Yad. Fiz. **13**, 441 (1971) [Sov. J. Nucl. Phys. **13**, 248 (1971)].

[29]L. Durand, P. M. Fishbane, and L. M. Simmons Jr., Wisconsin Preprint (1972).

Massive and massless supersymmetry: Multiplet structure and unitary irreducible representations

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UIR's of the supersymmetry algebra for the massive and massless cases are analyzed covariantly (without the use of induced representations) in terms of their component spins. For the massive case normalized basis vectors $|p^2>0,\ j_0;\ \sigma;\ pj\lambda\rangle$ are constructed, where j_0 is the "superspin" and σ is an additional quantum number serving to distinguish the different $|pj\lambda\rangle$, the constituent $p^2>0$, spin-j UIR's of the Poincaré group. For the massless case, normalized basis vectors $|p^2=0,\ \lambda_0;\ p\lambda\rangle$ are similarly constructed, where λ_0 is the "superhelicity." Matrix elements of the supersymmetry generators, in these bases, are explicitly given. The "σ basis" is used to define weight diagrams for the massive UIR's of supersymmetry, and their properties are briefly described. Eigenfunctions $\omega_\sigma(\theta)$ are also defined, and their connection with the reduction of higher spin massive superfields $\Phi^j(x,\theta)$ is discussed. Finally, it is shown how gauge dependence necessarily arises with certain massless superfields. The massless scalar superfield, both gauge-dependent and gauge-independent, is discussed as an example.

1. INTRODUCTION

The concept of a fermion–boson mixing symmetry was first formulated globally in four-dimensional space–time by Wess and Zumino.[1] The particular "supersymmetry," with which we are concerned in this article, was studied in detail by Salam and Strathdee,[2] and some of its UIR's were constructed. The generators, the ordinary Poincaré group generators P_μ, $J_{\mu\nu}$, together with a 4-spinor charge S_α, form a "generalized Lie algebra,"[3] with the following commutation and anticommutation relations, in addition to the usual Lie algebra of the P_μ and $J_{\mu\nu}$:

$$\begin{aligned}&\{S_\alpha, S_\beta\} = -(\gamma_\mu C)_{\alpha\beta} P^\mu,\\ &[S_\alpha, J_{\mu\nu}] = \tfrac{1}{2}(\sigma_{\mu\nu})_\alpha{}^\beta S_\beta,\\ &[S_\alpha, P_\mu] = 0.\end{aligned} \tag{1.1}$$

(We follow the notation of Ref. 4. Further notations and identities are collected in Appendix A.) A representation in which the P_μ, $J_{\mu\nu}$ are Hermitian, and the S_α satisfies the reality condition of a Majorana spinor:

$$S_\alpha = C_{\alpha\beta}\bar{S}^\beta \tag{1.2}$$

will be called a unitary representation.

Supersymmetric Lagrangian models have recently received considerable attention, in view of their renormalization properties.[5] Such models are very conveniently described using the "superfield" techniques of Salam and Strathdee.[4] A superfield $\Phi_a(x,\theta)$ is defined on an eight-dimensional space labelled by (x_μ, θ_α), where x_μ is ordinary space–time, θ_α is a Majorana 4-spinor, with anticommuting components, and a is a spin index. Such a field transforms under supersymmetry as

$$[S_\alpha, \Phi_a(x,\theta)] = i\left\{\frac{\partial}{\partial\theta} + \tfrac{1}{2}[i\gamma_\mu\partial^\mu]\theta\right\}_\alpha \Phi_a(x,\theta). \tag{1.3}$$

Thus on superfields the generators S_α are given a differential representation in terms of the anticommuting spinor θ_α.

Supersymmetry having been introduced, it is natural to seek its possible implications outside of a strictly field-theoretical context. For example, is some type of supersymmetry scheme, albeit badly broken, of any relevance at all for particle classification?[2b,6] If so, how are scattering amplitudes constrained? What is their Regge behavior? What is the nature of supersymmetric bound states?[7]

The differential representations of the supersymmetry algebra, while appropriate for field theory, are inappropriate in these other contexts. The aim of this article is to investigate the UIR's of the supersymmetry algebra (1.1), and to construct corresponding normalized bases and matrix elements, which will be naturally suited to such other applications.

In Sec. 2, we analyze the supersymmetry algebra in the timelike (massive) case in terms of its spin content, and find a normalized basis for the UIR's of the form $|p^2>0,\ j_0;\sigma;pj\lambda\rangle$, where j_0 is the "superspin," $j_0 = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, each $|pj\lambda\rangle$ specifies a UIR of the Poincaré group with mass $p^2>0$ and spin $j=j_0,\ j_0\pm\frac{1}{2}$, and $\sigma = 0,\ \pm\frac{1}{2}$ is an additional quantum number serving to distinguish the different spins occurring. The basis vectors are constructed with the help of a set of σ-shifting tensor operators $R^\pm_\kappa$, $\kappa = \pm\frac{1}{2}$, equivalent to the S_α. The matrix elements of the $R^\pm_\kappa$ in the "σ-basis" are also given. The σ-basis is used to define weight diagrams for the $(p^2>0,\ j_0)$ UIR's, and their properties are briefly described. Finally, it is shown how, in the superfield representation, σ-eigenfunctions $\omega_\sigma(\theta)$ may be defined, which can be used in the reduction of higher-spin superfields.

In Sec. 3, we analyze the supersymmetry algebra in the lightlike case, restricting ourselves to those UIR's containing only physical massless spin constituents, with invariant helicity. It is shown that this constraint also necessitates a contraction of the supersymmetry algebra, such that the UIR's contain just two helicities λ_0, $\lambda_0 - \frac{1}{2}$. A normalized basis of the form $|p^2=0,\ \lambda_0; p\lambda\rangle$ is constructed, where λ_0 is the "superhelicity," $\lambda_0 = 0, \pm\frac{1}{2}, \pm 1, \cdots$ and each $|p\lambda\rangle$ specifies a UIR of the Poincaré group with mass $p^2=0$ and invariant helicity $\lambda = \lambda_0$ or $\lambda_0 - \frac{1}{2}$. Matrix elements of the S_α in this basis are written down. It should be emphasized that the techniques of Secs. 2 and 3 involves no induced representation theory.

Finally, we apply our results for the $(p^2=0,\ \lambda_0)$ massless UIR's of supersymmetry, to massless superfields. It is shown that free, massless, irreducible superfields are of two types, gauge-independent or gauge-dependent. The discussion is illustrated by massless scalar superfields of each type.

In Appendix A the notation conventions are established, and some supersymmetry algebra identities are given. In Appendix B the properties of the σ-shifting tensor operators $R_\kappa^\pm$ are listed, together with their matrix elements in the σ-basis.

2. THE TIMELIKE CASE $P^2>0$

A. Analysis of spin content

It follows from (1.1) that P^2 is a Casimir not only of the Poincaré subalgebra $\mathcal{P}$, generated by the P_μ and $J_{\mu\nu}$, but also of the complete supersymmetry algebra $\mathcal{S}$, generated by the P_μ, $J_{\mu\nu}$, and S_α. (The supersymmetry algebra $\mathcal{S}$, "generated by P_μ, $J_{\mu\nu}$, and S_α", is not a group, but contains the subalgebra "generated by the P_μ and $J_{\mu\nu}$", namely the Lie group $\mathrm{ISL}(2,\mathbb{C})\equiv\mathcal{P}$, as a subgroup. We consider the algebra merely over $\mathbb{C}$ and make no appeal to Grassman algebras for our analysis of the UIR's.) Hence the UIR's of $\mathcal{S}$ may be classified by the eigenvalue of P^2. In this section we consider the timelike case $P^2>0$, and $\mathrm{sgn}(P_0)=\pm1$. The invariance of P^2 means that all components of a supersymmetry multiplet have the same mass.[2b]

A UIR of $\mathcal{S}$ provides a representation, possibly reducible, of $\mathcal{P}$, so that we may characterize the structure of the former by analyzing its spin content, or the UIR's of $\mathcal{P}$ which it contains. If the reduction is degenerate, then we require one or more additional quantum numbers to specify completely the spin content.

Before proceeding with this analysis, however, we investigate the algebra of operators commuting with the S_α. The square of the Pauli-Lubanski vector

$$W_\mu=-\tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}P^\nu J^{\rho\sigma}, \tag{2.1}$$

is a Casimir of $\mathcal{P}$, but not of $\mathcal{S}$. However, if we define[4]

$$\Sigma_\mu=-\tfrac{1}{4}\bar{S}i\gamma_\mu\gamma_6 S, \tag{2.2}$$

$$K_\mu=W_\mu-\Sigma_\mu,$$

$$K_\mu^\perp=K_\mu-P_\mu P^{-2}P\circ K, \tag{2.3}$$

then we find that $K_\mu^\perp$ commutes with S_α and P_μ, so that $(K^\perp)^2$ is a Casimir of $\mathcal{S}$. In fact, the tensors

$$K_{\mu\nu}=K_\mu P_\nu-K_\nu P_\mu,$$

$$M_{\mu\nu}=K_{\mu\nu}+\tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}K^{\rho\sigma} \tag{2.4}$$

also commute with S_α and P_μ, and, moreover,

$$[M_{\mu\nu},M_{\rho\sigma}]=iP^2(\eta_{\mu\sigma}M_{\nu\rho}+\eta_{\nu\rho}M_{\mu\sigma}-\eta_{\nu\sigma}M_{\mu\rho}-\eta_{\mu\rho}M_{\nu\sigma}), \tag{2.5}$$

so that the $M_{\mu\nu}$ generate a group $\mathcal{L}'$, isomorphic to the Lorentz group, $\mathrm{SL}(2,\mathbb{C})\equiv\mathcal{L}$, generated by the $J_{\mu\nu}$. If we denote by $\mathcal{T}$ the algebra generated by the S_α and P_μ, then we can describe the structure of $\mathcal{S}$ as follows[8]:

$$\mathcal{S}\cong\mathcal{L}\wedge\mathcal{T}\supset\mathcal{L}'\times\mathcal{T}, \tag{2.6}$$

where $\wedge$, $\times$ denote semidirect product and direct product, respectively.

The subalgebra $\mathcal{L}'\times\mathcal{T}$ provides an alternative means of analyzing the structure of UIR's of $\mathcal{S}$. In particular, since the Casimirs of $\mathcal{L}'$ also commute with $\mathcal{S}$, it follows that a UIR of $\mathcal{S}$ contains precisely one UIR of $\mathcal{L}'$. In fact[9]

$$\tfrac{1}{2}M_{\mu\nu}M^{\mu\nu}=P^2(K^\perp)^2=(P^2)^2(\lambda^2-\nu^2+1),$$

$$\tfrac{1}{4}\epsilon_{\mu\nu\rho\sigma}M^{\mu\nu}M^{\rho\sigma}=0=(P^2)^2\lambda\nu, \tag{2.7}$$

whence

$$\nu=0\ \text{ and }\ (K^\perp)^2=P^2(\lambda^2+1). \tag{2.8}$$

In order to analyze a UIR of $\mathcal{S}$ into its component spins, we must consider the algebra of $\mathcal{P}$ invariants constructed from its generators. If we define, in addition to W_μ and Σ_μ, a 4-vector

$$U_\mu=P^{-2}\epsilon_{\mu\nu\rho\sigma}P^\nu\Sigma^\rho W^\sigma, \tag{2.9}$$

then the $\mathcal{P}$-invariant subalgebra is generated by the set

$$\{W^2,\Sigma^2,U^2,\bar{S}S_\pm,P\circ\Sigma,\Sigma\circ W,W\circ U,\Sigma\circ U\}, \tag{2.10}$$

which are, however, not all algebraically independent. In fact, from the polynomial identities (A8) and (A9) satisfied by these invariants in any representation, it follows that, to any order, the independent invariants are W^2, $P\cdot\Sigma$, and $\bar{S}S_\pm$, where

$$[P\cdot\Sigma,W^2]=0=[\bar{S}S_\pm,W^2], \tag{2.11}$$

$$[P\cdot\Sigma,S_\pm]=\pm\tfrac{1}{2}P^2P\circ\Sigma,$$

$$[P\circ\Sigma,\bar{S}S_\pm]=\pm P^2P\cdot\Sigma. \tag{2.12}$$

We can now use (A9) and the invariance of

$$(K^\perp)^2=W^2-2\Sigma\cdot W+\Sigma^2-P^{-2}(P\circ\Sigma)^2, \tag{2.13}$$

to determine the allowed spin components of a $P^2>0$ UIR of $\mathcal{S}$, in terms of the eigenvalues

$$W^2=-P^2j(j+1),$$

$$P\cdot\Sigma=\sigma P^2=(0,\pm\tfrac{1}{2})P^2, \tag{2.14}$$

$$\Sigma\cdot W=\tau P^2.$$

If $\sigma=\pm\frac{1}{2}$, then (A9) and (2.13) reduce to $\tau=0$, and $W^2=(K^\perp)^2=P^2(\lambda^2+1)$, so that the $\sigma=\pm\frac{1}{2}$ sectors contain just one allowed spin value, say j_0. If $\sigma=0$, then (A9) and (2.13) reduce to

$$[\tau+\tfrac{1}{2}(j+1)](\tau-\tfrac{1}{2}j)=0,$$

$$-j_0(j_0+1)=-j(j+1)-2\tau-\tfrac{3}{4}.$$

The $j\geq0$ solutions for $\tau=-\frac{1}{2}(j+1)$, $\frac{1}{2}j$, are $j=j_0\pm\frac{1}{2}$, respectively.

To summarize, UIR's of $\mathcal{S}$ for the timelike case may be labelled $(p^2>0,\ j_0)$, where $j_0=0,\frac{1}{2},1,\cdots$ is the superspin. They contain UIR's of $\mathcal{P}$ with $P^2>0$ and possible allowed spins $j=j_0$, j_0, and $j_0\pm\frac{1}{2}$.

Explicit realization of these UIR's, using the σ-basis, are constructed in the next section. In particular, we show that the $(p^2>0,\ j_0)$ UIR's of $\mathcal{S}$ contain $4(2j_0+1)$ helicity states, the spin content being precisely

$$4(2j_0+1)=2(2j_0+1)+[2(j_0+\tfrac{1}{2})+1]+[2(j_0-\tfrac{1}{2})+1],$$

in agreement with Refs. 2b and 10. We also verify (1.2) as a matrix equation, showing that the representations are indeed unitary.

B. Matrix elements in the $|p^2 > 0, j_0; \sigma; pj\lambda\rangle$ basis

In this section we verify covariantly in the σ-basis the methods used in Refs. 2b and 10 in constructing the $(p^2 > 0, j_0)$ UIR's. No induced representation theory is needed. The vacuum states used in the induced representation method in constructing UIR's of the little algebra, correspond instead to a UIR of $\mathcal{P}$ with spin j_0 and "lowest weight" $\sigma = -\frac{1}{2}$. Then (2.12) shows that the $S_\pm$ and $\bar{S}S_\pm$ are raising and lowering operators for σ, so that the lowest weight states $|\sigma = -\frac{1}{2}\rangle$ satisfy

$$S_{-\alpha}\,|\sigma = -\tfrac{1}{2}\rangle = 0. \tag{2.15}$$

We shall use σ-raising operators acting on such lowest-weight states to define covariantly normalized basis states $|p^2 > 0, j_0; \sigma; pj\lambda\rangle$,

$$\langle\sigma'; p'j'\lambda'\,|\,\sigma; pj\lambda\rangle = \delta_{\sigma'\sigma}\delta_{j'j}\delta_{\lambda'\lambda}\langle p'\,|\,p\rangle, \tag{2.16}$$

where

$$\langle p'\,|\,p\rangle = 2p_0(2\pi)^3\,\delta^3(\mathbf{p}' - \mathbf{p})$$

and where the $|pj\lambda\rangle$ states of the various σ-sectors belong to induced UIR's of $\mathcal{P}$, with $p^2 = m^2 > 0$, spin j, and helicity λ:

$$|pj\lambda\rangle = U(L_p)\,|\hat{p}j\lambda\rangle,$$
$$\mathbf{J}^2\,|\hat{p}j\lambda\rangle = j(j+1)\,|\hat{p}j\lambda\rangle,$$
$$J_3\,|\hat{p}j\lambda\rangle = \lambda\,|\hat{p}j\lambda\rangle.$$

Having constructed the σ-basis, we then give explicitly the corresponding $4(2j_0+1)^2$-matrix representatives of the supersymmetry generators. {Rühl and Yunn[10] have given $[4^2\times(2j_0+1)^2]$-matrix representatives, without, however, introducing the σ-basis.}

The operators $S_{\pm\alpha}$ have a complicated effect on helicity states, and are not the most convenient σ-shifting operators. Instead, we pass to an equivalent set $Q^\pm_\kappa(p)$, defined[10] by

$$Q^\pm_\kappa(p) = \bar{u}_\kappa(p)\,S_\pm, \quad S_\pm = \frac{1}{m}\sum_\kappa u_{\kappa\pm}(p)\,Q^\pm_\kappa, \tag{2.17}$$

where $u_\kappa(p)_\alpha$, $\kappa = \pm\frac{1}{2}$ are a set of normalized positive-frequency c-number spinor solutions of the Dirac equation, with mass m, and helicity κ. Their properties are given in (B1). The algebra of the $Q^\pm_\kappa$ may be derived from that of the S_α.[4] In particular, they satisfy

$$Q^\pm_\kappa Q^\pm_{\kappa'} = \pm\kappa m\delta_{\kappa,-\kappa'}\bar{S}S_\pm,$$
$$\{Q^+_\kappa, Q^-_{\kappa'}\} = 2\kappa m^2\delta_{\kappa,-\kappa'}, \tag{2.18}$$

and

$$(Q^\pm_\kappa)^\dagger = \pm 2\kappa Q^\mp_{-\kappa}, \tag{2.19}$$

in a unitary representation. Their transformation property under Lorentz transformations is

$$U(\Lambda)\,Q^\pm_\kappa(p)\,U(\Lambda^{-1}) = Q^\pm_{\kappa'}(\Lambda p)\,D^{1/2*}_{\kappa'\kappa}(\hat{\Lambda}), \tag{2.20}$$

where $\hat{\Lambda} = L^{-1}_{\Lambda p}\Lambda L_p$ is a little group rotation, the $D^{1/2}$ (Wigner) matrix represents finite rotations for spin-$\frac{1}{2}$, and the $U(\Lambda)$ are unitary (reducible) operators representing Lorentz transformations. Using the reality property of the D-matrices,[11] we conclude that the tensor operators, $R^\pm_\kappa = (-1)^\kappa Q^\pm_{-\kappa}$, applied to basis vectors $|\sigma pj\lambda\rangle$, lead to the following transformation property under $U(\Lambda)$:

$$U(\Lambda)R^\pm_\kappa(p)\,|\sigma pj\lambda\rangle = R^\pm_{\kappa'}(\Lambda p)\,|\Lambda pj\lambda'\rangle\,D^{1/2}_{\kappa'\kappa}(\hat{\Lambda})\,D^j_{\lambda'\lambda}(\hat{\Lambda}).$$

Application of the Wigner-Eckart Theorem then gives

$$R^+_\kappa|\,-\tfrac{1}{2}; p\,j_0\lambda\rangle = \sum_{j\lambda'} c_j\,|\,0; pj\lambda'\rangle\langle j\lambda'\,|\,\tfrac{1}{2}\kappa; j_0\lambda\rangle, \tag{2.21}$$

where $\langle j\lambda'\,|\,\frac{1}{2}\kappa; j_0\lambda\rangle^* = \langle\frac{1}{2}\kappa; j_0\lambda\,|\,j\lambda'\rangle$ are Clebsch-Gordan coefficients, and where the c_j are independent of $\lambda' = \lambda + \kappa$.

The algebra of $R^\pm_\kappa$, (B2), and that of the $\bar{S}S_\pm$, and $P\circ\Sigma$, may now be used to determine the c_j, and hence the normalized basis vectors which are given in (B3). The nonzero matrix elements of $R^\pm_\kappa$ are given by

$$\langle 0; p'j\ \lambda+\kappa\,|\,R^\pm_\kappa|\,\mp\tfrac{1}{2}; p\,j_0\lambda\rangle$$
$$= m\,\langle j\ \lambda+\kappa\,|\,\tfrac{1}{2}\kappa; j_0\lambda\rangle\langle p'\,|\,p\rangle,$$
$$\langle\pm\tfrac{1}{2}; p'j_0\ \lambda+\kappa\,|\,R^\pm_\kappa|\,0; pj\lambda\rangle \tag{2.22}$$
$$= \pm 2m(j_0 - j)\left(\frac{2j+1}{2j_0+1}\right)^{1/2}\,\langle j_0\ \lambda+\kappa\,|\,\tfrac{1}{2}\kappa; j\lambda\rangle\langle p'\,|\,p\rangle,$$

(2.22)

and (2.19) holds as a matrix identity.

The $(p^2 > 0, j_0)$ UIR's of $\mathcal{S}$ may be extended to UIR's of $\mathcal{S}$ augmented by parity, $\mathbb{P}$, in a straightforward manner. If we assume[4]

$$U_{\mathbb{P}}\,S_\alpha\,U^{-1}_{\mathbb{P}} = (i\gamma_0 S)_\alpha, \tag{2.23}$$

then it follows that $P\cdot\Sigma$ is a pseudoscalar, and we deduce[12]

$$U_{\mathbb{P}}\,|\sigma; pj\lambda\rangle = (-1)^{-j}\eta^*_{\mathbb{P}}\,|-\sigma; \mathbb{P}pj-\lambda\rangle. \tag{2.24}$$

Note that for superfields, with nonunitary IR's of $\mathcal{P}$, parity doubling is generally necessary, since a spin component (j_1, j_2) transforms to (j_2, j_1) under parity.

C. Weight diagrams

The structure of the $(p^2 > 0, j_0)$ UIR's of supersymmetry is conveniently describes by means of "weight diagrams." O'Raifeartaigh[13] has proposed similar diagrams, with an interpretation only in terms of superfields. We shall represent the general $(p^2 > 0, j_0)$ UIR's by a two-dimensional plot of spin j vs σ. Diagrams for superspins 0, j_0 are given in Fig. 1. Their structure is actually the same as that of the "small diagrams" used in Ref. 13 for the chiral scalar superfields.[4]

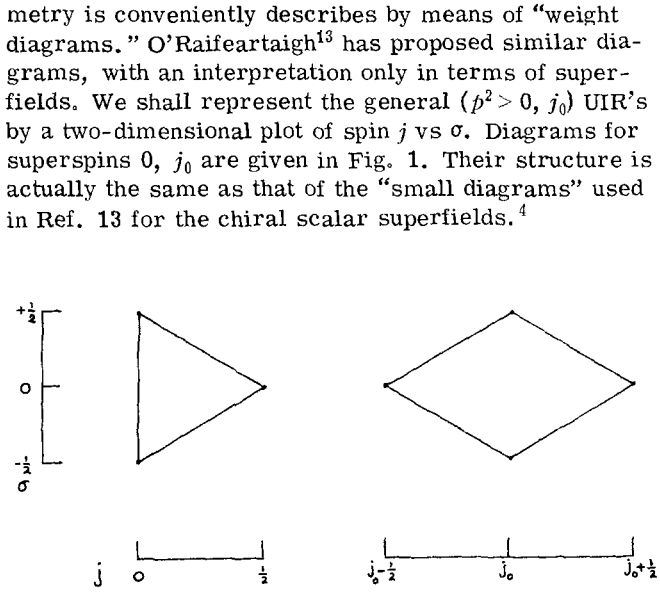

FIG. 1.

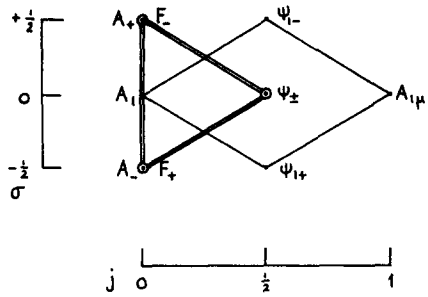

FIG. 2.

The diagrams are also useful in describing the spin and superspin constituents of superfields. Figure 2 gives the weight diagram for the general scalar superfield $\Phi_{\pm}(x,\theta)$. The irreducible constituents, the general chiral supermultiplets $\Phi_{\pm}(x,\theta)$, and the vector supermultiplet $\Phi_1(x,\theta)$ are readily distinguished.[4] Finally, Sokatchev[14] has shown that a massive, symmetrical, traceless, divergence-free superfield $\Phi_{\mu_1\cdots\mu_J}(x,\theta)$ or $\Phi_{\mu_1\cdots\mu_{J-1/2}\alpha}(x,\theta)$ of spin J has superspin content J^2, $J\pm\frac{1}{2}$. The corresponding weight diagram, Fig. 3, is that for the scalar superfield, Fig. 2, plus its mirror image.

A more intimate connection between weight diagrams and superfields is established if we expand the latter in the σ-basis, in the differential representation (1.3), using the definition (2.2). An arbitrary function of θ may be expanded in terms of a complete set of σ-eigenfunctions $e(\theta)$, $\bar{u}(\theta)$, and $\omega(\theta)$, of lowest power 0, 1, and 2 in θ, respectively (Table I). As $P\circ\Sigma\,\omega_0^{\mu}(\theta)\propto P^{\mu}$, the latter eigenfunction must occur in the form $\omega_0^{\mu}(\theta)X_{\mu}$, where $P^{\mu}X_{\mu}=0$. For example, for a general scalar superfield we have simply

$$\begin{aligned}\Phi(x,\theta)=&\,e_+(\theta)A_+(x)+\bar{u}_0(\theta)\psi_+(x)+\omega_-(\theta)F_+(x)\\&+e_-(\theta)A_-(x)+\bar{u}_0(\theta)\psi_-(x)+\omega_+(\theta)F_-(x)\\&+e_0(\theta)A_1(x)+\bar{u}(\theta)\psi_1(x)+\omega_0^{\mu}(\theta)A_{1\mu}(x),\end{aligned}\qquad(2.25)$$

from which we can label the nodes of the weight diagram, Fig. 2, with the appropriate fields.

The expansion (2.25) is clearly valid for a superfield of arbitrary spin. Evidently, the constraints $(D_{\mp})_{\alpha}\Phi_{\pm}=0$, where $(D_{\mp})_{\alpha}=(\gamma_{\mp})_{\alpha}{}^{\beta}D_{\beta}$ and D_{α} is the "covariant derivative,"[4] still project out irreducible chiral constituents, of superspin J. The nonlinear constraint $\bar{D}D\Phi_1=0$ now projects out a reducible, nonchiral superfield Φ_1, with constituent superspins $J+1$, $J-1$. Its reduction is effected by applying the appropriate Clebsch–Gordan coefficients to the component fields. For example, for spin 1, the field $\psi_{1\alpha\mu}$ may be written

$$\psi_{1\alpha\mu}=[\psi_{1\alpha\mu}-\tfrac{1}{4}(\gamma_{\mu})_{\alpha}{}^{\beta}(\gamma\circ\psi_1)_{\beta}]+\tfrac{1}{4}(\gamma_{\mu})_{\alpha}{}^{\beta}(\gamma\circ\psi_1)_{\beta},$$

indicating a reduction into a spin-$\frac{3}{2}$ component (belonging to the superspin-2 constituent), and a spin-$\frac{1}{2}$ component (belonging to superspin-0). Sokatchev[14] shows that the highest superspin $-(J+1)$ constituent is projected out by means of the additional differential conditions $\bar{D}^{\alpha}\Phi_{1\alpha}=0$, for spin $\frac{1}{2}$, and $(\gamma^{\mu}D)_{\alpha}\Phi_{1\beta\mu}=0$, for spin $>\frac{1}{2}$, applied to the nonchiral part Φ_1.

TABLE I.

	$\sigma=0$	$\sigma=\pm\frac{1}{2}$
0	$e_0(\theta)=1+\frac{1}{32}\bar{\theta}\theta^2\partial^2$	$e_{\pm}(\theta)=1\mp\frac{1}{4}\bar{\theta}\not{p}\gamma_5\theta-\frac{1}{32}\bar{\theta}\theta^2\partial^2$
1	$\bar{u}_0(\theta)=\bar{\theta}-\frac{1}{4}\bar{\theta}\theta\,\bar{\theta}i\not{p}$	$\bar{u}_{\pm}(\theta)=\bar{u}(\theta)\gamma_{\mp}=(\bar{\theta}+\frac{1}{4}\bar{\theta}\theta\,\bar{\theta}i\not{p})\gamma_{\mp}$
2	$\omega_0^{\mu}(\theta)=\frac{1}{4}\bar{\theta}i\gamma^{\mu}\gamma_5\theta$	$\omega_{\pm}(\theta)=\frac{1}{4}\bar{\theta}\theta_{\mp}$

3. THE LIGHTLIKE CASE $P^2=0$

A. Analysis of spin content

In this section we repeat, for the lightlike case, the analysis carried out in Sec. 2 of timelike UIR's of $\mathcal{S}$. Physical massless particles correspond to UIR's of $\mathcal{P}$ for which $P^2=W^2=0$. In this case the helicity Λ becomes a Casimir of $\mathcal{P}$, and the generators satisfy the constraint

$$W_{\mu}=\Lambda P_{\mu},\qquad(3.1)$$

where

$$\Lambda=P_0^{-1}\epsilon_{0\rho\sigma\tau}P^{\rho}J^{\sigma\tau}.\qquad(3.2)$$

Here we restrict ourselves to the analysis of those lightlike UIR's of $\mathcal{S}$ for which (3.1) holds in each spin sector. In fact, this constraint necessitates a contraction of the supersymmetry generators S_{α} as well. For we have

$$\begin{aligned}[S_{\alpha},W_{\mu}]&=\tfrac{1}{4}\epsilon_{\mu\rho\sigma\tau}P^{\rho}(\sigma^{\sigma\tau}S)_{\alpha}\\&=[S_{\alpha},\Lambda P_{\mu}]=\tfrac{1}{4}P_0^{-1}P_{\mu}\epsilon_{0\rho\sigma\tau}P^{\rho}(\sigma^{\sigma\tau}S)_{\alpha},\end{aligned}$$

and using (A4), we find that (3.1) implies

$$(\not{P})_{\alpha}{}^{\beta}S_{\beta}=0.\qquad(3.3)$$

Also, since in general

$$[S_{\alpha},W^2]=(i\gamma_5\not{W}\not{P})_{\alpha}{}^{\beta}S_{\beta}-\tfrac{3}{4}P^2S_{\alpha},$$

then (3.3) is consistent with the requirement $[S_{\alpha},W^2]=0$.

It follows from (3.3) that S_{α} may be represented as $S=i\not{P}S'$, for some Majorana spinor S'. Then we have explicitly, for the Poincaré invariants (2.10), that $\bar{S}S_{\pm}=0$, and $P\circ\Sigma=0$. Furthermore, we have

$$\Sigma_{\mu}=NP_{\mu},\qquad(3.4)$$

where $N=\frac{1}{2}\bar{S}'i\gamma_5\not{P}S'$ must be a Poincaré invariant. From (A6d) it follows that $N^2=\frac{1}{4}$, whence N has eigenvalues $\nu=\pm\frac{1}{2}$. Moreover, from (3.2) and (3.4), the operator

$$K=\Lambda-\tfrac{1}{2}(N-\tfrac{1}{2})\qquad(3.5)$$

is a Casimir of $\mathcal{S}$.

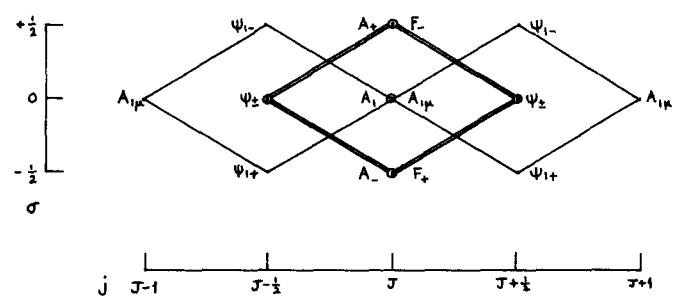

FIG. 3.

In summary, this class of lightlike UIR's of $\mathcal{S}$ may be labelled $(p^2=0,\ \lambda_0)$, where $\lambda_0=0,\ \pm\frac{1}{2},\ \pm1,\cdots$ is the superhelicity. They contain two spin sectors, carrying lightlike UIR's of $\mathcal{P}$ with invariant helicities λ_0, $\lambda_0-\frac{1}{2}$ corresponding to the eigenvalues $\nu=+\frac{1}{2},\ -\frac{1}{2}$, respectively. By constructing explicit realizations of these UIR's in the next section, we verify in fact that the $(p^2=0,\ \lambda_0)$ UIR of $\mathcal{S}$ contains precisely one lightlike UIR of $\mathcal{P}$ of each allowed helicity. We also explicitly verify the condition (1.2) as a matrix equation.

B. Matrix elements in the $|p^2=0,\lambda_0;p\lambda\rangle$ basis

In this section we follow the methods of Sec. 2B and construct the $(p^2=0,\lambda_0)$ UIR's of $\mathcal{S}$. Once again, no induced representation theory is needed, and we utilize as cyclic states a lightlike UIR of $\mathcal{P}$ with "lowest weight" $\nu=-\frac{1}{2}$, and therefore with invariant helicity $\lambda=\lambda_0-\frac{1}{2}$. From (3.3) and (A7), raising and lowering operators for N are again just the $(S_\pm)_\alpha$:

$$[N,(S_\pm)_\alpha]=\pm(S_\pm)_\alpha. \tag{3.6}$$

We shall act with the $(S_+)_\alpha$ on the lowest-weight states to define covariantly normalized basis vectors of the form $|p^2=0,\lambda_0;p\lambda\rangle$:

$$\langle p\lambda|p'\lambda'\rangle=\delta_{\lambda\lambda'}\langle p|p'\rangle, \tag{3.7}$$

where the $|p\lambda\rangle$ states in each ν sector belong to (induced) lightlike UIR's of $\mathcal{P}$, with $P^2=0=W^2$, and $P_\mu=\lambda W_\mu$.

We cannot here define shift operators analogous to the the $Q_\kappa^\pm$ introduced in the massive case, since the condition $\not{p}S_\pm=0$ ensures the vanishing of combinations like $\bar{u}S_\pm$ in the massless case. However, the effect of $(S_\pm)_\alpha$ is to change the helicity by $\pm\frac{1}{2}$, and to leave p_μ unchanged, so that we may immediately write down

$$\begin{aligned}(S_+)_\alpha|p\ \lambda_0-\tfrac{1}{2}\rangle&=u_{+\alpha}(p)|p\ \lambda_0\rangle,\\ (S_-)_\alpha|p\ \lambda_0\rangle&=u_{-\alpha}(p)|p\ \lambda_0-\tfrac{1}{2}\rangle,\end{aligned} \tag{3.8}$$

where the spinor normalization constants $u_{\pm\alpha}(p)$ must also satisfy

$$\not{p}u_\pm(p)=0,\quad \gamma_\mp u_\pm(p)=0, \tag{3.9}$$

and so may be written $u_\pm(p)=\gamma_\pm u(p)$ as the chiral projections of a spinor wavefunction solution of the Dirac equation in the massless case.

The algebra of the $(S_\pm)_\alpha$ in the massless case may be deduced from Ref. 4 and (3.4). One finds

$$\begin{aligned}&(S_\pm)_\alpha(S_\pm)_\beta=0,\\ &(S_\pm)_\alpha(S_\mp)_\beta=\mp(\not{p}\gamma_\mp c)_{\alpha\beta}(N\pm\tfrac{1}{2}),\end{aligned} \tag{3.10}$$

and applying (3.8) and (3.8) and (3.10) to states $|p\ \lambda_0-\frac{1}{2}\rangle$ gives

$$(S_-)_\alpha(S_+)_\beta|p\ \lambda_0-\tfrac{1}{2}\rangle=u_{-\alpha}(p)u_{+\beta}(p)|p\ \lambda_0-\tfrac{1}{2}\rangle,$$

$$(S_-)_\alpha(S_+)_\beta|p\ \lambda_0-\tfrac{1}{2}\rangle=-(\not{p}\gamma_+c)_{\alpha\beta}|p\ \lambda_0-\tfrac{1}{2}\rangle.$$

By using the completeness of the algebra of γ matrices, we deduce that

$$\bar{u}^c\gamma_\mu\gamma_+u=2p_\mu. \tag{3.11}$$

Finally, the representation will be unitary, satisfying

$$\overline{(S_+)}^\alpha=(c^{-1})^{\alpha\beta}(S_-)_\beta, \tag{3.12}$$

if

$$u(p)=u^c(p)=c\bar{u}(p), \tag{3.13}$$

that is, if $u(p)$ is a Majorana spinor. Conditions (3.9), (3.11), and (3.13) are sufficient to determine $u(p)$, and hence $|p\ \lambda_0\rangle$, up to a phase. The nonzero matrix elements in this basis are therefore

$$\begin{aligned}\langle p\ \lambda_0|(S_+)_\alpha|p'\ \lambda_0-\tfrac{1}{2}\rangle&=u_{+\alpha}(p)\langle p|p'\rangle,\\ \langle p\ \lambda_0-\tfrac{1}{2}|(S_-)_\alpha|p'\ \lambda_0'\rangle&=u_{-\alpha}(p)\langle p|p'\rangle.\end{aligned} \tag{3.14}$$

The $\langle p^2=0,\ \lambda_0\rangle$ UIR's of $\mathcal{S}$ may be extended in a straightforward manner to UIR's of $\mathcal{S}$ augmented by parity $\mathbb{P}$. Λ is a pseudoscalar in the massless case, and, with S_α transforming according to (2.23), so also is N, so that from (3.5)

$$U_{\mathbb{P}}KU_{\mathbb{P}^{-1}}=-K+\tfrac{1}{2}, \tag{3.15}$$

and therefore we deduce[12]:

$$U_{\mathbb{P}}|p^2=0,\ \lambda_0;p\lambda\rangle=(-1)^{-|\lambda|}\eta^*_{\mathbb{P}}|p^2=0,\ -\lambda_0+\tfrac{1}{2};\mathbb{P}p,-\lambda\rangle, \tag{3.16}$$

and hence the lightlike UIR's of $\mathcal{S}$ augmented by $\mathbb{P}$ have the form of a direct sum $(p^2=0,\ \lambda_0)\oplus(p^2=0,-\lambda_0+\frac{1}{2})$, with helicity content $\pm\lambda_0,\ \pm(\lambda_0-\frac{1}{2})$, viz. four helicity states. This result was stated in Ref. 4.

C. Massless superfields

We now use the results of the previous sections above to analyze massless superfields $\Phi_a(x,\theta)$. For conventional massless fields $\Phi_a(x)$, the triviality condition (3.1), ensuring only physical massless particles with an invariant helicity, is imposed either by carefully choosing the finite-dimensional IR(j_1,j_2) of the Lorentz group under which $\Phi_a(x)$ transforms, or if the M functions give amplitudes which remain invariant under certain "gauge transformations" of the external wavefunction. For spin 1, an example of the first kind is $F_{\mu\nu}(x)$, the electromagnetic tensor, and of the second kind is a vector field $A_\mu(x)$, with invariance under the gauge transformation,

$$A_\mu(x)\to A_\mu(x)+\partial_\mu\Lambda(x),$$

where $\Lambda(x)$ may be restricted in particular gauges, but is in general arbitrary.

For UIR's of supersymmetry in the lightlike case, we established (3.3) as a necessary consequence of imposing the triviality condition (3.1) on each spin component separately. We therefore infer that the corresponding free, massless, irreducible superfield $\Phi_a(x,\theta)$ satisfies

$$(\not{P}S)\,\Phi_a(x,\theta)=0. \tag{3.17}$$

This condition is clearly Lorentz-covariant. By applying an infinitesimal supertranslation $U(\epsilon)$, we have

$$\begin{aligned}\not{P}S'\Phi'(x',\theta')&=U(\epsilon)^{-1}\not{P}S\Phi(x,\theta)U(\epsilon)\\ &=(\not{P}S+2i\not{P}^2\epsilon)\,\Phi(x,\theta)+o(\epsilon^2),\end{aligned}$$

so it is indeed supercovariant, provided that $P^2=0$. Moreover, (3.17) commutes with the covariant derivative constraints on superfields, introduced to project out further the irreducible parts.[4,15]

Consider, for example, a free, massless, scalar superfield $\Phi(x,\theta)$. To discover which gauge-independent, free, massless, irreducible superfields it contains, it is consistent to impose the necessary condition (3.17). Using (1.3), we find that (3.17) holds if and only if

$$\Phi(x,\theta)=A(x)+\bar{\theta}\psi(x)+\tfrac{1}{4}\bar{\theta}i\not{\partial}X\gamma_s\theta,$$
$$\partial^2 A=0=\partial^2 X,\quad i\not{\partial}\psi=0. \tag{3.18}$$

Applying the further constraints $D_\pm\Phi_\mp(x,\theta)=0$, we find that $\Phi=\Phi_+ +\Phi_-$, and the irreducible parts are

$$\Phi_\pm(x,\theta)=A_\pm+\bar{\theta}\psi_\pm\pm\tfrac{1}{4}\bar{\theta}i\gamma_\nu\gamma_s\theta(i\partial^\nu A_\pm). \tag{3.19}$$

We may also write down basis functions $\Omega_\nu(\theta)$, as was done in Sec. 2C, for massive superfields in the σ-basis. Using the relation $\Sigma^\mu=NP^\mu$, (1.3) and (2.2), we have

$$N(1\pm\tfrac{1}{4}\bar{\theta}i\not{P}\gamma_s\theta)=\pm\tfrac{1}{2}(1\pm\tfrac{1}{4}\bar{\theta}i\not{P}\gamma_s\theta),$$
$$N\bar{\theta}_\pm=\mp\tfrac{1}{2}\theta_\pm. \tag{3.20}$$

We conclude that a reducible, free, massless, scalar superfield contains gauge-independent, irreducible, chiral parts $\Phi_+(p^2=0,\ \lambda_0=0)$ and $\Phi_-(p^2=0,\ \lambda_0=+\tfrac{1}{2})$. This type of reduction may obviously be generalized to higher-spin massless superfields.

If (3.1) fails on some component of a massless superfield, for example, if it contains a vector field $A_\mu(x)$, then necessarily $\not{P}S\Phi\neq 0$, and the superfield cannot be reduced by the above method of imposing (3.17). Nevertheless, the triviality condition (3.3) must still be implemented, in this case through gauge invariance of the M functions under gauge transformations of the superfield. A more detailed exposition of these applications of our work will be published elsewhere. Here we consider as an example again just the general massless scalar superfield, where now (3.17) is not imposed. The ensuing gauge dependence means that the chiral parts $\Phi_\pm$ can be gauged away, and that the non-chiral part Φ_1 effectively contains just two components, the vector $A_{1\mu}$, and the spinor ψ_1. This claim is manifest in the noncovariant "remarkable gauge" cited in Ref. 4 and elsewhere.

4. CONCLUDING REMARKS

The techniques of this article have yielded convenient bases, with diagonal component spins, and explicit matrix elements, for massive and massless UIR's of supersymmetry, with many possible applications, such as to the calculation of Clebsch–Gordan coefficients for supersymmetry, and to the supersymmetric bound state problem. The analysis has been restricted to those UIR's which describe physical elementary particles. However, for applications such as partial wave analysis, other UIR's, containing infinitely many spin components, are relevent. The techniques used here may also be applied in these cases. They may also be extended to handle the general question of algebraic generalizations of supersymmetry. Work is currently in progress in these directions.

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APPENDIX A: NOTATION AND ALGEBRAIC IDENTITIES

Notation and γ matrices

We use a Lorentz metric $\eta_{\mu\nu}=\mathrm{diag}(+---)$, $\mu,\nu=0,1,2,3$ and define $\epsilon_{0123}=+1$. The adjoint and conjugate matrices are denoted $A^\dagger$ and C, respectively. Adjoint and conjugate spinors are defined by

$$\bar{S}^\alpha=(A^{-1})^{\alpha\beta}S^\dagger_\beta,\quad \bar{S}^{c\alpha}=(C^{-1})^{\alpha\beta}S_\beta, \tag{A1}$$

respectively. The chiral projections $(S_\pm)_\alpha$ are defined by

$$S_{\pm\alpha}=(\gamma_\pm)_\alpha{}^\beta S_\beta=\tfrac{1}{2}(1\pm i\gamma_5)_\alpha{}^\beta S_\beta, \tag{A2}$$

where the γ-matrix algebra is generated by

$$\{\gamma_\mu,\gamma_\nu\}=2\eta_{\mu\nu},$$
$$\sigma_{\mu\nu}=\tfrac{1}{2}i[\gamma_\mu,\gamma_\nu]=i(\gamma_\mu\gamma_\nu-\eta_{\mu\nu}), \tag{A3}$$
$$\gamma_5=\gamma_0\gamma_1\gamma_2\gamma_3.$$

We note the following useful identities:

$$\epsilon_{\mu\nu\rho\sigma}\sigma^{\rho\sigma}=2\sigma_{\mu\nu}\gamma_5,$$
$$\epsilon_{\mu\nu\rho\sigma}\gamma^\sigma=i\gamma_5\gamma_\mu\sigma_{\nu\rho}. \tag{A4}$$

Supersymmetry algebra

The commutation relations (1.1) are in addition to the usual Lie algebra of the Poincaré group:

$$[P_\mu,P_\nu]=0,$$
$$[P_\mu,J_{\rho\sigma}]=i(\eta_{\mu\rho}P_\sigma-\eta_{\mu\sigma}P_\rho), \tag{A5}$$
$$[J_{\mu\nu},J_{\rho\sigma}]=i(\eta_{\mu\sigma}J_{\nu\rho}+\eta_{\nu\rho}J_{\mu\sigma}-\eta_{\nu\sigma}J_{\mu\rho}-\eta_{\mu\rho}J_{\nu\sigma}).$$

The W_μ and Σ_μ, defined by (2.1) and (2.2), satisfy the following commutation relations, which can be proved using the identities given in Ref. 4:

$$[W_\mu,W_\nu]=i\epsilon_{\mu\nu\rho\sigma}P^\rho W^\sigma,$$
$$[\Sigma_\mu,\Sigma_\nu]=i\epsilon_{\mu\nu\rho\sigma}P^\rho\Sigma^\sigma,$$
$$[\Sigma_\mu,W_\nu]=i\epsilon_{\mu\nu\rho\sigma}P^\rho\Sigma^\sigma, \tag{A6}$$
$$\{\Sigma_\mu,\Sigma_\nu\}=\tfrac{1}{2}\eta_{\mu\nu}(\Sigma^2-\tfrac{1}{4}P^2)+\tfrac{1}{2}P_\mu P_\nu;$$
$$[S_\alpha,W_\mu]=\tfrac{1}{2}(\sigma_{\mu\nu}P^\nu)\gamma_5 S_\alpha,$$
$$[S_\alpha,\Sigma_\mu]=-\tfrac{1}{2}i(\not{P}\gamma_\mu\gamma_5 S)_\alpha. \tag{A7}$$

Polynomial identities

The following identities satisfied by the P invariants in any UIR, can be proved using the identities of Ref. 4:

$$(\bar{S}S_\pm)^3=4P^2\bar{S}S_\pm,$$
$$(P\cdot\Sigma)^3=\tfrac{1}{4}P^2P\cdot\Sigma, \tag{A8}$$
$$\Sigma\cdot\Sigma=4P^{-2}(P\cdot\Sigma)^2-\tfrac{3}{4}P^2;$$
$$(P\cdot\Sigma)(\Sigma\cdot W)=0=(\Sigma\cdot W)(P\cdot\Sigma),$$
$$(\Sigma\cdot W)^2=\tfrac{1}{4}W^2(\Sigma^2-\tfrac{1}{4}P^2)-\tfrac{1}{2}P^2(\Sigma\cdot W). \tag{A9}$$

APPENDIX B: THE TENSOR SHIFT OPERATORS $R^{\pm}_{\kappa}(p)$

Normalized Dirac wavefunctions

$$
\begin{aligned}
&(\not{p}-m)\,u_{\kappa}(p)=0=\bar{u}_{\kappa}(p)(\not{p}-m),\\
&\tfrac{1}{2}(\underline{\sigma}\cdot\underline{p})\,u_{\kappa}(p)=\kappa\,|\underline{p}|\,u_{\kappa}(p),\\
&\bar{u}_{\kappa}u_{\kappa'}(p)=2m\delta_{\kappa,\kappa'},\\
&\sum_{\kappa}u_{\kappa}(p)\,\bar{u}_{\kappa}(p)=(\not{p}+m),\\
&u^{c}_{\kappa}=(-1)^{-\kappa}\gamma_{5}u_{-\kappa}=C\bar{u}_{\kappa}.
\end{aligned}
\tag{B1}
$$

Algebra of $R^{\pm}_{\kappa}(p)$

$$
\begin{aligned}
&R^{\pm}_{\kappa}(p)\,R^{\pm}_{\kappa'}(p)=\mp\kappa m\delta_{\kappa,-\kappa'}\overline{S}S_{\pm},\\
&\{R^{\pm}_{\kappa}(p),R^{\pm}_{\kappa'}(p)\}=0,\\
&\{R^{\pm}_{\kappa}(p)\,R^{\pm}_{\kappa'}(p)\}=\pm 2\kappa m^{2}\delta_{\kappa,-\kappa'}.
\end{aligned}
\tag{B2}
$$

Normalized basis vectors

$$
\begin{aligned}
&|+\tfrac{1}{2};p\,j_{0}\lambda\rangle=\frac{1}{2m}\,\overline{S}S_{+}\,|-\tfrac{1}{2};p\,j_{0}\,\lambda\rangle\\
&|0;pj\lambda\rangle=\sum_{\kappa}\frac{1}{m}\,R^{+}_{\kappa}\,|-\tfrac{1}{2};pj_{0}\lambda-\kappa\rangle\langle\tfrac{1}{2}\kappa;j_{0}\,\lambda-\kappa\,|j\lambda\rangle
\end{aligned}
\tag{B3}
$$

Matrix elements of $R^{\pm}_{\kappa}(p)$

$$
\begin{aligned}
&\langle 0;p'j\;\lambda+\kappa\,|R^{\pm}_{\kappa}|\mp\tfrac{1}{2};pj_{0}\lambda\rangle=m\langle j\;\lambda+\kappa\,|\tfrac{1}{2}\kappa;j_{0}\lambda\rangle\langle p'\,|p\rangle\\
&\langle\pm\tfrac{1}{2};p'j_{0}\;\lambda+\kappa\,|R^{\pm}_{\kappa}|\,0;pj\lambda\rangle\\
&\quad=\pm 2m(j_{0}-j)\left(\frac{2j+1}{2j_{0}+1}\right)^{1/2}\langle j_{0}\;\lambda+\kappa\,|\tfrac{1}{2}\kappa;j\lambda\rangle\langle p'\,|p\rangle.
\end{aligned}
\tag{B4}
$$

[1] J. Wess and B. Zumino, Nucl. Phys. B **70**, 39 (1974).
[2] Abdus Salam and J. Strathdee, Nucl. Phys. B **76**, 477 (1974); Abdus Salam and J. Strathdee, Nucl. Phys. B **80**, 499 (1974).
[3] F. A. Berezin and G. I. Kac, Mat. Sbornik **82**, 124 (1970) [Math. USSR Sbornik **11**, 311 (1970)].
[4] Abdus Salam and J. Strathdee, Phys. Rev. D **11**, 1509 (1975).
[5] J. Wess and B. Zumino, Phys. Lett. B **49**, 52 (1974); A. A. Slavnov, Theor. Math.-Phys. USSR **23**, 3 (1975); A. A. Slavnov, Nucl. Phys. B **97**, 155 (1975); S. Ferrara, and O. Piguet, CERN Preprint TH1995 (1975).
[6] D. Grosser, Lett. Nuovo Cimento **12** 649 (1975).
[7] R. Delbourgo and P. Jarvis, J. Phys. G **1**, 791 (1975).
[8] M. A. Naimark, *Linear Representations of the Lorentz Group* (Pergamon, Oxford, 1964).
[9] D. Grosser, Lett. Nuovo Cimento **12**, 455 (1975).
[10] W. Rühl, and B. C. Yunn, Kaiserslautern Preprint (1974).
[11] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U. P., Princeton, N. J., 1960).
[12] M. Jacob and G. C. Wick, Ann. Phys. (N.Y.) **7**, 404 (1959).
[13] L. O'Raifeartaigh, Nucl. Phys. B **89** 48 (1975).
[14] E. Sokatchev, Dubna Preprint E2-8681 (1975).

Classic theory of direct intermembrane interaction

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The theory of action-at-a-distance interaction between objects of two dimensions is studied. The theory developed has some similarities to the corresponding theory of one-dimensional objects (strings). The fundamental invariants of the theory are found. A particular interaction is studied, and it is found that the interaction between closed membranes takes place via a pseudoscalar field.

I. INTRODUCTION

In a recent paper[1] the idea of Feynman and Wheeler electrodynamics[2] (FWE) was used to build an action-at-a-distance theory of interaction between strings.[3] The strings are described by their world sheets, i.e., two-dimensional manifolds. The purpose of this paper is to extend the theory to the case of direct interaction between two-dimensional strings which we more properly called membranes. Now the membranes are described by their world tubes, i.e., three-dimensional manifolds.

Some of the interesting facts of the theory of direct interaction between strings are (a) for a simple case of interaction the interaction takes place via a massless scalar field, (b) the behavior of open and closed strings is different. These facts can be used[4] to give nice interpretations of both the Virasoro–Shapiro model[5] and the Pomeron sector of the Veneziano model.[6] We find that some of the above mentioned facts also have analogs in the theory of direct interaction between membranes, e.g., for a simple case of interaction we find that the interaction takes place via a massless pseudoscalar field. The behavior of open, semiopen, and closed membranes is in each case different.

In Secs. 2 and 3 we discuss the general theory. We find the set of invariants on which the action must depend to be Poincaré invariant. We also find a formal analogy between the equations of motion of particles, strings and membranes. In Sec. 4 we study an explicit type of interaction that is the obvious generalization of the interaction of FWE. We discuss the field theory that can be extracted from the given interaction. We find that the interaction takes place via a massless pseudoscalar field. Also we find that the field equations in a pseudovectorial representation are a sort of dual system of equations to Maxwell's equations in the Lorentz gauge. In an appendix we study some of the properties of the free membrane equation of motion.

2. FREE MEMBRANES

The three-dimensional world tube of a membrane is described by $x^\nu(\zeta, \xi, \eta)$ where ζ, ξ and η are invariant parameters.

The volume element of the world tube is

$$d\sigma^{\mu\nu\rho} = d\zeta\, d\xi\, d\eta\, \sigma^{\mu\nu\rho}, \tag{2.1}$$

where

$$\sigma^{\mu\nu\rho} = 3!\, \dot{x}^{[\mu} x'^{\nu} \hat{x}^{\rho]} \tag{2.2}$$

and

$$\dot{x}^\mu \equiv \frac{\partial}{\partial\zeta} x^\mu, \quad x'^\mu \equiv \frac{\partial}{\partial\xi} x^\mu \quad \text{and} \quad \hat{x}^\mu \equiv \frac{\partial}{\partial\eta} x^\mu. \tag{2.3}$$

The symbol $[\cdots]$ means antisymmetrization in the indicated indices. Note that $\sigma^{\mu\nu\rho}$ is invariant under a cyclic permutation of its indices,

$$\sigma^{\mu\nu\rho} = \sigma^{\nu\rho\mu} = \sigma^{\rho\mu\nu}. \tag{2.4}$$

The space in which the membrane world tube is embedded is the Minkowski space with metric $g_{\mu\nu}$ and signature -2. Also significant is the intrinsic metric of the membrane, γ_{AB}. Note this 3-space will in general have a nonzero curvature.

The Greek indices run from 0 through 3, the small Latin indices from 1 through n, n being the number of membranes, and the capital Latin indices from 0 through 2.

The action for a free membrane is given by

$$S^{(f)} = \mu^2 \int_{\zeta=\zeta_i}^{\zeta=\zeta_f} \int_{\xi=0}^{\xi=l} \int_{\eta=0}^{\eta=d} (d\sigma^{\alpha\beta\gamma}\, d\sigma_{\alpha\beta\gamma})^{1/2}. \tag{2.5}$$

We will consider only spacelike membranes, so the quantity between parentheses is positive. The integration domain is such that the spatial extension of the membrane is finite, evidently this action is manifestly parametrization independent.

The equation of motion is obtained by imposing the condition that the action (2.5) be stationary under the variation

$$x^\mu(\zeta, \xi, \eta) \to x^\mu(\zeta, \xi, \eta) + \delta x^\mu(\zeta, \xi, \eta), \tag{2.6}$$

$$\delta x^\mu(\zeta_i, \xi, \eta) = \delta x^\mu(\zeta_f, \xi, \eta) = 0. \tag{2.7}$$

From the above requirement we get

$$\delta S^{(f)} = \mu^2 \int d^3\zeta\, \frac{\sigma^{\alpha\beta\gamma}}{(\sigma\cdot\sigma)^{1/2}}\, \delta\sigma_{\alpha\beta\gamma} = 0, \tag{2.8}$$

where $d^3\zeta$ means $d\zeta\, d\xi\, d\eta$. The variation $\delta\sigma^{\mu\nu\rho}$ can be nicely expressed in terms of a linear differential operator as follows. Defining $D^{\mu\nu}$ as

$$D^{\mu\nu} = 2\left(\dot{x}^{[\mu} x'^{\nu]} \frac{\partial}{\partial\eta} - \dot{x}^{[\mu} \hat{x}^{\nu]} \frac{\partial}{\partial\xi} + x'^{[\mu} x^{\nu]} \frac{\partial}{\partial\zeta}\right). \tag{2.9}$$

the variation $\delta\sigma^{\mu\nu\rho}$ is

$$\delta\sigma^{\mu\nu\rho} = D^{\mu\nu}\delta x^\rho + D^{\rho\mu}\, \delta x^\nu + D^{\nu\rho}\delta x^\mu. \tag{2.10}$$

The operator $D^{\mu\nu}$ has the following properties:

$$D^{\mu\nu}(\alpha f+\beta g)=\alpha D^{\mu\nu}f+\beta D^{\mu\nu}g, \tag{2.11a}$$

$$D^{\mu\nu}(fg)=fD^{\mu\nu}g+gD^{\mu\nu}f, \tag{2.11b}$$

$$D^{\mu\nu}f(x)=\sigma^{\mu\nu\rho}\frac{\partial}{\partial x^{\rho}}f(x), \tag{2.11c}$$

$$D^{\mu\nu}g=-D^{\nu\mu}g. \tag{2.11d}$$

From (2.8), (2.10), (2.11), and (2.4) we find

$$\delta S^{(f)}=-3\mu^2\int d^3\xi\left[D^{\mu\nu}\frac{\sigma_{\mu\nu\rho}}{(\sigma\cdot\sigma)^{1/2}}\right]\delta x^{\rho}+6\mu^2\int d\xi\,d\xi\left[\frac{\sigma^{\mu\nu\rho}}{(\sigma\cdot\sigma)^{1/2}}\dot{x}_{\mu}\acute{x}_{\nu}\,\delta\hat{x}_{\rho}\right]_{\eta=0}^{\eta=d}+6\mu^2\int d\xi\,d\eta\left[\frac{\sigma^{\mu\nu\rho}}{(\sigma\cdot\sigma)^{1/2}}\dot{x}_{\mu}\hat{x}_{\nu}\,\delta\acute{x}_{\rho}\right]_{\xi=0}^{\xi=l}=0. \tag{2.12}$$

The surface term that does not appear in (2.12) vanishes by (2.7); the others do not vanish automatically if δx^{μ} is an arbitrary variation that satisfies (2.7). Moreover, $\delta x^{\mu}(\xi,\xi=0,\eta)$, $\delta x^{\mu}(\xi,\xi=l,\eta)$, etc., can still be arbitrary variations depending on the nonfixed parameters. We have several posibilities to kill the remaining surface terms, which we will analyze in detail. If the surface terms are zero, (2.12) implies

$$3\mu^2D^{\alpha\beta}\frac{\sigma_{\alpha\beta\gamma}}{(\sigma\cdot\sigma)^{1/2}}=0. \tag{2.13}$$

The surface terms vanish if one of the following sets of conditions holds:

$$\frac{\sigma^{\mu\nu\rho}}{(\sigma\cdot\sigma)^{1/2}}\dot{x}_{\mu}\hat{x}_{\nu}=0,\quad(\xi=0,l), \tag{2.14a}$$

$$\frac{\sigma^{\mu\nu\rho}}{(\sigma\cdot\sigma)^{1/2}}\dot{x}_{\mu}\acute{x}_{\nu}=0,\quad(\eta=0,d), \tag{2.14b}$$

$$\delta x^{\mu}(\xi,\xi=0,\eta)\neq\delta x^{\mu}(\xi,\xi=l,\eta), \tag{2.14c}$$

$$\delta x^{\mu}(\xi,\xi,\eta=0)\neq\delta x^{\mu}(\xi,\xi,\eta=d), \tag{2.14d}$$

$$\frac{\sigma^{\mu\nu\rho}}{(\sigma\cdot\sigma)^{1/2}}x_{\mu}x_{\nu}=0,\quad(\xi=0,l) \tag{2.15a}$$

$$x^{\mu}(\xi,\xi,\eta=0)=x^{\mu}(\xi,\xi,\eta=d), \tag{2.15b}$$

$$\hat{x}^{\mu}(\xi,\xi,\eta=0)=\hat{x}^{\mu}(\xi,\xi,\eta=d), \tag{2.15c}$$

$$\delta x^{\mu}(\xi,\xi,\eta=0)=\delta x^{\mu}(\xi,\xi,\eta=d), \tag{2.15d}$$

$$\delta x^{\mu}(\xi,\xi=0,\eta)\neq\delta x^{\mu}(\xi,\xi=l,\eta), \tag{2.15e}$$

$$\frac{\sigma^{\mu\nu\rho}}{(\sigma\cdot\sigma)^{1/2}}\dot{x}_{\mu}\acute{x}_{\nu}=0,\quad(\eta=0,d), \tag{2.16a}$$

$$x^{\mu}(\xi,\xi=0,\eta)=x^{\mu}(\xi,\xi=l,\eta), \tag{2.16b}$$

$$\acute{x}^{\mu}(\xi,\xi=0,\eta)=\acute{x}^{\mu}(\xi,\xi=l,\eta), \tag{2.16c}$$

$$\delta x^{\mu}(\xi,\xi=0,\eta)=\delta x^{\mu}(\xi,\xi=l,\eta), \tag{2.16d}$$

$$\delta x^{\mu}(\xi,\xi,\eta=0)\neq\delta x^{\mu}(\xi,\xi,\eta=d), \tag{2.16e}$$

$$x^{\mu}(\xi,\xi=0,\eta)=x^{\mu}(\xi,\xi=l,\eta), \tag{2.17a}$$

$$x^{\mu}(\xi,\xi,\eta=0)=x^{\mu}(\xi,\xi,\eta=d), \tag{2.17b}$$

$$\acute{x}^{\mu}(\xi,\xi=0,\eta)=\acute{x}^{\mu}(\xi,\xi=l,\eta), \tag{2.17c}$$

$$\hat{x}^{\mu}(\xi,\xi,\eta=0)=\hat{x}^{\mu}(\xi,\xi,\eta=d), \tag{2.17d}$$

$$\delta x^{\mu}(\xi,\xi=0,\eta)=\delta x^{\mu}(\xi,\xi=l,\eta), \tag{2.17e}$$

$$\delta x^{\mu}(\xi,\xi,\eta=0)=\delta x^{\mu}(\xi,\xi,\eta=d). \tag{2.17f}$$

When the set of conditions (2.14) is fulfilled, we name the membrane open. When (2.15) or (2.16) is fulfilled we name it semiopen or semiclosed interchangeably. When (2.17) is fulfilled we name it closed or "bag." Note that Chodos *et al.*[7] have discussed a model of bags in a completely different context. However, their interaction takes place in a different form.

Condition (2.14a) can be interpreted as follows, multiplying the mentioned condition by $\acute{x}^{\alpha}(\xi,\xi=0,\eta)$ and $x(\xi,\xi=l,\eta)$ we end up with $\sigma\cdot\sigma=0$ in $\xi=0,l$. Then we have that the edges defined by $\xi=0,l$ travel with the speed of light. In the same way we can interpret (2.14b). Then we have that in an open membrane its four edges travel with the speed of light, whereas for a semiclosed only two of them do. We will see that this is not the case when we have interactions. In that case the edges also interact and the relations (2.14a), (2.14b) are no longer valid.

Relation (2.13) is a system of second-order nonlinear differential equations that gives us the evolution of the membrane world-tube $x^{\mu}=x^{\mu}(\xi,\xi,\eta)$. This system of equations will be discussed in the appendix.

3. COUPLED MEMBRANES

We will take a Fokker type of action[8] for the system of membranes

$$S=\sum_a S_a^{(f)}+\tfrac{1}{2}\sum_{\substack{a,b\\a\neq b}}\int d^3\xi_a\int d^3\xi_b\times R_{ab}(x_a,x_b,\dot{x}_a,\acute{x}_a,\hat{x}_a,\dot{x}_b,\acute{x}_b,\hat{x}_b). \tag{3.1}$$

In general this action will not be adequate to describe all types of membrane–membrane interactions, due to the fact that it depends only on x^{μ} and its first derivatives. But a large class of interesting interactions will be well described, e.g., the generalization of the action that gives FWE.[2]

If we demand that S be Poincaré invariant, the dependence of R_{ab} on the indicated variables can take place only via the following set of 16 independent invariants,

$$s_{ab}=(x_{ab}\cdot x_{ab})^{1/2},\quad\text{where } x_{ab}=x_a-x_b, \tag{3.2a}$$

$$x_{ab}\cdot\dot{x}_a,\ x_{ab}\cdot\dot{x}_b,\ x_{ab}\cdot\acute{x}_a,\ x_{ab}\cdot\acute{x}_b,\ x_{ab}\cdot\hat{x}_a,\ x_{ab}\cdot\hat{x}_b, \tag{3.2b}$$

$$\dot{x}_a\cdot\dot{x}_b,\ \acute{x}_a\cdot\acute{x}_b,\ \hat{x}_a\cdot\hat{x}_b, \tag{3.2c}$$

$$\dot{x}_a\cdot\acute{x}_b,\ \acute{x}_a\cdot\dot{x}_b,\ \dot{x}_a\cdot\hat{x}_b,\ \hat{x}_a\cdot\dot{x}_b,\ \acute{x}_a\cdot\hat{x}_b,\ \hat{x}_a\cdot\acute{x}_b. \tag{3.2d}$$

Note that we get the corresponding set for strings setting $\hat{x}_a=\hat{x}_b=0$. In this case we have only nine invariants. Putting $\acute{x}_a=\acute{x}_b=\hat{x}_a=\hat{x}_b=0$ we recover the set of four independent invariants for a system of two particles[9] a and b.

If we demand

$$R_{ab}=R_{ba}, \tag{3.3}$$

i.e., symmetric interaction, the set (3.2) reduces to the ten independent invariants

$$s_{ab}, \tag{3.4a}$$

$$x_{ab}\cdot\dot{x}_{ab},\quad x_{ab}\cdot\acute{x}_{ab},\quad x_{ab}\circ\hat{x}_{ab}, \tag{3.4b}$$

$$\dot{x}_a\cdot\dot{x}_b,\quad \acute{x}_a\cdot\acute{x}_b,\quad \hat{x}_a\cdot\hat{x}_b, \tag{3.4c}$$

$$\dot{x}_a\cdot\acute{x}_b+\dot{x}_b\circ\acute{x}_a,\ \dot{x}_a\cdot\hat{x}_b+\dot{x}_b\circ\hat{x}_a,\ \acute{x}_a\cdot\hat{x}_b+\acute{x}_b\circ\hat{x}_a. \tag{3.4d}$$

Imposing the condition that the action (3.1) be stationary under the variation (2.6) and condition (3.3), we find

$$3\mu_a^2 D_a^{\mu\nu}\frac{\sigma_{a\mu\nu\rho}}{(\sigma_a\cdot\sigma_a)^{1/2}}=\sum_{b\neq a}\int d^3\zeta_b\left[\frac{\partial R_{ab}}{\partial x_a^\rho}-\frac{\partial}{\partial\xi_a}\frac{\partial R_{ab}}{\partial\dot{x}_a^\rho}-\frac{\partial}{\partial\xi_a}\frac{\partial R_{ab}}{\partial\acute{x}_a^\rho}-\frac{\partial}{\partial\eta_a}\frac{\partial R_{ab}}{\partial\hat{x}_a^\rho}\right] \tag{3.5}$$

and for the edges,

$$6\mu_a^2\frac{\sigma_{a\mu\nu\rho}}{(\sigma_a\cdot\sigma_a)^{1/2}}\dot{x}_a^\mu\hat{x}_a^\nu+\sum_{b\neq a}\int d^3\zeta_b\frac{\partial R_{ab}}{\partial x_a^\rho}=0,\quad(\xi=0,l), \tag{3.6a}$$

$$6\mu_a^2\frac{\sigma_{a\mu\nu\rho}}{(\sigma_a\cdot\sigma_a)^{1/2}}\dot{x}_a^\mu\acute{x}_a^\nu+\sum_{b\neq a}\int d^3\zeta_b\frac{\partial R_{ab}}{\partial\hat{x}_a^\rho}=0,\quad(\eta=0,d). \tag{3.6b}$$

For an open membrane we have that the edges have their own interactions and no longer travel with the speed of light. For a semiclosed membrane we have that only one condition, (3.6), must be satisfied, depending which are the open edges. For a bag conditions (3.6) do not apply.

Multiplying Eq. (3.5) by $\dot{x}_a$, $\acute{x}_a$, and $\hat{x}_a$ we find, after some algebra, the following "conservation laws":

$$\left[\frac{\partial}{\partial\zeta_a}\left(1-\dot{x}_a^\rho\frac{\partial}{\partial\dot{x}_a^\rho}\right)-\frac{\partial}{\partial\xi_a}\left(\dot{x}_a^\rho\frac{\partial}{\partial\acute{x}_a^\rho}\right)-\frac{\partial}{\partial\eta_a}\left(\dot{x}_a^\rho\frac{\partial}{\partial\hat{x}_a^\rho}\right)\right]\times\sum_{b\neq a}\int d^3\zeta_b R_{ab}=0, \tag{3.7a}$$

$$\left[\frac{\partial}{\partial\xi_a}\left(1-\acute{x}_a^\rho\frac{\partial}{\partial\acute{x}_a^\rho}\right)-\frac{\partial}{\partial\eta_a}\left(\acute{x}_a^\rho\frac{\partial}{\partial\hat{x}_a^\rho}\right)-\frac{\partial}{\partial\zeta_a}\left(\acute{x}_a^\rho\frac{\partial}{\partial\dot{x}_a^\rho}\right)\right]\times\sum_{b\neq a}\int d^3\zeta_b R_{ab}=0, \tag{3.7b}$$

$$\left[\frac{\partial}{\partial\eta_a}\left(1-\hat{x}_a^\rho\frac{\partial}{\partial\hat{x}_a^\rho}\right)-\frac{\partial}{\partial\zeta_a}\left(\hat{x}_a^\rho\frac{\partial}{\partial\dot{x}_a^\rho}\right)-\frac{\partial}{\partial\xi_a}\left(\hat{x}_a^\rho\frac{\partial}{\partial\acute{x}_a^\rho}\right)\right]\times\sum_{b\neq a}\int d^3\zeta_b R_{ab}=0. \tag{3.7c}$$

In the same way we find from (3.6)

$$\dot{x}_a^\rho\frac{\partial}{\partial\acute{x}_a^\rho}\sum_{b\neq a}\int d^3\zeta\, R_{ab}=0,\quad(\xi=0,l), \tag{3.8a}$$

$$\hat{x}_a^\rho\frac{\partial}{\partial\acute{x}_a^\rho}\sum_{b\neq a}\int d^3\zeta\, R_{ab}=0,\quad(\xi=0,l), \tag{3.8b}$$

$$\mu_a^2(\sigma_a\cdot\sigma_a)^{1/2}+\acute{x}_a^\rho\frac{\partial}{\partial\acute{x}_a^\rho}\sum_{b\neq a}\int d^3\zeta R_{ab}=0,\quad(\xi=0,l) \tag{3.8c}$$

$$\dot{x}_a^\rho\frac{\partial}{\partial\hat{x}_a^\rho}\sum_{b\neq a}\int d^3\zeta_b R_{ab}=0,\quad(\eta=0,d), \tag{3.9a}$$

$$\acute{x}_a^\rho\frac{\partial}{\partial\hat{x}_a^\rho}\sum_{b\neq a}\int d^3\zeta_b R_{ab}=0,\quad(\eta=0,d), \tag{3.9b}$$

$$\mu_a^2(\sigma_a\cdot\sigma_a)^{1/2}+\hat{x}_a^\rho\frac{\partial}{\partial\hat{x}_a^\rho}\sum_{b\neq a}\int d^3\zeta_b R_{ab}=0,\quad(\eta=0,d). \tag{3.9c}$$

We can conclude that R_{ab} must be chosen in such a way that it satisfies (3.7) in order to have a consistent set of equations of motion. If the membrane is open R_{ab} must satisfy (3.8) and (3.9). If the membrane is semiclosed, R_{ab} must satisfy either (3.8) or (3.9), depending on which are the open edges.

Equations (3.7)–(3.9) can also be found by demanding that the action (3.1) be invariant under the reparametrization

$$\zeta_a\to\zeta_a+\delta\zeta_a,\quad \xi_a\to\xi_a+\delta\xi_a,$$
$$\eta_a\to\eta_a+\delta\eta_a. \tag{3.10}$$

This fact implies that if we choose R_{ab} in such way that it satisfies (3.7)–(3.9) we are free to perform the change of parametrization

$$\bar{\zeta}_a=\bar{\zeta}_a(\zeta_a,\xi_a,\eta_a),\quad \bar{\xi}_a=\bar{\xi}_a(\zeta_a,\xi_a,\eta_a),$$
$$\bar{\eta}_a=\bar{\eta}_a(\zeta_a,\xi_a,\eta_a). \tag{3.11}$$

We can define the internal metric of each membrane as follows:

$$dm^2\equiv\gamma_{AB}\,d\zeta^A d\zeta^B\equiv dx^\mu\,dx_\mu(\zeta,\xi,\eta), \tag{3.12a}$$

$$dm^2=\dot{x}\cdot\dot{x}\,d\zeta^2+\acute{x}\cdot\acute{x}\,d\xi^2+\hat{x}\cdot\hat{x}\,d\eta^2+2\dot{x}\circ\acute{x}\,d\zeta\,d\xi+2\dot{x}\circ\hat{x}\,d\zeta\,d\eta+2\acute{x}\circ\hat{x}\,d\xi\,d\eta. \tag{3.12b}$$

The parametrization can be fixed by imposing three conditions on γ_{AB}. For example, we can choose a parametrization that diagonalizes γ_{AB}, i.e.,

$$\dot{x}\cdot\acute{x}=\dot{x}\cdot\hat{x}=\acute{x}\circ\hat{x}=0. \tag{3.13}$$

Note that $\dot{x}^\mu$ is a timelike vector and $\acute{x}^\mu$ and $\hat{x}^\mu$ are spacelike vectors, hence the signature of γ_{AB} is -1.

Given an arbitrary space with metric γ_{AB}, it is not always possible to solve the system of differential equations that relate γ_{AB} with x^μ. This is a consequence of the well-known fact that the number of dimensions of a flat space in which a pseudo-Riemannian space of three dimensions can be embedded[10] is six. But there exist simple criteria that tell us when we can embed pseudo-Riemannian spaces in flat spaces of one dimension higher (embedding of the class one).[11]

The three relations between $\dot{x},\acute{x},\hat{x}$ that fix the parametrization will in the general case be not sufficient to linearize the free membrane equation of motion (see the Appendix). In the case of strings the situation is totally

different, because, without loss of generality, the metric of the world sheet can always be chosen to be conformally flat. This fact is enough to linearize the free string equation of motion.[12,13]

If we assume that the dependence of R_{ab} on the invariants (3.4c) and (3.4d) takes place only through the combination of σ_a and σ_b, we can cast the equation of motion (3.5) in the form

$$3\mu_a^2 D_a^{\mu\nu} \frac{\sigma_{\mu\nu\rho}}{(\sigma_a \circ \sigma_a)^{1/2}} = \sum_{b\neq a} \int d^3\zeta_b \left(\frac{\partial}{\partial x_a^\rho} - 3D_a^{\mu\nu} \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} \right) R_{ab} \tag{3.14}$$

and Eqs. (3.6) in the form

$$\mu_a^2 \frac{\sigma_{a\mu\nu\rho}}{(\sigma_a \circ \sigma_a)^{1/2}} \dot{x}_a^\nu \hat{x}_a^\mu + \sum_{b\neq a} \int d^3\zeta \, \dot{x}_a^\mu \hat{x}_a^\nu \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} R_{ab} = 0, \quad (\xi = 0, l) \tag{3.15a}$$

$$\mu_a^2 \frac{\sigma_{a\mu\nu\rho}}{(\sigma_a \circ \sigma_a)^{1/2}} \dot{x}_a^\nu \acute{x}_a^\mu + \sum_{b\neq a} \int d^3\zeta_b \dot{x}_a^\mu \acute{x}_a^\nu \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} R_{ab} = 0, \quad (n = 0, d). \tag{3.15b}$$

The conservation laws (3.7), in this case, reduce to

$$\frac{\partial}{\partial \xi_a} \left(1 - \sigma_a^{\mu\nu\rho} \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} \right) \sum_{b\neq a} \int d^3\zeta_b R_{ab} = 0, \tag{3.16a}$$

$$\frac{\partial}{\partial \xi_a} \left(1 - \sigma_a^{\mu\nu\rho} \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} \right) \sum_{b\neq a} \int d^3\zeta_b R_{ab} = 0, \tag{3.16b}$$

$$\frac{\partial}{\partial \eta_a} \left(1 - \sigma_a^{\mu\nu\rho} \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} \right) \sum_{b\neq a} \int d^3\zeta_b R_{ab} = 0. \tag{3.16c}$$

And the equations for the edges (3.8) and (3.9) reduce to only one,

$$\mu_a^2 (\sigma_a \circ \sigma_a)^{1/2} + \sigma_{a\mu\nu\rho} \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} \sum_{b\neq a} \int d^3\tau_b R_{ab} = 0, \quad (\xi = 0, l, \ \eta = 0, d). \tag{3.17}$$

The system of equations (3.16) gives the following constant of motion:

$$E(\zeta_i, \zeta_f, l, d) = \left(\sigma_a^{\mu\nu\rho} \frac{\partial}{\partial \sigma_a^{\mu\nu\rho}} - 1 \right) \sum_{b\neq a} \int d^3\zeta_b R_{ab}. \tag{3.18}$$

The equation of motion (3.14) has the same form that the corresponding equation in the FWE[14] and in the action-at-a-distance theory of strings.[15] We can pass from one to another by the substitutions

$$\frac{d}{ds} \longleftrightarrow 2D^\nu \longleftrightarrow 3D^{\mu\nu},$$

$$u_\mu \longleftrightarrow \sigma_{\mu\nu} \longleftrightarrow \sigma_{\mu\nu\rho}.$$

This analogy only holds for the equations of motion.

4. A PARTICULAR CASE OF INTERACTION

In this section we explicitly consider the symmetric interaction between membranes given by

$$R_{ab} = g_a g_b \sigma_a^{\mu\nu\rho} \sigma_{b\mu\nu\rho} G(s_{ab}^2), \tag{4.1}$$

where g_a, g_b are coupling constants with the same units as μ. G is a Green's function describing time symmetric interactions.

First we will study the interaction for a general type of membrane. Then we will study some aspects of the field theory that can be extracted from the direct interaction between closed membranes.

A. The direct interaction

Action (3.1) with the interaction term (4.1) fulfills all the requirements mentioned for a consistent set of equations of motion if the Green's function is

$$G(s^2) = \delta(s^2) - \theta(s^2) \frac{m}{2s} J_1(ms), \tag{4.2}$$

i.e., the solution of the Klein–Gordon equation

$$\Box \, G(s^2) + m^2 G(s^2) = -4\pi \delta^4(x). \tag{4.3}$$

In this case the equation of motion (3.14) can be cast in the form

$$3\mu_a^2 D^{\alpha\beta} \frac{\sigma_{a\alpha\beta\rho}}{(\sigma_a \circ \sigma_a)^{1/2}} = g_a \sigma_a^{\alpha\beta\gamma} \sum_{b\neq a} F_{b\rho\alpha\beta\gamma}. \tag{4.4}$$

For the interaction of the edges we find

$$\mu_a^2 \frac{\sigma_{a\mu\nu\rho}}{(\sigma_a \circ \sigma_a)^{1/2}} \dot{x}_a^\nu \hat{x}_a^\mu + g_a \dot{x}_a^\mu \hat{x}_a^\nu \sum_{b\neq a} \Phi_{b\mu\nu\rho} \tag{4.5a}$$

$$\mu_a^2 \frac{\sigma_{a\mu\nu\rho}}{(\sigma_a \circ \sigma_a)^{1/2}} \dot{x}_a^\nu \acute{x}_a^\mu + g_a \dot{x}_a^\mu \acute{x}_a^\nu \sum_{b\neq a} \Phi_{b\mu\nu\rho}, \tag{4.5b}$$

where the sums run only over semiopen and open membranes with the same restrictions that we state for Eqs. (3.6).

The quantities $F^{\alpha\beta\gamma\delta}$ and $\Phi^{\alpha\beta\gamma}$ are defined by

$$F_{\alpha\beta\gamma\delta} \equiv \partial_\alpha \Phi_{\beta\gamma\delta} - \partial_\beta \Phi_{\alpha\gamma\delta} + \partial_\gamma \Phi_{\delta\alpha\beta} - \partial_\delta \Phi_{\gamma\alpha\beta}, \tag{4.6a}$$

$$\Phi_{\alpha\beta\gamma}(y) \equiv g \int d^3\zeta \, \sigma_{\alpha\beta\gamma}(\zeta^A) G\{[y - x(\zeta^A)]^2\}. \tag{4.7}$$

Note that $\Phi^{\alpha\beta\gamma}$ has the same symmetry as $\sigma^{\alpha\beta\gamma}$. From (4.6a) we find that $F^{\alpha\beta\gamma\delta}$ is completely antisymmetric in its four indices, and that it can be written as

$$F_{\alpha\beta\gamma\delta} = \epsilon_{\alpha\beta\gamma\delta} \epsilon^{\mu\nu\rho\sigma} \partial_\mu \Phi_{\nu\rho\sigma}. \tag{4.6b}$$

From the explicit form of $\Phi^{\alpha\beta\gamma}$ it follows that

$$\partial_\alpha \Phi^{\alpha\beta\gamma} = 2g\{ \int d\zeta \, d\xi [\dot{x}^{[\gamma} \acute{x}^{\beta]} G]_{\eta=0}^{\eta=d} + \int d\zeta \, d\eta [\dot{x}^{[\gamma} \hat{x}^{\beta]} G]_{\xi=0}^{\xi=l} \}, \tag{4.8}$$

where the right-hand side of the above equation is zero only for a closed membrane.

From (4.3) and (4.7) we get

$$\Box \, \Phi_{\alpha\beta\gamma} + m^2 \Phi_{\alpha\beta\gamma} = -4\pi J_{\alpha\beta\gamma}, \tag{4.9}$$

where

$$J_{\alpha\beta\gamma}(y) \equiv g \int d^3\zeta \sigma_{\alpha\beta\gamma}(\zeta^A)\, \delta^4\{[y - x(\zeta^A)]^2\}. \tag{4.10}$$

The field $F^{\alpha\beta\gamma\delta}$ defined by (4.6) is invariant under the gauge transformation

$$\Phi_{\alpha\beta\gamma} \to \Phi_{\alpha\beta\gamma} + \partial_\alpha \Psi_{\beta\gamma} + \partial_\beta \Psi_{\gamma\alpha} + \partial_\gamma \Psi_{\alpha\beta}, \tag{4.11a}$$

if $\Psi^{\alpha\beta}$ is such that

$$\Psi^{\alpha\beta} = -\Psi^{\beta\alpha}. \tag{4.11b}$$

Equation (4.4) is the generalization of Dirac's equations of motion. The potential $\Phi^{\alpha\beta\gamma}$ has a retarded and an advanced part. We expect to recover causality by the requirement that no net radiation exists. This procedure then yields the radiative reaction force on the membrane due to our coupling. In FWE the above procedure gives the reaction terms that appear in Dirac's equation of motion.[16]

B. The field theory of the interaction

If we assume that only closed membranes take part in the interaction, the field equation

$$\partial_\alpha F^{\alpha\beta\gamma\delta} + m^2 \Phi^{\beta\gamma\delta} = -4\pi J^{\beta\gamma\delta}$$

is equivalent to (4.9) whenever we impose for a closed membrane the gauge condition (4.8). Moreover, if we impose the condition of gauge invariance to the above field equation, we find that this requirement can only be fulfilled if the field is massless. Then we end up with

$$\partial_\alpha F^{\alpha\beta\gamma\delta} = -4\pi J^{\beta\gamma\delta}. \tag{4.12}$$

Furthermore, the relation (4.6) is the solution of

$$\partial_\epsilon F_{\alpha\beta\gamma\delta} + \partial_\alpha F_{\beta\epsilon\gamma\delta} + \partial_\beta F_{\epsilon\alpha\delta\gamma} + \partial_\gamma F_{\delta\epsilon\alpha\beta} + \partial_\delta F_{\epsilon\gamma\alpha\beta} = 0. \tag{4.13}$$

At this point we can abandon the action-at-a-distance formalism and study the field $F^{\alpha\beta\gamma\delta}$ as been produced by a given current $J^{\alpha\beta\gamma}$ due to other closed membranes. Equations (4.12) and (4.13) that define $F^{\alpha\beta\gamma\delta}$ are analogs to Maxwell's equations. For a closed membrane the field $F^{\alpha\beta\gamma\delta}$ is the physical observable, the analog to the electromagnetic tensor in EM. Also we know that the solution of (4.13) is (4.6) and that (4.6) is invariant under the gauge transformation (4.11).

It is a well-known fact that in a four-dimensional space–time a complete antisymmetric tensor of rank three is univocally associated with a vector density (pseudovector).[17] Hence we can obtain a pseudovectorial representation of the field equations. Defining

$$A^\alpha = 3!\, \epsilon^{\alpha\beta\gamma\delta} \Phi_{\beta\gamma\delta}, \tag{4.14a}$$

we have

$$\Phi_{\alpha\beta\delta} = \epsilon_{\delta\alpha\beta\gamma} A^\delta. \tag{4.14b}$$

From (4.14a), (4.9), and the condition $m = 0$ we get

$$\Box A^\alpha = -4\pi J^\alpha, \tag{4.15}$$

where J^α is defined by a relation similar to (4.14a). The gauge condition (4.8) (for a close membrane) in terms of A^α is

$$\partial^\alpha \Phi_{\alpha\beta\gamma} = \tfrac{1}{2}(\partial^\mu A^\nu - \partial^\nu A^\mu)\epsilon_{\mu\nu\beta\gamma} = 0. \tag{4.16}$$

Also

$$\partial^\alpha J_{\alpha\beta\gamma} = \tfrac{1}{2}(\partial^\mu J^\nu - \partial^\nu J^\mu)\epsilon_{\mu\nu\beta\gamma} = 0. \tag{4.17}$$

The last two equations are equivalent to

$$\partial^\mu A^\nu - \partial^\nu A^\mu = 0, \tag{4.18}$$

$$\partial^\mu J^\nu - \partial^\nu J^\mu = 0. \tag{4.19}$$

The field $F^{\alpha\beta\gamma\delta}$ can be expressed in terms of A^α as follows:

$$F^{\alpha\beta\gamma\delta} = \epsilon^{\alpha\beta\gamma\delta} \partial_\mu A^\mu. \tag{4.20}$$

The gauge transformation (4.11) now reads

$$A^\alpha \to A^\alpha + \partial_\beta \overset{*}{\Psi}{}^{\alpha\beta}, \tag{4.21a}$$

where

$$\overset{*}{\Psi}{}^{\alpha\beta} = 18\epsilon^{\alpha\beta\gamma\delta} \Psi_{\gamma\delta}. \tag{4.21b}$$

From (4.20) we find that

$$\tfrac{1}{4}\epsilon_{\alpha\beta\gamma\delta} F^{\alpha\beta\gamma\delta} = \partial_\mu A^\mu \neq 0. \tag{4.22}$$

Note that $\partial_\mu A^\mu$ is invariant under the gauge transformation (4.21). It is interesting to notice here that Eqs. (4.15), (4.18), and (4.22) give formally a sort of dual theory of Maxwell electromagnetism in the Lorentz gauge.

It is clear from (4.18) that we have a field with only one degree of freedom; moreover, (4.18) and (4.19) tell us that A^μ derives from a pseudoscalar potential Λ and J^μ from a pseudoscalar potential ρ, i.e.,

$$A^\mu = \partial^\mu \Lambda, \quad J^\mu = \partial^\mu \rho. \tag{4.23}$$

Equation (4.15) tells us that ρ and Λ are related by

$$\Box \Lambda = -4\pi(\rho + \rho_0), \tag{4.24}$$

where ρ_0 is an integration constant.

The field $F^{\alpha\beta\gamma\delta}$ is related to Λ by

$$F^{\alpha\beta\gamma\delta} = \epsilon^{\alpha\beta\gamma\delta} \Box \Lambda, \tag{4.25a}$$

and to ρ by

$$F^{\alpha\beta\gamma\delta} = -4\pi\epsilon^{\alpha\beta\gamma\delta}(\rho + \rho_0). \tag{4.25b}$$

From (4.25b) we conclude that ρ_0 represents the pseudoscalar version of the free-field solution to (4.12) and (4.13). Thus the free-field solution is a constant field. The free-field theory that we can extract from interaction (4.1) for the case of closed membranes is rather trivial (we do not have radiation as in EM).

Two derivatives are necessary to relate Λ with $F^{\alpha\beta\gamma\delta}$. This situation is similar to the Hertz potential of EM. But a physical interpretation of this field Λ is difficult—perhaps it can be related to a field that should exist inside the closed membrane (bag).

It is surprising that for the interaction (4.1), which is the obvious generalization of the interaction that gives the FWE, we end up, in the case of closed membranes, with a pseudoscalar type of interaction.

The situation in the case of open and semiopen membranes is such that we do no longer have a conserved current $J^{\alpha\beta\gamma}$. There is a loss of current at the edges.

This situation can be fixed by adding an extra interaction to the action (3.1). This extra interaction can be constructed in such a way that gives a change in the equation of motion only for the edges. In effect, the procedure here is analogous to the procedure followed for open strings.[1]

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APPENDIX

In this appendix we study some aspects of the free membrane equation of motion

$$D_{\beta\gamma}\frac{\sigma^{\beta\gamma\alpha}}{(\sigma\circ\sigma)^{1/2}}=0. \tag{A1}$$

When the parametrization

$$\dot{x}\circ x'=\dot{x}\cdot\hat{x}=x'\cdot\hat{x}=0 \tag{A2}$$

is imposed to (A1) this equation is reduced to

$$\frac{\partial}{\partial\xi}\frac{\dot{x}^\alpha}{\dot{x}\circ\dot{x}}+\frac{\partial}{\partial\eta}\frac{x'^\alpha}{x'\circ x'}+\frac{\partial}{\partial\eta}\frac{\hat{x}^\alpha}{\hat{x}\cdot\hat{x}}+\left(\frac{\dot{x}^\alpha}{\dot{x}\circ\dot{x}}\frac{\partial}{\partial\xi}+\frac{x'^\alpha}{x'\circ x'}\frac{\partial}{\partial\xi}+\frac{\hat{x}^\alpha}{\hat{x}\circ\hat{x}}\frac{\partial}{\partial\eta}\right)\ln\sqrt{\det\gamma_{AB}}=0. \tag{A3}$$

This equation can be cast in the more appealing form

$$\Box_{\gamma_{AB}}x^\alpha\equiv\frac{1}{\sqrt{\det\gamma_{AB}}}\frac{\partial}{\partial\xi^C}\left(\sqrt{\det\gamma_{EF}}\,\gamma^{CD}\frac{\partial}{\partial\xi^D}x^\alpha\right)=0. \tag{A4}$$

Note that $\Box_{\gamma_{AB}}$ is the d'Alambertian operator for *scalar functions* in the intrinsic space of the membrane. Also note that (A4) is not a linear equation, because γ_{AB} is defined by (3.12). Due to the fact that (A4) is invariant under the change of "coordinates"

$$\bar{\xi}=\bar{\xi}(\xi,\xi,\eta),\quad \bar{\xi}=\bar{\xi}(\xi,\xi,\eta),\quad \bar{\eta}=\bar{\eta}(\xi,\xi,\eta), \tag{A5}$$

we conclude that (A4) is equivalent to (A1).

Obviously Eq. (A4) cannot be cast in a linear form using only the change of paramentrization (A5). Therefore, we will not have a general solution to the free membrane equation of motion. But we can study particular solutions.

The trivial solution to (A1) is

$$x^\alpha=a^\alpha\xi+b^\alpha\xi+c^\alpha\eta+d^\alpha, \tag{A6}$$

where a^α, b^α, c^α, and d^α are constant vectors. This solution unhappily does not fulfill the requirements to represent the motion of a membrane because it does not satisfy any of the sets of conditions (2.14)–(2.17).

An interesting particular case is the one that is obtained by imposing the requirement that γ_{AB} be conformally flat, i.e., the condition (A2) and

$$\dot{x}\circ\dot{x}=x'\cdot x'=\hat{x}\cdot\hat{x}=f(\zeta,\xi,\eta)>0. \tag{A7}$$

In this case Eqs. (A3) and (A2) imply

$$\frac{\partial}{\partial\zeta}(3f+\ln f)=0,\qquad \frac{\partial}{\partial\xi}(f+\ln f)=0,\qquad \frac{\partial}{\partial\eta}(f+\ln f)=0, \tag{A8}$$

i.e., f is a constant that can be chosen without loss of generality to be equal to one. Then Eq. (A3) is reduced to

$$\frac{\partial^2x^\alpha}{\partial\zeta^2}-\frac{\partial^2x^\alpha}{\partial\xi^2}-\frac{\partial^2x^\alpha}{\partial\eta^2}=0. \tag{A9}$$

Hence, if one finds a solution to (A9) that satisfies (A2) in some range of its variables and condition (A7) (with $f=1$) at a point belonging to that range, then the equations of motion propagates the condition (A7) (with $f=1$) through the entire range of the variables where (A2) holds.

Note that corresponding to Eq. (A9) in the string case is the general free string equation of motion, and that this equation of motion propagates the condition $\dot{x}\cdot\dot{x}+x'\cdot x'=0$ through the entire range of the variables where $\dot{x}\circ x'=0$ holds.

A solution to (A9) that satisfies the conditions (2.17), (A2), and (A7) at a point can easily be found as a series of circular functions. These latter conditions are expressed as conditions on the coefficients of the series, in a manner analogous to the one found by Scherk in the case of strings.[12] But here it is not so clear that all the obtained conditions are consistent. This point together with a more sophisticated approach to Eq. (A1) using embedding techniques will be studied in a future paper.

[1]M. Kalb and P. Ramond, Phys. Rev. D 9, 2273 (1974).
[2]R. P. Feynman and J. A. Wheeler, Rev. Mod. Phys. 21, 425 (1949).
[3]A good review of action-at-a-distance theories can be found in *Classical Dynamics: A Modern Perspective*, by E. C. G. Sudarshan and N. Makunda (Wiley, New York, 1974), Chap. 22.
[4]See, for instance, J. H. Schwarz, Phys. Rev. C 8, 269 (1973) and the references contained therein.
[5]M. Virasoro, Phys. Rev. 177, 2309 (1969); J. A. Shapiro, Phys. Lett. B 33, 361 (1970).
[6]P. Olive and J. Scherk, Phys. Lett. B 44, 295 (1973); P. Ramond, Phys. Lett. B 47, 152 (1973).
[7]A. Chodos *et al.*, Phys. Rev. D 9, 3471 (1974).
[8]A. D. Fokker, Z. Phys. 58, 386 (1929).
[9]P. Havas, *Problems in the Foundation of Physics*, edited by M. Bunge (Springer, New York, 1971), p. 38.
[10]L. P. Eisenhart, *Riemannian Geometry* (Princeton U. P., New Jersey, 1961), p. 188.
[11]T. Y. Thomas, Acta Math. 67, 169 (1936).
[12]J. Scherk, Rev. Mod. Phys. 47, 123 (1975).
[13]For a general discussion of theories involving constraints see, for instance, "P. A. M. Dirac Lectures in Quantum Mechanics" (Yeshiva University, New York, 1964), lectures 3 and 4.
[14]See, for instance, in Ref. 1, Eq. (2.8).
[15]Ref. 1, Eq. (2.55).
[16]P. A. M. Dirac, Proc. R. Soc. A 167, 148 (1938).
[17]J. A. Schouten, *Tensor Analysis for Physicists* (Oxford U. P., London, 1951), p. 32.

Excitation of horizontally polarized waves in critical-coupling regions where the permittivity gradient approaches zero—Full wave solutions

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Maxwell's equations for inhomogeneous isotropic media are transformed into coupled ordinary differential equations for the wave amplitudes. To facilitate the solutions of these equations for dielectric layers with critical coupling regions, a generalized WKB approach is used. To this end, sets of auxiliary functions that are solutions to the wave equation for homogeneous or linearly varying permittivity profiles are employed. By introducing an additional set of auxiliary, parabolic cylindrical functions, the generalized WKB approach is extended to obtain suitable solutions for critical coupling regions of the dielectric layer where the gradient of the permittivity profile also approaches zero. Expressions for the reflection and transmission coefficients and the characteristic surface impedance for an inhomogeneous dielectric layer are derived as functions of the transverse wavenumber. Realizability and reciprocity relationships are also derived.

1. INTRODUCTION

Propagation of electromagnetic waves in inhomogeneous media has been analyzed extensively in the technical literature.[1–5] Rigorous closed form analytical solutions for the electromagnetic fields have been derived for special permittivity profiles. In the general case, for which no closed form analytical solutions are known, various numerical and analytical methods have been developed. Thus, for example, for horizontally polarized waves, the inhomogeneous dielectric layer is subdivided into strips of finite thickness in which the dielectric coefficient is assumed to be uniform or assumed to vary linearly as a function of position.[6] The solutions for the fields in each strip satisfy the boundary conditions for the electromagnetic fields at the interface between two adjacent strips. Another method employs Green's function techniques to rigorously formulate the electromagnetic fields in terms of integral equations[5] which are solved using standard iterative techniques. However approximate results obtained by a perturbation method do not necessarily obey all the conditions (such as energy conservation) satisfied by the exact solution.

Using a generalized WKB technique Maxwell's equations are transformed into coupled ordinary differential equations for a new set of dependent variables, the wave amplitudes.[7] The wave amplitudes are related to the transverse components of the electric and magnetic fields through the transverse wave admittances which locally depict the principal characteristics of the inhomogeneous permittivity profile. Thus for horizontally polarized waves in a slowly varying medium, devoid of critical coupling regions, the wave admittances are determined by regarding the medium to be locally homogeneous. For critical coupling regions, the permittivity profile is regarded to be linearly varying and the corresponding local wave admittances are expressed in terms of Airy integral functions. The formulation of the solution in terms of the coupled wave amplitudes is rigorous[7] and a program has been written to compute the electromagnetic fields and the reflection and transmission coefficients. The results are shown to be consistent with energy conservation and reciprocity relationships up to five significant figures. However, this analysis[7] is not suitable in its present form when the inhomogeneous dielectric contains critical coupling regions where the gradient of the refractive index also vanishes since the coupling coefficients become singular.

To apply this generalized WKB technique to critical coupling regions where the gradient of the refractive index also vanishes, in our present analysis the permittivity profile is regarded to be locally parabolic and the wave admittances are expressed in terms of parabolic cylindrical functions. Two different local characterizations of the permittivity profile in this region are considered and their relative merits are discussed.

Energy conservation and reciprocity relationships for evanescent waves and uniform plane waves propagating through an inhomogeneous dielectric slab are derived. Expressions for the reflection and transmission coefficients and the characteristic surface impedance are also derived as functions of the transverse wavenumber.

2. FORMULATION OF THE PROBLEM

The nonvanishing components of the horizontally polarized electromagnetic field due to a y directed electric line source $\bar{J}$, parallel to a horizontally stratified dielectric slab (see Fig. 1) are

$$-\frac{\partial E_y}{\partial z} = -i\omega\mu H_x, \tag{2.1a}$$

$$\frac{\partial E_y}{\partial x} = -i\omega\mu H_z, \tag{2.1b}$$

and

$$\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = i\omega\epsilon E_y + J_y, \tag{2.1c}$$

in which

$$\bar{J} = J_y \bar{a}_y = I\delta(x - x_s)\delta(z - z_s)\bar{a}_y, \tag{2.2}$$

where $\delta(x - x_s)$ and $\delta(z - z_s)$ are Dirac delta functions, and I is the intensity of the current filament. An $\exp(i\omega t)$ time dependence is assumed and ϵ and μ, the permittivity and permeability of the medium of propagation, are assumed to be independent of the variables x and y. The dual problem, excitation of vertically polarized waves,

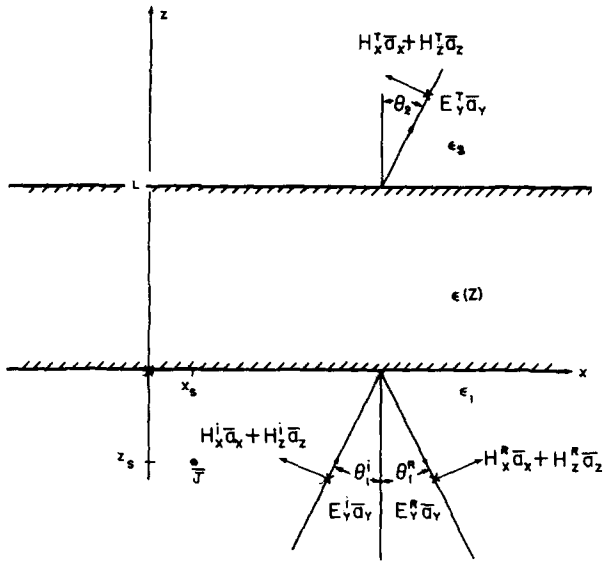

FIG. 1. Excitation of horizontally polarized waves by an electric line source parallel to an inhomogeneous dielectric slab.

may be treated in a similar way by replacing the electric line source $\bar{J}$ by a magnetic line source $\bar{J}_m$.

On eliminating H_x and H_z from (2.1) we obtain the wave equation for E_y, i.e.,

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}+\mu\frac{\partial}{\partial z}\left(\frac{1}{\mu}\right)\frac{\partial}{\partial z}+k^2\right)E_y \equiv L_T(E_y)=i\omega\mu J_y, \tag{2.3}$$

in which $k=\omega(\mu\epsilon)^{1/2}$ is the wave number. We assume that no known analytic solution for (2.3) exists in closed form for the particular inhomogeneous medium considered. Instead of solving the second-order differential equation (2.3) for E_y we proceed by transforming Maxwell's Eq. (2.1) for the transverse components E_y and H_x into a suitable set of ordinary differential equations for a new pair of dependent variables, the wave amplitudes ϕ_1 and ϕ_2. To this end we express the transverse components $E_y(x,z)$ and $H_x(x,z)$ in terms of their respective Fourier transforms $E(\beta,z)$ and $H(\beta,z)$. Thus

$$E_y(x,z)=\int_{-\infty}^{\infty}\exp[-i\beta(x-x_s)]E(\beta,z)\,d\beta, \tag{2.4a}$$

in which

$$E(\beta,z)=(1/2\pi)\int_{-\infty}^{\infty}\exp[i\beta(x-x_s)]E_y(x,z)\,dx, \tag{2.4b}$$

and a similar relationship exists between $H_x(x,z)$ and $H(\beta,z)$. The completeness relationship associated with (2.4) is

$$\delta(x-x_s)=(1/2\pi)\int_{-\infty}^{\infty}\exp[-i\beta(x-x_s)]\,d\beta. \tag{2.5}$$

Eliminating H_z from (2.1b) and (2.1c) we get

$$\frac{\partial H_x}{\partial z}=i\omega\epsilon\left(E_y+\frac{1}{k^2}\frac{\partial^2}{\partial x^2}E_y\right)+J_y. \tag{2.6}$$

Multiply (2.1a) and (2.6) by $\exp[-i\beta(x-x_s)]\,dx/2\pi$ and integrate with respect to x, $[-\infty,\infty]$, to get the ordinary differential equations for the transforms $E(\beta,z)$ and $H(\beta,z)$ of the transverse field components $E_y(x,z)$ and $H_x(x,z)$ respectively; i.e.,

$$\frac{d}{dz}E(\beta,z)=i\omega\mu H(\beta,z), \tag{2.7a}$$

$$\frac{d}{dz}H(\beta,z)=\frac{-1}{i\omega\mu}k_0^2q^2E(\beta,z)+J(\beta,z), \tag{2.7b}$$

in which $J(\beta,z)$ is the Fourier transform for the electric current distribution

$$J(\beta,z)=I\delta(z-z_s)/2\pi \tag{2.7c}$$

and

$$k_0^2q^2=k^2-\beta^2=k^2(1-s^2)=k^2c^2,\quad \mathrm{Im}c\leq 0, \tag{2.8a}$$

and in view of Snell's law,

$$\beta=k(z)s(z)=k_0S \tag{2.8b}$$

in which k_0 is the free space wavenumber. Thus

$$q^2=n^2-S^2=C^2+n^2-1,\quad \mathrm{Im}(C)\leq 0, \tag{2.8c}$$

and the refractive index is $n=k/k_0$.

3. THE DIFFERENTIAL EQUATIONS FOR THE WAVE AMPLITUDES

To facilitate the solution of (2.7) for the field transforms $E(\beta,z)$ and $H(\beta,z)$, we express them in terms of two new dependent variables, the wave amplitudes $\phi_1(\beta,z)$ and $\phi_2(\beta,z)$ defined by the following equations:

$$E=\phi_1+\phi_2 \tag{3.1a}$$

and

$$H=-(Y_1\phi_1-Y_2\phi_2),$$

in which Y_1 and Y_2 are local transverse wave admittances associated with the wave amplitudes ϕ_1 and ϕ_2 respectively, i.e.,

$$Y_1(\beta,z)=-(1/i\omega\mu)\ln'g_1(\beta,z) \tag{3.2a}$$

and

$$Y_2(\beta,z)=(1/i\omega\mu)\ln'g_2(\beta,z), \tag{3.2b}$$

in which $\ln'g=(dg/dz)/g$ and the auxiliary, local wave solutions, g_1 and g_2, are yet to be chosen.[7] Thus on substituting (3.1) into (2.7) we get

$$\phi_1'+\phi_2'=-i\omega\mu(Y_1\phi_1-Y_2\phi_2) \tag{3.3a}$$

and

$$-Y_1\phi_1'+Y_2\phi_2'=Y_1'\phi-Y_2'\phi_2-(1/i\omega\mu)k_0^2q^2(\phi_1+\phi_2)+J. \tag{3.3b}$$

In (3.3) the primes denote differentiation with respect to z. After some algebraic manipulations we obtain from (3.3),

$$\phi_1'=\frac{g_1'}{g_1}\phi_1+\frac{g_2L(g_1)}{W(g_1,g_2)}\phi_1+\frac{g_1L(g_2)}{W(g_1,g_2)}\phi_2-\frac{J}{Y^T}, \tag{3.4a}$$

$$\phi_2'=\frac{g_2'}{g_2}\phi_2+\frac{g_2L(g_1)}{W(g_2,g_1)}\phi_1+\frac{g_1L(g_2)}{W(g_2,g_1)}\phi_2+\frac{J}{Y^T}, \tag{3.4b}$$

in which the second-order differential operator L is given by

$$L(g)\equiv\left[\frac{d^2}{dz^2}+\mu\frac{d}{dz}\left(\frac{1}{\mu}\right)\frac{d}{dz}+k^2q^2\right]g. \tag{3.5a}$$

The Wronskian $W(g_1,g_2)$ and Y^T, the total wave admittance, are defined by

$$W(g_1, g_2) = g_1 g_2' - g_2 g_1' \tag{3.5b}$$

and

$$Y^T = Y_1 + Y_2 = (1/i\omega\mu) W(g_1, g_2)/g_1 g_2. \tag{3.5c}$$

Equations (3.4) can also be expressed in matrix notation as follows:

$$\Phi' = (G + C)\Phi + K, \tag{3.6a}$$

in which

$$\Phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad G = \begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} \end{pmatrix}$$

and

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}, \quad K \equiv \frac{I}{2\pi Y^T}\,\delta(z - z_s)\begin{pmatrix} -1 \\ 1 \end{pmatrix} \tag{3.6b}$$

where

$$G_{ii} = g_i'/g_i, \quad i = 1, 2 \text{ and } G_{ij} = 0, \quad i \neq j, \tag{3.7a}$$

and for $i \neq j$,

$$C_{ij} = -C_{jj} = g_i L(g_j)/W(g_i, g_j), \quad i = 1 \text{ or } 2, \quad j = 1 \text{ or } 2. \tag{3.7b}$$

The coupling coefficients C_{ij} can be made to vanish only if solutions to (2.3) are known in which case $\phi_i = g_i$ $(i = 1, 2)$. However, this is not the case of interest in our present investigations. Hence, a judicious choice for the local auxiliary wavefunctions g_1 and g_2 is such that the coupling coefficients C_{ij} are small compared to the local propagation coefficients G_{11} and G_{22}. The coupled differential equations (3.4) or (3.6) may be solved analytically using iterative approaches. One such method expresses the solution in terms of an infinite sum whose individual terms are associated with multiple reflections in the inhomogeneous layer.[1] Using another approach, the solution is expressed in terms of an infinite product. Thus,[7]

$$\phi_1 = g_1^0 \prod_{n=0}^{\infty} \exp\left(\int^z C_{11}^n\, dz\right)$$

$$= g_1^0 \exp\left(\sum_{n=0}^{\infty} \int^z C_{11}^n\right) dz, \tag{3.8a}$$

in which g_1^0 is the initial expression for the auxiliary wavefunctions and

$$C_{11}^n = L(g_1^n) g_2^n / W(g_1^n, g_2^n), \tag{3.8b}$$

where the recurrence formula

$$g_{1,2}^{n+1} = g_{1,2}^n \exp \int^z C_{11}^n\, dz \tag{3.8c}$$

is used to determine the successive expressions for the auxiliary wavefunctions. A similar expression can be written for ϕ_2.

Numerical solutions to the coupled differential equations (3.4) have also been obtained using the Runge–Kutta method.[8] In general, it is necessary to choose g_i such that the coupling coefficients are not singular functions of z.

4. CHOICE OF THE LOCAL WAVEFUNCTIONS FOR CRITICAL COUPLING REGIONS WHERE $|q^2| \to 0$ AND $d(q^2)/dz \to 0$

In this section we generate suitable expressions for the auxiliary wavefunctions, $g_i(z)$, for critical coupling regions of the inhomogeneous dielectric, $\epsilon(z)$, where

$$|q^2(z)| \to 0 \tag{4.1a}$$

and the gradient of the permittivity profile vanishes, hence

$$\alpha(z) = d[q^2(z)]/dz = d[n^2(z)]/dz \to 0. \tag{4.1b}$$

We assume here that for all z, $\mu = \mu_0$, and, for example, for dissipative ionized media, $q^2(z)$ can be expressed as[2]

$$q^2(z) = C^2 - X(z)/[1 - iZ(z)], \tag{4.2a}$$

in which

$$X = (\omega_p/\omega)^2 \text{ and } Z = \nu/\omega, \tag{4.2b}$$

where the plasma frequency ω_p and the collision frequency ν are functions of z.

For regions that do not contain turning points $(q^2 \to 0)$ the auxiliary wavefunctions g_i are determined by the following local propagation coefficients[8]:

$$G_{11} = -ik_0 q, \quad G_{22} = ik_0 q. \tag{4.3a}$$

The coupling coefficients associated with (4.3a) are for $i \neq j$,

$$C_{ij} = -C_{jj} = \frac{\alpha}{4q^2} = \frac{dq}{dz}\frac{1}{2q}, \quad i = 1 \text{ or } 2, \quad j = 1 \text{ or } 2. \tag{4.3b}$$

Substitution of (4.18) into (3.4) yields the familiar coupled WKB equations.[2] For critical coupling regions the auxiliary wavefunctions, g_i, are determined by the following local propagation coefficients[7]:

$$G_{ii} = -\alpha(k_0/\alpha)^{2/3} w_i'(\xi)/w_i(\xi), \quad i = 1, 2, \tag{4.4a}$$

in which w_1 and w_2 are independent solutions to the Airy differential equations, the prime denotes differentiation with respect to the argument

$$\xi = -(k_0/\alpha)^{2/3} q^2, \tag{4.4b}$$

and α is given by (4.1b). The coupling coefficients associated with (4.4) are

$$C_{ij} = -C_{jj} = \tfrac{2}{3} w_i w_j [(k/\alpha)^{4/3} q^4 + (k/\alpha)^{2/3} q^2 (w_j'/w_j)^2 - (w_j'/2w_j)]\alpha'/\alpha W(w_j, w_i). \tag{4.4c}$$

Numerical solutions to (3.6) for permittivity profiles with turning points have been obtained. The coefficients G_{ii} and C_{ij} in (3.6) are given by (4.3) for regions where $|\xi(z)| \geq 0.5$, and they are given by (4.4) for regions where $|\xi(z)| < 0.5$.[8] It can be shown that the reciprocity and the energy conservation relationships are satisfied, in general, only when the expressions for the coupling terms C_{ij} $(i \neq j)$ in (3.4) are not neglected.

For critical coupling regions in which α also vanishes (the q^2 profile has two neighboring simple zeros or when q^2 and α vanish at the same point), substitution of (4.4) into (3.6) yields a set of coupled differential equations that are not suitable for numerical computations since the coupling coefficients C_{ij} in (4.4c) are singular for $\alpha = 0$. Thus in these cases it is necessary to choose a different set of auxiliary wavefunctions. To this end we recast $k_0^2 q^2$ as follows:

$$k_0^2 q^2 \equiv k_0^2[q_m^2 + q_m^{2\prime\prime}(z - z_0)^2/2] \equiv K^2(\nu + \tfrac{1}{2} - \xi^2/4), \tag{4.5a}$$

in which

$$q_m^2 = q^2(z_m), \quad q_m^{2\prime\prime} = \frac{d^2}{dz^2} q^2(z)\Big|_{z_m}, \tag{4.5b}$$

and z_m is the value of z where α vanishes, thus

$$q_m^{2\prime} = q^{2\prime}(z_m) = 0. \tag{4.5c}$$

For a parabolic permittivity profile $z_0 = \text{const} = z_m$, however, in general, z_0 in (4.5a) is given by

$$\zeta = K(z - z_0) \equiv K[2(q^2 - q_m^2)/q_m^{2\prime\prime}]^{1/2}. \tag{4.6a}$$

In order to obtain the proper square root, (4.6a) is expressed as follows:

$$(z - z_0) = (z - z_m)[2(q^2 - q_m^2)/q_m^{2\prime\prime}(z - z_m)^2]^{1/2}, \tag{4.6b}$$

where the principal square root is assumed in (4.6b). Thus $z_0(z_m) = z_m$ and in general z_0 and z_m may be complex. The constants K and ν are given by

$$K = (-2k_0^2 q_m^{2\prime\prime})^{1/4} \tag{4.7a}$$

and

$$\nu + \tfrac{1}{2} = k_0^2 q_m^2 / K^2. \tag{4.7b}$$

The fourth root in (4.7a) is chosen such that ζ lies in the first or fourth quadrant when $\mathrm{Re}(z - z_m) > 0$. The derivative of z_0 with respect to z is

$$\frac{dz_0}{dz} = \left[q_m^{2\prime\prime}(z - z_0) - \frac{dq^2}{dz}\right] \Big/ q_m^{2\prime\prime}(z - z_0). \tag{4.8a}$$

On examining the Taylor series expansion of (4.8) about $z = z_m$ it follows that

$$\lim_{z \to z_m} \frac{dz_0}{dz} \to 0. \tag{4.8b}$$

The function $k_0^2 q^2$ can also be recast as follows:

$$k_0^2 q^2 = k_0^2[K_1 + q^{2\prime\prime}(z)\,(z - z_0)^2/2] \equiv K^2(\nu + \tfrac{1}{2} - \zeta^2/4), \tag{4.9a}$$

in which

$$\zeta = K(z - z_0) = K q^{2\prime}(z)/q^{2\prime\prime}(z) \tag{4.9b}$$

and

$$K_1 = q^2(z) - [q^{2\prime}(z)]^2/2q^{2\prime\prime}(z). \tag{4.9c}$$

Thus in this case,

$$K = [-2k_0^2 q^{2\prime\prime}(z)]^{1/4}, \tag{4.10a}$$

$$\nu + \tfrac{1}{2} = k_0^2 K_1 / K^2, \tag{4.10b}$$

and

$$\frac{dz_0}{dz} = q^{2\prime}(z) q^{2\prime\prime\prime}(z)/[q^{2\prime\prime}(z)]^2; \tag{4.10c}$$

hence

$$\frac{dz_0}{dz} \to 0 \quad \text{as} \quad \frac{dq^2(z)}{dz} \to 0. \tag{4.10d}$$

Both (4.5) and (4.8) reduce to the same form when the given q^2 profile is parabolic. In general this is not the case. When (4.5) is used to define the constant parameters K and ν (4.7), it is necessary to determine the value of z_m (which may be complex) (4.5c). However, when (4.8) is used though it is not necessary to determine the value of z_m, the parameters K and ν are functions of position z.

To obtain the expressions for the local propagation coefficients G_{ii} in the region, where $q^2 \to 0$ and $\alpha \to 0$, we recast q^2 as in (4.5) or (4.9) and regard K, ν, and z_0 as constants. Thus in view of (4.5a), the local propagation coefficients are

$$G_{ii} = K \frac{d}{d\zeta} \ln U_\nu^i(\zeta) = \ln' g_i, \tag{4.11a}$$

in which $U_\nu^1(\zeta)$ and $U_\nu^2(\zeta)$ are linearly independent parabolic cylindrical functions. For constant K, ν, and z_0, $U_\nu^i(\zeta)$ are exact solutions of the differential equation (3.5a) with $\mu = \text{const}$. Thus

$$\left[\frac{d^2}{d\zeta^2} + \left(\nu + \frac{1}{2} - \frac{\zeta^2}{4}\right)\right] U_\nu^i(\zeta) = 0, \quad i = 1, 2. \tag{4.11b}$$

A suitable choice for $U_\nu^i(\zeta)$ is given in terms of the Whittaker function, thus[9,2,4]

$$U_\nu^1(\zeta) = D_\nu(\zeta) \quad \text{and} \quad U_\nu^2(\zeta) = D_{-\nu-1}(-i\zeta). \tag{4.11c}$$

The coupling coefficients, C_{ij}, associated with the local wave solutions, g_i, (4.11a) are evaluated in the next section where the consequences of casting q^2 in forms (4.5) and (4.9) are discussed further.

5. DERIVATION OF THE COUPLING COEFFICIENTS FOR THE LOCAL PARABOLIC CYLINDRICAL WAVEFUNCTIONS

The auxiliary, local wavefunctions, g_i, (4.11a) for the critical coupling regions where $|q^2| \to 0$ and $dq^2/dz \to 0$ are

$$g_i = \exp\left(\int \frac{\partial}{\partial z} \ln U_\nu^i(\zeta)\, dz\right). \tag{5.1}$$

For the general case considered, K, ν, and z_0 are functions of z; thus

$$\frac{d}{dz} U_\nu^i(\zeta) = \frac{d}{dz} U_\nu^i[K(z - z_0)] = \left[\frac{d\zeta}{dz}\frac{\partial}{\partial \zeta} + \frac{d\nu}{dz}\frac{\partial}{\partial \nu}\right] U_\nu^i(\zeta), \tag{5.2a}$$

in which

$$\frac{d\zeta}{dz} = K\left(1 - \frac{dz_0}{dz}\right) + (z - z_0)\frac{dK}{dz}. \tag{5.2b}$$

Thus for regions of the inhomogeneous medium where the permittivity profile is parabolic, (5.1) reduces to

$$g_i = U_\nu^i(\zeta), \quad i = 1, 2, \tag{5.3}$$

and $L(g_i) = 0$. However, for the general case considered

$$\frac{1}{g_i}\frac{d^2 g_i}{dz^2} = \frac{1}{g_i}\frac{d}{dz}(g_i G_{ii}) = (G_{ii})^2 + \frac{d}{dz} G_{ii}, \tag{5.4a}$$

where G_{ii} is given by (4.11) and d/dz is interpreted as in (5.2). Thus it can be shown that

$$\begin{aligned}\frac{1}{g_i} L(g_i) = &\left[k^2 q^2 + K^2\left(\frac{U_\nu^{i\prime}}{U_\nu^i}\right)^2\right]\frac{dz_0}{dz} \\ &+ \left\{\frac{U_\nu^{i\prime}}{U_\nu^i} - \left[\frac{k^2 q^2}{K^2} + \left(\frac{U_\nu^{i\prime}}{U_\nu^i}\right)^2\right]\zeta\right\}\frac{dK}{dz} \\ &+ K\left(\frac{\partial U_\nu^{i\prime}}{\partial \nu}\frac{1}{U_\nu^i} - \frac{\partial U_\nu^i}{\partial \nu}\frac{U_\nu^{i\prime}}{(U_\nu^i)^2}\right)\frac{d\nu}{dz},\end{aligned}$$

in which the primes denote differentiation with respect to the argument ζ. The Wronskian $W_z(g_1, g_2)$ can be shown to reduce to

$$W_z(g_i, g_j) = K g_i g_j W_\zeta(U_\nu^i, U_\nu^j)/U_\nu^i U_\nu^j. \quad (5.4c)$$

The coupling coefficients $C_{ij} = -C_{jj} = g_i L(g_j)/W_z(g_i, g_j)$, (3.7b), can now be written explicitly in terms of the derivatives dz_0/dz, dK/dz, and $d\nu/dz$. These derivates vanish only for regions where the permittivity profile is parabolic. Casting the q^2 profile in the form (4.5) we determine dz_0/dz for a particular permittivity profile by using (4.8a) while dK/dz and $d\nu/dz$ are zero. When the q^2 profile is cast in the form (4.9), the derivatives $dK/d\nu$, $d\nu/dz$, and dz_0/dz are determined for a given permittivity profile by using (4.10a), (4.10b), and (4.11c) respectively. Thus, when the value of the critical point $z = z_m$ given by (4.5c) can be readily determined, it is more convenient to cast q^2 in the form (4.5). In this case the coupling coefficients reduce to

$$C_{ij} = -C_{jj} = U_\nu^i U_\nu^j [k^2 q^2 + K^2 (U_\nu^{j\prime}/U_\nu^j)^2](dz_0/dz) K W_\zeta(U_\nu^i, U_\nu^j) \quad (5.5a)$$

with dz_0/dz given by (4.8a), and for the particular choice of the parabolic cylindrical functions given in (4.11c) the Wronskian W_ζ is

$$W_\zeta(U_\nu^1, U_\nu^2) = -W_\zeta(U_\nu^2, U_\nu^1)$$

$$= W(D_\nu(\xi), D_{-\nu-1}(-i\xi)) = \exp[i(\nu+1)\pi/2]. \quad (5.5b)$$

For the q^2 profile given by (4.2),

$$q^{2\prime} = -\frac{X'(z) + i[X(z)Z'(z) - Z'(z)Z(z)]}{[1 - iZ(z)]^2}. \quad (5.5c)$$

Thus if Z is a constant or if $X'/X = Z'/Z$, z_m is real and $X'(z_m) = 0$. In general, however, z_m may be complex.

6. TRANSITION REGIONS OF THE COUPLED DIFFERENTIAL EQUATIONS

In Secs. 4 and 5 a choice of three sets of auxiliary local wavefunctions, $g_i(\beta, z)$, is considered to facilitate the solutions of the coupled differential equation (3.6). The first choice which is suitable for slowly varying media devoid of critical coupling regions ($q^2 \neq 0$) leads to the familiar coupled WKB equations. The wave amplitudes ϕ_i, the local propagation coefficients G_{ii}, and the coupling coefficients C_{ij} associated with this choice of the local wavefunctions g_i are identified by the superscript 1. Similarly for critical coupling regions where $(q^2)' = \alpha$ does not approach zero the local wavefunctions are expressed in terms of Airy integral functions Ai and Bi. The quantities ϕ_i, G_{ii}, and C_{ij} associated with the second choice are identified by the superscript 2. For critical coupling regions in which both q^2 and $(q^2)'$ approach zero, the local wavefunctions are expressed in terms of parabolic cylindrical functions $U_\nu^i(\zeta)$. The quantities ϕ_i, G_{ii}, and C_{ij} associated with this choice are identified by the superscript 3. Thus (3.6a) is written as

$$\phi_i^m = (G_{ij}^m + C_{ij}^m)\phi_j^m, \quad i, j = 1, 2 \text{ and } m = 1, 2, 3. \quad (6.1)$$

To determine precisely which of the three formulations is to be used in (3.6) for a particular region of the inhomogeneous dielectric, we examine the uniform asymptotic expansions for the parabolic cylindrical functions, $D_\nu(\zeta)$, derived by Olver.[10] For $|\nu + \frac{1}{2}| \gg 1$,

$$D_\nu(\zeta) \approx (2\pi)^{1/2}(\nu+\tfrac{1}{2})^{\nu/2} \exp[-\nu/2 - \tfrac{1}{4}]\left[\frac{t}{x^2-1}\right]^{1/4} \mathrm{Ai}(t), \quad (6.2a)$$

in which

$$\tfrac{2}{3}t^{3/2} = 2(\nu+\tfrac{1}{2})\int_1^x [x^2-1]^{1/2}\,dx$$

$$= (\nu+\tfrac{1}{2})[x(x^2-1)]^{1/2} - \ln[x + (x^2-1)^{1/2}] \quad (6.2b)$$

and

$$x = \zeta/2(\nu+\tfrac{1}{2})^{1/2}. \quad (6.2c)$$

Thus

$$\tfrac{2}{3}t^{3/2} = \int_{z_c}^{z} (-k_0^2 q^2)^{1/2}\,dz = ik_0 \int_{z_c}^{z} q\,dz, \quad (6.2d)$$

where the lower limit z_c (corresponding to $x = 1$) is the critical point defined by

$$q^2(z_c) = 0. \quad (6.2e)$$

On employing the uniform asymptotic expansion for $\mathrm{Ai}(t)$ we obtain for $x \not\approx 1$ and $|\arg t| \leq 2\pi/3$,

$$D_\nu(\zeta) \approx (\nu+\tfrac{1}{2})^{\nu/2}[4(x^2-1)]^{-1/4} \exp[-(\tfrac{2}{3}t^{3/2} + \nu/2 + \tfrac{1}{4})]. \quad (6.3a)$$

For $2\pi/3 \leq \arg t \leq 4\pi/3$

$$D_\nu(\zeta) = (\nu+\tfrac{1}{2})^{\nu/2}\exp(-\nu/2 - \tfrac{1}{4})$$

$$\times [4(x^2-1)]^{-1/4}[\exp(-\tfrac{2}{3}t^{3/2}) + i\exp(\tfrac{2}{3}t^{3/2})]. \quad (6.3b)$$

In critical coupling regions where $x \to 1$ and $t \to 0$ it can be shown that

$$t \approx (\nu+\tfrac{1}{2})^{2/3}(x^2-1) = -[k_0/q^{2\prime}(z_c)]^{2/3} q^2. \quad (6.4a)$$

Thus for $x \to 1$, $t \approx \xi$, where ξ is defined by (4.4b), and

$$D_\nu(\xi) \approx (2\pi)^{1/2}(\nu+\tfrac{1}{2})^{\nu/2+1/6}\exp[-\nu/2 - \tfrac{1}{4}]\mathrm{Ai}(\xi). \quad (6.4b)$$

For $|x| \to \infty$, $\frac{2}{3}t^{3/2} - (\nu+\frac{1}{2})(x^2 - \frac{1}{2}) - \ln(2x)$ and

$$D_\nu(\zeta) = \zeta^\nu \exp(-\zeta^2/4), \quad |\arg\zeta| \leq \pi/2, \quad (6.5a)$$

$$D_\nu(\zeta) = [\zeta^\nu \exp(-\zeta^2/4) - (2\pi)^{1/2}\exp(\nu\pi i)\zeta^{-(\nu+1)}$$

$$\times \exp(\zeta^2/4)/(-\nu-1)!\,], \quad \pi/2 \leq \arg\zeta \leq \pi. \quad (6.5b)$$

Using Stirling's formula for $|\nu+1| \gg 1$ it can be shown that

$$(-\nu-1)! = (2\pi)^{1/2}\left(\frac{-e}{\nu+\frac{1}{2}}\right)^{\nu+1/2}. \quad (6.5c)$$

Hence the solutions of (3.6) identified with the superscript $m = 3$ merge with the solutions identified by the superscript 2 for critical coupling regions where $q^2 \to 0$ and $(q^2)' \not\approx O(x-1)$. These solutions merge with the solutions identified with the superscript 1 for regions where $q^2 \not\approx 0$ even when $q^{2\prime} \to O(x-0)$. For regions where both $q^2 \to 0$ and $q^{2\prime} \to 0$, $\zeta \to 0$ and $\nu + \frac{1}{2} \to 0$, thus the asymptotic expansions (6.2)—(6.5) are not applicable. The coupling coefficients C_{ij}^1 and C_{ij}^2 are singular in this region and (6.1) is solved with $m = 3$. The parabolic cylindrical functions $U_\nu^j(\zeta)$ for $\zeta \to 0$ and $\nu + \frac{1}{2} \to 0$ are readily evaluated in terms of a series of ascending power of ζ.[9]

To determine which of the 3 formulations of (6.1) is

used to solve for the wave amplitudes ϕ_i in any particular region, it is necessary to examine the independent variables ξ, (4.6a) or (4.9b) and ξ, (4.4b).[8] For $|\zeta| < 0.5$ we set $m=3$ in (6.1) when $|\nu+\frac{1}{2}|<0.5$, and $m=1$ when $|\nu+\frac{1}{2}|>0.5$. However, for $|\zeta|>0.5$, we set $m=2$ when $|\xi|<0.5$, and $m=1$ when $|\xi|>0.5$.

At an interface $z=z_T$ where a change is made from one formulation of (6.1) to another it is necessary to impose the continuity conditions for the transverse components of the electromagnetic field. Thus for $m, l = 1, 2, 3$,

$$\phi_1^m + \phi_2^m = \phi_1^l + \phi_2^l \tag{6.6a}$$

and

$$G_{11}^m\phi_1^m + G_{22}^m\phi_2^m = G_{11}^l\phi_1^l + G_{22}^l\phi_2^l. \tag{6.6b}$$

Hence at $z=z_T\neq z_s$,

$$\begin{pmatrix}\phi_1^m\\ \phi_2^m\end{pmatrix}=\frac{1}{G_{22}^m-G_{11}^m}\begin{pmatrix}G_{22}^m-G_{11}^l & G_{22}^m-G_{22}^l\\ G_{11}^l-G_{11}^m & G_{22}^l-G_{11}^m\end{pmatrix}\begin{pmatrix}\phi_1^l\\ \phi_2^l\end{pmatrix}. \tag{6.6c}$$

The source term J in (3.4) results in a jump in the value of ϕ_i at the plane $z=z_s$ passing through the line source. Thus on integrating (3.4) with respect to z in the infinitesimal region about $z=z_s$, we get for $m=1$, 2 or 3,

$$\phi_1^m(z_s^+) - \phi_1^m(z_s^-) = I/2\pi Y^T \tag{6.7a}$$

and

$$\phi_2^m(z_s^+) - \phi_2^m(z_s^-) = -I/2\pi Y^T. \tag{6.7b}$$

In solving (3.4) numerically the source term J is set equal to zero and conditions (6.7) are imposed at $z=z_s$.

7. CHARACTERISTIC WAVE PARAMETERS FOR AN INHOMOGENEOUS DIELECTRIC SLAB

We consider here an inhomogeneous dielectric slab of thickness L bounded by semi-infinite homogeneous media $\epsilon=\epsilon_1$ for $z\leq 0$ and $\epsilon=\epsilon_2$ for $z\geq L$ and assume that the slab is excited by a horizontally polarized wave incident from below the slab ($z<0$) at an angle θ_1 given by

$$\sin\theta_1 = S_1 = \beta/k_1. \tag{7.1}$$

From the continuity conditions for the transverse electromagnetic fields at $z=0$ and $z=L$ we get

$$\begin{pmatrix}a(\beta,0)\\ b(\beta,0)\end{pmatrix}=\frac{1}{2ik_1C_1}\times\begin{pmatrix}ik_1C_1-G_1(\beta,0) & ik_1C_1-G_2(\beta,0)\\ ik_1C_1+G_1(\beta,0) & ik_1C_1+G_2(\beta,0)\end{pmatrix}\begin{pmatrix}\phi_1(\beta,0)\\ \phi_2(\beta,0)\end{pmatrix} \tag{7.2}$$

and

$$\begin{pmatrix}\phi_1(\beta,L)\\ \phi_2(\beta,L)\end{pmatrix}=\frac{a(\beta,L)}{G_2(\beta,L)-G_1(\beta,L)}\begin{pmatrix}G_2(\beta,L)+ik_2C_2\\ -G_1(\beta,L)-ik_2C_2\end{pmatrix}, \tag{7.3}$$

in which $a(\beta,0)$ and $b(\beta,0)$ are the amplitudes of the incident and specularly reflected waves at $z=0$, $a(\beta,L)$ is the amplitude of the transmitted wave at $z=L$, and

$$\beta = k_i(1-C_i^2)^{1/2},\quad k_i=\omega(\mu_0\epsilon_i)^{1/2},$$

$$\mathrm{Im}(k_i)\leq 0,\quad \mathrm{Im}(\beta)\leq 0,\quad \mathrm{Im}(C_i)\leq 0,\quad i=1,2. \tag{7.4}$$

Thus the reflection coefficient at the reference surface $z=0$ is

$$R(\beta) = b(\beta,0)/a(\beta,0), \tag{7.5a}$$

and the transmission coefficient is

$$T(\beta) = a(\beta,L)/a(\beta,0). \tag{7.5b}$$

The characteristic surface impedance is defined as the ratio $-E_y/H_x$, thus for $z=0$,

$$\begin{aligned}Z_s(\beta) &= (\eta_1/C_1)[1+R(\beta)]/[1-R(\beta)]\\ &= [\phi_1(\beta,0)+\phi_2(\beta,0)]/[Y_1(\beta,0)\phi_1(\beta,0)\\ &\quad - Y_2(\beta,0)\phi_2(\beta,0)],\end{aligned} \tag{7.6}$$

in which $\eta_i=\sqrt{\mu_0\epsilon_i}$ is the intrinsic impedance. When the layered dielectric structure supports trapped waveguide modes (conditions for total internal reflection within the slab are satisfied) the reflection coefficient $R(\beta)$ is a singular function of β. Thus the wave parameters β_s associated with the guided waves satisfy

$$1/R(\beta_s)=0,\quad \mathrm{Im}(C_i)\leq 0\ (i=1,2), \tag{7.7a}$$

and the surface wave contributions to the fields are obtained by evaluating the residues of the integrand in (2.4a) at the singular points $\beta=\beta_s$. The surface waves can be excited by an electric line source (2.2) or by an incident plane wave provided there are lateral inhomogeneities in the dielectric slab.[11]

Since the coupled differential equations (3.6) can be solved numerically with $z=L$ as the initial point we can set $a(\beta,L)=1$ for convenience, thus $T(\beta)=1/a(\beta,0)$ and condition (7.7) reduces to

$$a(\beta_s,0)=1/T(\beta_s)=0. \tag{7.7b}$$

The realizability condition, when the sources are below the dielectric slab, is obtained from energy considerations. For all $z\geq 0$,

$$\mathrm{Re}(-E_yH_x^*)=\mathrm{Re}\,|\phi_1+\phi_2|^2/Z_s^*\geq 0, \tag{7.8a}$$

hence $\mathrm{Re}(Z_s)=R_s\geq 0$ is consistent with the definition of Z_s (7.6) and

$$\mathrm{Re}\left(1-|R|^2+R-R^*\right)\frac{C_1^*}{\eta_1^*}\geq \mathrm{Re}\left(|T|^2\frac{C_2^*}{\eta_2^*}\right)\geq 0, \tag{7.8b}$$

in which the symbol * denotes complex conjugate. If ϵ_1 and ϵ_2 are real and both $S_1=\beta/k_1$ and $S_2=\beta/k_2$ are real and less than unity (uniform plane waves above and below the slab), (7.8b) reduces to

$$(1-|R|^2)\,C_1/\eta_1 \geq |T|^2\,C_2/\eta_2, \tag{7.8c}$$

in which C_i and η_i are real, and for a nondissipative dielectric slab the equal sign is used. When $S_1<1$ and $S_2>1$, C_2 is imaginary and (7.8b) becomes

$$(1-|R|^2)\geq 0. \tag{7.8d}$$

For a nondissipative slab this case corresponds to total internal reflection of the incident power and

$$|R|^2=1. \tag{7.8e}$$

When the source is near the lower boundary of the dielectric slab it is necessary to account for the excitation of evanescent waves characterized by $S_1 > 1$. In this case C_1 is imaginary, and, if $S_2 > 1$, (7.8b) becomes

$$\mathrm{Im}(R) \leq 0, \tag{7.8f}$$

with $\mathrm{Im}(R) = 0$ for a nondissipative slab. However, for $S > 1$ and $S_2 < 1$ some energy is transmitted to the region $z > L$, even though the incident wave is evanescent. In this case (7.8b) reduces to

$$(2|C_1|/\eta_1)\mathrm{Im}(-R) \geq |T|^2 C_2/\eta_2, \tag{7.8g}$$

in which the equal sign is used for nondissipative slabs.

In view of the normalization used in (2.4) and (3.1) the reciprocity relationship in electromagnetic theory is

$$T_1(\beta)\, C_1/\eta_1 = T_2(\beta) C_2/\eta_2, \tag{7.9}$$

in which $T_1(\beta)$ and $T_2(\beta)$ are the transmission coefficients for waves incident from below and above the dielectric slab respectively.

We conclude this section with an illustrative example. Consider a horizontally stratified ionized slab of permittivity,

$$\epsilon(z) = \epsilon_0 n^2(z) = \epsilon_0(1 - X(z)), \quad 0 \leq z \leq L, \tag{7.10a}$$

and assume that $\epsilon = \epsilon_0$ for $z < 0$ and $z > L$. Thus (2.8c), i.e.,

$$q^2(z) = C^2 - X(z), \tag{7.10b}$$

where

$$X(z) = (\omega_p/\omega)^2 = X_1 \sin \tau z, \tag{7.10c}$$

and ω_p is the plasma frequency. Thus by setting

$$X_1 = C^2, \quad \tau = \pi/2L, \tag{7.10d}$$

the permittivity profile (7.10) contains a critical coupling point at $z_c = L$ where both $q^2 = 0$ and $q^{2\prime} = 0$. The dielectric slab is assumed to be excited from below ($z < 0$) by uniform plane waves at angles of incidence θ. Thus

$$0 \leq C^2 = \cos^2\theta \leq 1. \tag{7.10e}$$

The computer program used to calculate the reflection and transmission coefficients $R(\beta)$ and $T(\beta)$ respectively, (7.5), and the surface impedance $Z_s(\beta)$, (7.6), is based on the representation of q^2 in terms of K, ν, and ξ as given by Eqs. (4.5)—(4.7). Thus the coupling coefficients C_{ij}, (3.7b), are obtained from (5.4) using (4.8a) for dz_0/dz and setting $dK/dz = 0$ and $d\nu/dz = 0$. The numerical solutions are subjected to the energy conservation test, (7.8c), and the reciprocity test, (7.9). For the special case considered, $\epsilon_1 = \epsilon_2 = \epsilon_0$, and $\mathrm{Im}[\epsilon(z)] = 0$, thus (7.8c) reduces to

$$1 - |R|^2 = |T|^2, \tag{7.11a}$$

and (7.9) reduces to

$$T_1(\beta) = T_2(\beta). \tag{7.11b}$$

To obtain $T_2(\beta)$, instead of exciting the dielectric slab from above ($z > L$) it is simpler to invert the permittivity profile. Thus (7.10c) is replaced by

$$X(z) = X_1 \sin\tau(L - z), \tag{7.12}$$

and therefore for this case the critical coupling point is at $z_c = 0$. These computations are shown to satisfy both reciprocity and energy conservation relationships to at least three significant figures. For the profile considered with $L = 0.5$ wavelengths, the computer program uses all three formulations ($m = 1, 2, 3$) of the coupled differential equations, the transition equations (6.6c), and the boundary conditions (7.2) and (7.3) (see Sec. 6). The electromagnetic field components E_y and H_x and the propagation parameters $R(\beta)$, $T(\beta)$, and $Z_s(\beta)$ for each angle of incidence θ are computed in 2.5 seconds. Results of these computations are given in Table I.

TABLE I. Numbers in parentheses are for inverted permittivity profile (7.12).

θ	$R(\beta)$	$T(\beta)$	$Z_s(\beta)/\eta$
0	$.197 - i.575$ $(.492 + i.357)$	$-.240 - i.757$ $(-.240 - i.757)$	$.646 - i1.18$ $(1.64 + i1.85)$
$9\pi/100$	$.254 - i.543$ $(.478 + i.363)$	$-.192 - i.776$ $(-.192 - i.776)$	$.752 - i1.28$ $(1.58 + i1.79)$
$19\pi/100$	$.405 - i.396$ $(.422 + i.378)$	$-.019 - i.824$ $(-.019 - i.824)$	$1.33 - i1.55$ $(1.43 + i1.59)$
$29\pi/100$	$.475 - i.094$ $(.305 + i.376)$	$.297 - i.823$ $(.297 - i.823)$	$2.69 - i.659$ $(1.23 + i1.20)$
$39\pi/100$	$.262 + i.169$ $(.125 + i.285)$	$.721 - i.617$ $(.721 - i.617)$	$1.57 + i.588$ $(1.07 + i.673)$

8. CONCLUDING REMARKS

A generalized WKB approach has been applied to determine the excitation of horizontally polarized waves by an electric line source in an inhomogeneous dielectric with critical coupling regions in which the gradient of the permittivity profile also vanishes. This method is based on the conversion of Maxwell's equations into a set of ordinary first-order differential equations for the wave amplitudes ϕ_i which are related to the electromagnetic field transforms through the wave admittances Y_i, (3.1). To facilitate the solution of these equations, the expressions chosen for the wave admittances locally depict the principal characteristics of the permittivity profile. To this end the inhomogeneous dielectric is subdivided, in general, into three regions. For slowly varying media devoid of critical coupling regions $|\zeta| > 0.5$ and $|\xi| > 0.5$, we set $Y_i = q/\eta_0$ where η_0 is the free space intrinsic impedance. For critical coupling regions ($q^2 \approx 0$) where $\alpha = (q^2)'$ does not approach zero, $|\zeta| > 0.5$ and $|\xi| < 0.5$, the local wave admittances are given by (3.2) with (4.4a) substituted for $\ln' g_i = G_{ii}$. These two regions were dealt with in an earlier analysis of the problem.[7] Since the formulation of the solution in terms of the coupled wave amplitudes (3.4) is rigorous, numerical solutions for the reflection and transmission coefficients $R(\beta)$ and $T(\beta)$ have been computed accurately to five significant figures as evidenced by reciprocity and energy conservation tests.[8] A program has been written to compute the electromagnetic fields in an inhomogeneous dielectric slab together with the surface impedance and the reflection and transmission

coefficients for an incident plane wave. The exection time for a single incident plane wave is less than one second for either nondissipative or dissipative dielectrics. If the coupling terms C_{ij} are neglected (as is done when approximate procedures are used), good agreement with energy conservation and reciprocity relationships is not achieved.

The earlier analysis of the problem[7] and the computer program based upon it is not suitable for inhomogeneous dielectrics with critical coupling regions ($q^2 \to 0$) where $\alpha = (q^2)' \to 0$, since the coupling coefficients C_{ij} become singular. This limitation has been removed in our present analysis through an appropriate choice of the local wave admittances Y_i. Thus for critical coupling regions where $q^2 \to 0$ and $\alpha \to 0$, $|\xi| < 0.25$, Y_i is given by (3.2) upon substituting (4.11a) for $G_{ii} = \ln' g_i$. Two different local characterizations of the q^2 profile [(4.5a) and (4.9a)] are considered in detail and the corresponding coupling coefficients C_{ij} are derived (Sec. 5). By using (4.5a), for instance, it is shown that $C_{ij} \to 0$ as both q^2 and α approach zero. Thus the present formulation of the first-order differential equations (3.4), for the wave amplitudes is readily solved using standard numerical techniques,[8] even for regions where $q^2 \to 0$ and $\alpha \to 0$. (Sec. 7).

In Sec. 6 several uniform asymptotic expansions for the parabolic cylindrical function $D_\nu(\xi)$ have been presented to demonstrate that the local wave solutions for parabolic permittivity profiles merge with those derived earlier for regions where $q^{2\prime} \not\approx 0$. However, to numerically solve (3.6), it is not necessary to evaluate any of these asymptotic expressions. The parabolic cylindrical functions $D_\nu(\xi)$ are used only in regions of the permittivity profiles where $|\nu + \frac{1}{2}| < 0.5$ and $|\xi| < 0.5$ ($q^2 \to 0$, $q^{2\prime} \to 0$) and the Airy integral functions $w_i(\xi)$ are used only in regions where $\xi \to 0$ ($q^2 \to 0$, $q^{2\prime} \neq 0$). Thus only series expansions of $D_\nu(\xi)$ and $w_i(\xi)$ in ascending power of the arguments ξ and ξ respectively are needed for the purpose of the numerical computations. Realizability and reciprocity relationships for inhomogeneous dielectric slabs are examined and expressions for the reflection and transmission coefficients and the characteristic surface impedance have been derived as functions of the transverse wavenumber β. The surface waves supported by the inhomogeneous dielectric are shown to be characterized by the wave parameters β_s given by $1/R(\beta_s) = 0$, (7.7a).

It is interesting to note that the technique used to transform Maxwell's equations into sets of ordinary first-order differential equations for the wave amplitudes is also used in solving problems of propagation in irregular waveguide structures.[12] The advantages of employing basis functions (and corresponding wave admittances) that locally depict the principal characteristics of the irregular guiding structure have been examined for waveguide bends and transition sections.[13,14]

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[1] H. Bremmer, *Terrestrial Radio Waves* (Elsevier, Amsterdam, 1949).
[2] K.G. Budden, *Radio Waves in the Ionosphere* (Cambridge U.P., London, 1961).
[3] J.R. Wait, *Electromagnetic Waves in Stratified Media* (Pergamon, Oxford, England, 1962).
[4] D.S. Jones, *The Theory of Electromagnetism* (Pergamon, New York, 1964).
[5] L. Felsen and N. Marcuvitz, *Radiation and Scattering of Waves, Microwave and Fields Series*, edited by N. Marcuvitz (Prentice-Hall, Englewood Cliffs, New Jersey, 1973).
[6] Y. Inoue and S. Horowitz, Radio Sci. 1 (New Series), 957 (1966).
[7] E. Bahar, J. Math. Phys. 8, 1735 (1967).
[8] E. Bahar, G. Govindarajan, and B.S. Agrawal, Radio Sci. 10, 197 (1975).
[9] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*, Appl. Math. Ser. 55, (Natl. Bur. Stand. U.S. GPO, Washington, D.C., 1964).
[10] F.W.J. Olver, J. Res. Natl. Bur. Stand. Sect. 63B, 131 (1959).
[11] E. Bahar and G. Govindarajan, J. Geophys. Res. 78, 393 (1973).
[12] S.A. Schelkunoff, Bell Sys. Tech. J. 34, 995 (1955).
[13] E. Bahar and G. Govindarajan, IEEE Trans. Microwave Theory Tech. MTT-21, 819 (1973).
[14] E. Bahar and G. Govindarajan, Proc. IEE 121, 443 (1974).

Generalized molecular distribution functions for fluids and occupation probabilities for lattice gases

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The generalized distribution functions $\sigma_n(\omega)$ specify the probability of finding a subset of n molecules in a specified configuration and simultaneously a subvolume empty of all other molecules, whereas the conventional distribution functions ρ_n specify only the configuration. The Mayer integral equation theory for the ρ_n is generalized assuming short-range intermolecular forces to express both the ρ_n and σ_n as sums of integrals over the σ_n and a kernel dependent on the forces. For the nearest-neighbor lattice gas, certain of these relations are equivalent to those obtained by Widom and Van Leeuwen for the probabilities f_n that an empty site is surrounded by n filled sites. The intimate relation of these relations, the Kirkwood–Salsburg integral equations, and the generalized distribution functions is thus displayed.

1. INTRODUCTION

The distribution functions usually employed in equilibrium classical statistical mechanics are defined by the statement that $\rho_n(\{n\})$ is the probability of finding a set of n molecules in the arbitrary configuration $\{n\}$. Occasionally certain generalized distribution functions have been used. An example is the function $\sigma_n(\{n\}|\,\omega)$, which is the probability of finding a set of n molecules in the arbitrary configuration $\{n\}$ and simultaneously a particular subvolume ω of the system empty of all molecules except possibly for members of set n with specified configurations. A further example is the occupation probability obtained by averaging σ_n over all configurations of set n within ω. Such quantities sometimes appear as adjuncts in the derivation of results involving the conventional distribution functions, for example in the derivation of fluctuation theorems.[1,2] They have also been studied in their own right in order to obtain alternative descriptions of the properties of classical fluids.[3–5]

In Secs. 2 and 3 of the present paper we use the methods of Mayer's theory of integral equations[6] to give a compact derivation of various integral relations between the two kinds of distribution functions assuming short-range intermolecular forces. The results express each ρ_n as a sum of integrals containing σ_m functions and a kernel dependent on the forces. The set of formal relations derived here is more complete than that presented in earlier papers, and the derivation allows a clearer view of how the generalized distribution functions fit into the ordinary integral equation theory. One advantage of the development is that it leads in an obvious way to new integral relations involving only σ distribution functions. These are given in Sec. 4.

It is shown in Sec. 5 that for the particular case of a nearest-neighbor lattice gas some of the results in Secs. 3 and 4 reduce to equations derived by Widom[7] using an unconventional method of studying certain averages of the potential energy of a test particle. The equations contain the probability f_n that an empty site is surrounded by exactly n filled sites. For a lattice with Z nearest neighbors per site the four equations relate the $Z+1$ occupation probabilities to the internal energy function, the activity, the concentration, and to ϵ/kT, where $-\epsilon$ is the nearest neighbor interaction energy. For $Z=3$ the thermodynamic functions determine the f_n completely and for $Z=2$ they imply a certain partial differential equation for the grand partition function. Van Leeuwen[8] rederived these results in a more conventional manner and obtained additional results including a relation between next-nearest-neighbor correlations and the functions f_n. We refer to his paper for a full discussion of the significance of these results. There appear to have been no other studies of this very economical and graphic description of a lattice gas, perhaps partly because the functions f_n do not seem to occur naturally in conventional statistical mechanical procedures. One of the main objectives of the present formalism is to display the intimate relationship of the Widom results both to the Kirkwood–Salsburg integral equations,[9] which are a subset of the Mayer equations, and to the theory of generalized distribution functions for fluids.

2. DISTRIBUTION FUNCTIONS IN THE PRESENCE OF AN EXTERNAL FIELD

A. Molecular distribution functions $\rho_n(\varphi)$

We consider a system of volume V, temperature T, and activity z in the presence of an external field φ. The potential energy due to this field of a set of n molecules in configuration $\{n\}$ is denoted by $\varphi_n(\{n\})$. The grand canonical ensemble results for the partition function $\Xi(\varphi)$ and the conventional distribution function $\rho_n(\{n\}|\,\varphi)$ giving the probability that there is a set of n molecules at the coordinates $\{n\}$ within the volume element $d\{n\}$ are summarized by[6]

$$G_n(\varphi)=\sum_{m\geq 0}(z^m/m!)\int_V G^0_{n+m}(\varphi)\,d\{m\}, \tag{2.1}$$

where

$$G_n(\varphi)=\Xi(\varphi)\rho_n(\{n\}|\,\varphi)/z^n, \tag{2.2}$$

$$G^0_n(\varphi)=G^0_n\exp[-\varphi_n(\{n\})/kT], \tag{2.3}$$

$$G^0_n=\exp[-U_n(\{n\})/kT]. \tag{2.4}$$

U_n is the potential energy of the set of n molecules apart

from the contribution from the external field φ. The convention used here that $G_n^0(\varphi=0)$ is written simply as G_n^0 is applied to all functions φ. The convention $\rho_0=1$ is also used. The inverse of (2.1) is

$$G_n^0(\varphi)=\sum_{m\geq 0}[(-z)^m/m!]\int_V G_{n+m}(\varphi)\,d\{m\}. \tag{2.5}$$

The generalization to multicomponent systems of these equations and the ones which follow can be made very simply following Mayer's method.[6]

Equations (2.1) and (2.5) can be combined to give

$$G_n(\varphi)=\sum_{m\geq 0}\frac{z^m}{m!}\int_V \frac{G_{n+m}^0(\varphi)}{G_{n+m}^0}\times\left(\sum_{l\geq 0}\frac{(-z)^l}{l!}\int_V G_{n+m+l}\,d\{l\}\right)d\{m\}. \tag{2.6}$$

In this equation we next replace l by $p-m$ and note that

$$\sum_{m\geq 0}\sum_{p-m\geq 0}\cdots=\sum_{p\geq 0}\sum_{m=0}^{p}\cdots \tag{2.7}$$

so that the result is

$$G_n(\varphi)=\sum_{p\geq 0}(z^p/p!)\int_V G_{n+p}K^0_{p+n,n,0}(\varphi)\,d\{p\}, \tag{2.8}$$

where the kernels are defined by

$$K^0_{p+n,n,k}(\varphi)=(\sum\{m\}_p)(-)^{p-m}G^0_{m+n+k}(\varphi)/G^0_{m+n}. \tag{2.9}$$

The summation $(\sum\{m\}_p)$ is over all the possible subsets $\{m\}_p$ of the set p. There are $p!/m!(p-m)!$ different distinct subsets of size m.

When φ_n for any set of n molecules has the form

$$\varphi_n(\{n\})=\sum_{i\subset n}\varphi_1((i)), \tag{2.10}$$

then Eq. (2.8) reduces to the basic equation of the functional formalism as used by Münster and others.[10,11] Here (i) denotes the configuration of molecule i and the summation is over all molecules of the set n. Equation (2.8) is not one of the Mayer equations[6] but is a convenient generalization.

B. Generalized distribution functions σ_n (ω,φ)

We define $\sigma_n(\{n\}|\,\omega,\varphi)$ to be the probability that in a system in the field a set of n molecules will be found at the coordinates $\{n\}$ and simultaneously a particular subvolume ω be empty of all molecules except possibly for members of set n. By arguments similar to those which lead to Eq. (2.1) we can obtain

$$Q_n(\omega,\varphi)=\sum_{m\geq 0}(z^m/m!)\int_{V-\omega}G^0_{n+m}(\varphi)\,d\{m\}, \tag{2.11}$$

where the abbreviation

$$Q_n(\omega,\varphi)=\text{≋}(\varphi)\sigma_n(\{n\}|\,\omega,\varphi)/z^n \tag{2.12}$$

has been used. The positions of the molecules of set m in the integral are constrained by the limits of integration to the volume V minus its subvolume ω.

C. Relationships between ρ_n and σ_n functions

Now suppose that an external field is applied which is nonzero only within the subvolume ω. We denote such a field by $\varphi(\omega)$ and the potential energy due to this field of a set of n molecules in configuration $\{n\}$ by $\varphi_n(\{n\}|\,\omega)$. It is straightforward to show that the kernel $K^0_{p+n,n,0}(\varphi(\omega))$ is zero if any molecule of the set p is outside of the subsubvolume ω. Hence the integral equation (2.8) can be written in the form

$$G_n(\varphi(\omega))=\sum_{p\geq 0}(z^p/p!)\int_\omega G_{n+p}K^0_{p+n,n,0}(\varphi(\omega))\,d\{p\}, \tag{2.13}$$

where the range of integrations is restricted to the subvolume ω.

For the purposes of the present paragraph only consider a particular external field $\varphi(\omega)$ such that the potential energy due to this field of any set of molecules assumes the form in Eq. (2.10). It follows from Eq. (2.1) that the function

$$G'_n(\varphi(\omega))\equiv G_n(\varphi(\omega))/\exp[-\varphi_n(\omega)/kT] \tag{2.14}$$

can be calculated from

$$G'_n(\varphi(\omega))=\sum_{m\geq 0}(z^m/m!)\int_V G^0_{n+m}\exp[-\varphi_m(\omega)/kT]\,d\{m\}. \tag{2.15}$$

For the case of a field such that $\varphi_1(\omega)\to\infty$ everywhere with ω for any molecule, the right-hand side of Eq. (2.15) is seen, by comparison with (2.11), to be equal to $Q_n(\omega)$. Hence, by dividing both sides of Eq. (2.13) by $\exp[-\varphi_n(\omega)/kT]$ and considering the same kind of field one obtains an expression for $Q_n(\omega)$. The function $K^0_{p+n,n,0}(\varphi(\omega))/\exp[-\varphi_n(\omega)/kT]$ therein is equal to $(-1)^p$ when the members of set p are all within ω and so the result is

$$Q_n(\omega)=\sum_{p\geq 0}[(-z)^p/p!]\int_\omega G_{n+p}\,d\{p\}. \tag{2.16}$$

The inverse of the last equation is

$$G_n=\sum_{m\geq 0}(z^m/m!)\int_\omega Q_{n+m}(\omega)\,d\{m\} \tag{2.17}$$

as can be verified by substitution for Q in (2.17) using (2.16).

The functions G_{n+p} can now be eliminated from the expansion of $G_n(\varphi(\omega))$, Eq. (2.13), by substituting the definition of the kernel functions K^0 and the identity for summations in Eq. (2.7). By employing Eq. (2.16) one obtains the result

$$G_n(\varphi(\omega))=\sum_{m\geq 0}(z^m/m!)\int_\omega \exp[-\varphi_{n+m}(\omega)/kT]Q_{n+m}(\omega)\,d\{m\}. \tag{2.18}$$

The inverse is

$$\exp[-\varphi_n(\omega)/kT]Q_n(\omega)=\sum_{m\geq 0}[(-z)^m/m!]\int_\omega G_{n+m}(\varphi(\omega))\,d\{m\}. \tag{2.19}$$

The principle results of this section are Eqs. (2.18) and (2.19) which reduce to (2.17) and (2.16) for $\varphi=0$. The latter equations were previously obtained by Squire and Salsburg[4] in a different way.

3. INTEGRAL RELATIONS BETWEEN THE ρ_n AND σ_n

Integral equations for the various distribution functions can be obtained by identifying the external field of the previous section as being due to a set of k molecules fixed in configuration $\{k\}$. In that case we have

$$\varphi_n(\{n\}) = U_{n:k}(\{n\}:\{k\}), \tag{3.1}$$

where

$$U_{n:k}(\{n\}:\{k\}) = U_{n+k}(\{n+k\}) - U_n(\{n\}) - U_k(\{k\}). \tag{3.2}$$

Equations (2.1) and (2.8) then give

$$G_k^0 G_n(\varphi) = G_{n+k} = \sum_{p\geq 0} (z^p/p!) \int_V G_{n+p} K^0_{p+n,n,k}\, d\{p\}. \tag{3.3}$$

These are the Mayer integral equations[6] for the distribution functions G. For a system with pairwise intermolecular forces the set of equations with $n=0$ and $k \geq 1$ is equivalent to the Mayer–Montroll hierarchy[3] and the set with $k=1$ and $n \geq 0$ is equivalent to the Kirkwood–Salsburg hierarchy.[9]

The same identification of the external field as being due to a set of k fixed molecules can be used in Eq. (2.18). In this case we assume that the range of interactions has a cutoff so that for a set of k molecules in configuration $\{k\}$ we may define a subvolume, $\omega(\{k\})$, such that any other molecule has nonzero energy of interaction with set k if and only if it is within the subvolume. Equation (2.18) then reduces to

$$G_{n+k} = \sum_{m\geq 0} (z^m/m!) \int_V Q_{n+m}(\omega(\{k\})) \times (G^0_{n+m+k}/G^0_{n+m}) \Delta_m(\omega(\{k\}))\, d\{m\}, \tag{3.4}$$

where the function $\Delta_m(\omega(\{k\}))$, which is unity when all molecules of set m are within $\omega(\{k\})$ and is zero otherwise, has been introduced to avoid a complicated subscript on the integral sign.

The last equation can also be derived directly from the Mayer equations (3.3) by similar steps to those used to obtain (2.18) from (2.13). An equation equivalent to (3.4) with $k=1$ and $n=0$ has been obtained by Squire and Salsburg[4] from the corresponding Kirkwood–Salsburg equation for pairwise forces. The attraction of Eqs. (3.4) compared with the Mayer equations is that the number of nonzero terms on the right is much less at least for short-range forces.[4] The strikingly compact results of Widom for the lattice gas[7,8] are an example of this as we shall see in Sec. 5. The difficulty is to find a self-contained method for calculating the functions Q_n, and this has never been satisfactorily solved. It is interesting that the present method leads to certain relations involving only the Q_n functions as follows.

4. INTEGRAL RELATIONS BETWEEN THE FUNCTIONS σ_n ALONE

The steps which lead from (2.1) to (2.8) and (2.16)–(2.19) can be applied to the basic equation for Q_n, Eq. (2.11). The results are

$$Q_n(\omega, \varphi) = \sum_{p\geq 0} (z^p/p!) \int_{V-\omega} Q_{n+p}(\omega) K^0_{p+n,n,0}(\varphi)\, d\{p\}, \tag{4.1}$$

$$Q_n(\omega, \varphi(\omega')) = \sum_{m\geq 0} (z^m/m!) \int_{\omega'-\omega} \exp[-\varphi_{n+m}(\omega')/kT] \times Q_{n+m}(\omega+\omega')\, d\{m\}, \tag{4.2}$$

$$\exp[-\varphi_n(\omega')/kT] Q_n(\omega+\omega') = \sum_{m\geq 0} [(-z)^m/m!] \times \int_{\omega'-\omega} Q_{n+m}(\omega, \varphi(\omega'))\, d\{m\}, \tag{4.3}$$

$\omega' - \omega$ denotes the subvolume ω' minus any part of it which is common to the subvolume ω. Equations (4.1)–(4.3) with $\omega = 0$ are equivalent to Eqs. (2.8), (2.18), and and (2.19), respectively. Equations (4.2) and (4.3) with $\varphi = 0$ give two further equations which are equivalent to (2.17) and (2.16) for $\omega = 0$.

5. WIDOM'S RELATIONS FOR A LATTICE GAS

We consider an homogeneous lattice gas in which the interaction potential for a pair of particles is $-\epsilon$ ($\epsilon > 0$) when they are nearest neighbors, ∞ when they are on the same site, and zero otherwise. Integration signs are now interpreted as appropriate lattice summations. The subvolume $\omega(\{k\})$ for a single particle i in configuration (i) will be written

$$\omega(i) = S(i) + Z(i), \tag{5.1}$$

where $S(i)$ denotes the particular site occupied by the atom and $Z(i)$ denotes the Z sites nearest-neighbor to that site. Finally, we define

$$x = \exp(\epsilon/kT), \quad u = -U/N\epsilon, \tag{5.2}$$

where U is the mean potential energy.

Two of Widom's relations follow almost at once from Eq. (3.4). When set k comprises a single particle labelled (i), Eq. (3.4) reduces to

$$\rho_{n+1}(\{n\}, (i))/z = \exp[-U_{n:1}(\{n\}:(i))/kT] \times \Big(\sum_{m=0} x^m p_{m/n}(\{n\}|(i))\Big), \tag{5.3}$$

where

$$p_{m/n}(\{n\}|(i)) = (m!)^{-1} \int_V \sigma_{m+n}(\{m+n\}|\, \omega(i)) \times \Delta_m(Z(i))\, d\{m\}. \tag{5.4}$$

$\Delta_m(Z(i))$ is unity when all members of set m are on the specified Z nearest-neighbor sites and is zero otherwise. Thus $p_{m/n}(\{n\}|(i))$ is the probability of finding n particles in configuration $\{n\}$ and simultaneously a particular site $S(i)$ empty and with exactly m nearest-neighbor particles in addition to any members of set n which are nearest neighbors.

For $n=0$ Eq. (5.3) is equivalent to the Widom relation

$$\rho/z(1-\rho) = \Big(\sum_{m=0}^{z} x^m f_m\Big), \tag{W1}$$

where $f_m = p_{m/0}(1-\rho)^{-1}$ is the probability that a vacant site has exactly m particles as nearest neighbors and ρ is the fraction of sites occupied by particles.

When the particle of set 1 is a nearest neighbor to $S(i)$, one can obtain from (5.4)

$$Zp_{m/1}=(m+1)p_{(m+1)/0}. \tag{5.5}$$

For $n=1$ Eq. (5.3) for the pair distribution function ρ_2 for two nearest-neighbor particles can then be reduced to

$$\rho_2=z(1-\rho)(\sum_{m=0}^{Z} mx^m f_m)/Z. \tag{5.6}$$

This leads to Widom's relation for the internal energy

$$2\rho u/z(1-\rho)=(\sum_{m=0}^{Z} mx^m f_m). \tag{W2}$$

For $Z>2$ one cannot, of course, express $p_{m/n}$ $(n\geq 2)$ in terms of the f_m, and so the theory of the higher order distribution functions introduces parameters additional to the f_m. However, from (5.3), one average can always be calculated from the f_m:

$$\int_V \rho_{n+1}(\{n\},(i))\Delta_n(Z(i))\,d\{n\}$$
$$=z\sum_{l=0}^{Z} l(l-1)\cdots(l-n+1)x^l p_{l/0}, \quad n\leq Z. \tag{5.7}$$

For $n=0,1$ this is equivalent to (W1) and (5.6).

The two remaining Widom relations and an additional result due to van Leeuwen follow in the present context from (4.2) with $\varphi=0$:

$$\sigma_n(\omega)=\sum_{m=0} (m!)^{-1}\int_{\omega'-\omega} \sigma_{n+m}(\omega+\omega')\,d\{m\}. \tag{5.8}$$

The choice $n=0$, $\omega=S(i)$, $\omega'-\omega=Z(i)$ leads at once to the obvious normalization condition

$$\sum_{m=0}^{Z} f_m=1 \tag{W3}$$

when it is recalled that $\sigma_0(S(i))$ is $(1-\rho)$. The derivation of the remaining equations can be simplified by introducing[8,12]

$$\begin{aligned}\rho g_m&=(m!)^{-1}\int_V \sigma_{1+m}((i),\{m\}|\,\omega(i))\Delta_m(Z(i))\,d\{m\},\\ h_m&=(m!)^{-1}\int_V \sigma_m(\{m\}|\,Z(i))\Delta_m(Z(i))\,d\{m\}.\end{aligned} \tag{5.9}$$

g_m is the probability that a particle has exactly m nearest neighbor particles and h_m the probability that a site has exactly m nearest-neighbor particles no matter whether the side is filled or empty. By definition one has

$$h_m=\rho g_m+(1-\rho)f_m \tag{5.10}$$

as can also be derived formally from (5.8). The additional relation

$$\rho g_m=zx^m(1-\rho)f_m \tag{5.11}$$

follows by substituting

$$\sigma_{1+m}((i),\{m\}|\,\omega(i))=$$
$$=z\exp[-U_{m;1}(\{m\}:(i))/kT]\sigma_m(\{m\}|\,\omega(i)) \tag{5.12}$$

into the definition of g_m. The last equation follows directly from the definition of σ functions, Eq. (2.11).

The remaining relations express the fact that the average defined by

$$S_n=\int \rho_n(\{n\})\Delta_n(Z(i))\,d\{n\}, \quad n\leq Z, \tag{5.13}$$

can be expressed in terms of the f_m functions when i is not a member of set n. Substituting for $\rho_n=\sigma_n(0)$ from (5.6) with $\omega=0$ and $\omega'=Z(i)$, one obtains

$$\begin{aligned}S_n&=\sum_{m=0}^{Z} m(m-1)\cdots(m-n+1)h_m\\ &=\sum_{m=0}^{Z} m(m-1)\cdots(m-n+1)\\ &\quad\times[1+zx^m]f_m(1-\rho).\end{aligned} \tag{5.14}$$

For $n=1$ one has $S_1=Z\rho$, and then the last equation combined with (W2) leads to

$$\sum_{m=0}^{Z} mf_m=(Z-2u)\rho/(1-\rho). \tag{W4}$$

For $n=2$ Eq. (5.13) involves at least nearest-neighbor pair correlations. The consequences of this for $Z=3,4$ have been discussed.[8]

The emphasis in the papers on the Widom relations[7,8] was very much on exact properties of the Ising model. The most important missing element is a generalization of the virial theorem to lattice gases which would relate the pressure to ρ_2 or the generalized distribution functions. The present scheme suggests no way of doing this this. It does give integral equations, (4.1)–(4.3), which could be solved approximately for the functions $p_{m/n}$ and hence for the Widom functions f_m. This is a more economic procedure than solving the Kirkwood–Salsburg equations for the ρ_n because it removes the kernel K^0 which has the inconvenient property of being nonzero in configurations in which particles are assigned to the same site.[13] However, as far as we have been able to discover, the functions do not lend themselves to making approximations which appear radically more attractive than those employed in other methods, and the equations are still very unwieldy. Since there are already many approximate methods for the classical lattice gas problems, we do not discuss this further. We have, however, found the scheme relatively advantageous in treating the properties of *dilute* systems of interacting lattice defects such as impurities and vacancies in systems which show order–disorder phenomena in the absence of the defects. This aspect is being studied further because conventional methods for lattice defects[14] are not suited to such systems.

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[1]D. J. Vezzetti, J. Math. Phys. **16**, 31 (1975).
[2]M. Kac and J. M. Luttinger, J. Math. Phys. **14**, 583 (1973).
[3]J. E. Mayer and E. Montroll, J. Chem. Phys. **9**, 2 (1941).
[4]D. R. Squire and Z. W. Salsburg, J. Chem. Phys. **40**, 2364 (1964).
[5]M. S. Green, in *Lectures in Theoretical Physics* (Interscience, New York, 1960), Vol. 3, p. 195.
[6]J. E. Mayer, J. Chem. Phys. **15**, 187 (1947).
[7]B. Widom, J. Chem. Phys. **39**, 2808 (1963).
[8]J. M. J. Van Leeuwen, J. Chem. Phys. **41**, 2959 (1964).
[9]J. G. Kirkwood and Z. W. Salsburg, Discuss. Faraday Soc. **15**, 28 (1953).
[10]E. Lux and A. Münster, Z. Phys. **199**, 465 (1967).
[11]A. Münster, *Statistical Thermodynamics* (Springer-Verlag, Berlin, and Academic, New York, 1969), Vol. 1.
[12]h_n is denoted $\langle 1\rangle_n$ in Ref. 8.
[13]An attempt to solve the Kirkwood–Salsburg equations for a lattice gas leads one fairly rapidly to the invention of the generalized distribution functions $p_{m/n}$!
[14]A. R. Allnatt, Advan. Chem. Phys. **11**, 1 (1966).

The Galilei group and its connected subgroups

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All the connected subgroups of the Galilei group G—and of its central extension $\tilde{G}$—are determined and classified up to a conjugation of G—respectively $\tilde{G}$—and also up to an isomorphism. In order to construct these subgroups, some general properties on subalgebras of a given Lie algebra have been proved. It is interesting to note that the subgroups of $\tilde{G}$ are derived from the subgroups of G.

1. INTRODUCTION

Recently the classification, up to a conjugation, of the connected subgroups of the Poincaré group P has been achieved.[1] As an application of this study, it has been possible to select the connected subgroups of P invariance groups of electromagnetic fields—and also to determine explicitly these fields.[2]

Here a similar classification is undertaken for the Galilei group G.[3] In fact we must distinguish G (ten-parameter group) from its physical extension[4] $\tilde{G}$ (eleven-parameter group).

The knowledge of the connected subgroups of G and $\tilde{G}$ can be used in several types of physical problems, in particular:

(i) A study similar to the one given in Ref. 2 in the relativistic case could be considered, i.e., the classification of the connected Galilei subgroups which are invariance groups of electromagnetic fields and the determination of these corresponding fields.[5] Cases of physical systems placed in an external field have already been studied by the help of representations of their corresponding invariance groups: let us mention the study concerning a nonrelativistic particle in the field of a constant and uniform electromagnetic field[6] and also in the field of an electromagnetic wave in the dipole approximation.[7] The conclusions which are drawn from these group theoretical analyses of elementary particles in an external electromagnetic field gives rise to the interest of a complete study of these invariance groups.

(ii) As is well known, the free Schrödinger equation is invariant under the Galilei group. More precisely, it has been shown by Niederer[8] that the greatest invariance group—acting on space—time—of the free Schrödinger equation is what has been called the Schrödinger group, Sch, a twelve parameter Lie group, which, of course, contains G as a subgroup.[9] Then, the knowledge of the subgroups of G allows us to compute the different types of interaction potentials invariant under subgroups of G and therefore to classify the Schrödinger equations corresponding to systems of particles in interaction, and carrying a symmetry, according to their invariance groups. It must be noticed that, for such an investigation, it is more interesting to know the subgroups of G up to a conjugation under Sch. than up to a conjugation under G itself. However, it can be added that the table of the subgroups of G will project light on the classification of the subgroups of Sch.[10]

(iii) It is worth noticing Ref. 7, in which an interesting use of some subgroups of G is considered in order to find the evolution operator allowing to go from the Schrödinger picture to the Heisenberg one, for systems the Hamiltonian of which possesses as invariance group a subgroup of G whose subgroups have particular properties.

We must add that studies of the closed subgroups H of the Euclidean group E and of the Galilean group G have already been achieved[11]: In these works the authors are interested in the corresponding homogeneous spaces E/H and G/H bearing a bounded invariant measure in view of the description of ergodic states of a C^*-algebra.

Now concerning the following study, let us point out the three following points already mentioned in Ref. 1:

(a) The classification of all the connected subgroups of a connected Lie group G is given by the classification of all the Lie subalgebras of the Lie algebra $\mathcal{G}$ of G.

(b) It is clear that we are interested in subgroups *up to a conjugation*. In fact the subgroups (subalgebras) of G ($\mathcal{G}$) and $\tilde{G}$ ($\tilde{\mathcal{G}}$) will be given + up to a conjugation of G, + up to an isomorphism.

(c) One can remark that if the set of the subalgebras of a Lie algebra $\mathcal{G}$ is a *lattice*, the set of the conjugacy classes is not (in general) a lattice, but only a partially ordered set (p. o. s.) $\Pi(\mathcal{G})$ (order = inclusion).

This paper is built as follows: After recalling some essential properties of the Lie algebras $\mathcal{G}$ and $\tilde{\mathcal{G}}$ (Sec. 2), a general theorem describing the maximal subalgebras of a real Lie algebra is settled (the proof of which is given in Appendix A) and applied to the determination of the maximal subalgebras (sons) of $\mathcal{G}$ (and $\tilde{\mathcal{G}}$) and of the maximal subalgebras of these maximal subalgebras (grandsons) of $\mathcal{G}$ (and $\tilde{\mathcal{G}}$) (Sec. 3).

The classification of the one-dimensional subalgebras of $\mathcal{G}$ and $\tilde{\mathcal{G}}$ by the help of invariants is given in Sec. 4.

It is then shown in Sec. 5 how to deduce simply the subalgebras of $\tilde{\mathcal{G}}$ from the knowledge of the subalgebras of $\mathcal{G}$.

The two last sections are devoted to the determination and classification of the $\mathcal{G}$-subalgebras of dimension between two and six, and of the $\tilde{\mathcal{G}}$-subalgebras of dimension between two and seven. All the results are gathered in several tables.

The Euclidean groups in $\mathcal{G}$ (and $\tilde{\mathcal{G}}$) are specially studied in Appendix B.

2. STRUCTURE OF THE LIE ALGEBRAS $\mathcal{G}$ AND $\tilde{\mathcal{G}}$

A. Group law of G and commutation relations of $\mathcal{G}$ (and $\tilde{\mathcal{G}}$)

Let us write the most general element g of G, $g = (d, \mathbf{c}, \mathbf{b}, R)$, R being a rotation, $\mathbf{b}$ a pure Galilean transformation, $(d, \mathbf{c})$ a space–time translation.[3]

The group law is then

$$g' \cdot g = (d', \mathbf{c}', \mathbf{b}', R)\,(d, \mathbf{c}, \mathbf{b}, R)$$
$$= (d' + d, \mathbf{c}' + R'\mathbf{c} + d\mathbf{b}', \mathbf{b}' + R'\mathbf{b}, R'R). \qquad (2.1)$$

By considering an infinitesimal transformation

$$(d, c, b, R) = 1 - i(\delta, \gamma, \beta, \alpha),$$

the action of G on its Lie algebra $\mathcal{G}$ can be written

$$(d, c, b, R)(\delta, \gamma, \beta, \alpha)(d, \mathbf{c}, \mathbf{b}, R)^{-1}$$
$$= (\delta, \gamma', \beta', \alpha')$$
$$= (\delta, R\gamma + \delta\mathbf{b} - d\,R\beta - (R\alpha) \wedge (\mathbf{c} - d\mathbf{b}), R\beta - (R\alpha) \wedge \mathbf{b}, R\alpha). \qquad (2.2)$$

By the help of the representation (2.1), one deduces the commutation relations of the Lie algebra $\mathcal{G}$ of G. Denoting by J_j, K_j, P_j $(j = 1, 2, 3)$ the rotation, Galilean boosts, space translation generators respectively and by H the time-translation one, the nonzero CR are

$$[J_j, J_k] = i\epsilon_{jkl}J_l, \quad [J_j, K_k] = i\epsilon_{jkl}K_l,$$
$$[J_j, P_k] = i\epsilon_{jkl}P_l, \quad [K_j, H] = iP_j.$$

The CR of $\tilde{\mathcal{G}}$ differ from that of $\mathcal{G}$ only by

$$[K_j, P_l] = i\delta_{jl}mI = i\delta_{jl}M.$$

For the action of $\tilde{G}$ on $\tilde{\mathcal{G}}$, the modification to bear in Eq. (2.2) concerns only the extension part.

$$(\mu, \delta, \gamma, \beta, \alpha)$$
$$\to (\mu + \tfrac{1}{2}d\,\mathbf{b}^2 + R\gamma \cdot \mathbf{b} - R\beta \cdot \mathbf{c} + R\alpha \cdot (\mathbf{b} \wedge \gamma), \delta, \gamma', \beta', \alpha').$$

B. Remarkable decompositions of $\mathcal{G}$ (and $\tilde{\mathcal{G}}$)

It is interesting to remark that $\mathcal{G}$ $(\tilde{\mathcal{G}})$ can be written as a semidirect sum in several different ways (we denote by $\{X, Y, \ldots, Z\}$ the Lie algebra a basis of which is given by $X, Y, \ldots, Z$):

(i) $\mathcal{G} = \{\mathbf{P}, \mathbf{K}, H\} \square \{\mathbf{J}\}$ = Levi's decomposition.[13]

(ii) $\mathcal{G} = \{\mathbf{P}, H\} \square \{\mathbf{J}, \mathbf{K}\}$: This decomposition may remind us the Inonü–Wigner[14] contraction from the Poincaré algebra $\mathcal{P} = \mathcal{T} \square \mathcal{L}$ into the Galilean one, the contraction in which the Lorentz algebra $\mathcal{L}$ is transformed into the Euclidean algebra $E_b(3) = \{\mathbf{J}, \mathbf{K}\}$. (The subscripts τ, s, b mean respectively time, space, and boost.)

(iii) $\mathcal{G} = \{\mathbf{P}, \mathbf{K}, \mathbf{J}\} \square \{H\} = \mathcal{G}' \square \{H\}$, $\mathcal{G}'$ being the derived algebra, also called isochronous Galilean algebra.

(iv) $\mathcal{G} = \{\mathbf{K}, \mathbf{P}\} \square \{\mathbf{J}, H\}$.

Similar decompositions can be given for the extended Galilean algebra $\tilde{\mathcal{G}}$. Denoting by $\mathcal{H}(3)$ the Heisenberg algebra $\{\mathbf{P}, \mathbf{K}, M\}$, the last decomposition becomes $\tilde{\mathcal{G}} = \mathcal{H}(3) \square [\{\mathbf{J}\} \oplus \{H\}]$. We can note the inclusion

$$\tilde{\mathcal{G}} \subset \widetilde{\mathcal{S}ch} = \mathcal{H}(3) \square [\{\mathbf{J}\} \oplus \{H, C, D\}] \subset \mathcal{H}(3) \square \mathcal{S}p(6, R)$$

$\widetilde{\mathcal{S}ch}$ denoting the extended Schrödinger algebra,[9] already mentioned in the Introduction, $\mathcal{S}p(6, R)$ the symplectic algebra acting on the six-dimensional phase space.

All the CR of $\widetilde{\mathcal{S}ch}$ will be known by adding to the CR of $\tilde{\mathcal{G}}$ the following nonzero ones:

$$[C, P_j] = -iK_j, \quad [C, H] = -iD,$$
$$[D, K_j] = iK_j \quad [D, H] = -2iH,$$
$$[D, P_j] = -iP_j, \quad [D, C] = 2iC.$$

C. Ideals and exact sequences

An interesting property of an ideal is that it is *its own conjugacy class*. We note that

$\{\mathbf{J}, \mathbf{K}, \mathbf{P}\}$
$\{H, \mathbf{K}, \mathbf{P}\}$
$\{\mathbf{K}, \mathbf{P}\}$ are ideals of $\mathcal{G}$.
$\{H, \mathbf{P}\}$
$\{\mathbf{P}\}$

In $\tilde{\mathcal{G}}$ we find as ideals

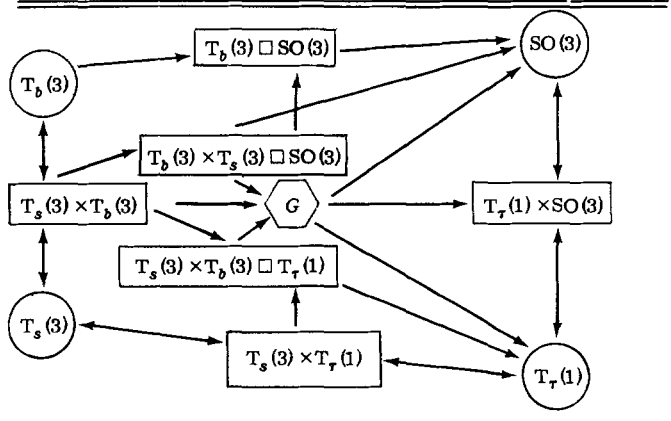
$\{\mathbf{J}, \mathbf{K}, \mathbf{P}, M\}$
$\{H, \mathbf{K}, \mathbf{P}, M\}$
$\{\mathbf{K}, \mathbf{P}, M\}$
$\{H, \mathbf{P}, M\}$
$\{\mathbf{P}, M\}$
$\{M\}$

The corresponding exact sequences[12] are gathered in Table I. Two subgroups do not appear in these decompositions

$$T_s(3) \to T_s(3) \square SO(3) \to SO(3),$$
$$T_\tau(1) \to T_\tau(1) \times T_s(3) \square SO(3) \to T_s(3) \square SO(3).$$

This commutative diagram contains only injective and surjective group homomorphisms.

TABLE I. Exact sequences and ideals of G.



D. Relations between the p.o.s. $\Pi(A)$ and $\Pi(C)$ with $C = B \square A$

Proposition: Let C be a Lie group, semidirect product of two Lie groups A and B, $C = B \square A$. Then two elements of the group A are conjugate under a transformation of C if and only if they are conjugate under a transformation of A. As a consequence the p. o. s. $\Pi(A)$ is a subset of $\Pi(C)$.

By definition of a semidirect product, the group law in $C = B \square A$ can be defined as

$$(b, a)(b', a') = (b * \sigma(a)b', a \cdot a')$$

for any (a, b) and $(a', b') \in C$, if we denote by $\cdot$ and $*$ the group laws in A and B respectively, σ being a homomorphism of A on the group of automorphisms of B. It is then obvious to remark that, denoting by 0 the identity element in B, if two elements $(0, a)$ and $(0, a')$ are conjugate under the element (b_0, a_0) in C, they are also conjugate under the element $(0, a_0)$.

Application: We deduce that

$\Pi(\{\mathbf{J}, \mathbf{K}\})$
$\Pi(\{\mathbf{J}, H\})$ are subsets of $\mathcal{G}$
$\Pi(\{\mathbf{J}\})$ of $\tilde{\mathcal{G}}$
$\Pi(\{H\})$

3. ON THE MAXIMAL SUBALGEBRAS OF A LIE ALGEBRA. APPLICATIONS: SONS AND GRANDSONS OF G AND $\tilde{G}$

A. Maximal subalgebras of a real Lie algebra

Theorem 3.1: Let $\mathcal{A}$ be a real Lie algebra, a Levi's decomposition of which being $\mathcal{A} = \mathcal{R} \square \mathcal{L}$, where $\mathcal{R}$ is the radical of $\mathcal{A}$ and $\mathcal{L}$ a Levi's factor. Then each maximal subalgebra $\mathcal{B}$ of $\mathcal{A}$ can be written, up to a conjugation, either as $\mathcal{B} = \mathcal{R} \square \mathcal{L}_B$ where $\mathcal{L}_B$ is some maximal subalgebra of $\mathcal{L}$, or as $\mathcal{B} = \mathcal{R}_B \square \mathcal{L}$, where $\mathcal{R}_B$ is an ideal of $\mathcal{A}$, maximal as subideal of $\mathcal{R}$. It follows that every maximal subalgebra $\mathcal{B}$ of $\mathcal{A}$ is symmorphic.

The proof is given in Appendix A. In fact, this theorem generalizes several properties proved in Ref. 1.

Let us recall here some definitions:

—$\mathcal{B}$ is said a maximal subalgebra of $\mathcal{A}$ iff $\mathcal{B}$ is a proper subalgebra of $\mathcal{A}$ ($\mathcal{B} \subsetneq \mathcal{A}$) such that there does not exist any subalgebra $\mathcal{C}$ of $\mathcal{A}$ with $\mathcal{B} \subsetneq \mathcal{C} \subsetneq \mathcal{A}$.

—The ideal $\mathcal{R}_B$ of $\mathcal{A}$ is said maximal as subideal of $\mathcal{R}$ iff there does not exist $\mathcal{R}_1$ ideal of $\mathcal{A}$ such that: $\mathcal{R}_B \subsetneq \mathcal{R}_1 \subsetneq \mathcal{R}$.

—Finally any subalgebra $\mathcal{B}$ of $\mathcal{A}$ can be written (as vector space):

$$\mathcal{B} = \mathcal{L}_B + \mathcal{M}_B + \mathcal{R}_B$$

with $\mathcal{L}_B = \mathcal{B} \cap \mathcal{L}$ and $\mathcal{R}_B = \mathcal{B} \cap \mathcal{R}$ and $\mathcal{M}_B$ denoting a complementary subspace of $\mathcal{L}_B + \mathcal{R}_B$ in $\mathcal{B}$:

$$m \in \mathcal{M}_B \Rightarrow m = l' + \tau', \quad l' \in \mathcal{L}, \notin \mathcal{L}_B,$$
$$m \neq 0 \qquad\qquad \tau' \in \mathcal{R}, \notin \mathcal{R}_B,$$
$$l', \tau' \text{ nonzero.}$$

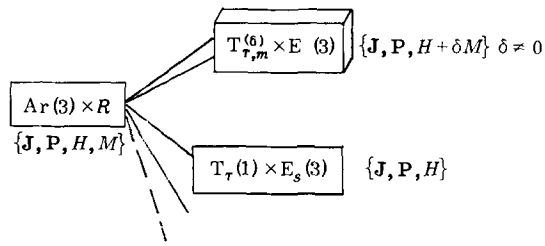
Then $\mathcal{B}$ is said symmorphic iff $\mathcal{M}_B = 0$, or if $\mathcal{B}$ is conjugate to $\mathcal{B}'$ such that $\mathcal{M}_{B'} = 0$.

B. Sons and grandsons of $\mathcal{G}$ (and $\tilde{\mathcal{G}}$)

By using the previous theorem, it is easy to deduce the maximal subalgebras (sons) and the maximal subalgebras of all the maximal subalgebras (grandsons) of $\mathcal{G}$, except those of the solvable one $\{\mathbf{K}, \mathbf{P}, H, J_z\}$, which need the use of Theorem 3. 5 of Ref. 1.

Sons and grandsons of $\tilde{\mathcal{G}}$ can be deduced by the same way, or by using techniques proposed in Sec. 5. Practically, the table of sons and grandsons of $\tilde{\mathcal{G}}$ can be obtained by adding the generator M of the extension to each subalgebra of Table II and also by drawing two new boxes corresponding to subalgebras of $\mathrm{Ar}(3) \oplus R$:

$\mathrm{Ar}(3) \oplus R$:



It may be noticed that the maximal algebras $\{\mathbf{K}, \mathbf{P}, H, J_z\}$ in $\mathcal{G}$ and $\{\mathbf{K}, \mathbf{P}, M, H, J_z\}$ in $\tilde{\mathcal{G}}$ are solvable and contain all the solvable subalgebras of $\mathcal{G}$ and $\tilde{\mathcal{G}}$ respectively. This last property is a direct consequence of the Borel—Morozov theorem for semisimple complex Lie algebras. (Indeed, let us recall that the Borel—Morozov theorem—valid for semisimple complex Lie algebras—has been easily extended in Sec. VI of Ref. 1 to the case of an inhomogeneous Lie algebra $\mathcal{T} \square \mathcal{L}$, with $\mathcal{T}$ Abelian and $\mathcal{L}$ isomorphic to a complex semisimple Lie algebra. We can use the same proof in which we replace $\mathcal{T}$ by a solvable algebra $\mathcal{R}$ to deduce that in $\mathcal{R} \square \mathcal{L}$ exists a subalgebra $\mathcal{R} \square \mathcal{B}$, $\mathcal{B}$ being the Borel algebra of $\mathcal{L}$, such that any solvable subalgebra of $\mathcal{R} \square \mathcal{L}$ is conjugate to a subalgebra of $\mathcal{R} \square \mathcal{B}$.)

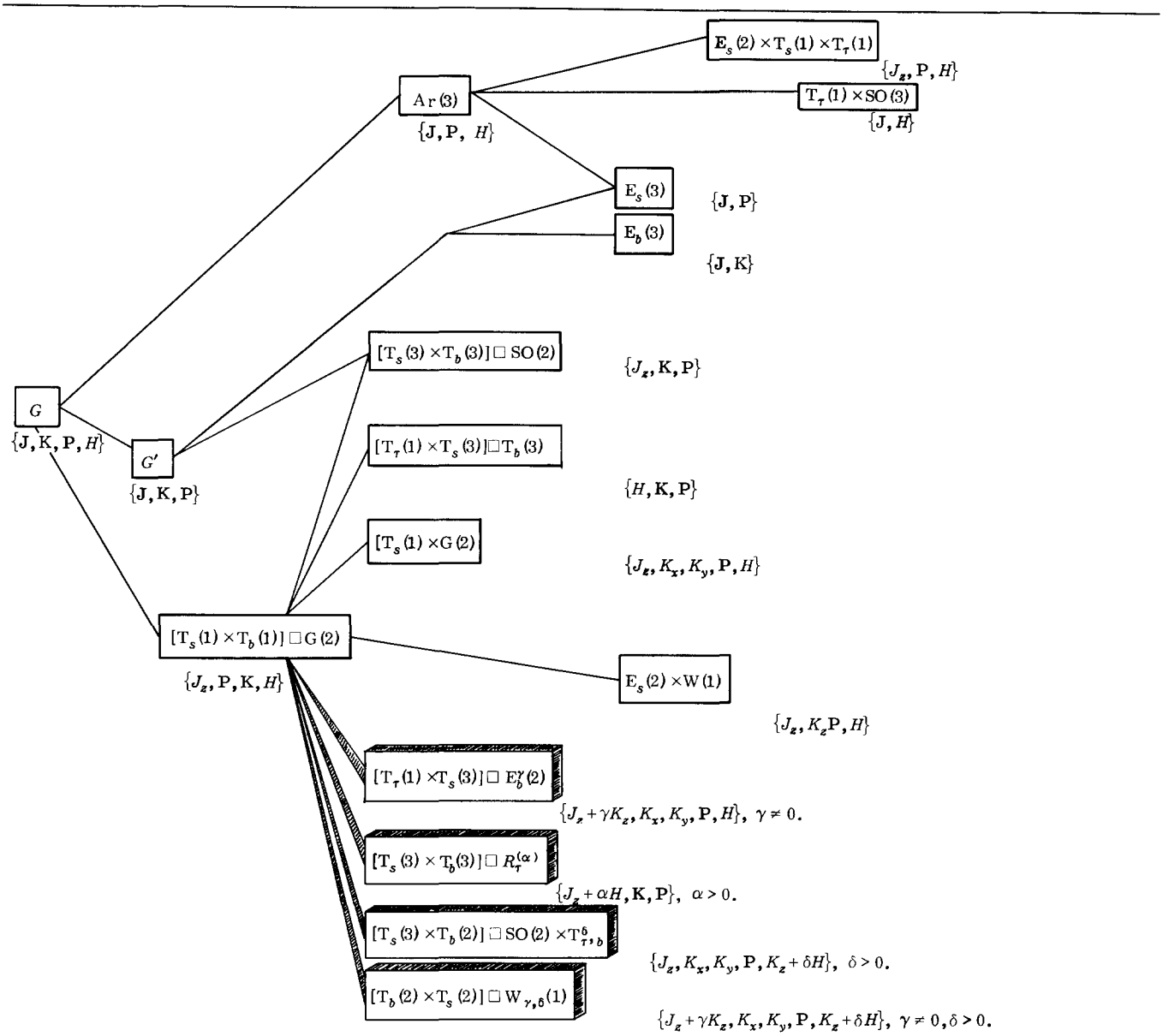
4. ONE-DIMENSIONAL SUBALGEBRAS OF $\mathcal{G}$ AND $\tilde{\mathcal{G}}$

The classification up to a conjugation of the one-dimensional subalgebras of $\mathcal{G}$ ($\tilde{\mathcal{G}}$) is only a problem of conjugation between the elements of the projective space $\hat{\mathcal{G}} = \mathcal{G}/\mathcal{R}$ of $\mathcal{G}$ (respectively $\hat{\tilde{\mathcal{G}}} = \tilde{\mathcal{G}}/\mathcal{R}$ of $\tilde{\mathcal{G}}$). More precisely, one can say that this problem is equivalent to *find the orbits of G on* $\hat{\mathcal{G}}$ (respectively $\tilde{G}$ on $\tilde{\mathcal{G}}$).

The actions of G on $\mathcal{G}$ and of $\tilde{G}$ on $\tilde{\mathcal{G}}$ have been given in Sec. 2 A.

The one-dimensional subalgebras of $\tilde{\mathcal{G}}$ are classified in Table III. An analogous classification for the one-dimensional subalgebras of $\mathcal{G}$ can be easily deduced by suppressing, in the above table, the families of sub-

TABLE II. Sons and grandsons of G.



algebras denoted IV and V and by taking away the condition $\mu = 0$ in I.

5. RELATIONS BETWEEN THE CONNECTED SUBGROUPS of G AND OF $\tilde{G}$

The p. o. s. $\Pi(\tilde{\mathcal{G}})$ can be deduced from $\Pi(\mathcal{G})$ without much difficulty owing to the following remarks.

Let us consider the exact sequence

$$0 \xrightarrow{\alpha} \mathcal{M} \xrightarrow{\mu} \tilde{\mathcal{G}} \xrightarrow{\theta} \mathcal{G} \xrightarrow{\beta} 0,$$

$\mathcal{M}$ being the one-dimensional subalgebra generated by the extension generator M. Then with each subalgebra $\tilde{H} \subset \tilde{\mathcal{G}}$ can be associated the subalgebra: $\theta(\tilde{H}) = H \subset \mathcal{G}$.

Conversely to each subalgebra $H \subset \mathcal{G}$ can be associated the subalgebra

$$\tilde{H} = \theta^{-1}(H) \subset \tilde{\mathcal{G}} \text{ with } \tilde{H} \supset \mathcal{M}.$$

It follows that we have the following relation between subalgebras of $\mathcal{G}$ and subalgebras of $\tilde{\mathcal{G}}$:

Subalgebras of $\mathcal{G}$	$\dashrightarrow$	*Subalgebras of* $\tilde{\mathcal{G}}$
H		(i) $\tilde{H} = \theta^{-1}(H)$, $\tilde{H} \supset \mathcal{M}$.
		(ii) $\tilde{K}$ subalgebras of $\tilde{H}$ such that $\tilde{K} \not\supset \mathcal{M}$, $\dim \tilde{K} = \dim \tilde{H} - 1$.

TABLE III. One-dimensional subalgebras of $\tilde{\mathcal{G}}$ ($\mathcal{G}$). General element: $X=\boldsymbol{\alpha}\cdot\mathbf{J}+\boldsymbol{\beta}\cdot\mathbf{K}+\boldsymbol{\gamma}\cdot\mathbf{P}+\delta H+\mu M$.

Representative element		Characterization by invariants			
J_z			$\varphi=0$	$\boldsymbol{\alpha}\cdot\boldsymbol{\beta}=0,\ \boldsymbol{\alpha}\cdot\boldsymbol{\gamma}=0$	
$J_z+\eta H$	Ⅰ	$\tau_g\varphi=\dfrac{\delta}{\lvert\boldsymbol{\alpha}\rvert}$	$\varphi=\arctan\eta$	$\boldsymbol{\alpha}\cdot\boldsymbol{\beta}=0$	$\mu=0$
H		$0\le\varphi\le\eta/2$	$\varphi=\eta/2$	$\boldsymbol{\beta}=0$	
$J_z+\beta K_z$					$\delta=0$
$J_z+\beta K_z+\delta H$			$\psi=\arctan\beta$		$\delta/\lvert\boldsymbol{\alpha}\rvert$
$J_z+\gamma P_z$	Ⅱ	$\tau_g\psi=\boldsymbol{\alpha}\cdot\boldsymbol{\beta}/\lvert\boldsymbol{\alpha}\rvert^2$	$\psi=0$	$\boldsymbol{\alpha}\cdot\boldsymbol{\gamma}/\lvert\boldsymbol{\alpha}\rvert$	$\delta=0$
$K_z+\zeta H$		$(0\le\psi<\pi;\psi\ne\pi/2)$			$\lvert\delta\rvert/\lvert\mathbf{P}\rvert$
K_z		$\boldsymbol{\alpha}=0$			
$K_z+\gamma P_x$	Ⅲ	$\boldsymbol{\alpha}=0$	$\tau_g\theta=\dfrac{\lvert\boldsymbol{\beta}\wedge\boldsymbol{\gamma}\rvert}{\lvert\boldsymbol{\beta}\rvert^2}$	$\theta=0$ / $\theta=\arctan\gamma$	$\delta=0$
P_z			$0\le\theta\le\dfrac{\pi}{2}$	$\theta=\dfrac{\pi}{2}$	
$J_z+\rho M$		Same characterization	$\lvert(\boldsymbol{\alpha}\wedge\boldsymbol{\beta})\cdot\boldsymbol{\gamma}+\mu\boldsymbol{\alpha}^2\rvert/\lvert\boldsymbol{\alpha}\rvert^3$		
$J_z+\eta H+\rho M$	Ⅳ	as in Ⅰ	$+\dfrac{(\boldsymbol{\alpha}\wedge\boldsymbol{\beta})\cdot\boldsymbol{\gamma}+\mu\boldsymbol{\alpha}^2+\frac{1}{2}\boldsymbol{\beta}^2-(\boldsymbol{\alpha}\cdot\boldsymbol{\gamma})^2/2\delta}{\lvert\boldsymbol{\alpha}\rvert^3}$		
$H+\rho M$			$(\gamma^2-2\mu\delta)/\delta^2$		
M	Ⅴ	$\boldsymbol{c}=\boldsymbol{\beta}+\boldsymbol{\gamma}=\delta=0$			

It is interesting to note that the problem of determination of subalgebras of $\tilde{\mathcal{G}}$ of type (ii) is *simplified* by the two properties, the proofs of which are straightforward.

Proposition 1:

$$\left.\begin{matrix}H\subset\mathcal{G}\\ [H,H]_{\tilde{\mathcal{G}}}=H\end{matrix}\right\}\Rightarrow\begin{cases}\text{the only subalgebra of type (ii) to be}\\ \text{considered from } \tilde{H}=\theta^{-1}(H) \text{ is } H \text{ itself.}\end{cases}$$

TABLE IV. Stability groups of the one-dimensional subalgebras of $\mathcal{G}$ and $\tilde{\mathcal{G}}$.

Representative element	Stability group in G	Stability group in $\tilde{G}$
J_z	$\{J_z,K_z,P_z,H\}$	$\{J_z,K_z,P_z,M,H\}$
$J_z+\eta H$	$\{J_z,P_z,H\}$	$\{J_z,P_z,H,M\}$
H	$\{\mathbf{J},\mathbf{P},H\}$	$\{\mathbf{J},\mathbf{P},H,M\}$
$J_z+\beta K_z$	$\{J_z,K_z,P_z\}$	$\{J_z,K_z,M\}$
$J_z+\beta K_z+\delta H$	$\{J_z,K_z+(\delta/\beta)H,P_z\}$	$\{J_z,K_z+(\delta/\beta)H,M\}$
$J_z+\gamma P_z$	$\{J_z,K_z,P_z,H\}$	$\{J_z,P_z,H,M\}$
$K+\zeta H$	$\{J_z,\mathbf{P},K_z+\zeta H\}$	$\{J_z,P_x,P_y,K_z+\zeta H,M\}$
K_z	$\{J_z,\mathbf{K},\mathbf{P}\}$	$\{J_z,\mathbf{K},P_x,P_y,M\}$
$K_z+\gamma P_x$	$\{\mathbf{K},\mathbf{P}\}$	$\{K_y,K_z,P_x,P_y,M\}$
P_z	$\{J_z,\mathbf{K},\mathbf{P},M\}$	$\{J_z,K_x,K_y,\mathbf{P},M\}$
$J_z+\rho M$		$\{J_z,K_z,P_z,M,H\}$
$J_z+\eta H+\rho M$		$\{J_z,P_z,H,M\}$
$H+\rho M$		$\{\mathbf{J},\mathbf{P},M,M\}$
M		$\{\mathbf{J},\mathbf{K},\mathbf{P},H,M\}$

Proposition 2:

$$\left.\begin{matrix}H\subset\mathcal{G}\\ \exists A\&B\in H \text{ s.t. } [A,B]_{\tilde{\mathcal{G}}}=M\end{matrix}\right\}\Rightarrow\begin{cases}\text{the algebra } \tilde{H}=\theta^{-1}(H) \text{ does not provide any}\\ \text{algebra of type (ii).}\end{cases}$$

Moreover, the problem of classification of subalgebras of $\tilde{\mathcal{G}}$ up to *a conjugation* becomes easy owing to the proposition:

Proposition 3: H and H' nonconjugate in $\mathcal{G}$:

$$\Rightarrow\begin{cases}(\alpha)\ \tilde{H}=\theta^{-1}(H) \text{ and } \tilde{H}'=\theta^{-1}(\tilde{H}') \text{ nonconjugate in } \tilde{\mathcal{G}}.\\ (\beta)\ \nexists\,\tilde{K} \text{ and } \tilde{K}' \text{ conjugate in } \tilde{\mathcal{G}} \text{ with } \tilde{K}\subset\tilde{H} \text{ and}\\ \quad\tilde{K}'\subset\tilde{H}',\ \tilde{K} \text{ and } \tilde{K}' \text{ satisfying (ii).}\end{cases}$$

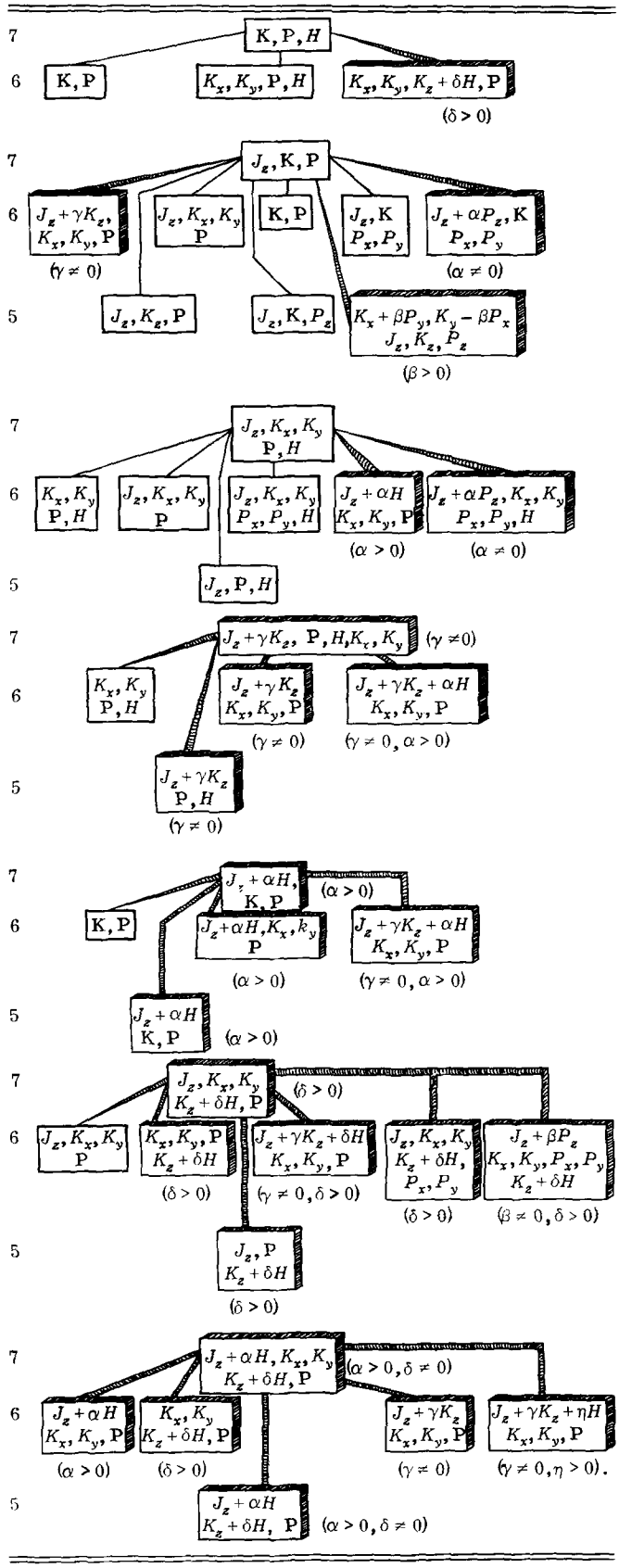
Indeed, let us suppose $\tilde{H}$ and $\tilde{H}'$ to be conjugate. Then there exists $\tilde{g}\in\tilde{G}$ such that $\tilde{g}\tilde{H}\tilde{g}^{-1}=\tilde{H}'$. Setting $g=\theta(\tilde{g})$ we shall obtain: $gHg^{-1}=H'$. By the same way, supposing the above defined subalgebras $\tilde{K}$ and $\tilde{K}'$ conjugate, then the existence of $\tilde{g}\in\tilde{G}$ such that: $\tilde{g}\tilde{K}\tilde{g}^{-1}=\tilde{K}'$ would imply: $gHg^{-1}=H'$, with $g=\theta(\tilde{g})$.

Thus, practically, the problem of conjugation in $\tilde{\mathcal{G}}$ has *only* to be examined between subalgebras $\tilde{K}$ coming from a same algebra $\tilde{H}=\theta^{-1}(H)$, if we know the p. o. s. $\Pi(\mathcal{G})$.

6. FOUR-, FIVE-, AND SIX-DIMENSIONAL SUBALGEBRAS IN $\mathcal{G}$. FIVE-, SIX-, AND SEVEN-DIMENSIONAL SUBALGEBRAS IN $\tilde{\mathcal{G}}$

The method we choose for the construction of the

TABLE V. Maximal subalgebras of the seven-dimensional grandsons of $\mathcal{G}$.



"middle" of $\Pi(G)$, i. e., the connected subgroups of dimension six, five, and four, is to continue the "top" of $\Pi(G)$ begun in Table II, more precisely to determine the sons, grandsons, and great-grandsons of the grandsons of G. This method is rather systematic and does not present great difficulty. Moreover, it has the advantage of exhibiting the relationships between the different subgroups (Tables V and VI).

By using then the properties mentioned in Sec. 5, the classification of the connected subgroups of $\tilde{G}$ of dimension five, six, and seven is given in the last part of this section.

A. Six-dimensional subalgebras in $\mathcal{G}$

Considering Table V we see that there exist three six-dimensional subgroups, namely the two Euclidean ones $\mathbf{E}_s(3)$ and $\mathbf{E}_b(3)$ generated respectively by $\{\mathbf{J}, \mathbf{P}\}$ and $\{\mathbf{J}, \mathbf{K}\}$ and the group $\mathbf{E}(2) \times \mathbf{W}(1)$ generated by $\{J_z, K_z, \mathbf{P}, H\}$, which are grandsons of G.

We can also note that the other six-dimensional connected subgroups have to be found among the maximal subgroups of seven-dimensional grandsons of G—each of them being seven-dimensional and son of the eight-dimensional group $R^2 \square G(2)$ generated by $\{J_z, \mathbf{K}, \mathbf{P}, H\}$.

The maximal subgroups of each of these seven groups are given in Table V.

Let us list below the nonconjugate algebras (or families of algebras) of dimension six, taking care to gather the isomorphic ones:

(i) Euclidean algebras:

$E_s(3)$ generated by $\{\mathbf{J}, \mathbf{P}\}$,

$E_b(3)$ generated by $\{\mathbf{J}, \mathbf{K}\}$.

(ii) Abelian algebra:

R^6 generated by $\{\mathbf{K}, \mathbf{P}\}$.

(iii) The (isomorphic) algebras:

generated by $\{K_x, K_y, \mathbf{P}, H\}$, $\{K_x, K_y, K_z + \delta H, \mathbf{P}\}$ ($\delta > 0$).

(iv) The (isomorphic) algebras generated by

$\{J_z + \gamma K_z, K_x, K_y, \mathbf{P}\}$ ($\gamma \neq 0$),

$\{J_z, K_x, K_y, \mathbf{P}\}$,

$\{J_z, P_x, P_y, \mathbf{K}\}$,

$\{J_z + \alpha P_z, P_x, P_y, \mathbf{K}\}$ ($\alpha \neq 0$).

(v) The (isomorphic) algebras generated by

$\{J_z, H, K_x, K_y, P_x, P_y\}$,

$\{J_z + \alpha P_z, H, K_x, K_y, P_x, P_y\}$ ($\alpha \neq 0$),

$\{J_z, K_z + \delta H, K_x, K_y, P_x, P_y\}$ ($\delta > 0$),

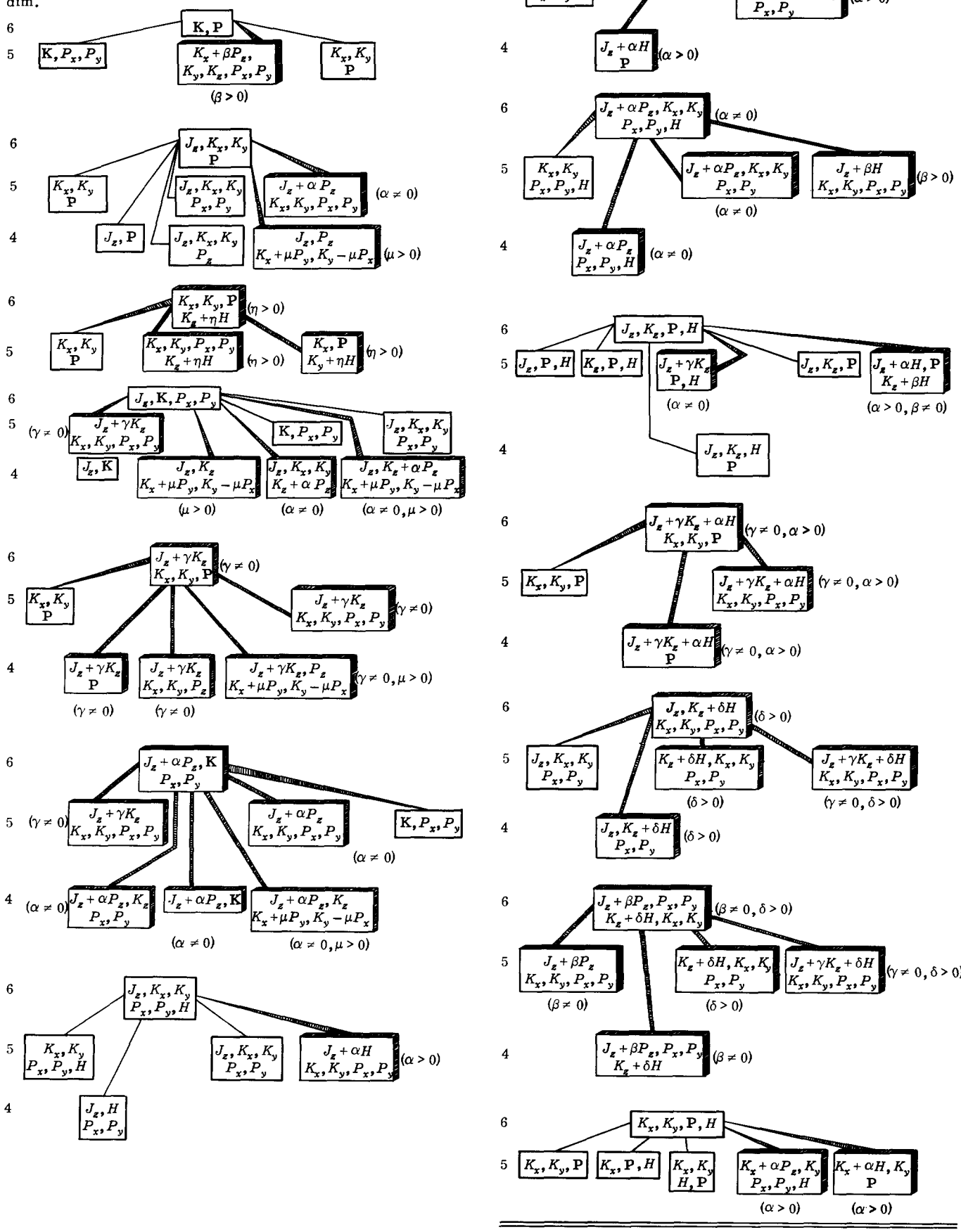
$\{J_z + \beta P_z, K_z + \delta H, K_x, K_y, P_x, P_y\}$ ($\beta \neq 0, \delta > 0$).

(vi) The (isomorphic) algebras generated by

$\{J_z + \alpha H, K_x, K_y, \mathbf{P}\}$ ($\alpha > 0$),

$\{J_z + \gamma K_z + \alpha H, K_x, K_y, \mathbf{P}\}$ ($\gamma \neq 0, \alpha > 0$).

TABLE VI. Maximal subalgebras of the six-dimensional algebras. In this table the maximal subalgebras of the Euclidean algebras, given in Table BI are not considered.



(vii) The algebra of $E(2)\times W(1)$ generated by

$\{J_z, K_z, \mathbf{P}, H\}$.

B. Five-dimensional subalgebras of $\mathcal{G}$

The five-dimensional subgroups will be obtained by considering the five-dimensional maximal subgroups of the seven-dimensional groups of $\Pi(G)$ (see Table V) and the maximal subgroups of the six-dimensional groups which are given in Table VI.

Let us remark that the Euclidean group $E_s(3)$ and $E_b(3)$ do not admit five-dimensional subgroups. We may also mention that the maximal subalgebras of the Abelian algebra $\{\mathbf{K}, \mathbf{P}\}$—which are obviously all five-dimensional—will be found without difficulty by noting that such a subalgebra admits a basis with either two P-pure generators or three P-pure generators.

Finally, we have obtained 21 nonconjugate five-dimensional subalgebras (or families of subalgebras) which we have classified below into seven sets of nonisomorphic algebras:

(i) The Abelian algebras generated by

$\{\mathbf{K}, P_x, P_y\}$,

$\{K_x, K_y, \mathbf{P}\}$,

$\{K_x + \beta P_z, K_y, K_z, P_x, P_y\}$ $(\beta > 0)$.

(ii) The (isomorphic) algebras generated by

$\{J_z, \mathbf{P}, H\}$,

$\{J_z, \mathbf{P}, K_z\}$,

$\{J_z, \mathbf{K}, P_z\}$,

$\{J_z, K_z + \delta H, \mathbf{P}\}$ $(\delta > 0)$,

$\{J_z, K_x + \beta P_y, K_y - \beta P_x, K_z, P_z\}$ $(\beta > 0)$.

(iii) The (isomorphic) algebras generated by

$\{K_x, \mathbf{P}, H\}$,

$\{K_y, \mathbf{P}, K_x + \alpha H\}$ $(\alpha > 0)$.

(iv) The (isomorphic) algebras generated by

$\{H, K_x, K_y, P_x, P_y\}$,

$\{H, K_x + \alpha P_z, K_y, P_x, P_y\}$ $(\alpha > 0)$,

$\{K_z + \delta H, K_x, K_y, P_x, P_y\}$ $(\delta > 0)$.

(v) The (isomorphic) algebras generated by

$\{J_z, K_x, K_y, P_x, P_y\}$,

$\{J_z + \alpha P_z, K_x, K_y, P_x, P_y\}$ $(\alpha \neq 0)$,

$\{J_z + \gamma K_z, K_x, K_y, P_x, P_y\}$ $(\gamma \neq 0)$.

(vi) The (isomorphic) algebras generated by

$\{J_z + \alpha H, K_x, K_y, P_x, P_y\}$ $(\alpha > 0)$,

$\{J_z + \gamma K_z + \alpha H, K_x, K_y, P_x, P_y\}$ $(\gamma \neq 0, \alpha > 0)$.

(vii) The (isomorphic) algebras generated by

$\{J_z + \gamma K_z, H, \mathbf{P}\}$ $(\gamma \neq 0)$,

$\{J_z + \alpha H, K_z, \mathbf{P}\}$ $(\alpha > 0)$,

$\{J_z + \alpha H, K_z + \beta H, \mathbf{P}\}$ $(\alpha \neq 0, \beta > 0)$.

C. Four-dimensional subalgebras in $\mathcal{G}$

The classification of the four dimensional subalgebras of $\mathcal{G}$ appears more fastidious than those given in the two previous paragraphs. This is due particularly to the large number of four-dimensional algebras contained in the Abelian one $\{\mathbf{K}, \mathbf{P}\}$. Note that each four-dimensional subalgebras of $\{\mathbf{K}, \mathbf{P}\}$ contains either one or two or three independent P-pure generators: We shall use this remark to classify these subalgebras.

Finally the four-dimensional subgroups of G can be gathered into four sets of nonisomorphic ones:

(i) $SO(3)\times R$ type: group generated by $\{\mathbf{J}, H\}$.

(ii) $E(2)\times R$ type: groups generated by

$\{J_z, K_x + \mu P_y, K_y - \mu P_x, K_z\}$ $(\mu > 0)$ $\Big|\{J_z, \mathbf{P}\}$,

$\{J_z, K_x + \mu P_y, K_y - \mu P_x, P_z\}$ $(\mu > 0)$

$\{J_z, K_x + \mu P_y, K_y - \mu P_x, K_z + \alpha P_z\}$ $(\alpha \neq 0,\ \mu > 0)$,

$\Big|\{J_z, K_x, K_y, P_z\}$

$\Big|\{J_z, \mathbf{K}\}$,

$\{J_z + \gamma K_z, \mathbf{P}\}$ $(\gamma \neq 0)$ $\Big|\{J_z, P_x, P_y, K_z\}$

$\{J_z + \gamma K_z, K_x, K_y, P_z\}$ $(\gamma \neq 0)$ $\Big|\{J_z, P_x, P_y, H\}$,

$\{J_z + \gamma K_z, K_x + \mu P_y, K_y - \mu P_x, P_z\}$ $(\gamma \neq 0,\ \mu > 0)$

$\{J_z + \alpha P_z, K_x, K_y, K_z + \beta P_z\}$ $(\alpha,\ \beta \neq 0)$

$\Big|\{J_z, K_x, K_y, K_z + \alpha P_z\}$ $(\alpha \neq 0)$

$\Big|\{J_z, P_x, P_y, K_z + \delta H\}$ $(\delta > 0)$,

$\{J_z + \alpha P_z, K_x + \mu P_y, K_y - \mu P_x, K_z\}$ $(\alpha \neq 0,\ \mu > 0)$

$\{J_z + \alpha P_z, K_x + \mu P_y, K_y - \mu P_x, K_z + \beta P_z\}$ $(\alpha, \beta \neq 0,\ \mu > 0)$

$\Big|\{J_z + \alpha P_z, \mathbf{K}\}$ $(\alpha \neq 0)$

$\Big|\{J_z + \alpha P_z, H, P_x, P_y\}$ $(\alpha \neq 0)$,

$\{J_z + \alpha H, \mathbf{P}\}$ $\Big|\{J_z + \alpha P_z, K_z, P_x, P_y\}$ $(\alpha \neq 0)$

$\{J_z + \gamma K_z + \alpha H, \mathbf{P}\}$ $\Big|\{J_z + \alpha P_z, K_z + \delta H, P_x, P_y\}$ $(\alpha \neq 0,\ \delta > 0)$.

(iii) $W(1)\times R$ type: groups generated by

$\{J_z, K_z, H, P_z\}$, $\{K_x, K_z + \delta H, P_x, P_y + \beta P_z\}$ $(\beta > 0,\ \delta > 0)$

$\{K_x, H, P_x, P_y\}$, $\{K_x + \alpha P_z, H, P_x, P_y\}$ $(\alpha > 0)$

$\{K_x, K_y + \delta H, P_x, P_y\}$ $(\delta > 0)$,

$\{K_x + \alpha P_z, K_y + \delta H, P_x, P_y\}$ $(\alpha > 0,\ \delta > 0)$

$\{K_z + \delta H, K_x, P_x, P_y\}$ $(\delta > 0)$,

$\{K_x + \alpha P_z, K_z + \delta H, P_x, P_y\}$ $(\alpha > 0,\ \delta > 0)$,

$\{K_x + \alpha P_y, K_z + \delta H, P_x, P_y + \beta P_z\}$ $(\alpha \neq 0,\ \beta > 0,\ \delta > 0)$.

(iv) R^4 type: groups generated by

$\{H, \mathbf{P}\}$, $\{\mathbf{K}, P_x\}$,

$\{K_x + \alpha P_y, K_y + \beta P_z, K_z + \gamma P_y + \delta P_z, P_x\}$

$(\alpha > 0,\ \beta > 0,\ \gamma, \delta \neq 0)$,

$\{K_x, K_y + \beta P_z, K_z + \gamma P_y + \delta P_z, P_x\}$ $(\beta > 0,\ \gamma, \delta \neq 0)$,

$\{K_x + \alpha P_y, K_y, K_z + \gamma P_y + \delta P_z, P_x\}$ $(\alpha > 0,\ \gamma > 0,\ \delta \neq 0)$,

$\{K_x, K_y, K_z + \gamma P_y + \delta P_z, P_x\}$ $(\gamma > 0,\ \delta \neq 0)$,

$\{K_x, K_y + \beta P_z, K_z + \gamma P_y, P_x\}$ $(\beta > 0,\ \gamma \neq 0)$,

$\{K_x, \alpha P_y, K_y, K_z, P_x\}$ $(\alpha > 0)$,

$\{K_x, K_y, K_z + \delta P_z, P_x\}$ $(\delta \neq 0)$,

TABLE VII. Two-dimensional subalgebras of $\mathcal{G}$.

SO(2) $\times R$ algebras
$\sim$[a] $\{J_z, K_z\}$
$\sim$ $\{J_z, P_z\}$
$\sim$ $\{J_z, H\}$
$\sim$ $\{J_z, K_z + \alpha H\}$ $(\alpha > 0)$
R^2 algebras
$\sim$ $\{P_x, P_y\}$
$\sim$ $\{P_x, H\}$
$\sim$ $\{K_x, K_y\}$
$\{K_z, P_z\}$
$\sim$ $\{K_z, P_x\}$
$\{K_y, P_x + \beta P_z\}$ $(\beta > 0)$
$\{K_z + \delta P_x, P_x + \beta P_y + \gamma P_z\}$ $(\delta > 0,\ \beta > 0,\ \gamma \neq 0)$
$\{K_z + \delta P_x, P_y + \gamma P_z\}$ $(\delta > 0,\ \gamma > 0)$
$\{K_z + \delta P_x, P_x + \gamma P_z\}$ $(\delta > 0,\ \gamma \neq 0)$
$\sim$ $\{K_z + \delta P_x, P_x + \beta P_y\}$ $(\beta > 0,\ \delta > 0)$
$\sim$ $\{K_z + \delta P_x, P_y\}$ $(\delta > 0)$
$\{K_z + \delta P_x, P_z\}$ $(\delta > 0)$
$\sim$ $\{K_z + \rho H, P_x\}$ $(\rho > 0)$
$\{K_z + \rho H, P_z\}$ $(\rho > 0)$
$\{K_z + \rho H, P_x + \gamma P_z\}$ $(\rho > 0,\ \gamma > 0)$
$\{K_z, K_x + \alpha P_x + \beta P_y + \gamma P_z\}$ $(\alpha \neq 0,\ \beta > 0,\ \gamma > 0)$
$\{K_z, K_x + \beta P_y + \gamma P_z\}$ $(\beta > 0,\ \gamma > 0)$
$\{K_z, K_x + \alpha P_x + \gamma P_z\}$ $(\alpha \neq 0,\ \gamma > 0)$
$\sim$ $\{K_z, K_x + \alpha P_x + \beta P_y\}$ $(\alpha \neq 0,\ \beta > 0)$
$\sim$ $\{K_z, K_x + \alpha P_x\}$ $(\alpha \neq 0)$
$\sim$ $\{K_z, K_x + \beta P_y\}$ $(\beta > 0)$
$\{K_z, K_x + \gamma P_z\}$ $(\gamma > 0)$
(if $\gamma = \delta$: $\sim$) $\{K_z + \delta P_x, K_x + \alpha P_x + \beta P_y + \gamma P_z\}$ $(\delta > 0,\ \alpha \neq 0,\ \beta > 0,\ \gamma \neq 0)$
(if $\gamma = \delta$: $\sim$) $\{K_z + \delta P_x, K_x + \beta P_y + \gamma P_z\}$ $(\delta > 0,\ \beta > 0,\ \gamma \neq 0)$
(if $\gamma = \delta$: $\sim$) $\{K_z + \delta P_x, K_x + \alpha P_x + \gamma P_z\}$ $(\delta > 0,\ \alpha \neq 0,\ \gamma > 0)$
$\{K_z + \delta P_x, K_x + \alpha P_x + \beta P_y\}$ $(\delta > 0,\ \alpha \neq 0,\ \beta > 0)$
(if $\gamma = \delta$: $\sim$) $\{K_z + \delta P_x, K_x + \gamma P_z\}$ $(\delta > 0,\ \gamma \neq 0)$
$\{K_z + \delta P_x, K_x + \beta P_y\}$ $(\delta > 0,\ \beta > 0)$
$\sim$ $\{J_z + \delta P_z, H\}$ $(\delta \neq 0)$
$\{J_z + \delta P_z, K_z\}$ $(\delta \neq 0)$
$\{J_z + \delta P_z, H + \rho K_z\}$ $(\delta \neq 0,\ \rho > 0)$
$\{J_z + \delta K_z, P_z\}$ $(\delta \neq 0)$
$\sim$ $\{J_z + \delta H, P_z\}$ $(\delta > 0)$
$\{J_z + \rho H + \delta K_z, P_z\}$ $(\rho > 0,\ \delta \neq 0)$

[a] The subalgebras preceded by the sign $\sim$ are subalgebras of $\mathcal{G}$ (See Table VIII).

TABLE VIII. Two-dimensional subalgebras of $\mathcal{G}$.

They can be gathered into three parts:

(i) the subalgebras obtained by adding the generator M to each one-dimensional subalgebra of $\mathcal{G}$ (see Table III);

(ii) the subalgebras preceded by the sign $\sim$ in the Table VII of the two-dimensional subalgebras of $\mathcal{G}$.

(iii) The subalgebras:

$$\{P_x, H + \beta M\} \quad (\beta \neq 0)$$
$$\{J_z + \delta P_z, H + \beta M\} \quad (\delta \neq 0,\ \beta \neq 0)$$
$$\{J_z + \delta P_z + \beta M, H\} \quad (\delta \neq 0,\ \beta > 0)$$
$$\{J_z + \delta P_z + \beta M, H + \gamma M\} \quad (\delta \neq 0,\ \beta > 0,\ \gamma \neq 0)$$
$$\{J_z + \delta H + \beta M, P_z\} \quad (\delta > 0,\ \beta \neq 0)$$
$$\{J_z + \beta M, K_z\} \quad (\beta > 0)$$
$$\{J_z + \beta M, P_z\} \quad (\beta > 0)$$
$$\{J_z + \alpha M, H\} \quad (\alpha > 0)$$
$$\{J_z, H + \beta M\} \quad (\beta \neq 0)$$
$$\{J_z + \alpha M, H + \beta M\} \quad (\alpha > 0,\ \beta \neq 0)$$
$$\{J_z + \alpha M, K_z + \beta M\} \quad (\alpha > 0,\ \beta \neq 0)$$
$$\{K_x, K_y, P_x, P_y\},\quad \{K_x, K_y, P_x, P_z\},$$
$$\{K_x, K_y, P_x, P_y + \gamma P_z\} \quad (\gamma > 0),$$
$$\{K_x + \gamma P_z, K_y, P_x, P_y\} \quad (\gamma > 0),$$
$$\{K_x + \alpha P_y, K_y, P_x, P_z\} \quad (\alpha > 0),$$
$$\{K_x + \alpha P_y, K_y, P_x, P_y + \gamma P_z\} \quad (\alpha > 0,\ \gamma > 0),$$
$$\{K_x, \mathbf{P}\},$$
$$\{K_x + \alpha P_y, K_y, K_z + \delta P_z, P_x\} \quad (\alpha > 0,\ \delta \neq 0).$$

D. Seven-, six-, and five-dimensional subalgebras in $\tilde{\mathcal{G}}$

As has been discussed in Sec. 5, we shall classify the subalgebras of a given dimension into two families: an algebra of the first family possessing M as a generator, and an algebra of the second family being such that M is not a generator of the algebra. Let us add that algebras of the first type are readily obtained by adding the generator M to each subalgebra of $\mathcal{G}$—and imposing then the commutation relations of $\tilde{\mathcal{G}}$. As for algebras of the second type, it has been shown that each such algebra appears as a (maximal) subalgebra of the algebra obtained by adding the generator M to the considered one, which induces a method of determination of these algebras.

There follows the classification below.

1. Seven-dimensional subalgebras of $\tilde{\mathcal{G}}$

(i) The subalgebras containing M as a generator: see the classification of the six-dimensional subalgebras of $\mathcal{G}$.

(ii) The subalgebras—whose corresponding groups are isomorphic to E(3)$\times R$—generated by

$$\{\mathbf{J}, \mathbf{P}, H\},\quad \{\mathbf{J}, \mathbf{P}, H + \delta M\} \quad (\delta \neq 0).$$

2. Six-dimensional subalgebras of $\tilde{\mathcal{G}}$

(i) The subalgebras containing M as a generator: see the classification of the five-dimensional subalgebras of $\mathcal{G}$.

(ii) The subalgebras—whose corresponding groups are isomorphic to E(3)—generated by

$$\{\mathbf{J}, \mathbf{K}\},\quad \{\mathbf{J}, \mathbf{P}\}.$$

3. Five-dimensional subalgebras of $\tilde{\mathcal{G}}$

(i) The subalgebras containing M as a generator: see the classification of the four-dimensional subalgebras of $\mathcal{G}$.

(ii) The subalgebras—whose corresponding groups are isomorphic to E(2)$\times R^2$—generated by

$$\{J_z, \mathbf{P}, H\},\quad \{J_z + \alpha M, \mathbf{P}, H\} \quad (\alpha > 0),$$
$$\{J_z, \mathbf{P}, H + \beta M\} \quad (\beta \neq 0),$$
$$\{J_z + \lambda H, \mathbf{P}, H + \mu M\} \quad (\lambda > 0,\ \mu \neq 0).$$

TABLE IX. Three-dimensional subalgebras of the ideal $\{\mathbf{K},\mathbf{P}\}$ in $\mathcal{G}$.

(i)

$\sim$[a]	$\{P_x, P_y, P_z\}$
	$\{K_x, P_x, P_y\}$
$\sim$	$\{K_x, P_y, P_z\}$
	$\{K_x, P_y, P_x+\alpha P_z\}$ $(\alpha>0)$
	$\{K_x+\delta P_y, P_x, P_z\}$ $(\delta>0)$
	$\{K_x, K_y, P_x\}$
	$\{K_x+\alpha P_y, K_y, P_x\}$ $(\alpha>0)$
	$\{K_x+\beta P_z, K_y, P_x\}$ $(\beta>0)$
	$\{K_x, K_y+\delta P_z, P_x\}$ $(\delta>0)$
	$\{K_x+\alpha P_y+\beta P_z, K_y, P_x\}$ $(\alpha>0,\beta>0)$
	$\{K_x+\alpha P_y, K_y+\delta P_z, P_x\}$ $(\alpha>0,\delta>0)$
	$\{K_x+\beta P_z, K_y+\delta P_z, P_x\}$ $(\beta>0,\delta>0)$
	$\{K_x+\alpha P_y+\beta P_z, K_y+\delta P_z, P_x\}$ $(\alpha>0,\beta>0,\delta\neq 0)$
$\sim$	$\{K_x, K_y, P_z\}$
	$\{K_x+bP_y, K_y, P_z\}$ $(b>0)$
$\sim$	$\{K_x, K_y+dP_y, P_z\}$ $(d\neq 0)$
(if $c=b$ $\sim$)	$\{K_x+bP_y, K_y+cP_x, P_z\}$ $(b>0,c\neq 0)$
	$\{K_x, K_y+cP_x+dP_y, P_z\}$ $(c>0,d\neq 0)$
(if $c=b$ $\sim$)	$\{K_x+bP_y, K_y+cP_x+dP_y, P_z\}$ $(b>0,c\neq 0,d\neq 0)$
	$\{K_x, K_y, P_x+\alpha P_z\}$ $(\alpha>0)$
	$\{K_x+aP_y, K_y, P_x+\alpha P_z\}$ $(a>0,\alpha>0)$
	$\{K_x+bP_z, K_y, P_x+\alpha P_z\}$ $(b\neq 0,\alpha>0)$.
	$\{K_x, K_y+dP_z, P_x+\alpha P_z\}$ $(d>0,\alpha>0)$
	$\{K_x+aP_y+bP_z, K_y, P_x+\alpha P_z\}$ $(a>0,b\neq 0,\alpha>0)$
	$\{K_x+aP_y, K_y+dP_z, P_x+\alpha P_z\}$ $(a>0,d\neq 0,\alpha>0)$
	$\{K_x+bP_z, K_y+dP_z, P_x+\alpha P_z\}$ $(b\neq 0,d>0,\alpha>0)$
	$\{K_x+aP_y+bP_z, K_y+dP_z, P_x+\alpha P_z\}$ $(a>0,b\neq 0,d\neq 0,\alpha>0)$

(ii) $\{K_x+\alpha P_y, K_y+aP_x+bP_y+cP_z, K_z+dP_x+jP_y+kP_z\}$ the values of α, a, b, c, d, j, k satisfying one of the following lines[b]—more precisely each line corresponds to a family of nonconjugate subalgebras, and two subalgebras belonging to two different lines being nonconjugate. [c]

	α	a	b	c	d	j	k	α	a	b	c	d	j	k	
$(a,b,c)\neq(d,j,k)$[d]	>			>				>	0		>			0	
	>	0		>				>		0	>	0			
	>		0	>				>		0	>		0		
	>			0	>			>		0	>			0	
	>			>	0			>			0	0	>		
	>			>		0		>			0	>	0		
	>			>			0	>			0	>		0	$(a,b)\neq(j,k)$
	>	0	0	>				>			>	0	0		
	>		0	0	>			>			>		0	0	
$(b,c)\neq(j,k)$	>	0		>	0			>	0	0	>	0			
	>	0		>		0		>	0	0	>		0		
	>	0	0	>			0	0	0	0	>	0			
	>	0		>	0	0		0	0	0	>	>	0		
	>		0	0	0	>		0	0	0	>	>		0	
	>	0		>		0	0	0	0		0	0	>		
	>		0	>		0	0	0	0		0	>	0		
	>	0	0	>		0	0	0	0		0	>	>	0	
	0							0	>	0	0	0	>		
	0	>		>				0	>	0	0	>	0		
	0	0		>	>			0	>	0	0	>		0	
	0	>	0	>				0	>	0	0	0	>	0	
	0	>		0	>			0	>	0	0	0	0		
	0	0	0	>	>			0	0		0	>	0	0	
	0	0		0	>	>		0	0		0	0	0		$(b)\neq(k)$
	0	>	0	0		>		0	0	0	>	>	0	0	
$(b,c)\neq(j,k)$	0	0		>	0			0	0	0	>	0		0	
$(a,c)\neq(d,k)$	0	>	0	>		0		0	>	0	0	0	0	0	
	0	0		>	>	0		0	0		0	0	0	0	
	0	0		>	>		0	0	>		0	0	0	0	
	0	>	0		>		0	0	0	0	0	0	0	0	
	0	>		0	>	0									

[a] The subalgebras preceded by the sign $\sim$ are subalgebras of $\mathcal{G}$ (see Table XI, 5).

[b] Inside a box, the signs >, 0 mean respectively positive and equal to 0. When a box is empty, the corresponding parameter takes all the values, except 0.

[c] Note that a subalgebra of the type (ii) belongs to $\tilde{\mathcal{G}}$ if $a=\alpha$, $d=0$, $j=c$.

[d] By $(a,b,c)\neq(d,j,k)$—or $(a,b)\neq(j,k)$—we mean that, in the three-dimensional Euclidean space R^3 the vector (a,b,c) is not parallel to the vector (d,j,k)—or in the two-dimensional Euclidean space R^2, the vector (a,b) is not parallel to the vector (d,j).

TABLE X. Three-dimensonal subalgebras in $\mathcal{G}$.

(i) SO(3) algebra: $\sim^{a}\{J_x, J_y, J_z\}$

(ii) Euclidean algebras E(2):

$$\sim\{J_z, P_x, P_y\}$$
$$\sim\{J_z, K_x, K_y\}$$
$$\{J_z, K_x+\mu P_y, K_y-\mu P_x\}\ (\mu>0)$$
$$\sim\{J_z+\gamma K_z, P_x, P_y\}\ (\gamma\neq 0)$$
$$\sim\{J_z+\gamma K_z, K_x, K_y\}\ (\gamma\neq 0)$$
$$\{J_z+\gamma K_z, K_x+\mu P_y, K_y-\mu P_x\}\ (\mu>0, \gamma\neq 0)$$
$$\sim\{J_z+\alpha P_z, P_x, P_y\}\ (\alpha\neq 0)$$
$$\sim\{J_z+\alpha P_z, K_x, K_y\}\ (\alpha\neq 0)$$
$$\{J_z+\alpha P_z, K_x+\mu P_y, K_y-\mu P_x\}\ (\mu>0, \alpha\neq 0)$$
$$\sim\{J_z+\beta H, P_x, P_y\}\ (\beta>0)$$
$$\sim\{J_z+\gamma K_z+\beta H, P_x, P_y\}\ (\gamma\neq 0, \beta>0)$$
$$\sim\{J_z+\gamma K_z+\alpha P_z, K_x, K_y\}\ (\gamma\neq 0, \alpha\neq 0)$$
$$\{J_z+\gamma K_z+\alpha P_z, K_x+\mu P_y, K_y-\mu P_x\}\ (\gamma\neq 0, \alpha\neq 0, \mu>0)$$

(ii) Weyl algebras W(1):

$$\{H, K_x, P_x\}$$
$$\{H, K_x+\alpha P_y, P_x\}\ (\alpha>0)$$
$$\{H+\beta K_z, K_x, P_x\}\ (\beta>0)$$
$$\{H+\beta K_z, K_x+\alpha P_y, P_x\}\ (\beta>0, \alpha\neq 0)$$
$$\{H+\beta K_z, K_x+\rho K_z+\alpha P_x, P_x+\rho P_z\}\ (\beta>0, \rho>0, \alpha\neq 0)$$
$$\{H+\beta K_z, K_x+\rho K_z+\alpha P_y, P_x+\rho P_z\}\ (\beta>0, \rho>0, \alpha\neq 0)$$
$$\{H+\beta K_z, K_x+\rho K_z+aP_x+bP_y, P_x+\rho P_z\}\ (\beta>0, \rho>0, a\neq 0, b\neq 0)$$
$$\{H, K_z+\gamma J_z, P_z\}\ (\gamma\neq 0)$$
$$\{H+\gamma J_z, K_z, P_z\}\ (\gamma>0)$$
$$\{H+\gamma J_z, K_z+\delta H, P_z\}\ (\gamma>0, \delta\neq 0)$$
$$\{H+\gamma K_z, K_z+\delta J_z, P_z\}\ (\gamma>0, \delta\neq 0)$$
$$\{H+\gamma J_z, J_z+\delta K_z, P_z\}\ (\gamma>0, \delta\neq 0).$$

(iv) Abelian algebras

$SO(2)\times R^2$ algebras:
$$\{J_z, K_z, P_z\}$$
$$\sim\{J_z, H, P_z\}$$
$$\{J_z, K_z+\delta H, P_z\}\ (\delta>0)$$

R^3 algebras: $\sim\{H, P_x, P_y\}$
all three-dimensional subalgebras of {K, P} (see Table XI).

[a]The subalgebras preceded by the sign ~ are subalgebras of $\tilde{\mathcal{G}}$ (see Table XI.)

7. TWO- AND THREE-DIMENSIONAL SUBALGEBRAS IN. TWO-, THREE-, AND FOUR-DIMENSIONAL SUBALGEBRAS IN $\tilde{\mathcal{G}}$

A. Construction of the subalgebras

Here is a rapid outline about the determination of the low dimensional subalgebras of $\mathcal{G}$.

So let A and B generate a two-dimensional subalgebra of $\mathcal{G}$. Then considering successively for A each element written in the three first boxes of Table III, we shall have to associated with it the elements B of $\mathcal{G}$ such that A, B form a basis of a two-dimensional Lie algebra not conjugate under G to an algebra already obtained. Note that B has to be taken only in the solvable part $\mathcal{R}$ of $\mathcal{G}$ since the simple part $\mathcal{L}\approx$SO(3) does not contain two-dimensional subalgebras.

Consider now the three-dimensional subalgebras of $\mathcal{G}$. From Theorem 3.1, one deduces that all these algebras are solvable except the simple part $\mathcal{L}\approx$SO(3). These solvable algebras will be studied following their type $\mathcal{B}=\mathcal{L}_B+\mathcal{R}_B$ (with $\dim\mathcal{L}_B=1$), $\mathcal{M}_B+\mathcal{R}_B$ (with $\dim\mathcal{M}_B=1$) and $\mathcal{R}_B$.

Let us add a remark about the two- and three-dimensional subalgebras of the Abelian ideal {K, P}. Indeed the classification of these algebras is equivalent to the study of the orbits of the group $SO(3)\times R$ generate by {J, H} in the sets of subspaces of {K, P} of dimension two and three, respectively.

Concerning the subalgebras of $\tilde{\mathcal{G}}$, we consider the techniques proposed in Sec. 5 and already used in Sec. 6.

Finally the classification up to an isomorphy of these algebras leads to

Proposition 7.1: All two-dimensional subalgebras of $\mathcal{G}$ and of $\tilde{\mathcal{G}}$ are Abelian. Any three-dimensional subalgebras of $\mathcal{G}$ and of $\tilde{\mathcal{G}}$ is either simple and of the rotation type SO(3), or solvable. In this last case, it is either Abelian, or of the Euclidean type E(2), or of the Weyl type W(1). (See, for example, Ref. 1 for the list of the nonisomorphic three-dimensional real Lie algebras.)

B. Tables of the subalgebras

The two-dimensional subalgebras of $\mathcal{G}$ and $\tilde{\mathcal{G}}$ are gathered in Tables VII and VII, respectively.

A special table (Table IX) is devoted to the three-dimensional subalgebras of $\mathcal{G}$ which are subalgebras of the ideal {K, P}. Tables X and XI give the three-dimensional subalgebras of $\mathcal{G}$ and $\tilde{\mathcal{G}}$ respectively. Finally, the four-dimensional subalgebras of $\tilde{\mathcal{G}}$ are given in Table XII.

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Paul Sorba

TABLE XI. Three-dimensional subalgebras of $\tilde{\mathcal{G}}$.

They can be gathered into three parts:

(i) the subalgebras obtained by adding the generator M to each two-dimensional subalgebra of $\mathcal{G}$ (see Table VII);

(ii) the subalgebras preceded by the sign ~ in the Tables IX and X of the three-dimensional subalgebras of $\mathcal{G}$;

(iii) the subalgebras:
$$\{J_z+\alpha M, P_x, P_y\}\ (\alpha>0)$$
$$\{J_z+\alpha M, K_x, K_y\}\ (\alpha>0)$$
$$\{J_z+\beta H+\gamma M, P_x, P_y\}\ (\beta>0, \gamma\neq 0)$$
$$\{J_z+\alpha M, H, P_z\}\ (\alpha>0)$$
$$\{J_z, H+\beta M, P_z\}\ (\beta\neq 0)$$
$$\{J_z+\alpha M, H+\beta M, P_z\}\ (\alpha>0, \beta\neq 0)$$
$$\{H+\alpha M, P_x, P_y\}\ (\alpha\neq 0)$$

TABLE XII. Four-dimensional subalgebras of $\tilde{\mathcal{G}}$.

They can be gathered into two parts:

(i) the subalgebras obtained by adding the generator M to each three-dimensional subalgebras of $\mathcal{G}$ (see Tables IX and X).

(ii) the subalgebras:

$\{\mathbf{J}, H\}$ (isomorphic to $SO(3)\times R$)
$\{\mathbf{J}, H+\delta M\}$ $(\delta \neq 0)$

$\{J_z+\alpha H, \mathbf{P}\}$ $(\alpha > 0)$ [isomorphic to $E(2)\times R$]:
$\{J_z+\alpha H+\beta M, \mathbf{P}\}$ $(\alpha > 0, \beta \neq 0)$
$\{J_z, \mathbf{P}\}$
$\{J_z+\alpha M, \mathbf{P}\}$ $(\alpha > 0)$
$\{J_z K_x, K_y, P_z\}$
$\{J_z+\alpha M, K_x, K_y, P_z\}$
$\{J_z, \mathbf{K}\}$
$\{J_z+\alpha M, \mathbf{K}\}$ $(\alpha > 0)$
$\{J_z, P_x, P_y, K_z+\delta H\}$ $(\delta > 0)$
$\{J_z+\alpha M, P_x, P_y, K_z+\delta H\}$ $(\alpha > 0, \delta \neq 0)$
$\{J_z+\alpha P_z, H, P_x, P_y\}$ $(\alpha \neq 0)$
$\{J_z+\alpha P_z+\beta M, H, P_x, P_y\}$ $(\alpha \neq 0, \beta > 0)$

$\{H, \mathbf{P}\}$ (isomorphic to R^4)
$\{H+\alpha M, \mathbf{P}\}$ $(\alpha \neq 0)$

$\{J_z+\alpha P_z+\beta M, H+\gamma M, P_x, P_y\}$ $(\alpha \neq 0, \beta > 0, \gamma \neq 0)$
$\{J_z+\alpha P_z, H+\beta M, P_x, P_y\}$ $(\alpha \neq 0, \beta \neq 0)$
$\{J_z+\beta M, K_x, K_y, K_z+\alpha P_z\}$ $(\beta > 0, \alpha \neq 0)$
$\{J_z, K_x, K_y, K_z+\alpha P_z\}$ $(\alpha \neq 0)$
$\{J_z+\alpha M, P_x, P_y, H+\beta M\}$ $(\alpha > 0, \beta \neq 0)$
$\{J_z, P_x, P_y, H+\beta M\}$ $(\beta \neq 0)$
$\{J_z+\alpha M, P_x, P_y, H\}$ $(\alpha > 0)$
$\{J_z, P_x, P_y, H\}$
$\{J_z+\alpha M, P_x, P_y, K_z\}$ $(\alpha > 0)$
$\{J_z, P_x, P_y, K_z\}$

APPENDIX A: PROOF OF THEOREM 3.1

Let $\mathcal{B} = \mathcal{L}_B + \mathcal{M}_B + \mathcal{R}_B$ a maximal subalgebra of $\mathcal{A}$. Two cases can be considered concerning the ideal $\mathcal{R}_B$.

(i) $\mathcal{R}_B = \mathcal{R}$; then $\mathcal{B} = \mathcal{R} + \mathcal{L}_B = \mathcal{R} \square \mathcal{L}_B$ and so $\mathcal{L}_B$ must be maximal in $\mathcal{L}$ if $\mathcal{B}$ is maximal in $\mathcal{A}$.

(ii) $\mathcal{R}_B \subsetneq \mathcal{R}$; considering the vector space $\mathcal{M}_B$, let us denote by $\mathcal{L}_B$ and $\mathcal{R}'_B$ the spaces spanned by the elements l' and r' respectively.

First one shows that $\mathcal{L}_B + \mathcal{L}'_B = \mathcal{L}$. Indeed assuming that the subalgebra $\mathcal{L}_B + \mathcal{L}'_B \neq \mathcal{L}$, the subalgebra $\mathcal{C} = \mathcal{R} + \mathcal{L}_B + \mathcal{L}'_B$ would be a proper subalgebra and would include $\mathcal{B}$:

$$\mathcal{B} \subsetneq \mathcal{C} \subsetneq \mathcal{A}.$$

It is then possible to prove that $\mathcal{L}_B + \mathcal{M}_B$ is a subalgebra of $\mathcal{B}$ and also that it is exactly $\mathcal{L}$ up to a conjugation.

Now if $\mathcal{R}_B = 0$, $\mathcal{L}_B + \mathcal{M}_B$ is an algebra. But if $\mathcal{R}_B \neq 0$, we can consider the quotient $\mathcal{Q} = \mathcal{B}/\mathcal{R}_B$. $\mathcal{Q}$ is a Lie algebra since $\mathcal{R}_B$ is an ideal. Moreover, $\mathcal{Q}$ is semisimple; indeed, the existence of an Abelian nonzero ideal in $\mathcal{Q}$ would induce the existence of an Abelian nonzero ideal in $\mathcal{L}$.

Since all the extensions of a semisimple Lie algebra are trivial,[15] we are insured that $\mathcal{L}_B + \mathcal{M}_B$ forms an algebra and that $\mathcal{B}$ can be written as the semidirect (or direct) sum $\mathcal{B} = \mathcal{R}_B \square (\mathcal{L}_B + \mathcal{M}_B)$. The same type of arguments showing the semisimplicity of $\mathcal{Q}$ allows to deduce that $\mathcal{L}_B + \mathcal{M}_B$ is semisimple. Thus $\mathcal{A}$ can be written

$$\mathcal{A} = \mathcal{R} \square (\mathcal{L}_B + \mathcal{M}_B)$$

with $\mathcal{L}_B + \mathcal{M}_B$ playing the role of a Levi's factor.

All of Levi's factors being conjugate in a real Lie algebra (Malcev's theorem), $\mathcal{L}_B + \mathcal{M}_B$ is $\mathcal{L}$ or conjugate to $\mathcal{L}$. It follows that $\mathcal{B} = \mathcal{R}_B \square \mathcal{L}$ or is conjugate to $\mathcal{B}_0 = \mathcal{R}_0 \square \mathcal{L}$.

Finally the maximality of $\mathcal{B}_0$ in $\mathcal{A}$ imposes the subalgebra $\mathcal{R}_0$ of $\mathcal{R}$ to be maximal as a subalgebra of $\mathcal{R}$ invariant under $\mathcal{L}$. Thus $\mathcal{R}_0$ is an ideal of $\mathcal{A}$ maximal as subideal of $\mathcal{R}$.

APPENDIX B: THE EUCLIDEAN GROUPS $E(3)$ IN G (AND $\tilde{G}$)

One finds in G two three-dimensional Euclidean groups E(3) which are not conjugate: the group generated by $\{\mathbf{J}, \mathbf{K}\}$ which will be denoted by $E_b(3)$ and the group generated by $\{\mathbf{J}, \mathbf{P}\}$ denoted by $E_s(3)$.

We know from Sec. II D that $\Pi(E_b(3))$ is exactly a subset of $\Pi(G)$. It can also proved that $\Pi(E_s(3))$ is a subset of $\Pi(G)$.

Indeed let us consider $g = (0, \mathbf{c}, 0, R)$, $g' = (0, \mathbf{c}', 0, R')$ and $g_0 = (d_0, \mathbf{c}_0, \mathbf{b}_0, R_0)$ such that

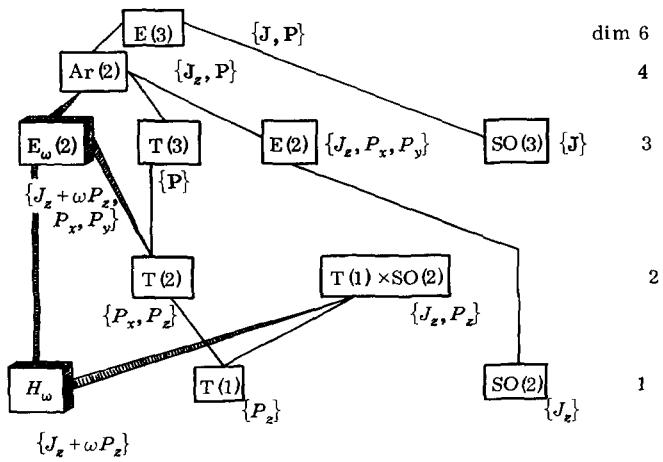
$$g_0 g g_0^{-1} = g'. \tag{B1}$$

One can compute

$$g_0 g g_0^{-1} = (0, \mathbf{c}_0 + R_0\mathbf{c} - R_0 R R_0^{-1}\mathbf{c}_0 - d_0(\mathbf{b}_0 - R_0 R R_0^{-1}\mathbf{b}_0), \mathbf{b}_0 - R_0 R R_0^{-1}\mathbf{b}, R_0 R R_0^{-1})$$

TABLE BI.[a] The p.o.s. $\pi(E(3))$

The p.o.s. $\pi(E(3))$.



[a] This table is for E(3) considered as subgroup of G as well as subgroup of $\tilde{G}$.

Using Eq. (B1), we get

$$\mathbf{c}' = \mathbf{c}_0 + R_0\mathbf{c} - R_0RR_0^{-1}\mathbf{c}_0, \quad R' = R_0RR_0^{-1}.$$

So, it follows that g and g' are also conjugate under

$$g_1 = (0, \mathbf{c}_0, 0, R_0) \in E_s(3).$$

By the same arguments one deduces that $\Pi(E_b(3))$ and $\Pi(E_s(3))$ are subsets of $\Pi(\tilde{G})$.

Although the p.o.s. $\Pi(E(3))$ had already been studied in Ref. 1, we rapidly draw its form in Table BI.

[1]H. Bacry, Ph. Combe, and P. Sorba, Rept. Math. Phys. **5**, 2, 145 (1974); **5**, 3, 361 (1974).
[2]Ph. Combe and P. Sorba, Physica A **80**, 271 (1975).
[3]J.M. Levy-Leblond, in *Group Theory and Applications, Vol.* 2, edited by E.M. Loebl (Academic, New York, 1972).
[4]V. Bargmann, Ann. Math. **59**, 1 (1954).
[5]J.M. Levy-Leblond and M. Le Bellac, Nuovo Cimento B **14**, 217 (1973).
[6]H. Bacry, Ph. Combe, and J.L. Richard, Nuovo Cimento A **70**, 289 (1970).
[7]J. Kubar-Andre, Nuovo Cimento A **15**, 577 (1973).
[8]U. Niederer, Helv. Phys. Acta **45**, 802 (1972).
[9]G. Burdet, M. Perrin, P. Sorba, J. Math. Phys. **15**, 1436 (1974); **15**, 2253 (1974); Lett. Nuovo Cimento **7**, 855 (1973).
[10]Let us note that the one-dimensional connected subgroups of the Schrödinger group Sch have been recently classified in, G. Burdet and M. Perrin, J. Math. Phys. **16**, 2172 (1975).
[11]D. Kastler, G. Loupias, M. Mebkhout, and L. Michel, Comm. Math. Phys. **27**, 195 (1972); G. Loupias and M. Mebkhout, J. Math. Phys. **14**, 777 (1973).
[12]L. Michel, *Relativistic Invariance and Internal Symmetries*, in *Brandeis Summer School* 1965 (Gordon and Breach, New York, 1966).
[13]N. Jacobson, *Lie Algebras* (Interscience, London, 1965).
[14]E. Inonu and E.P. Wigner, Proc. Nat. Acad. Sci. USA **39**, 510 (1953).
[15]D.J. Simms, "Projective Representations, Symplectic Manifolds and Extensions of Lie Algebras," lectures given in Marseilles (1969).

Wave operators for long-range hard-core potentials

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In a previous paper, we have proposed a definition of wave operators for hard-core potentials of long range from the standpoint of time-dependent single-channel quantum scattering theory. In the present note, we prove the existence of these operators for a large class of such potentials. The proof involves a combination of methods previously used to establich the existence of wave operators for short-range hard-core potentials and long-range potentials without hard cores.

1. INTRODUCTION

There have been a number of investigations of the existence of wave operators appropriate to short-range hard-core potentials and to long-range potentials without hard cores within the framework of time-dependent single-channel quantum scattering theory.[1] We have proposed[2] a definition of wave operators for long-range hard-core potentials within this framework. Roughly speaking, it is obtained from the pertinent definition for short-range potentials with hard cores by replacing the unitary operator describing the free evolution of the scattering system by a "renormalized" one familiar in the time-dependent approach to scattering by long-range potentials without such cores.

The purpose of the present note is to prove the existence of such wave operators for a large class of hard-core potentials of long range. The proof, given in Sec. 2, involves a combination of the methods of Ikebe[3] for short-range hard-core potentials and of Alsholm and Kato[4] and Alsholm[5] for long-range potentials with no hard cores.[6] Appendices A and B contain theorems on self-adjoint extensions of relevant operators.

Our existence result allows a rigorous and straightforward extension of an earlier approach[7] for determining potentials whose single-channel S operators are the same as that of a given potential of a suitable class to the case when this class is that of the long-range hard-core potentials defined in Sec. 2. This extension is important for constructing phase-equivalent proton–proton potentials.

2. WAVE OPERATORS FOR LONG-RANGE POTENTIALS WITH HARD CORES

We consider an arbitrary fixed integer $n \geq 2$, unless an explicit statement to the contrary is made. Let Γ be an open subset of R^n such that $\gamma = R^n \backslash \Gamma$, the hard core, is compact.

In this section, we shall be concerned with a potential V which is a fixed multiplication operator in $L^2(\Gamma)$ by a real-valued function $V(\cdot)$ having the following properties:

I. Let m denote a fixed positive integer and let there exist a decomposition

$$V(\cdot) = V_S(\cdot) + V_L(\cdot) \tag{1}$$

of $V(\cdot)$ into short-range and long-range parts, $V_S(\cdot)$ and $V_L(\cdot)$ being real-valued functions on Γ such that

$$(1 + |x|)^{1+\epsilon} V_S(\cdot) \in L^2(\Gamma) + L^\infty(\Gamma)$$

holds for some $\epsilon > 0$ and that all the partial derivatives $D^p V_L(x)$ of order $p = 1, \ldots, N \geq [m + \alpha_m] + m + 1$ exist on Γ and satisfy

$$|D^p V_L(x)| \leq \text{const } (1 + |x|)^{-p-\alpha_p} \tag{2}$$

thereon, where the α_p are positive constants fulfilling the conditions (L) stated in Theorem 3, Ref. 5, and where $[q]$ is the largest integer not exceeding a given real q.

The latter conditions are too complicated to state here, and we must refer the interested reader to Ref. 5. They are satisfied, in particular, if (2) holds in the stated sense with $\alpha_1 = \cdots = \alpha_{2m} = \alpha$, where $(m+1)^{-1} < \alpha \leq 1$.

The requirements I on $V_L(\cdot)$ entail that the following limit exists and is finite[8]:

$$V_0 = \lim_{|x| \to \infty} V_L(x).$$

From I and the finiteness of V_0, it is clear that $V_L(\cdot) \in L^\infty(\Gamma)$. Therefore, $V(\cdot) \in L^2(\Gamma) + L^\infty(\Gamma)$, whence Theorem A of Appendix A entails that the operator $-\Delta + V$ on $C_0^\infty(\Gamma)$[9] has a self-adjoint extension, Δ being the Laplacian operator in R^n. In this section, we denote by H a fixed, but arbitrary, self-adjoint extension of the penultimate operator. For the existence purposes of this paper, any such self-adjoint extension is as good as any other. However, it is an important fact physically that for $n = 3$, at least under certain additional hypotheses on Γ (which will not be made in the present section), there exists a self-adjoint extension H' of $-\Delta + V$ on $C_0^\infty(\Gamma)$ with the following property. The functions in the domain of H' satisfy the boundary condition usually associated with a hard core, namely, they are equivalent to continuous functions f on Γ such that $f(x) \to 0$ as x tends to any given point of the boundary of Γ. The existence of H' follows from Theorem B of Appendix B.

Without loss of generality, it will be assumed henceforth in the text that $V_L(\cdot)$ is the restriction to Γ of a real-valued function $\tilde{V}_L(\cdot)$ on R^n having the properties ascribed to $V_L(\cdot)$ in I, but with Γ replaced by R^n. In fact, if there exists a decomposition (1) of the type specified in I, then there also exists a decomposition $V(\cdot) = V'_S(\cdot) + V'_L(\cdot)$, where $V'_S(\cdot)$ and $V'_L(\cdot)$ satisfy the respective conditions imposed on the corresponding unprimed quantities in I and, additionally, $V'_L(\cdot)$ is the restriction of such a $\tilde{V}_L(\cdot)$.[10]

By an appropriate shift of the zero of the energy scale, we will set the constant V_0 pertaining to the present $V_L(\cdot)$ equal to zero from now on. It will also prove convenient to introduce an auxiliary multiplication operator $\tilde{V}$ in $L^2(R^n)$ by a real-valued function $\tilde{V}(\cdot) \in L^2_{\rm loc}(R^n)$ such that

$$\tilde{V}(x) = \tilde{V}_S(x) + \tilde{V}_L(x) \quad \text{on } R^n, \tag{3}$$

where $\tilde{V}_S(\cdot)$ is a real-valued extension of $V_S(\cdot)$ to R^n. *Therefore, I holds if we replace* $V(\cdot)$, $V_S(\cdot)$, $V_L(\cdot)$, *and* Γ *by* $\tilde{V}(\cdot)$, $\tilde{V}_S(\cdot)$, $\tilde{V}_L(\cdot)$, *and* R^n, *respectively*. This will allow us to use the pertinent results of Ref. 5 in this paper.

We define the wave operators $\Omega_\pm^{(m)}: L^2(R^n) \to L^2(\Gamma)$ for long-range potentials with hard cores by

$$\Omega_\pm^{(m)} = \text{s-lim}_{t \to \pm\infty} V_t^* \rho U_t^{(m)} \tag{4}$$

at each $-\infty < t < \infty$ when the limits exist.[11] The operator $\rho: L^2(R^n) \to L^2(\Gamma)$ is specified by

$$\rho f(x) = f(x) \quad \text{on } \Gamma$$

for each $f \in L^2(R^n)$ and $U_t^{(m)}: L^2(R^n) \to L^2(R^n)$ is the unitary operator

$$U_t^{(m)} = \exp(-itH_0 - iX_t^{(m)}).$$

Here $X_t^{(m)}$ is an operator of multiplication in the momentum-space representation of $L^2(R^n)$ by the function $X_t^{(m)}(\cdot)$ defined recursively by

$$\begin{aligned} &X_t^{(0)}(k) = 0, \\ &X_t^{(p)}(k) = \int_0^t \tilde{V}_L(sk + \nabla_k X_s^{(p-1)}(k))\, ds. \end{aligned} \tag{5}$$

The last definition in (5) can be readily seen to be effective for $p = 1, \ldots, m$.

On physical grounds, it is natural to require that

$$\tilde{V}_L(x) = 0 \quad \text{on } R^n \quad \text{when } V_L(x) = 0 \quad \text{on } \Gamma. \tag{3'}$$

Indeed, if (3′) and the remaining relevant hypotheses of the paper hold, then $\Omega_\pm^{(m)}$ reduce to the corresponding operators for short-range potentials with hard cores when $V_L(x) \equiv 0$. The condition (3′) is obviously compatible with the previous ones. If one replaces Γ and $\tilde{V}_L(\cdot)$ by R^n and $V_L(\cdot)$, respectively, then $\Omega_\pm^{(m)}$ agree with the corresponding operators for long-range potentials advocated by many authors,[1] provided that V_t is suitably reinterpreted.

Plainly, the decomposition (1) is not unique and hence neither are $\Omega_\pm^{(m)}$. For the case of long-range potentials, the nonuniqueness of the corresponding wave operators has been discussed by a number of authors.[12] A similar situation arises in the case under consideration.[13]

Our main result is the theorem which we proceed to state. This theorem is true independently of whether (3′) is satisfied.

Theorem 1: The operators $\Omega_\pm^{(m)}$ exist, are isometric on $L^2(R^n)$, and have the intertwining properties

$$\exp(itH)\Omega_\pm^{(m)} = \Omega_\pm^{(m)} \exp(itH_0). \tag{6}$$

Proof: To prove the existence of $\Omega_\pm^{(m)}$, we write

$$V_t^* \rho U_t^{(m)} = \Omega_t^{(1)} + \Omega_t^{(2)}$$

and show that the strong limits as $t \to \pm\infty$ of the operators

$$\begin{aligned} \Omega_t^{(1)} &= V_t^* \rho (I - \eta) U_t^{(m)}, \\ \Omega_t^{(2)} &= V_t^* \rho \eta U_t^{(m)} \end{aligned}$$

exist. Here I is the unit operator in $L^2(R^n)$ and η is a multiplication operator in this space by a function $\eta(\cdot) \in C^\infty(R^n)$ such that $\text{supp}\eta(\cdot) \subset \Gamma$, that $0 \leq \eta(x) \leq 1$, and that $\eta(x) = 1$ identically outside of some compact subset of R^n containing γ.

Now,[14]

$$\begin{aligned} &\| \zeta U_t^{(m)} f \|_{L^2(R^n)} \leq \text{const } |t|^{-1-\delta} \\ &\text{for all } \delta > 0, \ |t| \geq 1, \ f \in \mathcal{S}, \end{aligned} \tag{7}$$

where ζ is a multiplication operator in $L^2(R^n)$ by a function $\zeta(\cdot)$, for which $|\zeta(x)| \leq \text{const } (1 + |x|)^{-1-\delta}$ a.e. on R^n for some $\delta > 0$. In (7), $\mathcal{S}$ is the dense subset of $L^2(R^n)$ consisting of those functions $f \in L^2(R^n)$ having a Fourier transform $\hat{f} \in C_0^\infty(R^n)$ such that $\text{supp}\hat{f} \subset R^n \backslash \{0\}$. From this result, in combination with the relevant definitions and elementary arguments, we infer that (7) holds with $\zeta U_t^{(m)}$ replaced by $\Omega_t^{(1)}$ and $L^2(R^n)$ by $L^2(\Gamma)$. Hence, $\Omega_t^{(1)}$ tends strongly to zero on $\mathcal{S}$ as $t \to \pm\infty$, so that, by uniform boundedness, $\Omega_t^{(1)}$ has these same properties on the whole of $L^2(R^n)$.

By a standard argument, the existence of $\text{s-lim}_{t \to \pm\infty} \Omega_t^{(2)}$ will be proved if one shows that, as a function of t,

$$\left\| \frac{d\Omega_t^{(2)}}{dt} f \right\|_{L^2(\Gamma)} \in L^1(-\infty, -1) \cap L^1(1, \infty), \quad \text{if } f \in \mathcal{S}, \tag{8}$$

where the time derivative is understood here and henceforth in the strong sense.

In the remainder of the proof of the existence of $\Omega_\pm^{(m)}$, we shall assume that the decomposition $\tilde{V}(\cdot) = \tilde{V}_S(\cdot) + \tilde{V}_L(\cdot)$ considered is such that the additional properties $\tilde{V}_L(\cdot) \in C^\infty(R^n)$ and

$$\begin{aligned} &\left\| (\tilde{V} - \frac{dX_t^{(m)}}{dt})\, U_t^{(m)} f \right\|_{L^2(R^n)} \in L^1(-\infty, -1) \cap L^1(1, \infty) \\ &\quad \text{if } f \in \mathcal{S}, \end{aligned} \tag{9}$$

both hold. That this assumption entails no loss of generality should be clear from the following facts.[15] First, the existence of a decomposition (3) such that the properties in the italicized statement immediately after (3) obtain entails that there is also a decomposition (3) such that these properties and also those in the penultimate sentence are present. Second, if the operators (4) corresponding to the second decomposition exist, so do those pertaining to the first decomposition.

To prove (8), we focus our attention on a fixed $h \in \mathcal{S}$ and observe that

$$h \in D(H_0), \quad \rho \eta U_t^{(m)} h \in D(H). \tag{10}$$

The first assertion of (10) should be clear. The second follows by combining the fact that $\rho \eta U_t^{(m)} h \in \mathcal{S}(\Gamma)$ with Theorem A of Appendix A. Here $\mathcal{S}(\Gamma)$ is the set of functions on Γ, each of which is the restriction of a function $f \in \mathcal{S}(R^n)$, such that $\text{supp}\, f \subset \Gamma$, $\mathcal{S}(R^n)$ being the set of Schwartz functions of fast decrease on R^n. The membership statement in the penultimate sentence is deduced by

employing, in particular, the infinite differentiability and support properties of $\eta(\cdot)$, the infinite differentiability of $X_t^{(m)}(\cdot)$ [which follows from the validity of (5) over the pertinent ranges, couped with the assumption that $\tilde{V}_L(\cdot) \in C^\infty(R^n)$], that $\mathcal{S}(R^n)$ is invariant under Fourier transformation, and that $\mathcal{S}(R^n) \supset \mathcal{S}$.

Using (10), the definitions of the pertinent operators, and properties such as the one that $dX_t^{(m)}/dt$ exists and has domain $L^2(R^n)$, one concludes that $(d\Omega_t^{(2)}/dt)h$ exists and is given by

$$\frac{d\Omega_t^{(2)}}{dt} h = iV_t^* \left[H\rho\eta - \rho\eta\left(H_0 + \frac{dX_t^{(m)}}{dt}\right)\right] U_t^{(m)} h. \tag{11}$$

Keeping in mind, in particular, that (A2) of Appendix A holds for $f = \rho\eta U_t^{(m)} h$ and manipulating (11) by procedures analogous to ones in Ref. 3, one infers that

$$\begin{aligned}
\left\| \frac{d\Omega_t^{(2)}}{dt} h \right\|_{L^2(\Gamma)} &\leq \left\| \left(V\rho\eta - \rho\eta \frac{dX_t^{(m)}}{dt} \right) U_t^{(m)} h \right\|_{L^2(\Gamma)} \\
&\quad + \| \rho(\Delta\eta) U_t^{(m)} h \|_{L^2(\Gamma)} + 2 \sum_{i=1}^{n} \left\| \rho \left(\frac{\partial \eta}{\partial x_i} \right) U_t^{(m)} \frac{\partial h}{\partial x_i} \right\|_{L^2(\Gamma)} \\
&\leq \left\| \left(\tilde{V} - \frac{dX_t^{(m)}}{dt} \right) U_t^{(m)} h \right\|_{L^2(R^n)} + \| (\Delta\eta) U_t^{(m)} h \|_{L^2(R^n)} \\
&\quad + 2 \sum_{i=1}^{n} \left\| \left(\frac{\partial \eta}{\partial x_i} \right) U_t^{(m)} \frac{\partial h}{\partial x_i} \right\|_{L^2(R^n)},
\end{aligned} \tag{12}$$

where $\Delta\eta$ and $\partial\eta/\partial x_i$ are multiplication operators in $L^2(R^n)$ by $\Delta\eta(\cdot)$ and $\partial\eta(\cdot)/\partial x_i$, respectively, with x_i the ith component of $x \in R^n$. The significance of the remaining factors should be clear. Since $\Delta\eta(\cdot)$ and $\partial\eta(\cdot)/\partial x_i$ are in $C_0^\infty(R^n)$, h and $\partial h/\partial x_i$ are in $\mathcal{S}$, and (7), (9), and (12) hold, (8) follows directly.

Henceforth in this proof, we dispense with the assumptions made in the sentence containing (9).

In order to show that the $\Omega_\pm^{(m)}$ are isometric, we begin by observing that

$$\| V_t^* \rho U_t^{(m)} f \|_{L^2(\Gamma)}^2 = \| f \|_{L^2(R^n)}^2 - \| \chi_\gamma U_t^{(m)} f \|_{L^2(R^n)}^2 \tag{13}$$

at each $f \in L^2(R^n)$, where χ_γ is a multiplication operator in $L^2(R^n)$ by the characteristic function $\chi_\gamma(\cdot)$ of the hard-core region γ.

The second term on the rhs of (13) tends to zero as $t \to \pm\infty$ at every $f \in \mathcal{S}$, as one deduces with the aid of (7). Hence, this vanishing property holds for each $f \in L^2(R^n)$. Together, this result and (13) evidently imply the desired isometry property.

Finally, the intertwining relations (6) can be established by an approach analogous to the corresponding one in Ref. 5.[16] This completes the proof of Theorem 1.

APPENDIX A: SELF-ADJOINT EXTENSIONS FOR $n \geq 2$

In this appendix, V, V_1, and V_2 are multiplication operators in $L^2(\Gamma)$ by the respective real-valued functions $V(\cdot)$, $V_1(\cdot)$, and $V_2(\cdot)$ on Γ. The set $\mathcal{S}(\Gamma)$ mentioned below was defined in the third sentence after (10).

Theorem A[17]: The operator $-\Delta + V$ on $C_0^\infty(\Gamma)$ has a self-adjoint extension if $V(\cdot) \in L^2_{\text{loc}}(\Gamma)$. Moreover, let

$$\begin{aligned}
&V = V_1 + V_2, \\
&V_1(\cdot) \in L^2(\Gamma), V_2(\cdot) \in L^\infty(\Gamma).
\end{aligned} \tag{A1}$$

Then any such self-adjoint extension H has domain $D(H) \supset \mathcal{S}(\Gamma)$ and

$$Hf = -\Delta f + Vf, \quad \text{if } f \in \mathcal{S}(\Gamma). \tag{A2}$$

Proof: The operator $-\Delta + V$ on the set $C_0^\infty(\Gamma)$, dense in $L^2(\Gamma)$, is symmetric when $V(\cdot) \in L^2_{\text{loc}}(\Gamma)$. By an obvious extension of a theorem of Schecter[18] to $L^2(\Gamma)$, it follows that a self-adjoint extension of this real symmetric operator exists.

To complete the proof of Theorem A, we consider a fixed $f \in \mathcal{S}(\Gamma)$ and a fixed $\varphi \in C_0^\infty(R^n)$, where $\varphi(x) = 1$ for $|x| \leq 1$ and $0 \leq \varphi(x) \leq 1$ on R^n. We also define $f_\rho \in C_0^\infty(\Gamma)$ for each $0 < \rho < \infty$ by setting

$$f_\rho(x) = \varphi(x/\rho) f(x) \quad \text{on } \Gamma.$$

One finds that[19]

$$\lim_{\rho \to \infty} \| f - f_\rho \|_{L^\infty(\Gamma)} = 0, \tag{A3}$$

$$\begin{aligned}
&\lim_{\rho \to \infty} \| f - f_\rho \|_{L^2(\Gamma)} = 0, \\
&\lim_{\rho \to \infty} \| \Delta f - \Delta f_\rho \|_{L^2(\Gamma)} = 0.
\end{aligned} \tag{A4}$$

If V_1 and V_2 satisfy (A1), then

$$\begin{aligned}
\| V_1(f - f_\rho) \|_{L^2(\Gamma)} &\leq \| V_1(\cdot) \|_{L^2(\Gamma)} \| f - f_\rho \|_{L^\infty(\Gamma)}, \\
\| V_2(f - f_\rho) \|_{L^2(\Gamma)} &\leq \| V_2(\cdot) \|_{L^\infty(\Gamma)} \| f - f_\rho \|_{L^2(\Gamma)}.
\end{aligned} \tag{A5}$$

From (A3)—(A5), we see that for potentials V of the type (A1) one has

$$\lim_{\rho \to \infty} \| V(f - f_\rho) \|_{L^2(\Gamma)} = 0. \tag{A6}$$

Employing, in particular, (A4), (A5), and an elementary theorem,[20] we conclude that $f \in D(\mathring{H})$, where $\mathring{H}$ is the smallest closed symmetric extension of $-\Delta + V$ on $C_0^\infty(\Gamma)$ when V is of the latter type and that, in addition,

$$\mathring{H} f = -\Delta f + Vf.$$

Since $\mathring{H} \subset H$, where H is an arbitrary self-adjoint extension of $-\Delta + V$ on $C_0^\infty(\Gamma)$, it follows that $f \in D(H)$ and that (A2) holds for the present H and f.

APPENDIX B: SELF-ADJOINT EXTENSION FOR $n = 3$

In this appendix, we will limit ourselves to this value of n [21] and will assume that Γ is an open subset of R^3 whose boundary $\partial\Gamma$ is a closed surface of class C^2. Let $W^{2,2}(\Gamma)$ be the usual Sobolev space. Each element of this space is equivalent to a continuous function on $\Gamma \cup \partial\Gamma$ restricted to Γ. The operators V, V_1, and V_2 below are as described by the first sentence of Appendix A, but with $n = 3$.

Ikebe[22] has shown the existence of a positive self-adjoint extension H^0 of $-\Delta$ defined as follows. $D(H^0)$ is the set of those $f \in W^{2,2}(\Gamma)$ whose equivalent continuous functions $f(x)$ approach zero as x approaches any point of $\partial\Gamma$. For each $f \in D(H^0)$, $H^0 f = -\Delta f$, where $-\Delta$ is interpreted in the distribution sense.

The following theorem generalizes a theorem[23] of Ref. 22 to include a large class of long-range potentials.

Theorem B: Let V be such that (A1) holds for $n=3$. Then

$$H' = H^0 + V \tag{B1}$$

is self-adjoint and $\mathcal{S}(\Gamma) \subset D(H^0) = D(H') \subset D(V)$. In addition, (A2) holds for H' and this operator is lower semibounded.

Proof: Let $g \in D(H^0)$. Then

$$\|g\|_{L^\infty(\Gamma)} \leq \alpha \|H^0 g\|_{L^2(\Gamma)} + \beta \|g\|_{L^2(\Gamma)} < \infty, \tag{B2}$$

with an arbitrarily small constant $\alpha > 0$ and a constant $0 < \beta < \infty$.[24]

From (B2) and the assumed properties of V_1 and V_2, it is clear that $\| V_1 g\|_{L^2(\Gamma)}$ and $\|V_2 g\|_{L^\infty(\Gamma)}$ obey inequalities similar to (A5). Using these inequalities and the fact that (B2) holds in the stated sense, it is plain that V is relatively bounded with H^0-bound zero. Hence, the operator H' in (B1) is such that $D(H') = D(H^0) \subset D(V)$ and is also[25] self-adjoint and lower semibounded.

Finally, one proves the assertions that $\mathcal{S}(\Gamma) \subset D(H')$ and that the present H satisfies (A2) by invoking, in particular, the equality $D(H') = D(H^0)$ and the characterization of H^0 given earlier in this appendix.

[1]See, e.g., the review by W.O. Amrein, "Some Questions in Non-Relativistic Scattering Theory," in *Proceedings of the NATO Advanced Study Institute on Scattering Theory in Mathematics and Physics*, edited by J. LaVita and J.-P. Marchand (Reidel, Dordrecht, Holland, 1974).

[2]A.W. Sáenz and W.W. Zachary, J. Math. Phys. **17**, 409 (1976).

[3]T. Ikebe, J. Math. Kyoto Univ. **7**, 93 (1967).

[4]P. Alsholm and T. Kato, "Scattering with Long-Range Potentials," in *Proceedings of the Symposium on Pure Mathematics* (Am. Math. Soc., Providence, R.I., 1971), Vol. XXIII, pp. 393–399.

[5]P. Alsholm, "Wave Operators for Long-Range Scattering," thesis, University of California, Berkeley, 1972.

[6]For the important special case of Coulomb-like potentials with hard cores, the simpler analysis of Dollard can be used in place of that of Refs. 4 or 5, but we will not indicate the changes that this entails. See J.D. Dollard, J. Math. Phys. **5**, 729 (1964); Rocky Mountain J. Math. **1**, 5 (1971); **2**, 317 (1972) (E).

[7]A rigorous treatment of this approach is given in Ref. 2, where pertinent earlier references can be found. A.W. Sáenz and W.W. Zachary, Phys. Lett. **58B**, 13 (1975), have extended this method to multichannel scattering.

[8]Ref. 5, p. 71, Proposition 1.

[9]For each open subset M of R^n, $C_0^\infty(M)$ is defined as in, e.g., K. Yosida, *Functional Analysis* (Springer, New York, 1966), p. 26.

[10]Let the decomposition $V(\cdot) = V_S(\cdot) + V_L(\cdot)$ be as specified in I. Define $V_L'(x) = \xi(x) V_L(x)$ on Γ, $V_S'(\cdot) = V(\cdot) - V_L'(\cdot)$, and $\tilde{V}_L(x) = V_L'(x)$ (0) on $\Gamma(\gamma)$. Here $\xi \in C_0^\infty(R^n)$, with $\xi(x) = O(1)$ on Γ (outside of some compact set containing γ). Then $V_S'(\cdot)$ and $V_L'(\cdot)$ satisfy the conditions stated in the text.

[11]If nothing to the contrary is mentioned, all subsequent statements and equations involving operators with the subscript t should also be understood to hold for $-\infty < t < \infty$.

[12]See, e.g., W.O. Amrein, Ph.A. Martin, and B. Misra, Helv. Phys. Acta **43**, 313 (1970); E. Prugovečki, Nuovo Cimento B **4**, 105 (1971).

[13]For completeness, we mention two results connected with the nonuniqueness of the wave operators (4), similar results being well known for the wave operators appropriate for long-range potentials without hard cores. With the aid of conclusions of Sec. 4 of Ref. 5 and, in particular, the remarks on pp. 29 and 30 thereof, we arrive at the results which we now state. The wave operators of type (4), say $\Omega_\pm^{(m)}$ and $\Omega_\pm'^{(m)}$, pertaining to two decompositions $\tilde{V}(\cdot) = \tilde{V}_S(\cdot) + \tilde{V}_L(\cdot)$ and $\tilde{V}(\cdot) = \tilde{V}_S'(\cdot) + \tilde{V}_L'(\cdot)$ which fulfill the conditions stated in the second sentence of the paragraph containing (3) and of the paragraph preceding it, differ only by right multiplication by a unitary operator. This operator depends only on $\tilde{V}_L(\cdot)$ and $\tilde{V}_L'(\cdot)$. If the last two functions are spherically symmetric, then this unitary operator is a function of H_0. This entails that the S operators $\Omega_+^{(m)*}\Omega_-^{(m)}$ and $\Omega_+^{(m)'*}\Omega_-^{(m)'}$ corresponding to these respective decompositions are equal in this special case, as is clear from the validity of the intertwining relations (6) for the wave operators concerned.

[14]Ref. 5, p. 61, inequality (9.2).

[15]These facts follow from results in Secs. 4, 8, and 9 of Ref. 5. See, particularly, the remarks on pp. 29 and 30 thereof. That (9) is true under the desired conditions when α_1 in I is greater than unity can be shown by an approach similar to one on pp. 28 and 29 of Ref. 5.

[16]See Sec. 10 of this reference.

[17]The first assertion of this theorem can be immediately generalized to apply to an operator $L = P(D) + V$ on $C_0^\infty(M)$, where $P(D)$ denotes a linear partial differential operator of finite order with constant real coefficients and involving only even derivatives, V being a multiplication operator by $V(\cdot) \in L^2_{\text{loc}}(M)$ and M an open subset of R^n ($n \geq 2$). The second assertion of Theorem A can also be generalized to apply to L, provided that V fulfills (A1) with Γ replaced by M or that the conditions that $V(\cdot) \in L^2_{\text{loc}}(M)$ and that there exists a constant $0 < \sigma < \infty$ such that ess $\sup_{|x| \geq \sigma} |V(x)| < \infty$ are satisfied.

[18]M. Schechter, *Spectra of Partial Differential Operators* (North-Holland, Amsterdam, 1971), p. 152, Theorem 1.1.

[19]One can prove the second Eq. (A4) by the approach in pp. 58–59 of Ref. 18 (proof of Lemma 1.2).

[20]See, e.g., Ref. 18, p. 6, Theorem 2.1.

[21]The proof of Theorem B presented below fails for higher values of n because the Green's function of the analog of H^0 is then not of the Carleman type. For $n=2$, results analogous to Theorem B can probably be proved by combining our approach with that of Ikebe in Ref. 22. In the special case of short-range potentials, results on self-adjointness have been obtained by the eigenfunction expansion method for all $n \geq 2$. For this approach and for further references see N. Shenk and D. Thoe, J. Math. Anal. Appl. **36**, 313 (1971).

[22]T. Ikebe, Japanese J. Math. **36**, 33 (1967).

[23]Ref. 22, p. 49, Theorem 5.1.

[24]That (B2) holds for α and β of the stated type is entailed by two results on p. 49 of Ref. 22: inequality (5.4) and the Green's function property mentioned in the sentence following (5.4).

[25]See, e.g., T. Kato, *Perturbation Theory for Linear Operators* (Springer, New York, 1966), p. 291, Theorem 4.11.

High frequency approximations for elastic surface waves propagating along cylinders of general cross section*

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The propagation of high frequency elastic surface waves along the generators of a homogeneous isotropic cylinder of general cross section is considered. The boundary surface is stress-free and the surface waves, or Rayleigh waves, are disturbances whose amplitudes decay rapidly with depth into the cylinder. An approximate equation, and a refined one, are derived which describe the high frequency behavior of the surface wave modes. These approximate equations lead to the asymptotic results derived earlier by Wilson and the author for the case of an open boundary curve for which the curvature attains its algebraic maximum at a single point, and in fact they permit a more complete analysis of the higher order modes. Moreover, the refined approximate equation describes the behavior of the surface wave modes in the transition region, at high frequencies, between the case of cross-sectional boundary curves of nonconstant (and not "almost" constant) curvature, for which the modes are localized, and the case of constant curvature, for which they are not localized. Some particular examples are considered.

1. INTRODUCTION

Elastic surface waves, or Rayleigh waves, are disturbances which travel over the stress-free surface of an elastic solid, and whose amplitudes decay rapidly with depth into the solid. In a recent paper,[1] hereafter referred to as I, Wilson and the author investigated the high frequency propagation of such waves along a homogeneous isotropic cylinder which has a cross-sectional boundary of nonconstant curvature. In the case of an open boundary curve for which the curvature attains its algebraic maximum at a single point, it was shown that there are surface wave modes in which the disturbance is localized in the neighborhood of that point, as well as being confined close to the surface. The case of closed boundary curves was also discussed, in which the region under consideration may be either interior to the boundary cylinder, corresponding to a rod, or exterior to it, corresponding to a bore.

The analysis of the elastic problem involves a scalar wave equation, a vector wave equation, and rather complicated boundary conditions. Since the analysis is rather cumbersome, a simpler scalar "model problem" was first investigated by the author.[2] The techniques developed for that problem have counterparts for the elastic problem. The lowest order surface wave mode for the elastic problem was investigated in almost as much detail as that for the scalar problem, but because of the algebraic complexities the higher order elastic modes were less completely analyzed.

For the scalar problem,[2] an approximate equation was derived which describes the high frequency behavior of the surface wave modes. Moreover, it was pointed out that a refined approximation also describes their behavior in the transition region, at high frequencies, between the case of cross-sectional boundary curves of nonconstant (and not "almost" constant) curvature, for which the modes are localized, and the case of constant curvature, for which they are not localized.

The purpose of this paper is to derive the analogous approximate equations which describe the high frequency behavior of the elastic surface wave modes. In addition to describing the behavior in the transition region, the approximate equations also permit a more complete analysis of the higher order modes. Moreover, numerical solution of the approximate equations leads to a more satisfactory description of the modes in the case of closed cross-sectional boundary curves.

The elastic problem was formulated in I in terms of a right-handed coordinate system with unit vectors $\mathbf{n}$, $\mathbf{t}$, and $\mathbf{k}$ in the directions of the inward normal, tangent to the cross-sectional boundary curve, and along the generators of the cylinder, respectively, as depicted in I, Fig. 1. Then n will represent distance from the surface along the inward normal, while s will be signed arc length along the boundary curve, and z will be distance along the generators of the cylinder. Using appropriate units of length, and of frequency ω, we are interested in the case $\omega \gg 1$.

The displacement $\mathbf{u}$ is given in terms of a scalar potential and a vector potential: $\mathbf{u} = \nabla\varphi + \nabla \times \mathbf{A}$. We seek solutions of the resulting scalar and vector wave equations that satisfy the stress-free boundary condition, and have the form

$$\begin{aligned}\varphi &= \exp(-i\beta z - \omega\alpha_L n)\\ &\quad\times\left(G^{(0)}(s) + nG^{(1)}(s) + \frac{n^2}{2}G^{(2)}(s) + \frac{n^3}{6}G^{(3)}(s) + \cdots\right),\\ \mathbf{A} &= \exp(-i\beta z - \omega\alpha_T n)\\ &\quad\times\left(\mathbf{\Gamma}^{(0)}(s) + n\mathbf{\Gamma}^{(1)}(s) + \frac{n^2}{2}\mathbf{\Gamma}^{(2)}(s) + \frac{n^3}{6}\mathbf{\Gamma}^{(3)}(s) + \cdots\right),\end{aligned} \tag{1.1}$$

where α_L and α_T are positive numbers. The disturbance is confined close to the surface in the region $n = O(\omega^{-1})$.

In the Appendix we first write down six exact equations connecting the quantities in (1.1). Since more than six of the quantities occur in these equations, we seek an asymptotic approximation which reduces the number to exactly six. The assumptions that we make about the orders of $G^{(j)}$, and of the components $\Gamma_n^{(j)}$, $\Gamma_t^{(j)}$, and $\Gamma_k^{(j)}$ of $\mathbf{\Gamma}^{(j)}$, and the orders of their derivatives with respect to s, are motivated by the asymptotic results of

I. We also assume that $\beta=\omega\beta_0+\Lambda$, where $\Lambda=O(1)$. The validity of these assumptions may be verified *a posteriori*.

In Sec. 2 it is shown that β_0 satisfies the classical secular equation for Rayleigh waves on a plane infinite half-space. Also, the asymptotic assumptions are used to obtain six approximate equations for the quantities $G^{(0)}$, $G^{(1)}$, $\Gamma_t^{(0)}$, $\Gamma_t^{(1)}$, $\Gamma_n^{(0)}$, and $\Gamma_k^{(0)}$. From these six equations we derive the lowest order approximate equation for $G^{(0)}$, and relate the other quantities to $G^{(0)}$. It is found that

$$\frac{d^2G^{(0)}}{ds^2}+\omega[\gamma\kappa(s)-2\beta_0\Lambda]G^{(0)}=O(G^{(0)}), \tag{1.2}$$

where $\kappa(s)$ is the (sufficiently smooth) curvature of the cross-sectional boundary curve, and $\gamma>0$ is a constant given by I (3.17). Approximate expressions are given for the displacement on, and near, the surface.

In Sec. 3, ten asymptotically approximate equations for the quantities $G^{(0)}$, $G^{(1)}$, $G^{(2)}$, $\Gamma_t^{(0)}$, $\Gamma_t^{(1)}$, $\Gamma_t^{(2)}$, $\Gamma_n^{(0)}$, $\Gamma_n^{(1)}$, $\Gamma_k^{(0)}$, and $\Gamma_k^{(1)}$ are used to obtain a refined approximate equation (3.3) for $G^{(0)}$, which includes the terms of order $G^{(0)}$ omitted in (1.2), and a term involving $\omega^{-1}dG^{(0)}/ds$. The derivation involves the use of Eq. (1.2) to eliminate higher order derivatives. It is somewhat remarkable that the more involved elastic problem, with complicated boundary conditions, may be reduced to an eigenvalue problem for a single second order differential equation, which has the same structure as that for the scalar problem[2] with simple boundary condition.

In Sec. 4 we discuss some applications of the approximate equations for $G^{(0)}$ to cases not covered by the asymptotic analysis of I. The refined approximate equation may be used to describe the behavior of surface wave modes in the transition region mentioned earlier. In particular, we consider boundary curves of nearly constant curvature, the deviation from constancy being of order ω^{-1}. In general the refined approximate equation has to be solved numerically. An example is given corresponding to a nearly circular bore, for which the solution may be expressed in terms of Mathieu functions. We also consider a wedgelike object, similar to a hyperbolic cylinder, for which the solution may be given explicitly in closed form. There is a finite number of modes, and the lowest order mode always exists. If the maximum curvature is sufficiently small, then only the lowest order mode exists. The boundary becomes planar as the maximum curvature tends to zero, and in the limit the lowest order mode corresponds to a Rayleigh wave on a plane infinite half-space.

2. LOWEST ORDER APPROXIMATION

In the Appendix we write down six exact equations, (A1)–(A6), corresponding to the quantities in (1.1). Since more than six of the quantities occur in these equations, we seek an asymptotic approximation which reduces the number to exactly six. A close examination of the results in I leads us to assume the relative orders of magnitude

$$\begin{aligned} &G^{(j)}=O(M),\quad \Gamma_t^{(j)}=O(M),\\ &\Gamma_n^{(j)}=O(\omega^{-1}\Delta M),\quad \Gamma_k^{(j)}=O(\omega^{-1}\Delta M), \end{aligned} \tag{2.1}$$

where M depends on s and ω, and

$$\frac{d^jM}{ds^j}=O(\Delta^jM),\quad 1\le\Delta\le O(\omega^{1/2}). \tag{2.2}$$

The quantity M is introduced because of the factor $\exp[\omega^{1/2}\psi(s)]$, where $\psi(s)$ is given by I (3.19), which occurs in the potentials φ and **A**. We also assume that the propagation constant has the form

$$\beta=\omega\beta_0+\Lambda,\quad \Lambda=O(1). \tag{2.3}$$

The validity of the assumptions in (2.1)–(2.3) may be verified *a posteriori*.

It follows from (2.1)–(2.3), (A1), and (A2) that

$$\alpha_L^2+1/c_L^2-\beta_0^2=0,\quad \alpha_T^2+1/c_T^2-\beta_0^2=0, \tag{2.4}$$

and that

$$\frac{d^2G^{(0)}}{ds^2}+\omega(\alpha_L\kappa-2\beta_0\Lambda)G^{(0)}-2\omega\alpha_LG^{(1)}=O(M), \tag{2.5}$$

and

$$\frac{d^2\Gamma_t^{(0)}}{ds^2}+\omega(\alpha_T\kappa-2\beta_0\Lambda)\Gamma_t^{(0)}-2\omega\alpha_T\Gamma_t^{(1)}=O(M). \tag{2.6}$$

Also, from (A3)–(A6), we obtain

$$\omega\alpha_T\Gamma_n^{(0)}+i\omega\beta_0\Gamma_k^{(0)}-\frac{d\Gamma_t^{(0)}}{ds}=O(\omega^{-1}\Delta M), \tag{2.7}$$

$$\begin{aligned}\omega\left[\left(\beta_0^2-\frac{1}{2c_T^2}\right)G^{(0)}-i\beta_0\alpha_T\Gamma_t^{(0)}\right]-2\alpha_LG^{(1)}\\ -\alpha_T\frac{d\Gamma_k^{(0)}}{ds}+i\beta_0\Gamma_t^{(1)}-i\Lambda\alpha_T\Gamma_t^{(0)}=O(\omega^{-1}M),\end{aligned} \tag{2.8}$$

$$\begin{aligned}\omega\left[i\beta_0\alpha_LG^{(0)}+\left(\beta_0^2-\frac{1}{2c_T^2}\right)\Gamma_t^{(0)}\right]-2\alpha_T\Gamma_t^{(1)}+\alpha_T\kappa\Gamma_t^{(0)}\\ +\alpha_T\frac{d\Gamma_n^{(0)}}{ds}+i\Lambda\alpha_LG^{(0)}-i\beta_0G^{(1)}=O(\omega^{-1}M),\end{aligned} \tag{2.9}$$

and

$$\omega\left[\left(\beta_0^2-\frac{1}{2c_T^2}\right)\Gamma_k^{(0)}-i\beta_0\alpha_T\Gamma_n^{(0)}\right]+\alpha_L\frac{dG^{(0)}}{ds}=O(\omega^{-1}\Delta M). \tag{2.10}$$

We now have six approximate equations for the six quantities $G^{(0)}$, $G^{(1)}$, $\Gamma_t^{(0)}$, $\Gamma_t^{(1)}$, $\Gamma_n^{(0)}$, and $\Gamma_k^{(0)}$. But, from (2.1), (2.2), (2.8), and (2.9), we find

$$\begin{aligned}\left(\beta_0^2-\frac{1}{2c_T^2}\right)G^{(0)}-i\beta_0\alpha_T\Gamma_t^{(0)}=O(\omega^{-1}M),\\ i\beta_0\alpha_LG^{(0)}+\left(\beta_0^2-\frac{1}{2c_T^2}\right)\Gamma_t^{(0)}=O(\omega^{-1}M).\end{aligned} \tag{2.11}$$

We obtain the secular equation I (3.5) for β_0 by setting the determinant of the coefficients in (2.11) equal to zero.

We next multiply Eq. (2.8) by $(\beta_0^2-1/2c_T^2)$ and Eq. (2.9) by $i\beta_0\alpha_T$, add, and use I (3.5), to obtain

$$\left(\beta_0^2-\frac{1}{2c_T^2}\right)\left[-2\alpha_L G^{(1)}-\alpha_T\frac{d\Gamma_k^{(0)}}{ds}+i\beta_0\Gamma_t^{(1)}-i\Lambda\alpha_T\Gamma_t^{(0)}\right]$$
$$+i\beta_0\alpha_T\left[-2\alpha_T\Gamma_t^{(1)}+\alpha_T\kappa\Gamma_t^{(0)}+\alpha_T\frac{d\Gamma_n^{(0)}}{ds}\right.$$
$$\left.+i\Lambda\alpha_L G^{(0)}-i\beta_0 G^{(1)}\right]=O(\omega^{-1}M). \tag{2.12}$$

But, from (2.2) and (2.10),

$$\omega\left[\left(\beta_0^2-\frac{1}{2c_T^2}\right)\frac{d\Gamma_k^{(0)}}{ds}-i\beta_0\alpha_T\frac{d\Gamma_n^{(0)}}{ds}\right]$$
$$=-\alpha_L\frac{d^2G^{(0)}}{ds^2}+O(\omega^{-1}\Delta^2M). \tag{2.13}$$

If we substitute for $G^{(1)}$ and $\Gamma_t^{(1)}$ from (2.5) and (2.6), and use (2.13), then (2.12) yields an equation which involves $G^{(0)}$ and $\Gamma_t^{(0)}$, and their second order derivatives. The final step is to eliminate $\Gamma_t^{(0)}$ by using (2.11), from which it also follows, using (2.1) and (2.2), that

$$\left(\beta_0^2-\frac{1}{2c_T^2}\right)\frac{d^2G^{(0)}}{ds^2}-i\beta_0\alpha_T\frac{d^2\Gamma_t^{(0)}}{ds^2}=O(\omega^{-1}\Delta^2M). \tag{2.14}$$

Making some algebraic simplifications, with the help of (2.4) and I(3.5), and noting that $\Delta^2\le O(\omega)$, we obtain the lowest order approximate equation

$$\frac{d^2G^{(0)}}{ds^2}+\omega[\gamma\kappa(s)-2\beta_0\Lambda]G^{(0)}=O(M), \tag{2.15}$$

where the constant $\gamma>0$ is given by I(3.17). The quantity $\Gamma_t^{(0)}$ is given approximately in terms of $G^{(0)}$ by (2.11). Also, from (2.1), (2.2), (2.7), and (2.11), it follows that

$$\omega\alpha_T\Gamma_n^{(0)}+i\omega\beta_0\Gamma_k^{(0)}=\frac{-i\beta_0\alpha_L}{(\beta_0^2-1/2c_T^2)}\frac{dG^{(0)}}{ds}+O(\omega^{-1}\Delta M). \tag{2.16}$$

Hence, from (2.10) and (2.16), we have

$$\Gamma_n^{(0)}=O(\omega^{-2}\Delta M),\quad \Gamma_k^{(0)}=\frac{-\alpha_L}{\omega(\beta_0^2-1/2c_T^2)}\frac{dG^{(0)}}{ds}+O(\omega^{-2}\Delta M). \tag{2.17}$$

Expressions for $G^{(1)}$ and $\Gamma_t^{(1)}$ in terms of $G^{(0)}$ follow from (2.5), (2.6), (2.11), (2.14), and (2.15).

Corresponding to the expansion in (1.1), the displacement $\mathbf{u}=\nabla\varphi+\nabla\times\mathbf{A}$ may be written in the form

$$\mathbf{u}=\exp(-i\beta z)[\exp(-\omega\alpha_L n)(\mathbf{v}^{(0)}+n\mathbf{v}^{(1)}+\cdots)$$
$$+\exp(-\omega\alpha_T n)(\mathbf{w}^{(0)}+n\mathbf{w}^{(1)}+\cdots)]. \tag{2.18}$$

Using the curvilinear expressions for gradient and curl,[3] it is found, in particular, that

$$\mathbf{v}^{(0)}=(G^{(1)}-\omega\alpha_L G^{(0)})\mathbf{n}+\frac{dG^{(0)}}{ds}\mathbf{t}-i\beta G^{(0)}\mathbf{k}, \tag{2.19}$$

and

$$\mathbf{w}^{(0)}=\left(\frac{d\Gamma_k^{(0)}}{ds}+i\beta\Gamma_t^{(0)}\right)\mathbf{n}+(\omega\alpha_T\Gamma_k^{(0)}-\Gamma_k^{(1)}-i\beta\Gamma_n^{(0)})\mathbf{t}$$
$$-\left(\omega\alpha_T\Gamma_t^{(0)}-\Gamma_t^{(1)}+\kappa\Gamma_t^{(0)}+\frac{d\Gamma_n^{(0)}}{ds}\right)\mathbf{k}. \tag{2.20}$$

These quantities determine the surface displacement. It follows from the results of this section that

$$\mathbf{v}^{(0)}=-\omega\alpha_L G^{(0)}\mathbf{n}+\left(\frac{dG^{(0)}}{ds}\mathbf{t}-i\omega\beta_0 G^{(0)}\mathbf{k}\right)+O(M), \tag{2.21}$$

and

$$\mathbf{w}^{(0)}=\tfrac{1}{2}(\beta_0^2+\alpha_T^2)\left[\frac{\omega}{\alpha_T}G^{(0)}\mathbf{n}-\frac{1}{\beta_0^2}\left(\frac{dG^{(0)}}{ds}\mathbf{t}-i\omega\beta_0 G^{(0)}\mathbf{k}\right)\right]+O(M). \tag{2.22}$$

3. REFINED APPROXIMATION

We now consider a refinement of Eq. (2.15) which includes the $O(M)$ terms explicitly. This refinement is derived from five exact equations, (A1)–(A5), and five asymptotically approximate equations, (A7)–(A11), for the ten quantities $G^{(0)}$, $G^{(1)}$, $G^{(2)}$, $\Gamma_t^{(0)}$, $\Gamma_t^{(1)}$, $\Gamma_t^{(2)}$, $\Gamma_n^{(0)}$, $\Gamma_n^{(1)}$, $\Gamma_k^{(0)}$, and $\Gamma_k^{(1)}$. The procedure is to multiply Eq. (A4) by $(\beta_0^2-1/2c_T^2)$ and Eq. (A5) by $i\beta_0\alpha_T$, add, and then to express all the quantities in this equation in terms of $G^{(0)}$, to within the appropriate order of accuracy, with the help of the remaining equations. We omit the very laborious details, but remark that it is necessary, in particular, to obtain a refinement of (2.11), and it is found that

$$\Gamma_t^{(0)}=\frac{-i\beta_0\alpha_L}{(\beta_0^2-1/2c_T^2)}\left(1+\frac{\Lambda}{\omega\beta_0}-\frac{f\kappa}{\omega}\right)G^{(0)}+O(\omega^{-2}M), \tag{3.1}$$

where

$$2\beta_0^2\alpha_L^2\alpha_T f=[\beta_0^2(\alpha_L-\alpha_T)+\alpha_L\alpha_T^2]\gamma+\beta_0^2\alpha_L\alpha_T. \tag{3.2}$$

In deriving the refined approximate equation for $G^{(0)}$, repeated use is made of the lowest order approximate equation (2.15) to eliminate higher order derivatives.

The refined approximate equation is

$$\frac{d^2G^{(0)}}{ds^2}+\omega[\gamma\kappa(s)-2\beta_0\Lambda]G^{(0)}+\{d[\kappa(s)]^2+c\beta_0\Lambda\kappa(s)-\Lambda^2\}G^{(0)}$$
$$+2e\frac{\kappa'}{\omega}\frac{dG^{(0)}}{ds}=O(\omega^{-1}M), \tag{3.3}$$

where the constants c, d, and e are defined as follows. If we let

$$\Sigma=(\alpha_L-\alpha_T)[\beta_0^2(\alpha_L-\alpha_T)+2\alpha_L\alpha_T^2], \tag{3.4}$$

then d and c are determined by the relationship

$$\Sigma\{d[\kappa(s)]^2+c\beta_0\beta_1\kappa(s)\}=\rho(s), \tag{3.5}$$

where $\rho(s)$ is defined[1] below I(3.28), subject to I(3.17). Also,

$$\Sigma e=\frac{\beta_0^2}{2\alpha_L\alpha_T}(\alpha_L^3+\alpha_T^3-3\alpha_L^2\alpha_T)+\tfrac{1}{2}\alpha_L\alpha_T(7\alpha_L-6\alpha_T)$$
$$+\frac{\gamma(\alpha_L-\alpha_T)^2}{4\alpha_L^2\alpha_T^2}[4\alpha_L^2\alpha_T^2-\beta_0^2(\alpha_L+\alpha_T)^2]. \tag{3.6}$$

We remark that Eq. (3.3) has the same structure as the refined approximate equation that arises in the scalar problem.[2] Also, it follows from (3.1), with the help of (2.1) and (2.2), that $\Gamma_t^{(0)}$ satisfies a very similar equation, the only difference being that e is replaced by $e+f$ in (3.3), where f is given by (3.2). It is convenient to eliminate the term involving $dG^{(0)}/ds$ in (3.3) by letting

$$G^{(0)} = (1 - e\kappa/\omega)H + O(\omega^{-2}M). \tag{3.7}$$

Then, using (2.1), we obtain the (modified) refined approximate equation

$$\frac{d^2H}{ds^2} + [\omega(\gamma\kappa - 2\beta_0\Lambda) + d\kappa^2 + c\beta_0\Lambda\kappa - \Lambda^2]H = O(\omega^{-1}M). \tag{3.8}$$

The components of $\mathbf{v}^{(0)}$ and $\mathbf{w}^{(0)}$ in (2.19) and (2.20), which determine the surface displacement, are given in terms of H by

$$v_n^{(0)} = \left\{-\omega\alpha_L + \left[\alpha_L e + \frac{(\alpha_L - \gamma)}{2\alpha_L}\right]\kappa\right\}H + O(\omega^{-1}M), \tag{3.9}$$

$$v_t^{(0)} = \frac{dH}{ds} + O(\omega^{-1}\Delta M), \tag{3.10}$$

$$v_k^{(0)} = -i(\omega\beta_0 + \Lambda - \beta_0 e\kappa)H + O(\omega^{-1}M), \tag{3.11}$$

and

$$w_n^{(0)} = \frac{(\beta_0^2 + \alpha_T^2)}{2\alpha_T}\left\{\omega + \left[\frac{\gamma}{\beta_0^2} - (e+f)\right]\kappa\right\}H + O(\omega^{-1}M), \tag{3.12}$$

$$w_t^{(0)} = -\frac{(\beta_0^2 + \alpha_T^2)}{2\beta_0^2}\frac{dH}{ds} + O(\omega^{-1}\Delta M), \tag{3.13}$$

$$w_k^{(0)} = -\frac{(\beta_0^2 + \alpha_T^2)}{2i\beta_0^2}\left\{\omega\beta_0 + \Lambda + \beta_0\left[\frac{(\alpha_T + \gamma)}{2\alpha_T^2} - (e+f)\right]\kappa\right\}H + O(\omega^{-1}M). \tag{3.14}$$

4. APPLICATIONS

The asymptotic results obtained in I by Wilson and Morrison follow from the refined approximate equation (3.8), which in fact leads to some higher order terms in the expansions. The leading term in the asymptotic results follows from the lowest order approximate equation (2.15). These results apply in the case of an open boundary curve for which the curvature $\kappa(s)$ attains its algebraic maximum at a single point, $s = 0$, with $\kappa'(0) = 0$, $\kappa''(0) < 0$ and $\kappa(s)$ bounded away from $\kappa(0)$ as $|s| \to \infty$. We omit the details, since the results are obtained by deriving the asymptotic solution of (3.8) for $\omega \gg 1$ with the help of standard techniques. However, it is possible to analyze the higher order modes more completely than was done in I, and without the additional assumption $\kappa(-s) = \kappa(s)$ which was made there. We merely quote the result for the term β_2 in the expansion I(2.6) for the propagation constant β. It is found that

$$2\beta_0\beta_2 = \left(d + \frac{c\gamma}{2} - \frac{\gamma^2}{4\beta_0^2}\right)\kappa_0^2 + \frac{11\kappa_3^2}{16\kappa_2^2} - \frac{3\kappa_4}{4\kappa_2} + \tfrac{3}{8}m(m+1)\left(\frac{5\kappa_3^2}{\kappa_2^2} - \frac{4\kappa_4}{\kappa_2}\right),$$

where the κ_j are defined above I(3.32). For $m = 0$, corresponding to the lowest order mode, this agrees with the expression for β_2 in I(3.31).

We have so far considered open boundary curves for which the curvature attains its algebraic maximum at a single point, designated by $s = 0$. The disturbance, in addition to being confined close to the surface in the region $n = O(\omega^{-1})$, is also essentially confined to the region $|s| = O(\omega^{-1/4})$, and decays exponentially outside this region.[1] The application of these asymptotic results to closed boundary curves for which the curvature attains its algebraic maximum at a single point, and to closed boundary curves which are symmetric and for which the curvature attains its algebraic maximum at two points, was discussed in I. However, these results are not applicable unless the frequency is high enough, so that the disturbance is sufficiently localized in the neighborhood of the point of maximum curvature. Nor are the results applicable if the deviation of the curvature from a constant value is small. In both of these cases we may make use of the refined approximate equation (3.8), which in general has to be solved numerically.

Let us consider boundary curves of nearly constant curvature, the deviation from constancy being of order ω^{-1}. We assume that $\omega/\omega_0 = O(1)$, where $\omega_0 \gg 1$, and consider boundary curves for which the curvature has the form $\kappa(s) = k_0 + \omega_0^{-1}k_1(s)$, where k_0 is constant. Then,

$$\Lambda \sim \frac{\gamma k_0}{2\beta_0} + \omega_0^{-1}\Lambda_1, \quad H(s) \sim H_0(s), \tag{4.1}$$

where, from (3.8),

$$\frac{d^2H_0}{ds^2} + \left[\left(d + \frac{c\gamma}{2} - \frac{\gamma^2}{4\beta_0^2}\right)k_0^2 + \frac{\omega}{\omega_0}[\gamma k_1(s) - 2\beta_0\Lambda_1]\right]H_0 = 0. \tag{4.2}$$

This is an elgenvalue problem, with Λ_1 to be determined. In general, Eq. (4.2) has to be solved numerically in the region where $\gamma k_1(s) = O(1)$, $\omega/\omega_0 = O(1)$.

If we take $l\kappa(s) = -1 + 2\omega_0^{-1}k_1\cos(2s/l)$, corresponding to an almost circular bore with circumference $2\pi l$, then the periodic solutions of (4.2) may be expressed in terms of Mathieu functions,[4] and the values of Λ_1 are given in terms of the corresponding eigenvalues. An analogous discussion for the scalar problem was given in Ref. 2. For a circular bore, corresponding to $k_1 = 0$, the solutions of (4.2) which are periodic in s with period $2\pi l$ are simple harmonic functions, and

$$2\frac{\omega}{\omega_0}\beta_0\Lambda_1 l^2 = d + \frac{c\gamma}{2} - \frac{\gamma^2}{4\beta_0^2} - m^2, \tag{4.3}$$

where $m = 0, 1, 2, \cdots$. We have verified that the asymptotic solution of the known dispersion relation for the lowest order surface mode,[5] corresponding to $m = 0$, is consistent with (2.3), (4.1), and (4.2). An expression equivalent to that for the leading term in (4.1) was derived by Gregory,[6] in the case $m = 0$. The higher order surface modes correspond to those investigated by Ronnekleiv[7] and we have verified that the asymptotic solution of the dispersion relation gives the leading term in (4.1), independently of m.

We now take $k_0 = 0$ and $lk_1(s) = k_1\,\mathrm{sech}^2(s/l)$, with $k_1 > 0$, corresponding to a wedgelike object somewhat similar to a hyperbolic cylinder. In this case the solution of (4.2) may be written down explicitly.[8] The solutions which vanish for $|s| \to \infty$ are

$$H_0 = [\mathrm{sech}(s/l)]^{b_m}F(2b_m + m + 1, -m; b_m + 1; \tfrac{1}{2}[1 - \tanh(s/l)]), \tag{4.4}$$

where

$$b_m = [(\omega/\omega_0)\gamma k_1 l + \tfrac{1}{4}]^{1/2} - m - \tfrac{1}{2} > 0, \quad m = 0, \ldots, N, \tag{4.5}$$

and the corresponding eigenvalues are given by $2(\omega/\omega_0)\beta_0\Lambda_1 l^2 = b_m^2$. The hypergeometric function[9] in (4.4) terminates, and is a polynomial of degree m in its argument. There is a finite number of modes, and the lowest order mode, corresponding to $m = 0$, always exists. Note that for $m = 0$ the hypergeometric function in (4.4) is identically equal to 1. If $\omega\gamma k_1 l < 2\omega_0$, then only the lowest order mode exists. In the limiting case $k_1 \to 0$, corresponding to a planar boundary, $b_0 \to 0$ and $H_0 \to 1$. That is, the lowest order mode tends to a Rayleigh wave on a plane infinite half-space as $k_1 \to 0$.

In a subsequent paper[10] the results of the numerical solution of the refined approximate equation (3.8) for various cross-sectional shapes, corresponding to both open and closed boundary curves, will be presented. The mode behavior in the transition region between the case of cross-sectional boundary curves of constant (and not "almost" constant) curvature, for which the modes are localized, and the case of constant curvature, for which they are not, is vividly depicted by these results. Also, comparisons are made with numerical results based on the asymptotic formulas in I. In addition, some higher order modes are considered. The phase and group velocities are also computed.

APPENDIX

We first write down six exact equations which follow from (1.1) and the equations for φ and A derived in I. The terms independent of $\xi = \omega n$ in the first two equations of I(2.10) yield

$$\frac{d^2G^{(0)}}{ds^2} + \left[\omega^2\left(\alpha_L^2 + \frac{1}{c_L^2}\right) - \beta^2 + \omega\alpha_L\kappa\right]G^{(0)} - (2\omega\alpha_L + \kappa)G^{(1)} + G^{(2)} = 0, \tag{A1}$$

$$\frac{d^2\Gamma_t^{(0)}}{ds^2} + \left[\omega^2\left(\alpha_T^2 + \frac{1}{c_T^2}\right) - \beta^2 + \omega\alpha_T\kappa - \kappa^2\right]\Gamma_t^{(0)} - (2\omega\alpha_T + \kappa)\Gamma_t^{(1)} + \Gamma_t^{(2)} - 2\kappa\frac{d\Gamma_n^{(0)}}{ds} - \kappa'\Gamma_n^{(0)} = 0. \tag{A2}$$

The divergence condition I(2.15) and the boundary conditions I(2.12)–(2.14) yield

$$(\omega\alpha_T + \kappa)\Gamma_n^{(0)} - \Gamma_n^{(1)} + i\beta\Gamma_k^{(0)} - \frac{d\Gamma_t^{(0)}}{ds} = 0, \tag{A3}$$

$$\omega^2\left(\alpha_L^2 + \frac{1}{c_L^2} - \frac{1}{2c_T^2}\right)G^{(0)} - 2\omega\alpha_L G^{(1)} + G^{(2)} + \frac{d\Gamma_k^{(1)}}{ds} + (\kappa - \omega\alpha_T)\frac{d\Gamma_k^{(0)}}{ds} + i\beta(\Gamma_t^{(1)} - \omega\alpha_T\Gamma_t^{(0)}) = 0, \tag{A4}$$

$$\left[\omega^2\left(\alpha_T^2 + \frac{1}{2c_T^2}\right) + \omega\alpha_T\kappa - \kappa^2\right]\Gamma_t^{(0)} - (2\omega\alpha_T + \kappa)\Gamma_t^{(1)} + \Gamma_t^{(2)} - \frac{d\Gamma_n^{(1)}}{ds} + (\omega\alpha_T - \kappa)\frac{d\Gamma_n^{(0)}}{ds} + i\beta(\omega\alpha_L G^{(0)} - G^{(1)}) = 0, \tag{A5}$$

and

$$\omega^2\left(\alpha_T^2 + \frac{1}{2c_T^2}\right)\Gamma_k^{(0)} - 2\omega\alpha_T\Gamma_k^{(1)} + \Gamma_k^{(2)} + i\beta(\Gamma_n^{(1)} - \omega\alpha_T\Gamma_n^{(0)}) - \frac{dG^{(1)}}{ds} + (\omega\alpha_L - \kappa)\frac{dG^{(0)}}{ds} = 0. \tag{A6}$$

Four more equations may be obtained from the terms independent of $\xi = \omega n$ in the last two equations of I(2.10), and from the terms proportional to ξ in the first two equations of I(2.10). We do not write out the exact equations here, but merely state the asymptotic approximations to them which are obtained by making use of (2.1)–(2.4). It is found that

$$\frac{d^2\Gamma_n^{(0)}}{ds^2} + \omega(\alpha_T\kappa - 2\beta_0\Lambda)\Gamma_n^{(0)} - 2\omega\alpha_T\Gamma_n^{(1)} + 2\kappa\frac{d\Gamma_t^{(0)}}{ds} + \kappa'\Gamma_t^{(0)} = O(\omega^{-1}\Delta M), \tag{A7}$$

$$\frac{d^2\Gamma_k^{(0)}}{ds^2} + \omega(\alpha_T\kappa - 2\beta_0\Lambda)\Gamma_k^{(0)} - 2\omega\alpha_T\Gamma_k^{(1)} = O(\omega^{-1}\Delta M), \tag{A8}$$

$$\omega\alpha_L\kappa^2 G^{(0)} + \omega(\alpha_L\kappa - 2\beta_0\Lambda)G^{(1)} - 2\omega\alpha_L G^{(2)} + \frac{d^2G^{(1)}}{ds^2} + 2\kappa\frac{d^2G^{(0)}}{ds^2} + \kappa'\frac{dG^{(0)}}{ds} = O(M), \tag{A9}$$

and

$$\omega\alpha_T\kappa^2\Gamma_t^{(0)} + \omega(\alpha_T\kappa - 2\beta_0\Lambda)\Gamma_t^{(1)} - 2\omega\alpha_T\Gamma_t^{(2)} + \frac{d^2\Gamma_t^{(1)}}{ds^2} + 2\kappa\frac{d^2\Gamma_t^{(0)}}{ds^2} + \kappa'\frac{d\Gamma_t^{(0)}}{ds} = O(M). \tag{A10}$$

We also use the asymptotic approximation to (A6),

$$\omega^2\left(\beta_0^2 - \frac{1}{2c_T^2}\right)\Gamma_k^{(0)} - 2\omega\alpha_T\Gamma_k^{(1)} - i\omega\alpha_T(\omega\beta_0 + \Lambda)\Gamma_n^{(0)} + i\omega\beta_0\Gamma_n^{(1)} - \frac{dG^{(1)}}{ds} + (\omega\alpha_L - \kappa)\frac{dG^{(0)}}{ds} = O(\omega^{-1}\Delta M). \tag{A11}$$

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[1]L.O. Wilson and J.A. Morrison, J. Math. Phys. **16**, 1795 (1975).
[2]J.A. Morrison, J. Math. Phys. **16**, 1786 (1975).
[3]C.E. Weatherburn, *Advanced Vector Analysis* (Bell, London, 1949), p. 16.
[4]M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964), pp. 721—46.
[5]M.A. Biot, J. Appl. Phys. **23**, 997 (1952).
[6]R.D. Gregory, Proc. Cambridge Philos. Soc. **70**, 103 (1971).
[7]A. Ronnekleiv, E. Lab Report No. TE-141, Electronics Research Laboratory, Trondheim, Norway, April 1970.
[8]P.M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953) Part II. p. 1651.
[9]Ref. 4, p. 556.
[10]J.A. Morrison, J.B. Seery, and L.O. Wilson, "Propagation of high frequency elastic surface waves along cylinders with various cross-sectional shapes."

Derivation of an exact quantum-mechanical formula for the second term in the activity expansion of the correlation function $S(\mathbf{Q},\omega)$*

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We derive an exact expression for the second term in the activity expansion of $S(\mathbf{Q},\omega)$, the Fourier transform of Van Hove's correlation function, for a quantum system of bosons or fermions (spin neglected). The results for both the self and distinct parts of this function are given in terms of standard two-particle T matrices. The detailed-balance condition and zeroth and first moment relations are confirmed. An expression for the second term in the activity expansion of $S(\mathbf{Q})$, the structure factor, is obtained. The derivation follows directly from the definition of $S(\mathbf{Q},\omega)$ using formal operator techniques; in addition, we show that the *conserving T approximation* for two-particle Green's functions yields the same result.

I. INTRODUCTION

The function $S(\mathbf{Q},\omega)$, sometimes called the "scattering law" or "dynamical structure factor," is defined to be the space and time Fourier transform of the Van Hove pair correlation function[1] for a system of particles. It has been utilized in the study of inelastic neutron scattering, absorption of radiation in matter, and inelastic electron scattering from nuclei.[2-6] This function is characteristic of a particular system of particles; when the system is considered as a scattering medium the quantities $\hbar\mathbf{Q}$ and $\hbar\omega$ are the momentum and energy transfers, respectively, from the projectile to the medium. (We set $\hbar=1$ for convenience; to restore $\hbar$ in any formula replace m by $m\hbar^{-2}$ and ω by $\hbar\omega$.)

The definition from which we begin is

$$S(\mathbf{Q},\omega)=(2\pi n\Omega)^{-1}\int_{-\infty}^{\infty}dt\exp(iwt)\Big\langle\sum_{ij}\exp[-i\mathbf{Q}\cdot\mathbf{r}_i(t)]\times\exp[i\mathbf{Q}\cdot\mathbf{r}_j(0)]\Big\rangle, \tag{1.1}$$

where n is the density of particles, Ω is the volume of the system ($\lim\Omega\to\infty$ is to be taken), and the position operator $\mathbf{r}_i(t)$ in the Heisenberg representation is given by

$$\mathbf{r}_i(t)=\exp(-itH)\mathbf{r}_i\exp(itH) \tag{1.2}$$

where H is the many-body Hamiltonian; the grand canonical ensemble average is defined by

$$\langle\Theta\rangle=\mathrm{Tr}\{\exp[-\beta(H-\mu\hat{N})]\Theta\}/\mathrm{Tr}\exp[-\beta(H-\mu\hat{N})], \tag{1.3}$$

where β is the inverse temperature, μ the chemical potential of the system and $\hat{N}$ the number operator. The terms with $l=j$ in (1.1) yield the *self* part $S^{(s)}$ while those with $l\neq j$ yield the *distinct* part $S^{(d)}$, such that $S(\mathbf{Q},\omega)=S^{(s)}(\mathbf{Q},\omega)+S^{(d)}(\mathbf{Q},\omega)$. This separation is required in the analysis of coherent and incoherent scattering from systems having nonzero spin or a mixture of isotopes.

In this paper we derive an exact quantum mechanical expression for the next-to-leading term in the density or activity expansion of $S(\mathbf{Q},\omega)$. That is, we go one step beyond the familiar ideal gas expression for $S(\mathbf{Q},\omega)$ in the same sense that the second virial coefficient provides an improvement to the ideal gas equation of state. Our result is expressed in terms of on- and half-on-shell two-particle T matrices and, if apposite, two-particle bound state energies and wavefunctions. We demonstrate two methods for obtaining this result: in the main body of the text, (Secs. II and III), we proceed directly from definition (1.1) with the aid of certain operator relations[7] to obtain separately both $S^{(s)}(\mathbf{Q},\omega)$ and $S^{(d)}(\mathbf{Q},\omega)$; in Appendix C we use a Green function technique, starting from the expression for $S(\mathbf{Q},\omega)$ in terms of a certain two-particle Green's function. We show that these two approaches yield the same result provided that the latter includes the additional term in the *conserving T-approximation* for the two-particle Green's function.[8]

In Sec. IV we confirm that the condition of detailed balance is satisfied for our results and study the zeroth and first moment relations. From the zeroth moment of $S(\mathbf{Q},\omega)$ we obtain an exact expression for the coefficient of the linear term in the activity expansion of $S(\mathbf{Q})$, the structure factor.

II. PRELIMINARIES

We consider a quantum system containing spinless particles (bosons or fermions) of mass m which interact via a two-body potential V; the system is assumed to be dilute so that the activity, $z=\exp(\beta\mu)\ll 1$; let $\lambda=(2\pi\beta/m)^{1/2}$. The Hamiltonian is

$$H=H_0+H_1=\sum_i K_i+\sum_{i<j}V_{ij}, \tag{2.1}$$

where K represents the one-particle kinetic energy operator. The standard two-particle T operator is defined by

$$T(\zeta)=V+V(\zeta-H_0^{(2)})^{-1}T(\zeta), \tag{2.2}$$

where ζ is a complex variable (not purely real). The two-body system with Hamiltonian $H_0^{(2)}+V$ may possess bound states $|B)$ with energies $\epsilon_B<0$ after the center-of-mass energy has been removed. (For the sake of brevity we omit bound state contributions in presenting our results but indicate in Appendix A how they may be included if desired.)

Matrix elements of the T operator between eigenstates of $H_0^{(2)}$ are introduced: we write $(\mathbf{p}_1\mathbf{p}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2)$ where $H_0^{(2)}|\mathbf{p}_1\mathbf{p}_2)=(E_{p_1}+E_{p_2})|\mathbf{p}_1\mathbf{p}_2)$ and $E_{p_1}=p_1^2/2m$. Re-

duced matrix elements $(\mathbf{p}|T(\mathbf{P},\zeta)|\mathbf{k})$ and $(\mathbf{p}|T(\zeta)|\mathbf{k})$ are defined by (A6) and (A7) in Appendix A; $\mathbf{p}=(\mathbf{p}_1-\mathbf{p}_2)/2$, $\mathbf{P}=\mathbf{p}_1+\mathbf{p}_2$, etc. The function $(\mathbf{p}_1\mathbf{p}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2)$ is analytic in the complex ζ plane except on the real axis. We write $(\mathbf{p}_1\mathbf{p}_2|T(x^{\pm})|\mathbf{k}_1\mathbf{k}_2)$ for $\lim_{\epsilon\to 0^+}(\mathbf{p}_1\mathbf{p}_2|T(x\pm i\epsilon)|\mathbf{k}_1\mathbf{k}_2)$ where x is real: By property (A3) the real part of this function is continuous across the real axis, and we write, simply, $\mathrm{Re}(\mathbf{p}_1\mathbf{p}_2|T(x)|\mathbf{k}_1\mathbf{k}_2)$; the discontinuity in the imaginary part is given by (A8).

The density of particles in the system is given by a power series in the activity according to

$$n=\lambda^{-3}z+n_2z^2+\cdots, \tag{2.3}$$

where (neglecting bound-state effects),[9]

$$\begin{aligned}n_2=&\pm 2^{-3/2}\lambda^{-3}-2^{3/2}\lambda^{-3}\beta\int\frac{d\mathbf{p}}{(2\pi)^3}\exp(-\beta p^2/m)\\&\times\mathrm{Re}(\mathbf{p}|T(p^2/m)|\mathbf{p})_s+2^{3/2}\lambda^{-3}P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\\&\times\frac{\exp(-\beta k^2/m)-\exp(-\beta p^2/m)}{(k^2/m-p^2/m)^2}(\mathbf{p}|T(k^2/m^+)|\mathbf{k})\\&\times(\mathbf{k}|T(k^2/m^-)|\mathbf{p})_s\end{aligned} \tag{2.4}$$

with $|\mathbf{p})_s=|\mathbf{p})\pm|-\mathbf{p})$. Beginning with (2.4), upper and lower signs are used to denote Bose and Fermi statistics, respectively.

Let us define

$$F^{(s)}(\mathbf{Q},\omega)=2\pi nS^{(s)}(\mathbf{Q},\omega), \tag{2.5a}$$

$$F^{(d)}(\mathbf{Q},\omega)=2\pi nS^{(d)}(\mathbf{Q},\omega). \tag{2.5b}$$

These quantities possess expansions in z of the form

$$S(\mathbf{Q},\omega)=S_0(\mathbf{Q},\omega)+zS_1(\mathbf{Q},\omega)+\cdots, \tag{2.6}$$

$$F(\mathbf{Q},\omega)=zF_1(\mathbf{Q},\omega)+z^2F_2(\mathbf{Q},\omega)+\cdots, \tag{2.7}$$

where it is well known that, (for the ideal gas limit),

$$S_0(\mathbf{Q},\omega)=S_0^{(s)}(\mathbf{Q},\omega)=(\beta m/2\pi)^{1/2}Q^{-1}\exp\left[\frac{-\beta m}{2Q^2}\left(\omega-\frac{Q^2}{2m}\right)^2\right]. \tag{2.8}$$

The object of our attention is $S_1(\mathbf{Q},\omega)$ which, by combining (2.6), (2.5), (2.3), and (2.7), is given by

$$S_1^{(s)}(\mathbf{Q},\omega)=(2\pi)^{-1}\lambda^3F_2^{(s)}(\mathbf{Q},\omega)-\lambda^3n_2S_0(\mathbf{Q},\omega), \tag{2.9a}$$

$$S_1^{(d)}(\mathbf{Q},\omega)=(2\pi)^{-1}\lambda^3F_2^{(d)}(\mathbf{Q},\omega). \tag{2.9b}$$

Thus, our purpose is to derive exact expressions for $F_2^{(s)}(\mathbf{Q},\omega)$ and $F_2^{(d)}(\mathbf{Q},\omega)$: These will yield the first correction terms in the activity expansions of $S^{(s)}(\mathbf{Q},\omega)$ and $S^{(d)}(\mathbf{Q},\omega)$.

III. DERIVATION

We now derive exact expressions for $F_2^{(s)}(\mathbf{Q},\omega)$ and $F_2^{(d)}(\mathbf{Q},\omega)$ starting from Eqs. (2.5) and (1.1).[10] The grand canonical expectation appearing there may be evaluated by summing over an appropriately symmetrized orthonormal basis, $|M_1\cdots M_N)$, for fixed N, then summing over N. Thus,

$$\begin{aligned}F(\mathbf{Q},\omega)=\Omega^{-1}Z_{\mathrm{gr}}^{-1}\int_{-\infty}^{\infty}dt\exp(i\omega t)\sum_{N=1}^{\infty}\frac{z^N}{N!}\sum_P\epsilon^P\\\times\sum_{M_1\cdots M_N}\sum_{l,j=1}(M_1\cdots M_N|\exp[-(\beta-it)H^{(N)}]\\\times\exp(-i\mathbf{Q}\cdot\mathbf{r}_l)\exp(-itH^{(N)})\\\times\exp(i\mathbf{Q}\cdot\mathbf{r}_j)P|M_1\cdots M_N),\end{aligned} \tag{3.1}$$

so that $F^{(s)}(\mathbf{Q},\omega)$ corresponds to $l=j$ terms and $F^{(d)}(\mathbf{Q},\omega)$ to $l\neq j$ terms; $H^{(N)}$ is the Hamiltonian for the N particle system, P is the permutation operator and $\epsilon^P=1$ for bosons and ±1 for fermions according to whether P is an even or odd permutation, respectively; the grand partition function has the expansion

$$Z_{\mathrm{gr}}=1+z\Omega\lambda^{-3}+\cdots. \tag{3.2}$$

We choose a representation consisting of states $|\mathbf{p}_1\cdots\mathbf{p}_N)$ where each $|\mathbf{p}_i)$ is an eigenstate of the corresponding kinetic energy operator, i.e.,

$$K_i|\mathbf{p}_i)=E_{\mathbf{p}_i}|\mathbf{p}_i). \tag{3.3}$$

Each summation on M_i is replaced by an integral on $(2\pi)^{-3}d\mathbf{p}_i$; to be consistent each $|\mathbf{p}_i)$ has dimensions of $(\mathrm{volume})^{1/2}$ and $(\mathbf{p}_i|\mathbf{p}_i)=\Omega$. In this manner we obtain from (3.1):

$$\begin{aligned}F_1(\mathbf{Q},\omega)=&\int\frac{d\mathbf{p}}{(2\pi)^3}\exp\left(\frac{-\beta p^2}{2m}\right)\int_{-\infty}^{\infty}dt\\&\times\exp\left[it\left(\omega+\frac{p^2}{2m}-\frac{(\mathbf{p}+\mathbf{Q})^2}{2m}\right)\right]\\=&\frac{m^2}{2\pi\beta Q}\exp\left[\frac{-\beta m}{2Q^2}\left(\omega-\frac{Q^2}{2m}\right)^2\right],\end{aligned} \tag{3.4}$$

which agrees with the ideal gas result (2.8), and

$$\begin{aligned}F_2(\mathbf{Q},\omega)=&\Omega^{-1}\int_{-\infty}^{\infty}dt\exp(it\omega)\int\frac{d\mathbf{p}_1\,d\mathbf{p}_2}{(2\pi)^6}\\&\times(\mathbf{p}_1\mathbf{p}_2|\exp[-(\beta-it)H^{(2)}]\exp(-i\mathbf{Q}\cdot\mathbf{r}_1)\\&\times\exp(-itH^{(2)})[\exp(i\mathbf{Q}\cdot\mathbf{r}_1)+\exp(i\mathbf{Q}\cdot\mathbf{r}_2)]|\mathbf{p}_1\mathbf{p}_2)_s\\&-\Omega\lambda^{-3}F_1(\mathbf{Q},\omega),\end{aligned} \tag{3.5}$$

where $|\mathbf{p}_1\mathbf{p}_2)_s=|\mathbf{p}_1\mathbf{p}_2)\pm|\mathbf{p}_2\mathbf{p}_1)$ accounts for statistics. There are two different types of contributions to F_2 arising from the two terms in brackets in (3.5); the first term, $\exp(i\mathbf{Q}\cdot\mathbf{r}_1)$, yields $F_2^{(s)}$ while the second term gives $F_2^{(d)}$.

In evaluating (3.5) the essential problem is how to treat the operators $\exp[-(\beta-it)H^{(2)}]$ and $\exp(-itH^{(2)})$. Our approach leads to the introduction of the T operator (2.2). We use the operator relations[11]

$$\exp(-\tau H)=\frac{1}{2\pi i}\int_C d\zeta\exp(-\tau\zeta)(\zeta-H)^{-1}, \tag{3.6}$$

where the contour C encloses the real axis of the complex ζ plane in the positive sense, and

$$(\zeta-H)^{-1}=\sum_{r=0}^{\infty}(\zeta-H_0)^{-1}[H_1(\zeta-H_0)^{-1}]^r. \tag{3.7}$$

Combining these relations and isolating the $r=0$ term leads to

$$\begin{aligned}\exp(-\tau H^{(2)})=&\exp(-\tau H_0^{(2)})+\frac{1}{2\pi i}\int_C d\zeta\exp(-\tau\zeta)\\&\times\frac{1}{\zeta-H_0^{(2)}}T(\zeta)\frac{1}{\zeta-H_0^{(2)}}.\end{aligned} \tag{3.8}$$

This result is now employed to replace the operators $\exp[-(\beta - it)H^{(2)}]$ and $\exp(-itH^{(2)})$ occurring in (3.5). The two terms of (3.8) thus give rise to four terms in $F_2^{(s)}$ and four in $F_2^{(d)}$; in addition, each of these has a direct term and an exchange term arising from the two possible permutations of the final state labels. These contributions will be denoted by

$$F_2^{(s)} = \chi^{(0)} + \chi^{(T1)} + \chi^{(T2)} + \chi^{(TT)}, \tag{3.9}$$

$$F_2^{(d)} = \phi^{(0)} + \phi^{(T1)} + \phi^{(T2)} + \phi^{(TT)}, \tag{3.10}$$

where in (3.5) $\exp[-(\beta - it)H^{(2)}]$ is to be replaced by the corresponding first term of (3.8) in (0) and ($T1$) and by the second term of (3.8) in ($T2$) and (TT) while $\exp(-itH^{(2)})$ is replaced by its first term of (3.8) in (0) and ($T2$) and its second term of (3.8) in ($T1$) and (TT). We simply note that the various terms in the expansion of (3.1) can be represented by diagrams similar to these of Bloch[10]; however, there is little to be gained by presenting the diagrams for the $N=2$ terms and, therefore, we do not do so.

The interaction—independent contributions are

$$\begin{aligned}\chi^{(0)}(\mathbf{Q},\omega) &= 2\pi\Omega^{-1}\int \frac{d\mathbf{p}_1\,d\mathbf{p}_2}{(2\pi)^6}\exp\left[-\beta\left(\frac{p_1^2}{2m}+\frac{p_2^2}{2m}\right)\right]\\ &\quad\times\{\delta(\omega-\mathbf{p}_1\cdot\mathbf{Q}/m-Q^2/2m)\Omega^2\\ &\quad\pm\delta(\omega-\mathbf{p}_2\cdot\mathbf{Q}-Q^2/2m)\Omega(2\pi)^3\delta(\mathbf{p}_1-\mathbf{p}_2)\}\\ &\quad-\Omega\lambda^{-3}F_1(\mathbf{Q},\omega)\\ &= \pm\frac{m^2}{4\pi\beta Q}\exp\left[\frac{-\beta m}{Q^2}\left(\omega-\frac{Q^2}{2m}\right)^2\right],\end{aligned} \tag{3.11}$$

$$\begin{aligned}\phi^{(0)}(\mathbf{Q},\omega) &= \pm 2\pi\Omega^{-1}\int \frac{d\mathbf{p}_1\,d\mathbf{p}_2}{(2\pi)^6}\exp\left[-\beta\left(\frac{p_1^2}{2m}+\frac{p_2^2}{2m}\right)\right]\\ &\quad\times\delta(\omega-\mathbf{p}_1\cdot\mathbf{Q}/m-Q^2/2m)\Omega(2\pi)^3\delta(\mathbf{p}_1+\mathbf{Q}-\mathbf{p}_2)\\ &= \exp(-\beta\omega)\chi^{(0)}(\mathbf{Q},\omega).\end{aligned} \tag{3.12}$$

Note the cancellation which occurs in (3.11): the same result is obtained if one neglects the effect of Z_{gr} and considers only the *linked* diagrams for F_2.

The other components of F_2 are interaction-dependent, the interaction entering via the T matrices. The complex integral in the second term of (3.8) has matrix elements which, because of property (A4), can be expressed in terms of a real variable of integration,

$$\begin{aligned}&\frac{1}{2\pi i}\int_C d\zeta\exp(-\tau\zeta)(\mathbf{p}_1\mathbf{p}_2|\,(\zeta-H_0^{(2)})^{-1}T(\zeta)(\zeta-H_0^{(2)})^{-1}|\,\mathbf{k}_1\mathbf{k}_2)\\ &\quad=-\int_{-\infty}^{\infty}\frac{dx}{\pi}\exp(-\tau x)\,\mathrm{Im}\left\{\frac{(\mathbf{p}_1\mathbf{p}_2|\,T(x^+)|\,\mathbf{k}_1\mathbf{k}_2)}{(x^+-E_{p_1}-E_{p_2})(x^+-E_{k_1}-E_{k_2})}\right\}.\end{aligned} \tag{3.13}$$

The integration over t in (3.5) yields a delta function in every case. Accordingly, we obtain

$$\begin{aligned}\chi^{(T1)}(\mathbf{Q},\omega) &= -2\Omega^{-1}\int\frac{d\mathbf{p}_1\,d\mathbf{p}_2}{(2\pi)^6}\exp[-\beta(E_{p_1}+E_{p_2})\\ &\quad\times\int_{-\infty}^{\infty}dx\,\delta(\omega+E_{p_1}+E_{p_2}-x)\\ &\quad\times\mathrm{Im}\left\{\frac{(\mathbf{p}_1+\mathbf{Q},\mathbf{p}_2|\,T(x^+)|\,\mathbf{p}_1+\mathbf{Q},\mathbf{p}_2)}{(x^+-E_{p_1+Q}-E_{p_2})^2}\right.\\ &\quad\left.\pm\frac{(\mathbf{p}_1+\mathbf{Q},\mathbf{p}_2|\,T(x^+)|\,\mathbf{p}_2+\mathbf{Q},\mathbf{p}_1)}{(x^+-E_{p_1+Q}-E_{p_2})(x^+-E_{p_1}-E_{p_2+Q})}\right\},\end{aligned} \tag{3.14a}$$

$$\begin{aligned}\chi^{(T2)}(\mathbf{Q},\omega) &= -2\Omega^{-1}\int\frac{d\mathbf{p}_1\,d\mathbf{p}_2}{(2\pi)^6}\int_{-\infty}^{\infty}dx\exp(-\beta x)\\ &\quad\times\delta(\omega+x-E_{p_1+Q}-E_{p_2})\,\mathrm{Im}\left\{\frac{(\mathbf{p}_1\mathbf{p}_2|\,T(x^+)|\,\mathbf{p}_1\mathbf{p}_2)_s}{(x^+-E_{p_1}-E_{p_2})^2}\right\},\end{aligned} \tag{3.14b}$$

$$\begin{aligned}\chi^{(TT)}(\mathbf{Q},\omega) &= 2\Omega^{-1}\int\frac{d\mathbf{p}_1\,d\mathbf{p}_2\,d\mathbf{k}_1\,d\mathbf{k}_2}{(2\pi)^{12}}\int_{-\infty}^{\infty}\frac{dx'}{\pi}\exp(-\beta x')\\ &\quad\times\int_{-\infty}^{\infty}dx\,\delta(\omega+x'-x)\\ &\quad\times\mathrm{Im}\left\{\frac{(\mathbf{p}_1\mathbf{p}_2|\,T(x'^+)|\,\mathbf{k}_1\mathbf{k}_2)_s}{(x'^+-E_{p_1}-E_{p_2})(x'^+-E_{k_1}-E_{k_2})}\right\}\\ &\quad\times\mathrm{Im}\left\{\frac{(\mathbf{k}_1+\mathbf{Q},\mathbf{k}_2|\,T(x^+)|\,\mathbf{p}_1+\mathbf{Q},\mathbf{p}_2)}{(x^+-E_{k_1+Q}-E_{k_2})(x^+-E_{p_1+Q}-E_{p_2})}\right\},\end{aligned} \tag{3.14c}$$

$$\begin{aligned}\phi^{(T1)}(\mathbf{Q},\omega) &= -2\Omega^{-1}\int\frac{d\mathbf{p}_1\,d\mathbf{p}_2}{(2\pi)^6}\exp[-\beta(E_{p_1}+E_{p_2})]\\ &\quad\times\int_{-\infty}^{\infty}dx\,\delta(\omega+E_{p_1}+E_{p_2}-x)\\ &\quad\times\mathrm{Im}\left\{\frac{(\mathbf{p}_1+\mathbf{Q},\mathbf{p}_2|\,T(x^+)|\,\mathbf{p}_1,\mathbf{p}_2+\mathbf{Q})}{(x^+-E_{p_1+Q}-E_{p_2})(x^+-E_{p_1}-E_{p_2+Q})}\right.\\ &\quad\left.\pm\frac{(\mathbf{p}_1+\mathbf{Q},\mathbf{p}_2|\,T(x^+)|\,\mathbf{p}_2,\mathbf{p}_1+\mathbf{Q})}{(x^+-E_{p_1+Q}-E_{p_2})^2}\right\},\end{aligned} \tag{3.15a}$$

$$\begin{aligned}\phi^{(T2)}(\mathbf{Q},\omega) &= -2\Omega^{-1}\int\frac{d\mathbf{p}_1\,d\mathbf{p}_2}{(2\pi)^6}\int_{-\infty}^{\infty}dx\exp(-\beta x)\\ &\quad\times\delta(\omega+x-E_{p_1}-E_{p_2+Q})\\ &\quad\times\mathrm{Im}\left\{\frac{(\mathbf{p}_1\mathbf{p}_2|\,T(x^+)|\,\mathbf{p}_1-\mathbf{Q},\mathbf{p}_2+\mathbf{Q})_s}{(x^+-E_{p_1}-E_{p_2})(x^+-E_{p_1-Q}-E_{p_2+Q})}\right\},\end{aligned} \tag{3.15b}$$

$$\begin{aligned}\phi^{(TT)}(\mathbf{Q},\omega) &= 2\Omega^{-1}\int\frac{d\mathbf{p}_1\,d\mathbf{p}_2\,d\mathbf{k}_1\,d\mathbf{k}_2}{(2\pi)^{12}}\\ &\quad\times\int_{-\infty}^{\infty}\frac{dx'}{\pi}\exp(-\beta x')\int_{-\infty}^{\infty}dx\,\delta(\omega+x'-x)\\ &\quad\times\mathrm{Im}\left\{\frac{(\mathbf{p}_1\mathbf{p}_2|\,T(x'^+)|\,\mathbf{k}_1\mathbf{k}_2)_s}{(x'-E_{p_1}-E_{p_2})(x'^+-E_{k_1}-E_{k_2})}\right\}\\ &\quad\times\mathrm{Im}\left\{\frac{(\mathbf{k}_1+\mathbf{Q},\mathbf{k}_2|\,T(x^+)|\,\mathbf{p}_1,\mathbf{p}_2+\mathbf{Q})}{(x^+-E_{k_1+Q}-E_{k_2})(x^+-E_{p_1}-E_{p_2+Q})}\right\}.\end{aligned} \tag{3.15c}$$

The x-integration in each of these expressions may be readily performed. Then we introduce relative and center-of-mass momenta and the reduced T matrices as defined by (A6). Thus, we obtain, for example from (3.14a),

$$\chi^{(T1)}(\mathbf{Q},\omega) = -2\int \frac{d\mathbf{p}}{(2\pi)^3}\exp\left(\frac{-\beta p^2}{m}\right)\int \frac{d\mathbf{P}}{(2\pi)^3}\exp\left(\frac{-\beta P^2}{4m}\right)\exp\left[\frac{-\beta}{2m}\ (Q^2 - 2\mathbf{p}\cdot\mathbf{Q} - \mathbf{P}\cdot\mathbf{Q})\right]$$
$$\times \mathrm{Im}\left\{\frac{(\mathbf{p}|\,T(\mathbf{P},\omega + P^2/4m + p^2/m + Q^2/2m - \mathbf{p}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)\,|\mathbf{p})}{(\omega + Q^2/2m - \mathbf{p}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)^2}\right.$$
$$\left. \pm \frac{(\mathbf{p}|\,T(\mathbf{P},\omega + P^2/4m + p^2/m + Q^2/2m - \mathbf{p}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)\,|-\mathbf{p}+\mathbf{Q})}{(\omega + Q^2/2m - \mathbf{p}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)(\omega - Q^2/2m + \mathbf{p}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)}\right\}; \tag{3.16}$$

there are corresponding expressions arising from (3.14b), (3.15a) and (3.15b). The corresponding result for (3.14c) is

$$\chi^{(TT)}(\mathbf{Q},\omega) = 2\int \frac{d\mathbf{p}\,d\mathbf{k}\,d\mathbf{P}}{(2\pi)^9}\int_{-\infty}^{\infty}\frac{dx}{\pi}\exp(-\beta x)\,\mathrm{Im}\left\{\frac{(\mathbf{p}|\,T(\mathbf{P},x^+)\,|\mathbf{k})_s}{(x^+ - p^2/m - P^2/4m)(x^+ - k^2/m - P^2/4m)}\right\}$$
$$\times \mathrm{Im}\left\{\frac{(\mathbf{k}+\tfrac{1}{2}\mathbf{Q}|\,T(\mathbf{P}+\mathbf{Q},x^+ + \omega)\,|\mathbf{p}+\tfrac{1}{2}\mathbf{Q})}{(x^+ + \omega - (\mathbf{k}+\tfrac{1}{2}\mathbf{Q})^2/m - (\mathbf{P}+\mathbf{Q})^2/4m)(x^+ + \omega - (\mathbf{p}+\tfrac{1}{2}\mathbf{Q})^2/m - (\mathbf{P}+\mathbf{Q})^2/4m)}\right\}, \tag{3.17}$$

and there is an analogous result for (3.15c).

To perform the x-integration in (3.17) we require the formulas (B1) from Appendix B and (A8) from Appendix A; We obtain

$$\chi^{(TT)}(\mathbf{Q},\omega) = -4P\cdot V\cdot\int \frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\exp\left(-\frac{\beta p^2}{m}\right)\frac{\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{k})_s}{p^2/m - k^2/m}\int\frac{d\mathbf{P}}{(2\pi)^3}\exp\left(-\frac{\beta P^2}{4m}\right)$$
$$\times \mathrm{Im}\left\{\frac{(\mathbf{k}+\tfrac{1}{2}\mathbf{Q}|\,T(\mathbf{P}+\mathbf{Q},\omega + P^2/4m + p^2/m + i\epsilon)\,|\mathbf{p}+\tfrac{1}{2}\mathbf{Q})}{(\omega + p^2/m - k^2/m - Q^2/2m - \mathbf{k}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)(\omega - Q^2/2m - \mathbf{p}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)}\right\}$$
$$-2P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}\,d\mathbf{l}}{(2\pi)^9}\exp\left(-\frac{\beta l^2}{m}\right)\frac{(\mathbf{p}|\,T(l^2/m^+)\,|\mathbf{l})(\mathbf{l}|\,T(l^2/m^-)\mathbf{k})_s}{(l^2/m - p^2/m)(l^2/m - k^2/m)}\int\frac{d\mathbf{P}}{(2\pi)^3}\exp\left(-\frac{\beta P^2}{4m}\right)$$
$$\times \mathrm{Im}\left\{\frac{(\mathbf{k}+\tfrac{1}{2}\mathbf{Q}|\,T(\mathbf{P}+\mathbf{Q},\omega + P^2/4m + l^2/m + i\epsilon)\,|\mathbf{p}+\tfrac{1}{2}\mathbf{Q})}{(\omega + l^2/m - k^2/m - Q^2/2m - \mathbf{k}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/2m + i\epsilon)(\omega + l^2/m - p^2/m - Q^2/2m - \mathbf{p}\cdot\mathbf{Q}/m - \mathbf{P}\cdot\mathbf{Q}/m + i\epsilon)}\right\}, \tag{3.18}$$

and the corresponding expression for $\phi^{(TT)}(\mathbf{Q},\omega)$.

Finally, the center-of-mass momentum integration in (3.16), (3.18), and the corresponding expressions for $\chi^{(T2)}$, $\phi^{(T1)}$, $\phi^{(T2)}$, and $\phi^{(TT)}$ can be performed with the aid of Eqs. (B2), (B3), (A7), and (A8); we also use (A13) to replace a derivative of the T matrix where it appears. The results are:

$$\chi^{(T1)} = \chi_D^{(T1)} + \chi_E^{(T1)},$$

where

$$\chi_D^{(T1)}(\mathbf{Q},\omega) = \frac{4m^3}{\pi Q^3}\int\frac{d\mathbf{p}}{(2\pi)^3}\exp\left[-\frac{\beta}{m}(\mathbf{p}-\tfrac{1}{2}\mathbf{Q})^2\right]\left(\omega - \frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)\exp\left[-\frac{\beta m}{Q^2}\left(\omega - \frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)^2\right]\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{p})$$
$$+\frac{2m^2}{\pi\beta Q}P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\exp\left[-\frac{\beta}{m}(\mathbf{p}-\tfrac{1}{2}\mathbf{Q})^2\right]$$
$$\times\frac{\exp[-\beta m/Q^2(\omega - \mathbf{p}\cdot\mathbf{Q}/m + p^2/m - k^2/m)^2] - \exp[-\beta m/Q^2(\omega - \mathbf{p}\cdot\mathbf{Q}/m)^2]}{(k^2/m - p^2/m)^2}$$
$$\times(\mathbf{p}|\,T(k^2/m^+)\,|\mathbf{k})(\mathbf{k}|\,T(k^2/m^-)\,|\mathbf{p}), \tag{3.19a}$$

$$\chi_E^{(T1)}(\mathbf{Q},\omega) = \pm\frac{4m^2}{\pi\beta Q}P\cdot V\cdot\int\frac{d\mathbf{p}}{(2\pi)^3}\exp\left[-\frac{\beta}{m}(\mathbf{p}-\tfrac{1}{2}\mathbf{Q})^2\right]\exp\left[-\frac{\beta m}{Q^2}\left(\omega - \frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)^2\right]\frac{\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|-\mathbf{p}+\mathbf{Q})}{p^2/m - (-\mathbf{p}+\mathbf{Q})^2/m}$$
$$\pm\frac{2m^2}{\pi\beta Q}\int\frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\exp\left[-\frac{\beta}{m}(\mathbf{p}-\tfrac{1}{2}\mathbf{Q})^2\right]\exp\left[-\frac{\beta m}{Q^2}\left(\omega - \frac{\mathbf{p}\cdot\mathbf{Q}}{m} + \frac{p^2}{m} - \frac{k^2}{m}\right)^2\right]$$
$$\times\frac{(\mathbf{p}|\,T(k^2/m^+)\,|\mathbf{k})(\mathbf{k}|\,T(k^2/m^-)\,|-\mathbf{p}+\mathbf{Q})}{(k^2/m - p^2/m)(k^2/m - (-\mathbf{p}+\mathbf{Q})^2/m)}, \tag{3.19a'}$$

$$\chi^{(T2)}(\mathbf{Q},\omega) = -\frac{4m^2}{\pi Q^3}\int\frac{d\mathbf{p}}{(2\pi)^3}\exp\left(-\frac{\beta p^2}{m}\right)\left(\omega - \frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)\exp\left[-\frac{\beta m}{Q^2}\left(\omega - \frac{Q^2}{2m} - \frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)^2\right]\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{p})_s$$
$$+\frac{2m^2}{\pi\beta Q}P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\left\{\exp\left(-\frac{\beta k^2}{m}\right)\exp\left[-\frac{\beta m}{Q^2}\left(\omega - \frac{Q^2}{2m} - \frac{\mathbf{p}\cdot\mathbf{Q}}{m} + \frac{k^2}{m} - \frac{p^2}{m}\right)^2\right]\right.$$
$$\left. -\exp\left(-\frac{\beta p^2}{m}\right)\exp\left[-\frac{\beta m}{Q^2}\left(\omega - \frac{Q^2}{2m} - \frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)^2\right]\right\}(k^2/m - p^2/m)^{-2}(\mathbf{p}|\,T(k^2/m^+)\,|\mathbf{k})(\mathbf{k}|\,T(k^2/m^-)\,|\mathbf{p})_s, \tag{3.19b}$$

$$\chi^{(TT)}(\mathbf{Q},\omega)=\frac{4m^2}{\pi\beta Q}P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\exp\left(-\frac{\beta p^2}{m}\right)\frac{\mathrm{Re}(\mathbf{p}|T(p^2/m)|\mathbf{k})_s}{p^2/m-k^2/m}\left\{\exp\left[-\frac{\beta m}{Q^2}\left(\omega-\frac{Q^2}{2m}-\frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)^2\right]\right.$$
$$\times\frac{\mathrm{Re}(\mathbf{k}+\frac{1}{2}\mathbf{Q}|T((\mathbf{p}+\frac{1}{2}\mathbf{Q})^2/m)|\mathbf{p}+\frac{1}{2}\mathbf{Q})}{(\mathbf{p}+\frac{1}{2}\mathbf{Q})^2/m-(\mathbf{k}+\frac{1}{2}\mathbf{Q})^2/m}+\exp\left[-\frac{\beta m}{Q^2}\left(\omega-\frac{Q^2}{2m}-\frac{\mathbf{k}\cdot\mathbf{Q}}{m}+\frac{P^2}{m}-\frac{k^2}{m}\right)^2\right]$$
$$\times\frac{\mathrm{Re}(\mathbf{k}+\frac{1}{2}\mathbf{Q}|T((\mathbf{k}+\frac{1}{2}\mathbf{Q})^2/m)|\mathbf{p}+\frac{1}{2}\mathbf{Q})}{(\mathbf{k}+\frac{1}{2}\mathbf{Q})^2/m-(\mathbf{p}+\frac{1}{2}\mathbf{Q})^2/m}+\int\frac{d\mathbf{l}}{(2\pi)^3}\exp\left[-\frac{\beta m}{Q^2}\left(\omega-\frac{Q^2}{4m}-\frac{p^2}{m}-\frac{l^2}{m}\right)^2\right]$$
$$\left.\times\frac{(\mathbf{k}+\frac{1}{2}\mathbf{Q}|T(l^2/m^+)|\mathbf{l})(\mathbf{l}|T(l^2/m^-)|\mathbf{p}+\frac{1}{2}\mathbf{Q})}{(l^2/m-(\mathbf{k}+\frac{1}{2}\mathbf{Q})^2/m)(l^2/m-(\mathbf{p}+\frac{1}{2}\mathbf{Q})^2/m)}\right\}+\frac{2m^2}{\pi\beta Q}P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}\,d\mathbf{l}}{(2\pi)^9}\exp\left(-\frac{\beta l^2}{m}\right)$$
$$\times\frac{(\mathbf{p}|T(l^2/m^+)|\mathbf{l})(\mathbf{l}|T(l^2/m^-)|\mathbf{k})_s}{(l^2/m-p^2/m)(l^2/m-k^2/m)}\left\{2\exp\left[-\frac{\beta m}{Q^2}\left(\omega-\frac{Q^2}{2m}-\frac{\mathbf{p}\cdot\mathbf{Q}}{m}+\frac{l^2}{m}-\frac{p^2}{m}\right)^2\right]\right.$$
$$\times\frac{\mathrm{Re}(\mathbf{k}+\frac{1}{2}\mathbf{Q}|T((\mathbf{p}+\frac{1}{2}\mathbf{Q})^2/m)|\mathbf{p}+\frac{1}{2}\mathbf{Q})}{(\mathbf{p}+\frac{1}{2}\mathbf{Q})^2/m-(\mathbf{k}+\frac{1}{2}\mathbf{Q})^2/m}+\int\frac{d\mathbf{u}}{(2\pi)^3}\exp\left[-\frac{\beta m}{Q^2}\left(\omega-\frac{Q^2}{4m}+\frac{l^2}{m}-\frac{u^2}{m}\right)^2\right]$$
$$\left.\times\frac{(\mathbf{k}+\frac{1}{2}\mathbf{Q}|T(u^2/m^+)|\mathbf{u})(\mathbf{u}|T(u^2/m^-)|\mathbf{p}+\frac{1}{2}\mathbf{Q})}{(u^2/m-(\mathbf{k}+\frac{1}{2}\mathbf{Q})^2/m)(u^2/m-(\mathbf{p}+\frac{1}{2}\mathbf{Q})^2/m)}\right\},\tag{3.19c}$$

$\phi^{(T1)}=\phi_D^{(T1)}+\phi_E^{(T1)}$, where $\phi_D^{(T1)}(\mathbf{Q},\omega)=\pm\chi_E^{(T1)}(\mathbf{Q},\omega)$ with final state $|-\mathbf{p}+\mathbf{Q})$ replaced by $|\mathbf{p}-\mathbf{Q})$ in each term of (3.19a′), and $\phi_E^{(T1)}(\mathbf{Q},\omega)=\pm\chi_D^{(T1)}(\mathbf{Q},\omega)$ with final state $|\mathbf{p})$ replaced by $|-\mathbf{p})$ in each term of (3.19a), (3.20a)

$$\phi^{(T2)}(\mathbf{Q},\omega)=\frac{4m^2}{\pi\beta Q}P\cdot V\cdot\int\frac{d\mathbf{p}}{(2\pi)^3}\exp\left(-\frac{\beta p^2}{m}\right)\exp\left[-\frac{\beta m}{Q^2}\left(\omega-\frac{Q^2}{2m}+\frac{\mathbf{p}\cdot\mathbf{Q}}{m}\right)^2\right]\frac{\mathrm{Re}(\mathbf{p}|T(p^2/m)|\mathbf{p}-\mathbf{Q})_s}{p^2/m-(\mathbf{p}-\mathbf{Q})^2/m}$$
$$+\frac{2m^2}{\pi\beta Q}P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\exp\left(-\frac{\beta k^2}{m}\right)\exp\left[-\frac{\beta m}{Q^2}\left(\omega-\frac{Q^2}{2m}+\frac{\mathbf{p}\cdot\mathbf{Q}}{m}+\frac{k^2}{m}-\frac{p^2}{m}\right)^2\right]$$
$$\times\frac{(\mathbf{p}|T(k^2/m^+)|\mathbf{k})(\mathbf{k}|T(k^2/m^-)|\mathbf{p}-\mathbf{Q})_s}{(k^2/m-p^2/m)(k^2/m-(\mathbf{p}-\mathbf{Q})^2/m)},\tag{3.20b}$$

$\phi^{(TT)}(\mathbf{Q},\omega)$ is obtained from $\chi^{(TT)}(\mathbf{Q},\omega)$, as given by (3.19c), by replacing the states $(\mathbf{p}|$ by $(-\mathbf{p}|$ and $|\mathbf{p}+\frac{1}{2}\mathbf{Q})$ by $|-\mathbf{p}-\frac{1}{2}\mathbf{Q})$. (3.20c)

Now, combining (3.11) with (3.19), we obtain $F_2^{(s)}(\mathbf{Q},\omega)$, while (3.12) and (3.20) give $F_2^{(d)}(\mathbf{Q},\omega)$. Our final expressions for $S_1^{(s)}(\mathbf{Q},\omega)$ and $S_1^{(d)}(\mathbf{Q},\omega)$ are then given by (2.9).

IV. ADDITIONAL PROPERTIES

There are a few well-known properties which must be possessed by $S(\mathbf{Q},\omega)$; from our point of view these serve as checks on our calculation.

The detailed-balance condition is $S(-\mathbf{Q},-\omega)=\exp(-\beta\omega)S(\mathbf{Q},\omega)$. This relation is satisfied by $F_2(\mathbf{Q},\omega)$, but it is not true that $F_2^{(s)}(-\mathbf{Q},-\omega)=\exp(-\beta\omega)\times F_2^{(s)}(\mathbf{Q},\omega)$ because of the exchange terms. We can show from (3.11), (3.12), (3.19), and (3.20) that (if direct and exchange are denoted by subscripts D and E, respectively), the detailed-balance relation is satisfied individually by $\chi^{(0)}+\phi^{(0)}$, $\chi_D^{(T1)}+\chi_D^{(T2)}$, $\chi^{(TT)}$, $\phi_D^{(T1)}+\phi_D^{(T2)}$, $\phi^{(TT)}$, $\chi_E^{(T1)}+\phi_E^{(T2)}$, and $\chi_E^{(T2)}+\phi_E^{(T1)}$.

The familiar zeroth moment relations are

$$\int_{-\infty}^{\infty}d\omega\,S^{(s)}(\mathbf{Q},\omega)=1,\quad\int_{-\infty}^{\infty}d\omega\,S(\mathbf{Q},\omega)=S(\mathbf{Q}),\tag{4.1}$$

which defines the *structure facture*, $S(\mathbf{Q})$. Since

$$\int_{-\infty}^{\infty}d\omega\,S_0(\mathbf{Q},\omega)=1,\tag{4.2}$$

it is necessary, according to (2.9), that

$$\int_{-\infty}^{\infty}d\omega\,F_2^{(s)}(\mathbf{Q},\omega)=2\pi n_2,\tag{4.3}$$

where n_2 is given by (2.4); this acts as a check. On the other hand, if we define

$$S(\mathbf{Q})=1+zS_1(\mathbf{Q})+\cdots,\tag{4.4}$$

then the equation

$$S_1(\mathbf{Q})=(2\pi)^{-1}\lambda^3\int_{-\infty}^{\infty}d\omega\,F_2^{(d)}(\mathbf{Q},\omega),\tag{4.5}$$

gives a new result, namely, an exact expression for the first order term in the activity expansion of the structure factor.

Let us denote the zeroth moment of the various contributions to F_2 by a subscript 0. Confirmation of (4.3) is obtained from equations (3.11) and (3.19) by showing directly that $\chi_{D,0}^{(T1)}=0$ and $\chi_0^{(0)}+\chi_0^{(T2)}=2\pi n_2$; we require equation (A12) to show that $\chi_{E,0}^{(T1)}=\chi_0^{(TT)}=0$. Then we make use of (A12) to show that Eqs. (3.12) and (3.20) yield $\phi_0^{(T1)}=\phi_0^{(TT)}=0$; from $\phi_0^{(0)}$ and $\phi_0^{(T2)}$ we obtain the result

$$S_1(\mathbf{Q})=\pm2^{-3/2}\exp\left(-\frac{\beta Q^2}{4m}\right)+2^{5/2}\int\frac{d\mathbf{p}}{(2\pi)^3}$$
$$\times\exp\left(-\frac{\beta p^2}{m}\right)\frac{\mathrm{Re}(\mathbf{p}|T(p^2/m)|\mathbf{p}-\mathbf{Q})_s}{p^2/m-(\mathbf{p}-\mathbf{Q})^2/m}$$
$$+2^{3/2}P\cdot V\cdot\int\frac{d\mathbf{p}\,d\mathbf{k}}{(2\pi)^6}\exp\left(-\frac{\beta k^2}{m}\right)$$
$$\times\frac{(\mathbf{p}|T(k^2/m^+)|\mathbf{k})(\mathbf{k}|T(k^2/m^-)|\mathbf{p}-\mathbf{Q})_s}{(k^2/m-p^2/m)(k^2/m-(\mathbf{p}-\mathbf{Q})^2/m)}.\tag{4.6}$$

The first moment relations are usually written

$$\int_{-\infty}^{\infty}d\omega\,\omega S^{(s)}(\mathbf{Q},\omega)=Q^2/2m,\tag{4.7a}$$
$$\int_{-\infty}^{\infty}d\omega\,\omega S^{(d)}(\mathbf{Q},\omega)=0.\tag{4.7b}$$

We now confirm that (4.7a) and (4.7b) are satisfied by our result. We denote the first moments of the various contributions to F_2 by the subscript 1, and, using formulas (A14), (A15), (A16), and (A18), we can show

that Eqs. (3.11), (3.12), (3.19), and (3.20) yield the following (see Appendix A for notation):

$$\chi_1^{(0)} + \chi_1^{(T2)} = 2\pi n_2 \frac{Q^2}{2m} - 2^{5/2}\pi\lambda^{-3} \times \int \frac{d\mathbf{p}}{(2\pi)^3} (\mathbf{p}|\exp(-\beta\tilde{H})\tilde{V}|\mathbf{p})_s, \quad (4.8a)$$

$$\chi_1^{(T1)} = 2^{5/2}\pi\lambda^{-3} \int \frac{d\mathbf{p}}{(2\pi)^3} (\mathbf{p}|\exp(-\beta\tilde{H}_0)\tilde{V}|\mathbf{p})_s, \quad (4.8b)$$

$$\chi_1^{(TT)} = 2^{5/2}\pi\lambda^{-3} \int \frac{d\mathbf{p}}{(2\pi)^3} (\mathbf{p}|(\exp(-\beta\tilde{H}) - \exp(-\beta\tilde{H}_0))\tilde{V}|\mathbf{p})_s, \quad (4.8c)$$

$$\Phi_1^{(0)} = 0, \quad (4.9a)$$

$$\phi_1^{(T1)} = 2^{5/2}\pi\lambda^{-3} \int \frac{d\mathbf{p}}{(2\pi)^3} (\mathbf{p}|\exp(-\beta\tilde{H}_0)\tilde{V}|\mathbf{p}-\mathbf{Q})_s, \quad (4.9b)$$

$$\phi_1^{(T2)} = -2^{5/2}\pi\lambda^{-3} \int \frac{d\mathbf{p}}{(2\pi)^3} (\mathbf{p}|\exp(-\beta\tilde{H})\tilde{V}|\mathbf{p}-\mathbf{Q})_s, \quad (4.9c)$$

$$\phi_1^{(TT)} = 2^{5/2}\pi\lambda^{-3} \int \frac{d\mathbf{p}}{(2\pi)^3} (\mathbf{p}|(\exp(-\beta\tilde{H}_0) - \exp(-\beta\tilde{H}_0))\tilde{V}|\mathbf{p}-\mathbf{Q})_s. \quad (4.9d)$$

Thus, combining all of (4.8) and (4.9) we obtain

$$\int_{-\infty}^{\infty} d\omega\, \omega F_2^{(s)}(\mathbf{Q},\omega) = 2\pi n_2 (Q^2/2m), \quad (4.10a)$$

$$\int_{-\infty}^{\infty} d\omega\, \omega F_2^{(d)}(\mathbf{Q},\omega) = 0, \quad (4.10b)$$

which agree with (4.7a) and (4.7b).

V. DISCUSSION

We have obtained exact expressions for the coefficient of z in the activity expansions of $S^{(s)}(\mathbf{Q},\omega)$ and of $S^{(d)}(\mathbf{Q},\omega)$: These are given by (2.9), (3.9), (3.10), (3.11), (3.12), (3.19), and (3.20). These results are expressed in terms of on- and half-on-shell two-particle T matrices. It is assumed that the two-body interaction depend only on the relative coordinates and that this function be integrable over all space; no further restrictions are required. The effect of two-particle bound states was not included in our results but can be introduced by means of the second term in (A8). Statistics was included and spin can be quite simply if desired. Thus, our results are quite general.

An exact result for the coefficient of z in the activity expansion of the structure factor $S(\mathbf{Q})$ is given by (4.6). In Appendix A we obtain some properties of the T matrix which to our knowledge have not previously been recorded.

In Appendix C we demonstrate that Baym and Kadanoff's *conserving T approximation*[8] for the two-particle Green function gives the correct result for $S(\mathbf{Q},\omega)$ to first order in the activity. Note, however, that this technique does not allow $S^{(s)}(\mathbf{Q},\omega)$ and $S^{(d)}(\mathbf{Q},\omega)$ to be calculated separately. Moreover, the Green function theory requires a considerably more difficult calculation (not described in detail in Appendix C), than the method used in Sec. III. This suggests that the Green's function formalism is not the most convenient for activity expansion calculations.

We are aware of a derivation by Dashen and Ma[12] of part of the coefficient $S_1(\mathbf{Q},\omega)$: They obtained only the two lowest order terms in Q and ω. In that paper a more general class of correlation functions was considered and these were given in the low energy limit in terms of scattering amplitudes. Although their nonrelativistic formula (7.7) is simply related to part of $S_1(\mathbf{Q},\omega)$ we have been unable to make a detailed comparison of our result with theirs; in fact, it is not obvious that our formula for $S_1(\mathbf{Q},\omega)$ does possess such a series expansion.

APPENDIX A

The properties of the T matrices which are used in this paper are presented (and in some cases derived), here. The T operator is defined by (2.2), and its matrix elements in the momentum representation are

$$(\mathbf{p}_1\mathbf{p}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2) = (\mathbf{p}_1\mathbf{p}_2|V|\mathbf{k}_1\mathbf{k}_2) + \int \frac{d\mathbf{l}_1\, d\mathbf{l}_2}{(2\pi)^6} \frac{(\mathbf{p}_1\mathbf{p}_2|V|\mathbf{l}_1\mathbf{l}_2)(\mathbf{l}_1\mathbf{l}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2)}{\zeta - E_{l_1} - E_{l_2}}, \quad (A1)$$

where the complex variable ζ is not purely real. It follows immediately that[13]

$$\frac{\partial}{\partial\zeta}(\mathbf{p}_1\mathbf{p}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2) = -\int \frac{d\mathbf{l}_1\, d\mathbf{l}_2}{(2\pi)^6} \frac{(\mathbf{p}_1\mathbf{p}_2|T(\zeta)|\mathbf{l}_1\mathbf{l}_2)(\mathbf{l}_1\mathbf{l}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2)}{(\zeta - E_{l_1} - E_{l_2})^2}. \quad (A2)$$

The interaction V is assumed to be such that $V(\mathbf{r}_1,\mathbf{r}_2) = V(\mathbf{r}_1-\mathbf{r}_2) = V(\mathbf{r}_2-\mathbf{r}_1)$ and $\int d\mathbf{r}\tilde{V}(\mathbf{r})$ exists: It follows that

$$(\mathbf{p}_1\mathbf{p}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2) = (\mathbf{k}_1\mathbf{k}_2|T(\zeta)|\mathbf{p}_1\mathbf{p}_2) = (\mathbf{p}_2\mathbf{p}_1|T(\zeta)|\mathbf{k}_2\mathbf{k}_1). \quad (A3)$$

In addition, hermiticity of V implies that if x is real,

$$(\mathbf{p}_1\mathbf{p}_1|T(x^+)|\mathbf{k}_1\mathbf{k}_2)^* = (\mathbf{p}_1\mathbf{p}_2|T(x^-)|\mathbf{k}_1\mathbf{k}_2). \quad (A4)$$

Introducing the center-of-mass and relative momenta corresponding to each two-particle state we obtain

$$(\mathbf{p}_1\mathbf{p}_2|V|\mathbf{k}_1\mathbf{k}_2) = (2\pi)^3\delta(\mathbf{P}-\mathbf{K})(\mathbf{p}|\tilde{V}|\mathbf{k}), \quad (A5)$$

where $(\mathbf{p}|\tilde{V}|\mathbf{k}) = \tilde{V}(\mathbf{p}-\mathbf{k}) = \tilde{V}(\mathbf{k}-\mathbf{p})$. Thus, reduced or one-particle T matrices can be defined according to

$$(\mathbf{p}_1\mathbf{p}_2|T(\zeta)|\mathbf{k}_1\mathbf{k}_2) = (2\pi)^3\delta(\mathbf{P}-\mathbf{K})(\mathbf{p}|T(\mathbf{P},\zeta)|\mathbf{k}); \quad (A6)$$

the reduced matrix elements have symmetry properties corresponding to (A3) and (A4). It can also be shown from the definition that if α is independent of P, then

$$(\mathbf{p}|T(\mathbf{P}, P^2/4m + \alpha)|\mathbf{k}) = (\mathbf{p}|T(\alpha)|\mathbf{k}) \quad (A7)$$

does not depend on P. The latter quantity is said to be *half-on-shell* if $\alpha = p^2/m$ or $\alpha = k^2/m$. An expression for the discontinuity across the real axis of the T matrix can be derived[14]:

$$\mathrm{Im}(\mathbf{p}|T(\mathbf{P},x^+)|\mathbf{k}) = -\pi\int \frac{d\mathbf{l}}{(2\pi)^3}\delta(x - P^2/4m - l^2/m) \times (\mathbf{p}|T(l^2/m^+)|\mathbf{l})(\mathbf{l}|T(l^2/m^-)|\mathbf{k}) - \pi\sum_B \delta(x - P^2/4m - \epsilon_B)(\epsilon_B - p^2/m) \times (\epsilon_B - k^2/m)(\mathbf{p}|B)(B|\mathbf{k}), \quad (A8)$$

the right side containing *half-on-shell* T matrices, bound-state energies $\epsilon_B < 0$ and bound-state wavefunctions.

We now develop some additional properties which are based on the operator relation (3.8),

$$\exp(-\tau H^{(2)}) - \exp(-\tau H_0{}^{(2)}) = (2\pi i)^{-1}\int_C d\zeta \exp(-\tau\zeta)(\zeta - H_0{}^{(2)})^{-1}T(\zeta)(\zeta - H_0{}^{(2)})^{-1}, \tag{A9}$$

where the path of integration C surrounds the real axis of the ζ plane in the positive sense. By expanding both members of (A9) in powers of τ we obtain

$$\int_{-\infty}^{\infty} dx\, \mathrm{Im}\left[\frac{(\mathbf{p}_1\mathbf{p}_2|\,T(x^+)\,|\mathbf{k}_1\mathbf{k}_2)}{(x^+ - E_{p_1} - E_{p_2})(x^+ - E_{k_1} - E_{k_2})}\right] = 0, \tag{A10}$$

$$\int_{-\infty}^{\infty} dx\, x\, \mathrm{Im}\left[\frac{(\mathbf{p}_1\mathbf{p}_2|\,T(x^+)\,|\mathbf{k}_1\mathbf{k}_2)}{(x^+ - E_{p_1} - E_{p_2})(x^+ - E_{k_1} - E_{k_2})}\right] = -\pi(\mathbf{p}_1\mathbf{p}_2|\,V\,|\mathbf{k}_1\mathbf{k}_2). \tag{A11}$$

These formulas may be combined with (A8) (we neglect the bound state term for brevity, but there is no difficulty, in principle, to include this contribution if desired), to yield, with the help of (B1), such results as

$$\frac{\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{k})}{p^2/m - k^2/m} + \frac{\mathrm{Re}(\mathbf{p}|\,T(k^2/m)\,|\mathbf{k})}{k^2/m - p^2/m} + P\cdot V\cdot\int \frac{d\mathbf{l}}{(2\pi)^3} \times \frac{(\mathbf{p}|\,T(l^2/m^+)\,|\mathbf{l})(\mathbf{l}|\,T(l^2/m^-)\,|\mathbf{k})}{(l^2/m - p^2/m)(l^2/m - k^2/m)} = 0, \quad \text{if } p^2 \neq k^2, \tag{A12}$$

$$\frac{\partial}{\partial x}\,\mathrm{Re}(\mathbf{p}|\,T(x)\,|\mathbf{k})_{x=p^2/m} + \int \frac{d\mathbf{l}}{(2\pi)^3} \times \mathrm{Re}(l^2/m - p^2/m + i\epsilon)^{-2}(\mathbf{p}|\,T(l^2/m^+)\,|\mathbf{l})(\mathbf{l}|\,T(l^2/m^-)\,|\mathbf{k}) = 0, \quad \text{if } p^2 = k^2, \tag{A13}$$

$$\frac{(p^2/m)\,\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{k})}{p^2/m - k^2/m} + \frac{(k^2/m)\,\mathrm{Re}(\mathbf{p}|\,T(k^2/m)\mathbf{k})}{k^2/m - p^2/m} + P\cdot V\cdot\int \frac{d\mathbf{l}}{(2\pi)^3}(l^2/m)\frac{(\mathbf{p}|\,T(l^2/m^+)\,|\mathbf{l})(\mathbf{l}|\,T(l^2/m^-)\,|\mathbf{k})}{(l^2/m - p^2/m)(l^2/m - k^2/m)} = (\mathbf{p}|\,\tilde{V}\,|\mathbf{k}), \quad \text{if } p^2 \neq k^2, \tag{A14}$$

$$\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{k}) + P\cdot V\cdot\int \frac{d\mathbf{l}}{(2\pi)^3} \times \frac{(\mathbf{p}|\,T(l^2/m^+)\,|\mathbf{l})(\mathbf{l}|\,T(l^2/m^-)\mathbf{k})}{l^2/m - p^2/m} = (\mathbf{p}|\,\tilde{V}\,|\mathbf{k}), \quad \text{if } p^2 = k^2. \tag{A15}$$

Returning to (A9) and defining the single-particle operators $\tilde{H} = 2K + \tilde{V}$ and $\tilde{H}_0 = 2K$ we obtain the result

$$\exp\left(-\frac{\beta p^2}{m}\right)\frac{\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{k})}{p^2/m - k^2/m} + \exp\left(-\frac{\beta k^2}{m}\right)\frac{\mathrm{Re}(\mathbf{p}|\,T(k^2/m)\,|\mathbf{k})}{k^2/m - p^2/m} + P\cdot V\cdot\int \frac{d\mathbf{l}}{(2\pi)^3}\exp\left(-\frac{\beta l^2}{m}\right)\frac{(\mathbf{p}|\,T(l^2/m^+)\,|\mathbf{l})(\mathbf{l}|\,T(l^2/m^-)\,|\mathbf{k})}{(l^2/m - p^2/m)(l^2/m - k^2/m)} = (\mathbf{p}|\exp(-\beta\tilde{H}) - \exp(-\beta H_0)\,|\mathbf{k}), \quad \text{If } k^2 \neq p^2. \tag{A16}$$

Another operator relation, easily obtainable from (3.7), is

$$\exp(-\beta H^{(2)})V = (2\pi i)^{-1}\int_C d\zeta \exp(-\beta\zeta)(\zeta - H_0{}^{(2)})^{-1}T(\zeta), \tag{A17}$$

and this gives the formula

$$\exp\left(-\frac{\beta p^2}{m}\right)\mathrm{Re}(\mathbf{p}|\,T(p^2/m)\,|\mathbf{k}) + P\cdot V\cdot\int \frac{d\mathbf{l}}{(2\pi)^3} \times \exp\left(-\frac{\beta l^2}{m}\right)\frac{(\mathbf{p}|\,T(l^2/m^+)\,|\mathbf{l})(\mathbf{l}|\,T(l^2/m^-)\,|\mathbf{k})}{l^2/m - p^2/m} = (\mathbf{p}|\exp(-\beta\tilde{H})\tilde{V}\,|\mathbf{k}). \tag{A18}$$

APPENDIX B

The following formulas are used in this paper to evaluate certain integrals ($\lim\epsilon \to 0^+$ is implied in every case).

If the function f is such that $f(x + i\epsilon) = f^*(x - i\epsilon)$, then

$$\int_{-\infty}^{\infty} dx\, \mathrm{Im}\left(\frac{f(x + i\epsilon)}{(x - a + i\epsilon)(x - b + i\epsilon)}\right) = \begin{cases} -\pi(a-b)^{-1}[\mathrm{Re}f(a) - \mathrm{Re}f(b)] + P\cdot V\int_{-\infty}^{\infty} dx \times \dfrac{\mathrm{Im}f(x + i\epsilon)}{(x-a)(x-b)}, & \text{if } b \neq a, \\ -\pi\,\mathrm{Re}f'(a) + P\cdot V\cdot\int dx\,\dfrac{\mathrm{Im}f(x + i\epsilon) - \mathrm{Im}f(a + i\epsilon)}{(x-a)^2}, & \text{if } b = a. \end{cases} \tag{B1}$$

If g is a function of two variables and if g_1 and g_2 denote the two partial derivatives, then

$$\int_{-1}^{1} dX \int_0^{\infty} dP\, g(P^2, PX)\,\mathrm{Im}[(a - PX + i\epsilon)^{-1}(b - PX + i\epsilon)^{-1}] = \begin{cases} \pi(a-b)^{-1}\int_0^1 dX\, X^{-1}[g(a^2X^{-2}, a) - g(b^2X^{-2}, b)], & \text{if } b \neq a \\ \pi\int_0^1 dX[2aX^{-3}g_1(a^2X^{-2}, a) + X^{-1}g_2(a^2X^{-2}, a)], & \text{if } b = a \end{cases} \tag{B2}$$

and

$$\int_{-1}^{1} dX \int_0^{\infty} dP\, g(P^2, PX)\delta(a - PX) = \int_0^1 dX\, X^{-1}g(a^2X^{-2}, a). \tag{B3}$$

These formulas are used to perform the center-of-mass momentum integration leading to Eqs. (3.19) and (3.20). In particular, (B3) is used in connection with (A8).

APPENDIX C

Here we present an outline of how the theory of temperature Green's functions can be used to compute $S(\mathbf{Q}, \omega)$ to the same order in z as in the main text of this paper. The definitions of the one- and two-particle Green's functions, their boundary conditions and other properties are given by Kadanoff and Baym[15]; we conform to their notation.

Consider the two-particle Green's function $\mathcal{G}(\mathbf{r}_1 - \mathbf{r}_2, \tau_1 - \tau_2) = G_2(\mathbf{r}_1\tau_1, \mathbf{r}_2\tau_2; \mathbf{r}_1\tau_1{}^+, \mathbf{r}_2\tau_2{}^+)$ where the "times" here are imaginary and ordered from 0 to $-i\beta$. The Fourier transform with respect to the space variable and series with respect to the "time" variable gives the coefficients $\mathcal{G}(\mathbf{Q}, \omega_N)$ where the boundary con-

ditions require that $\omega_N = i\pi\beta^{-1}N$ where N is an even integer. For $N > 0$ these coefficients define by continuation a function $\mathcal{G}(\mathbf{Q}, \zeta)$ which is analytic in the upper half ζ plane. It has been shown that[16]

$$S(\mathbf{Q}, \omega) = -(\pi n)^{-1}[1 - \exp(-\beta\omega)]^{-1}\,\mathrm{Re}\mathcal{G}(\mathbf{Q}, \omega^+). \tag{C1}$$

Thus, $S(\mathbf{Q}, \omega)$ can be obtained from the Fourier coefficients of a certain two-particle temperature Green function.

An activity expansion of the coefficients can be carried out with the aid of operator relations (or diagram techniques), similar to those used in the body of the paper. However, it is customary to consider the equations of motion for the Green's functions. Since these form an infinite hierarchy of equations they cannot be solved exactly and various methods of approximating the solutions have been proposed. Here, we use the *conserving T matrix approximation*[8] which yields an approximate one-particle Green's function G and a particular two-particle correlation function which obey all the conservation laws and which, as we show, yield results exact to second order in the activity.

The *conserving T approximation for* G_2 is defined by Eq. (60) of Ref. 8. There, an integral equation is formulated for the quantity $L(12, 1'2') = G_2(12, 1'2') - G(11')G(22')$ in terms of G and a generalized T matrix for which the standard two-body T matrix is the $z \to 0$ limit. (In the present calculation the lowest order suffices; we have shown previously in a paper on the third virial coefficient how to use the next order of this T matrix.[9]) The G to be used in this integral equation (and in the equation defining the generalized T matrix), is that associated with the self-energy given by the T approximation; compare Eqs. (C6) and (C7) for the Fourier coefficients.

We follow the approach of Leribaux and Pope[17] who showed how to obtain the terms of order z^2 in $\mathcal{G}(\mathbf{Q}, \omega_N)$. [However, in their actual calculation certain approximations were made which precluded attainment of the exact result for $S_1(\mathbf{Q}, \omega)$.] These authors showed that, to order z^2, the coefficients $\mathcal{G}(\mathbf{Q}, \omega_N)$ can be obtained from the first iteration solution of the integral equation for $L(12, 1'2')$. The corresponding G_2 contains three terms which must be transformed to obtain the following first iteration contributions to $\mathcal{G}(\mathbf{Q}, \omega_N)$,[17]

$$\mathcal{G}^{(HF)}(\mathbf{Q}, \omega_N) = \pm i\beta^{-1}\int \frac{d\mathbf{p}}{(2\pi)^3}\sum_M G(\mathbf{p}, \gamma_M)G(\mathbf{p}+\mathbf{Q}, \gamma_M + \omega_N), \tag{C2}$$

$$\mathcal{G}^{(T)}(\mathbf{Q}, \omega_N) = -i\beta^{-2}\Omega^{-1}\int \frac{d\mathbf{p}_1\, d\mathbf{p}_2}{(2\pi)^6}\sum_{M_1 M_2} G(\mathbf{p}_1, \gamma_{M_1})G(\mathbf{p}_2, \gamma_{M_2}) \times (\mathbf{p}_1\mathbf{p}_2 \,|\, T(\gamma_{M_1} + \gamma_{M_2}) \,|\, \mathbf{p}_1 + \mathbf{Q}, \mathbf{p}_2 - \mathbf{Q}) \times G(\mathbf{p}_1 + \mathbf{Q}, \gamma_{M_1} + \omega_N)G(\mathbf{p}_2 - \mathbf{Q}, \gamma_{M_2} - \omega_N), \tag{C3}$$

$$\mathcal{G}^{(TT)}(\mathbf{Q}, \omega_N) = i\beta^{-3}\Omega^{-2}\int \frac{d\mathbf{p}_1\, d\mathbf{p}_2\, d\mathbf{p}_3}{(2\pi)^9}\sum_{M_1 M_2 M_3} G(\mathbf{p}_1, \gamma_{M_1}) \times G(\mathbf{p}_1 + \mathbf{Q}, \gamma_{M_1} + \omega_N)G(\mathbf{p}_2, \gamma_{M_2}) \times G(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3, \gamma_{M_1} + \gamma_{M_2} - \gamma_{M_3}) \times (\mathbf{p}_1\mathbf{p}_2 \,|\, T(\gamma_{M_1} + \gamma_{M_2}) \,|\, \mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3, \mathbf{p}_3) \times (\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_3, \mathbf{p}_3 + \mathbf{Q} \,|\, T(\gamma_{M_1} + \gamma_{M_2} + \omega_N) \,|\, \mathbf{p}_2, \mathbf{p}_1 + \mathbf{Q}) \times G(\mathbf{p}_3, \gamma_{M_3})G(\mathbf{p}_3 + \mathbf{Q}, \gamma_{M_3} + \omega_N), \tag{C4}$$

where $\gamma_M = i\pi\beta^{-1}M + \mu$, ($M = 0, \pm 2, \cdots$ for bosons, $\pm 1, \pm 3, \cdots$ for fermions); then,

$$\mathcal{G}(\mathbf{Q}, \omega_N) = \mathcal{G}^{(HF)}(\mathbf{Q}, \omega_N) + \mathcal{G}^{(T)}(\mathbf{Q}, \omega_N) + \mathcal{G}^{(TT)}(\mathbf{Q}, \omega_N). \tag{C5}$$

Note that the third term, corresponding to (C4), was introduced to guarantee conservation of particle number, momentum, angular momentum, and energy.

The one-particle Green's function coefficient here is

$$G(\mathbf{p}, \gamma_M) = (\gamma_M - p^2/2m - \Sigma(\mathbf{p}, \gamma_M))^{-1} \tag{C6}$$

where the *self-energy* is

$$\Sigma(\mathbf{p}, \gamma_M) = \mp\beta^{-1}\Omega^{-1}\lim_{\tau \to 0^+}\frac{d\mathbf{p}'}{(2\pi)^3}\sum_{M'}\exp(\tau\omega_{M'}) \times (\mathbf{p}\mathbf{p}' \,|\, T(\gamma_{M'} + \gamma_M) \,|\, \mathbf{p}\mathbf{p}')_s G(\mathbf{p}', \gamma_{M'}). \tag{C7}$$

The summations in (C2), (C3), (C4), and (C7) may be performed by a method of complex integration if we assume that $(\mathbf{p}_1\mathbf{p}_2 \,|\, T(\zeta) \,|\, \mathbf{p}_1\mathbf{p}_{2'})$ is analytic for nonreal ζ and bounded as $|\zeta| \to \infty$. In some cases this introduces certain integrals which involve T evaluated on the edges of the real-axis branch cut. In every case there emerges a power series in z arising from the μ which appears in γ_m. For example, (C7) to lowest order is

$$\Sigma(\mathbf{p}, \gamma_M) = z\Omega^{-1}\int \frac{d\mathbf{p}'}{(2\pi)^3}\exp\left(-\frac{\beta p'^2}{2m}\right) \times (\mathbf{p}\mathbf{p}' \,|\, T(\gamma_M + p'^2/2m) \,|\, \mathbf{p}\mathbf{p}')_s. \tag{C8}$$

In order to obtain the first two terms in an activity expansion of the first iteration result for the coefficients, $\mathcal{G}(\mathbf{Q}, \omega_N)$, it is sufficient to replace everywhere the generalized T matrix by its low activity limit (the ordinary T matrix), and to neglect completely the self-energy occurring in G or to replace it by its low activity limit which according to Eq. (C8) is of order z as $z \to 0$. On performing the summations in (C2), (C3), and (C4), the coefficients $\mathcal{G}(\mathbf{Q}, \omega_N)$ are given by the resulting power series in z. Thus, the lowest order contribution to each of (C2), (C3), and (C4) is obtained by replacing G by $G^{(0)}(\mathbf{p}, \gamma_m) = (\gamma_m - p^2/2m)^{-1}$. There will be a contribution of order z to $\mathcal{G}(\mathbf{Q}, \omega_N)$ coming from (C2) only: This gives the ideal gas result. We seek the contribution of order z^2 which comes from each term in (C5): In (C2) one must use (C6) for G; in (C3) and (C4) G must be replaced by $G^{(0)}$.

The calculations for (C2), (C3), and (C4) require extreme care so that the correct terms of order z^2 are obtained. Then, reduced T matrices are introduced according to (A6) and the branch cut integrations are performed with the aid of (B1) and (A8). Finally, the center-of-mass momentum integration is performed using (B2) and (B3).

The three results thus obtained are inserted into (C1) to produce three contributions to $S_1(\mathbf{Q}, \omega)$: Call these $S_1^{(HF)}$, $S_1^{(T)}$, and $S_1^{(TT)}$. Comparing these with the quantities derived in the main text we see that

$$S_1^{(HF)} = (2\pi)^{-1}\lambda^3[\chi^{(0)} + \phi^{(0)} + \chi_D^{(T1)} + \phi_E^{(T1)} + \chi^{(T2)}], \tag{C9}$$

$$S_1^{(T)} = (2\pi)^{-1}\lambda^3[\phi_D^{(T1)} + \chi_E^{(T1)} + \phi^{(T1)}], \quad \text{(C10)}$$

$$S_1^{(TT)} = (2\pi)^{-1}\lambda^3[\chi^{(TT)} + \phi^{(TT)}]. \quad \text{(C11)}$$

Thus, the conserving T approximation yields precisely the correct result for $S_1(\mathbf{Q}, \omega)$: Note that it was essential to include the extra term (C4).

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[1]L. Van Hove, Phys. Rev. 95, 249 (1954).
[2]D. E. Parks, M. S. Nelkin, J. R. Beyster, and N. F. Wikner, *Slow Neutron Scattering and Thermalization* (Benjamin, New York, 1970).
[3]P. A. Egelstaff, *An Introduction to the Liquid State* (Academic, New York, 1967).
[4]J. E. Enderby, in *Physics of Simple Liquids*, edited by H. N. V. Temperley, J. S. Rowlinson, and G. S. Rushbrooke (North-Holland, Amsterdam, 1968).
[5]A. Sjolander, in *Thermal Neutron Scattering*, edited by P. A. Egelstaff (Academic, London, 1965).
[6]W. Marshall and S. W. Lovesey, *Theory of Thermal Neutron Scattering* (Oxford, 1971).
[7]A. S. Reiner, Phys. 26, 700 (1960).
[8]G. Baym and L. P. Kadanoff, Phys. Rev. 124, 287 (1961).
[9]R. E. Johnson, N. K. Pope, and A. J. Barrett, J. Math. Phys. 15, 458 (1974).
[10]Here we follow the approach of C. Bloch, in *Studies in Statistical Mechanics* (North-Holland, Amsterdam, 1965), Vol. III.
[11]K. M. Watson, Phys. Rev. 89, 577 (1953); 103, 489 (1956).
[12]R. Dashen and S. Ma, J. Math. Phys. 12, 1449 (1971).
[13]B. J. Baumgartl, Z. Phys. 198, 148 (1967).
[14]C. Lovelace, in *Strong Interactions and High Energy Physics*, edited by R. G. Moorhouse (Oliver and Boyd, London, 1964).
[15]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).
[16]A. A. Abrikosov, L. P. Gorkov, I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, translated and edited by R. A. Silverman (Prentice-Hall, Englewood Cliffs, New Jersey, 1963), pp. 149, 151.
[17]H. R. Leribaux and N. K. Pope, Phys. Rev. A 3, 1752 (1971).

A class of conservative diffusion processes with delta function initial conditions

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A class of conservative one-dimensional diffusion processes is discussed which satisfy a delta function initial condition. A similarity relationship exists between the space and time variables. This class contains as special cases three well-known diffusion processes and another one that very recently became of interest in the theory of superradiant emission.

I. INTRODUCTION

Recent studies by Narducci, Coulter, and Bowden,[1] and by Narducci and Bluemel[2] of superradiant emission processes have led to a very useful and elegant description of such processes by means of the single Fokker–Planck equation,[2]

$$[z(1+z)G]_{zz}-[(1+Nz)G]_z=G_t,\quad z>0,\ t>0,$$

$N=2(r+1)$, $r=$Dicke cooperation number, for the density function $G(z,t)$. The corresponding lowest order equation[2]

$$zG_{zz}+(1-Nz)G_z-NG=G_t,\quad z>0,\ t>0, \tag{1.1}$$

which is also of the Fokker–Planck type,

$$[zG]_{zz}-[(1+Nz)G]_z=G_t,\quad z>0,\ t>0,$$

plays an essential role.

As verified in Ref. 2, Eq. (1.1) has the particular positive solution

$$G_0(z,t)=b^{-1}(t)\exp(-\xi),\quad \xi=zb^{-1}(t), \tag{1.2}$$

in the domain $z>0$, $t>0$, with

$$b(t)=N^{-1}(\exp(Nt)-1),\quad N\neq 0.$$

This function $G_0(z,t)$ has two important properties, namely,

$$\int_0^\infty G_0(z,t)\,dz=1,$$

and

$$G_0(z,t)\downarrow 0 \text{ as } t\downarrow 0 \text{ for fixed } z\in(0,\infty).$$

It represents an example of a conservative solution of a special parabolic equation corresponding to a completely concentrated initial state or, loosely speaking, under a delta function initial condition. In the work of Refs. 1 and 2, this solution describes the lowest order approximation of the process of spontaneous emission from the state of complete inversion.

In general, a solution $u(z,t)$ of the one-dimensional autonomous parabolic equation

$$A(z)u_{zz}+B(z)u_z+C(z)u=u_t \tag{1.3}$$

in the domain $z>0$, $t>0$, is called *conservative* (or norm preserving) if $u(z,t)\in L^1[0,\infty)$ for every $t>0$ {Riemann integrable on $[0,\infty)$} and if in particular,

$$0\le\int_0^\infty u(z,t)\,dz\equiv\text{const}<\infty.$$

The function $G_0(z,t)$ given in (1.2) has another remarkable property. It can be written in the form

$$G_0(z,t)=f(\xi)\frac{\partial\xi}{\partial z},\quad f(\xi)=\exp(-\xi),\quad \xi=zb^{-1}(t),$$

i.e., there exists a similarity relationship between the original independent variables z and t, and

$$\int_0^\infty G_0(z,t)\,dz=\int_0^\infty f(\xi)\,d\xi.$$

Conservative solutions involving a more general similarity relationship between z and t exist for other parabolic equations. For example, the Fokker–Planck equation

$$[\alpha u\exp(-\beta z)]_{zz}-[-\tfrac{1}{2}\alpha\beta u\exp(-\beta z)]_z=u_t,\quad \alpha>0,\ \beta>0$$

(which reduces to the heat equation as $\beta\downarrow 0$), has in $z>0$, $t>0$, the particular positive conservative δ function initial condition solution

$$u(z,t)=b^{-1}(t)\exp(\tfrac{1}{2}\beta z_e-\xi^2),$$

with

$$\xi=2\beta^{-1}[\exp(\tfrac{1}{2}\beta z)-1]b^{-1}(t),\quad b(t)=(4\alpha t)^{1/2},\ f(\xi)=\exp(-\xi^2).$$

In this note we are not going to discuss the general situation. Rather we are going to concentrate our attention on a particular class of equations (1.3) which contains three well-known diffusion equations as special cases, one of which in turn contains Eq. (1.1) for a special choice of parameter values. For this class we shall establish the conservative δ function initial condition solution which is of the form

$$u(z,t)=f(\xi)b^{-1}(t),\quad \xi=zb^{-1}(t)>0 \text{ in } z>0,\ t>0.$$

This particular class of parabolic equations plays an important role in physical as well as biological diffusion processes.

II. GENERAL CONDITIONS

Although the objective of this paper is the discussion of a special class of parabolic equations (1.3), it is nevertheless useful to present briefly conditions on the coefficient functions $A(z)$, $B(z)$, and $C(z)$ of the parabolic equation

$$A(z)u_{zz}+B(z)u_z+C(z)u=u_t,\quad u=u(z,t),$$
$$A(z)>0,\quad z>0,\quad t>0, \tag{2.1}$$

under which solutions of the form

$$u(z,t)=f(\xi)b^{-1}(t) \tag{2.2}$$

with

$$\xi=zb^{-1}(t)>0 \quad \text{in } z>0, \quad t>0 \tag{2.3}$$

exist. If $f(\xi)\in L^1[0,\infty)$, then

$$\int_0^\infty u(z,t)\,dz=\int_0^\infty f(\xi)\,d\xi.$$

We assume that $A(z)$, $B(z)$, and $C(z)$ are continuous in $(0,\infty)$, and that $b(t)$ is a positive once continuously differentiable function in $(0,\infty)$. Equation (2.1) is a Fokker–Planck equation, i.e., transformable into

$$[A(z)u]_{zz}-[\tilde{B}(z)u]_z=u_t \tag{2.4}$$

if and only if

$$C(z)=B'(z)-A''(z).$$

If this is the case, then $\tilde{B}=2A'-B$. With Eq. (2.4) one associates the function $h(z)=A^{-1}(z)\,W^{-1}(z)$ (which is due to Hille[3]) with

$$W(z)=\exp[-\int_1^z \tilde{B}(s)A^{-1}(s)\,ds]. \tag{2.5}$$

It satisfies the ordinary first-order equation

$$A(z)h'+[B(z)-A'(z)]h=0, \tag{2.6}$$

and plays a fundamental role in the semigroup theoretical approach to the parabolic equation problem (Feller[4]).

Substituting (2.2) into (2.1), we obtain the differential identity

$$Rf''+Sf'+Tf=0, \tag{2.7}$$

with $R=A$, $S=Bb+zb'$, $T=Cb^2+bb'$. A prime signifies differentiation with respect to t and ξ for the functions $b(t)$ and $f(\xi)$, respectively. For the identity (2.7) to specify f as a function of ξ only, it is necessary and sufficient that the ratios SR^{-1} and TR^{-1} be functions of ξ only, i.e., that

$$(Bb+zb')A^{-1}=\alpha_1(\xi), \tag{2.8}$$

$$b(Cb+b')A^{-1}=\alpha_0(\xi). \tag{2.9}$$

Then (2.7) changes into a differential equation for $f(\xi)$,

$$f''+\alpha_1(\xi)f'+\alpha_0(\xi)f=0. \tag{2.10}$$

From (2.8) and (2.9), we obtain the identity

$$\xi\alpha_0(\xi)-\alpha_1(\xi)=\xi^{-1}z(zC-B)A^{-1}.$$

Since its left-hand side is a function of ξ only, its right-hand side must also be explicitly independent of z, i.e., the factor of ξ^{-1} must be a constant $k\in(-\infty,\infty)$ and, hence,

$$\xi\alpha_0(\xi)-\alpha_1(\xi)=k\xi^{-1}. \tag{2.11}$$

This leads to the condition

$$kA(z)=z^2C(z)-zB(z) \tag{2.12}$$

on the coefficients A, B, and C of Eq. (2.1) for solutions to be of the form (2.2) in which ξ is given by (2.3). Furthermore, the relation (2.12) makes one of the conditions (2.8) and (2.9) superfluous. Using (2.8) and setting there $z=b$, we obtain the first-order equation for the function $b(t)$,

$$bb'+bB(b)-\alpha_1(1)A(b)=0. \tag{2.13}$$

III. A SPECIAL CLASS OF PARABOLIC EQUATIONS

We consider now Eq. (2.1) with the coefficient functions

$$\begin{aligned} &A(z)=\alpha z^{\lambda+1}, \quad \alpha>0, \ \lambda\in(-\infty,\infty),\\ &B(z)=\beta_1 z^\lambda+\beta_2 z, \quad \beta_{1,2}\in(-\infty,\infty),\\ &C(z)=(\alpha k+\beta_1)z^{\lambda-1}+\beta_2, \quad k\in(-\infty,\infty), \end{aligned} \tag{3.1}$$

which satisfy the condition (2.12). The corresponding equation is of Fokker–Planck type if and only if the parameter k in the coefficient $C(z)$ satisfies the equation

$$\alpha k+\beta_1=\lambda[\beta_1-\alpha(1+\lambda)], \tag{3.2}$$

which is independent of the parameter β_2 occurring in $B(z)$ and $C(z)$. We restrict our attention to this Fokker–Planck case.

Using the Hille function $h(z)=A^{-1}(z)\,W^{-1}(z)$, with $W(z)$ given by (2.5), which takes here the special form

$$h(z)=z^{1+\lambda-\alpha^{-1}\beta_1}\exp\left(-\frac{\alpha^{-1}\beta_2}{1-\lambda}z^{1-\lambda}\right), \quad \lambda\neq 1, \tag{3.3}$$

and

$$h(z)=z^{2-\alpha^{-1}(\beta_1+\beta_2)}, \quad \lambda=1,$$

we can characterize the properties of the z boundaries $r_1=0$ and $r_2=+\infty$ (Feller,[4] p. 516):

(1) $\lambda<1$, r_1 is regular if $1+2\lambda<\alpha^{-1}\beta_1<2+\lambda$ for every β_2

r_1 is exit if $2+\lambda\leq\alpha^{-1}\beta_1$ for every β_2,

r_1 is entrance if $\alpha^{-1}\beta_1<2+\lambda$ for every β_2,

r_2 is natural;

(2) $\lambda>1$, r_1 is natural,

r_2 is regular if $2+\lambda<\alpha^{-1}\beta_1<1+2\lambda$ for every β_2,

r_2 is exit if $\alpha^{-1}\beta_1\leq 2+\lambda$ for every β_2,

r_2 is entrance if $2+\lambda<\alpha^{-1}\beta_1$ for every β_2;

(3) $\lambda=1$, r_1 and r_2 are natural.

Since we are interested in conservative solutions that satisfy a δ function initial condition, we may immediately disregard the case $\lambda=1$. For, if $\lambda=1$, i.e., if both boundaries are natural, the pure initial value problem for the Eq. (2.4) is unique (Feller,[4] p. 517). This means that there exists no solution $u(z,t)$ with $u(z,t)\to 0$ as $t\downarrow 0$ for $z\in(0,\infty)$ except the trivial identically vanishing one. Therefore, we consider now the case $\lambda\neq 1$. We differentiate Eq. (2.6) once to obtain

$$h''+A^{-1}Bh'+A^{-1}Ch=0, \quad C=B'-A''. \tag{3.4}$$

Furthermore, we look at Eq. (2.10) with coefficients given in (2.8) and (2.9). We see that it becomes formally identical with Eq. (3.4) if

$$\begin{aligned}\alpha_1(\xi)&=[B(z)b(t)+zb'(t)]A^{-1}(z)=A^{-1}(\xi)B(\xi)\\ &=\alpha^{-1}[\beta_1\xi^{-1}+\beta_2\xi^{-\lambda}],\end{aligned}$$

$$\alpha_0(\xi) = b(t)[C(z)b(t) + b'(t)]A^{-1}(z) = A^{-1}(\xi)C(\xi)$$
$$= \alpha^{-1}[(\alpha k + \beta_1)\xi^{-2} + \beta_2\xi^{-\lambda-1}].$$

These two functions satisfy the relation (2.11).

Let us observe at this point that the character of the boundaries $r_1 = 0$ and $r_2 = +\infty$ is completely independent of the parameter β_2, i.e., that the nature of the corresponding solutions is independent of β_2. Therefore, instead of β_2 in the expressions for $\alpha_1(\xi)$ and $\alpha_0(\xi)$, we use a new parameter κ which will be disposed of later. Then

$$\alpha_1(\xi) = \alpha^{-1}[\beta_1\xi^{-1} + \kappa\xi^{-\lambda}]$$

and, in particular,

$$\alpha_1(1) = \alpha^{-1}(\beta_1 + \kappa). \tag{3.5}$$

The solution $f(\xi)$ of (2.10) is now identical with the function h of (3.3) if β_2 is replaced there by κ, i.e.,

$$f(\xi) = \xi^{1+\lambda-\alpha^{-1}\beta_1} \exp\left(-\frac{\alpha^{-1}\kappa}{1-\lambda}\ \xi^{1-\lambda}\right),\ \lambda \neq 1.$$

(This solution can also be found in Kamke,[5] C. 2·215.)

Furthermore, observing (3.5), we obtain from (2.13) the equation

$$b' = \kappa b^{\lambda} - \beta_2 b,$$

which has the solution

$$b(t) = \begin{cases} [\kappa(1-\lambda)t]^{(1-\lambda)^{-1}}, & \beta_2 = 0, \\ \{\kappa\beta_2^{-1} - \kappa\beta_2^{-1}\exp[-(1-\lambda)\beta_2 t]\}^{(1-\lambda)^{-1}}, & \beta_2 \neq 0. \end{cases}$$

To have now $b(t)$ positive for $t > 0$ as required earlier, we set

$$\kappa = \alpha(1-\lambda), \quad \alpha > 0.$$

This then gives us the positive solution

$$u(z,t) = b^{-1}(t)\xi^{1+\lambda-\alpha^{-1}\beta_1}\exp(-\xi^{1-\lambda}), \quad \lambda \neq 1,\ z > 0,\ t > 0, \tag{3.6}$$

of Eq. (2.1) with coefficients (3.1) for the Fokker–Planck case with

$$b(t) = \begin{cases} [\alpha(1-\lambda)^2 t]^{(1-\lambda)^{-1}}, & \beta_2 = 0, \\ \{\alpha(1-\lambda)\beta_2^{-1} - \alpha(1-\lambda)\beta_2^{-1}\exp[-(1-\lambda)\beta_2 t]\}^{(1-\lambda)^{-1}}, \\ \beta_2 \neq 0. \end{cases}$$

The solution (3.6) is of the form (2.2) with $\xi = zb^{-1}(t)$. The function

$$f(\xi) = \xi^{1+\lambda-\alpha^{-1}\beta_1}\exp(-\xi^{1-\lambda}), \quad \lambda \neq 1,$$

appearing in (3.6) will be in $L^1(0,\infty)$, i.e., the solution (3.6) will be conservative, if and only if $(2 + \lambda - \alpha^{-1}\beta_1)(1-\lambda)^{-1} > 0$. This is easily verified. It is only necessary to introduce the new variable $x = \xi^{1-\lambda}$ and to observe that

$$\int_0^{\infty} f(\xi)\,d\xi = |1-\lambda|^{-1}\int_0^{\infty} x^{(1+2\lambda-\alpha^{-1}\beta_1)(1-\lambda)^{-1}}\exp(-x)\,dx$$
$$= |1-\lambda|^{-1}\Gamma\left(\frac{2+\lambda-\alpha^{-1}\beta_1}{1-\lambda}\right)$$

if the argument of the gamma function is positive. In other words, (3.6) is conservative if either $\lambda < 1$ and $\alpha^{-1}\beta_1 < 2 + \lambda$ or if $\lambda > 1$ and $\alpha^{-1}\beta_1 > 2 + \lambda$. Comparing this result with the properties of the boundaries $r_1 = 0$ and $r_2 = +\infty$, we see that in both cases the conservativeness interval coincides with the entrance interval of r_1 and r_2 respectively, independent of the parameter β_2.

In diffusion theory the function $A(z)$ in (2.4) is called the diffusion coefficient and the function $\tilde{B}(z)$ is called the drift coefficient. In the special case we are considering here, $A(z) = \alpha z^{\lambda+1}$, $\tilde{B}(z) = \alpha[2(1+\lambda) - \alpha^{-1}\beta_1]z^{\lambda} - \beta_2 z$. We see, therefore, that, for given $\lambda \neq 1$, the conservativeness property of the solution (3.6) is exclusively determined by the ratio of the diffusion parameter α and the drift parameter β_1.

Furthermore, the solution (3.6) has always the property that

$$u(z,t) \downarrow 0 \ \text{ as } \ t \downarrow 0 \text{ for } z \in (0,\infty). \tag{3.7}$$

This can be seen immediately by noting that $\xi^{1-\lambda} \uparrow \infty$ as $t \downarrow 0$ $(\lambda \neq 1, z > 0)$.

The solution (3.6) corresponds to a δ function initial condition applied at $x = 0$ if $\lambda < 1$ and at $x = \infty$ if $\lambda > 1$.

We finally see that the solution (3.6) is even *singular* if either $\lambda > 1$ or if $\lambda < 1$ and $\alpha^{-1}\beta_1 < 1 + \lambda$. This terminology is due to Doetsch[6] and means that $u(z,t)$ does not only have the property (3.7), but that also

$$u(z,t) \not\to 0 \ \text{ as } z \downarrow 0 \text{ for } t \in (0,\infty).$$

If $\lambda > 1$, the solution (3.6) is always singular, independent of the diffusion and drift parameters. However, if $\lambda < 1$, (3.6) will be singular only if the ratio of the drift and diffusion parameters is sufficiently small. This requires a negative drift parameter if $\lambda \leq -1$. For $\lambda < 1$, the singularity interval of (3.6) never coincides with the entrance interval of the boundary $r_1 = 0$ whose right-hand end point is $2 + \lambda$. It may or may not, however, cover part of the regularity interval of r_1, according as $\lambda < 0$ or $0 \leq \lambda < 1$.

Singular solutions are of interest in the *general* initial-boundary value problem[7] with perpendicular approach to the boundaries of the domain $z > 0$, $t > 0$, which excludes the approach to $(0,0)$. The existence of such singular solutions is rather disturbing within the framework of diffusion theory and its applications. Whereas the existence of δ function initial condition solutions renders the pure initial-value problem nonunique, the existence of singular solutions makes the general initial-boundary value problem nonunique.

IV. SPECIAL CASES

The results of Sec. III for the Eq. (2.1) with coefficients (3.1) and k satisfying the Fokker–Planck condition (3.2) cover the following well-known equations.

(1) *Feller equation*[8]: $\lambda=0$, $k=-\alpha^{-1}\beta_1$, $\kappa=\alpha<0$,

$$u(z,t)=b^{-1}(t)\xi^{1-\alpha^{-1}\beta_1}\exp(-\xi), \quad \xi=zb^{-1}(t),$$

$$b(t)=\begin{cases}\alpha t & \text{if } \beta_2=0,\\ \alpha\beta_2^{-1}(1-\exp[-\beta_2 t]) & \text{if } \beta_2\neq 0.\end{cases} \tag{4.1}$$

Its solution (4.1) is conservative if $\alpha^{-1}\beta_1<2$ and singular if $\alpha^{-1}\beta_1<1$.

Equation (1.1) of Ref. 2 is clearly a special Feller equation: $\alpha=\beta_1=1$, $\beta_2=-N$, $k=-1$, $\kappa=1$. Its solution is conservative but *not* singular.

(2) *Heat equation*: $\lambda=-1$, $\beta_1=\beta_2=0$, $k=0$, $\kappa=2\alpha>0$;

$$u(z,t)=b^{-1}(t)\exp(-\xi^2), \quad \xi=zb^{-1}(t), \tag{4.2}$$

$$b(t)=(4\alpha t)^{1/2}.$$

Its solution (4.2) is conservative but not singular.

(3) *Kepinski equation*[9]: $\lambda=0$, $\alpha=n^{-1}$, $\beta_1=n^{-1}(m+1)$,

$\beta_2=0$, $k=-(m+1)$, $\kappa=n^{-1}>0$,

$$n^{-1}zu_{zz}+n^{-1}(1+m)u_z=u_t,$$

or, in Fokker–Planck form,

$$[n^{-1}zu]_{zz}-[n^{-1}(1-m)u]_z=u_t,$$

$$u(z,t)=b^{-1}(t)\xi^{-m}\exp(-\xi), \quad \xi=zb^{-1}(t),$$

$$b(t)=n^{-1}t. \tag{4.3}$$

This equation is another special case of the general Feller equation. Its solution (4.3) is conservative for $m<1$ and singular for $m<0$.

[1]L. M. Narducci, C. A. Coulter, and C. M. Bowden, Phys. Rev. A **9**, 829 (1974).
[2]L. M. Narducci and V. Bluemel, Phys. Rev. A **11**, 1354 (1975).
[3]E. Hille, C.R. Acad. Sci. Paris **230**, 34 (1950).
[4]W. Feller, Ann. Math. **55**, 468 (1952).
[5]E. Kamke, *Differentialgleichungen, Lösungsmethoden und Lösungen* (Chelsea, New York, 1959), 3rd ed., Vol. 1.
[6]G. Doetsch, Math. Z. **22**, 293 (1925).
[7]G. Doetsch, *Handbuch der Laplace-Transformation* (Birkhäuser, Basel, 1956), Vol. 3.
[8]W. Feller, Ann. Math. **54**, 173 (1951).
[9]S. Kepinski, Math. Ann. **61**, 397 (1905).

Subgroups of the Poincaré group and their invariants*

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The continuous subgroups of the Poincaré group, classified into conjugacy classes in a previous article, are here classified into isomorphism classes. For each isomorphism class of Lie subalgebras all invariants are found, with a distinction made between Casimir operators (polynomials in the generators), rational invariants (rational functions of the generators), and general invariants (irrational and transcendental functions of the generators). All results are summarized in tables. The meaning of nonpolynomial invariants is briefly discussed and illustrated in examples.

1. INTRODUCTION

In a previous paper[1] (further to be referred to as I) a classification was given of all continuous subgroups of the Poincaré group (the inhomogeneous Lorentz group). Representatives were given for each conjugacy class of subgroups, where conjugacy was considered under the group of inner automorphisms, more specifically under the connected component of the Poincaré group (proper orthochronous Poincaré transformation).

In the present article we continue the investigation of the properties of the subgroups of the Poincaré group. First of all we present all isomorphisms between different subgroups, i.e., modify the tables of conjugacy classes, found in I, into a table of isomorphism classes. Secondly, for each subgroup we find all of its invariants, or to be more precise, find a basis for the algebra of invariants, such that all invariants can be written as functions of those found in this article. The term "invariant" in this article is to be understood as a generalization of the concept of a Casimir operator which is a polynomial in the generators and thus an element of the enveloping algebra of the corresponding Lie algebra, commuting with all the generators of the group.

We distinguish between three types of invariants. The first are Casimir operators, as defined above. The second can be called harmonics or rational invariants; they are also left invariant by transformations of the group; however, they do not lie in the enveloping algebra, but rather in the quotient field of the enveloping algebra (i.e., they are rational functions of the generators). Finally, general invariants will be more general functions of the generators. The significance of Casimir operators is clear—in group representation theory they can be used to label irreducible representations and to split reducible representations into irreducible ones. In physical applications the Casimir operators are usually associated with quantities characterizing a certain physical system, rather than a specific state of this system. It is our opinion that the more general invariants can be used and interpreted in a similar manner.

The present article is part of a series in which we study the subgroup structure of groups of importance in physics, analyze their properties, and consider applications of such a subgroup classification.[2–6] Much of the motivation for this study was presented earlier.[1–6]

Fields associated with enveloping algebras of Lie algebras, relevant to the discussion of harmonics that are not Casimir operators, were discussed e.g., by Gel'fand and Kirillov[7] and Chow.[8] A relevant discussion of an operator calculus involving nonpolynomial functions of operators is given, e.g., by Maslov.[9]

In Sec. 2 we discuss the general methods which we use to classify subalgebras of the Poincaré Lie algebra into isomorphism classes and also to calculate invariants of these algebras. Section 3 contains the main result, namely a list of all subalgebras of the Poincaré algebra with their invariants. The algebras are organized first by dimension and then for each given dimension they are divided into isomorphism classes characterized in each case by a certain standard algebra. Physical comments on the subgroups and their invariants are concentrated in Sec. 4.

2. GENERAL METHODS AND COMMENTS

Our starting point is Tables III and IV of I in which we list representatives for all conjugacy classes of continuous subgroups of the Poincaré group. Conjugacy was considered under the proper orthochronous Poincaré group. In this article we shall allow for a larger group of automorphisms, in that we also include parity and time reversal in the group.

We wish to organize all the subalgebras into isomorphism classes and also to find all invariants of the subalgebras. The invariants themselves provide a useful tool for identifying isomorphisms.

The method to be used for calculating invariants of Lie algebras consists of reducing the problem to that of solving a set of linear first order partial differential equations. The method goes back to the original work of Lie, has been discussed in detail and applied to all real Lie algebras of dimension $d \leq 5$ in a previous paper,[10] and has recently received considerable attention in the physical literature.[11–15] We shall just summarize a few points.

Consider a real Lie algebra L with a basis $\{X_1, \ldots, X_n\}$ satisfying the commutation relations

$$[X_i, X_k] = \sum_l C_{ik}^l X_l, \quad i,k,l = 1, \ldots, n. \tag{1}$$

Consider functions $f(x_1, \ldots, x_n)$ of n real variables and construct the differential operators

$$X_i = \sum_{l,k=1}^{n} C_{ik}^{l} x_l \frac{\partial}{\partial x_k} \tag{2}$$

acting on the considered space of functions. Obviously the operators X_i satisfy relations (1) and thus provide a representation of the Lie algebra. We must now find all independent functions $F(x_1, \ldots, x_n)$ satisfying

$$X_i F(x_1, \ldots, x_n) = 0, \quad i = 1, \ldots, n. \tag{3}$$

If a solution is a polynomial in x_i, then we obtain a Casimir operator by first symmetrizing the polynomial with respect to all x_i involved and then replacing x_i by the generator X_i {it is easy to check after symmetrization the requirement $X_i F(x_1, \ldots, x_n) = 0$ is isomorphic to the requirement $[X_i, F(X_1, \ldots, X_n)] = 0$}. If a solution is the ratio of two polynomials, then we symmetrize the denominator and numerator separately (the denominator must commute with the numerator) and then again replace all x_i by X_i and obtain rational invariants. General invariants are obtained from general (not necessarily polynomial or rational) solutions of of Eqs. (3) in an analogous manner.

Let us note that each of Eqs. (3) can be solved in a simple manner. Indeed, the partial differential equation

$$\sum_{k,l=1}^{n} C_{ik}^{l} x_l \frac{\partial}{\partial x_k} F = 0 \tag{4}$$

leads to the subsidiary equations

$$\frac{dx_1}{\sum_l C_{i1}^l x_l} = \frac{dx_2}{\sum_l C_{i2}^l x_l} = \cdots = \frac{dx_n}{\sum_l C_{in}^l x_l} \equiv \frac{ds}{s}. \tag{5}$$

Clearly Eqs. (5) can be replaced by a set of equivalent equations, putting

$$\frac{ds}{s} = \frac{d(\alpha_1 x_1 + \cdots + \alpha_n x_n)}{\sum_{l,b} \alpha_b C_{ib}^l x_l}, \tag{6}$$

where $\alpha_1, \ldots, \alpha_n$ are arbitrary constants. This allows us to choose n linearly independent combinations of $x_1, \ldots, x_n$ in a convenient manner, so as to reduce the matrix of coefficients $C_{ia}^l \equiv (C_i)_a^l$ to a standard form, in particular to the Jordan canonical form. This reduces Eqs. (5) to a manageable form and thus provides a general solution of Eq. (4).

It is well known that the space of all invariants of a semisimple Lie algebra is spanned by a set of independent polynomials (the Casimir operators). The same can be shown to be true for nilpotent algebras. An even (odd) dimensional Lie algebra must have an even (odd) number of functionally independent invariants.

As an example of the method consider a three-dimensional Lie algebra with the basis $\{Y_1, Y_2, Y_3\}$ satisfying

$$[Y_1, Y_2] = 0, \quad [Y_2, Y_3] = Y_1 + pY_2, \quad [Y_3, Y_1] = -pY_1 + Y_2, \quad p > 0 \tag{7}$$

(this algebra is isomorphic to $P_{5,4}$ of I). Following (2), we have

$$Y_1 = (py_1 - y_2)\frac{\partial}{\partial y_3}, \quad Y_2 = (y_1 + py_2)\frac{\partial}{\partial y_3}$$

TABLE I. One-dimensional subalgebras.

Notation	Generator	Range of parameters under $P_0^\uparrow$	Range of parameters under P
$P_{11,6}$	$\cos cL_3 + \sin cK_3$	$0 < c < \pi$, $c \neq \pi/2$	$0 < c < \pi/2$
$P_{12,10}$	L_3		
$P_{13,9}$	K_3		
$P_{14,9}$	$L_2 + K_1$		
$P_{15,8}$	$P_0 - P_3$		
$P_{15,9}$	P_3		
$P_{15,10}$	P_0		
$\tilde{P}_{12,23}$ and $\tilde{P}_{12,24}$	$L_3 + \epsilon(P_0 + P_3)$	$\epsilon = \pm 1$	$\epsilon = 1$
$\tilde{P}_{12,25}$	$L_3 + aP_0$	$a > 0$	
$\tilde{P}_{12,26}$	$L_3 + aP_3$	$a \neq 0$	$a > 0$
$\tilde{P}_{13,15}$	$K_3 + aP_1$	$a > 0$	$a > 0$
$\tilde{P}_{14,24}$	$L_2 + K_1 + P_0 + P_3$		
$\tilde{P}_{14,25}$ and $\tilde{P}_{14,26}$	$L_2 + K_1 + \epsilon P_2$	$\epsilon = \pm 1$	$\epsilon = 1$

$$Y_3 = -(py_1 - y_2)\frac{\partial}{\partial y_1} - (y_1 + py_2)\frac{\partial}{\partial y_2}. \tag{8}$$

Clearly $Y_i F(y_1 y_2 y_3) = 0$ $(i = 1, 2)$ implies that F does not depend on y_3. The equation $Y_3 F = 0$ provides us with the subsidiary equations

$$\frac{dy_1}{py_1 - y_2} = \frac{dy_2}{y_1 + py_2} \equiv \frac{ds}{s}. \tag{9}$$

We follow the procedure (6) and put

$$\frac{ds}{s} = \frac{d(\alpha_1 y_1 + \alpha_2 y_2)}{\alpha_1(py_1 - y_2) + \alpha_2(y_1 + py_2)}. \tag{10}$$

To simplify (10), we request that

$$\frac{ds}{s} = \frac{d(\alpha_1 y_1 + \alpha_2 y_2)}{\lambda(\alpha_1 y_1 + \alpha_2 y_2)}. \tag{11}$$

This leads to an eigenvalue problem for λ and two solutions for α_i, namely,

$$\lambda_1 = p - i, \quad \alpha_1 = 1, \quad \alpha_2 = -i, \tag{12a}$$

and

$$\lambda_2 = p + i, \quad \alpha_1 = 1, \quad \alpha_2 = i. \tag{12b}$$

Equation (9) is thus replaced by the equivalent equation

$$\frac{d(y_1 - iy_2)}{(p - i)(y_1 - iy_2)} = \frac{d(y_1 + iy_2)}{(p + i)(y_1 + iy_2)}. \tag{13}$$

The obvious solution can be transformed into the form

$$(y_1^2 + y_2^2)\left(\frac{y_1 + iy_2}{y_1 - iy_2}\right)^{ip} = c \tag{14}$$

so that the general invariant can be written as

$$(Y_1^2 + Y_2^2)\left(\frac{Y_1 + iY_2}{Y_1 - iY_2}\right)^{ip} = \text{inv}. \tag{15}$$

Notice that Y_1 and Y_2 commute and that in any representation we can choose a basis where Y_1 and Y_2 are diagonal. The operator (15) can thus be given a perfectly legitimate meaning and can be used to characterize irreducible representations of the considered Lie algebra and the corresponding group.

In order to find all isomorphisms between subalgebras of the Poincaré algebra, we proceed as follows. We first consider the algebras of dimension $1 \leq d \leq 5$.

TABLE II. Two-dimensional subalgebras.

Type	Notation	Generators	Range of parameters under P_0'	Range of parameters under P	Invariants
Abelian $2A_1$	$P_{9,6}$	L_3, K_3;			both generators
"	$P_{10,5}$	L_2+K_1, L_1-K_2;			"
"	$P_{12,7}$	L_3, P_0-P_3;			"
"	$P_{12,8}$	L_3, P_3;			"
"	$P_{12,9}$	L_3, P_0;			"
"	$P_{13,8}$	K_3, P_1;			"
"	$P_{14,7}$	L_2+K_1, P_0-P_3;			"
"	$P_{14,8}$	L_2+K_1, P_2;			"
"	$P_{15,5}$	P_0-P_3, P_1;			"
"	$P_{15,6}$	P_0, P_3;			"
"	$P_{15,7}$	P_1, P_2;			"
"	$\tilde{P}_{10,16}$	$L_2+K_1, L_1-K_2+P_2$;			"
"	$\tilde{P}_{12,19}$ and $\tilde{P}_{12,20}$	$L_3+\epsilon(P_0+P_3), P_0-P_3$;	$\epsilon=\pm 1$	$\epsilon=1$	"
"	$\tilde{P}_{12,21}$	L_3+aP_0, P_3;	$a>0$	$a>0$	"
"	$\tilde{P}_{12,22}$	L_3+aP_3, P_0;	$a\neq 0$	$a>0$	"
"	$\tilde{P}_{13,14}$	K_3+aP_2, P_1;	$a>0$	$a>0$	"
"	$\tilde{P}_{14,20}$	$L_2+K_1+P_0+P_3, P_0-P_3$;			"
"	$\tilde{P}_{14,21}$ and $\tilde{P}_{14,22}$	$L_2+K_1+\epsilon P_2, P_0-P_3$;	$\epsilon=\pm 1$	$\epsilon=1$	"
"	$\tilde{P}_{14,23}$	$L_2+K_1+P_0+P_3, P_2$;			
A_2	$P_{8,9}$	$K_3; L_2+K_1$			none
	$P_{11,5}$	$\cos cL_3+\sin cK_3; P_0-P_3$	$0<c<\pi$, $c\neq\pi/2$	$0<c<\pi/2$	"
	$\tilde{P}_{13,7}$	$K_3; P_0-P_3$			"
	$\tilde{P}_{8,17}$	$K_3+aP_2; L_2+K_1$	$a>0$	$a>0$	"
	$P_{13,13}$	$K_3+aP_2; P_0-P_3$	$a>0$	$a>0$	"

All one-dimensional algebras are isomorphic and we denote them by A_1 (we leave aside the question of the different groups corresponding to the algebras). Only two different two-dimensional real Lie algebras exist: A decomposable one $A_1 \otimes A_1 \equiv 2A_1$ and an indecomposable one A_2 (with basis elements satisfying $[a_1, a_2] = a_1$). Each of the two-dimensional subalgebras of the Poincaré algebra can at a glance be identified as $2A_1$ or A_2. All three-, four-, and five-dimensional real Lie algebras have been classified by Mubarakzyanov[16] and we make use of his classification, which we have slightly modified for our purposes. Thus, decomposable three dimensional algebras will be denoted $3A_1$ and A_1+A_2, indecomposable ones $A_{3,1}, \ldots, A_{3,9}$. Among these $A_{3,1}, \ldots, A_{3,4}$ and $A_{3,6}$, $A_{3,8}$ and $A_{3,9}$ are individual algebras, and $A^h_{3,5}$ and $A^p_{3,7}$ are actually infinite classes of nonisomorphic algebras, depending on a real parameter indicated by a superscript. Similarly four- and five-dimensional algebras can decompose into sums of lower-dimensional algebras. The indecomposable ones will be denoted $A_{4,1}, \ldots, A_{4,12}$ and $A_{5,1}, \ldots, A_{5,1}, \ldots, A_{5,40}$ respectively. Dependence of a class of algebras on certain real parameters will be indicated by superscripts. For further details and standard forms of the commutation relations we refer to a previous paper.[10]

Thus, to classify subalgebras of the Poincaré algebra with $1 \leq d \leq 5$, all we have to do is to find a basis which reduces each one to one of the known standard forms and this turns out to be a simple task.

To our knowledge, no complete classification of real algebras with $d \geq 6$ exists. However, only one eight-dimensional algebra occurs in our list. We have six seven-dimensional subalgebras, all of them mutually nonisomorphic. This can be seen immediately by comparing their largest Abelian ideals and the corresponding factor algebras. To find possible isomorphisms among the 11 different types of six-dimensional algebras, we consider the derived algebras. Three of the algebras are perfect, namely SL(2,C), E(3), and E(2,1) (these are clearly all nonisomorphic). The other subalgebras have lower-dimensional derived algebras. If any among these derived subalgebras are isomorphic, then the corresponding algebras are candidates for being isomorphic. If they are indeed isomorphic, then they must have the same number of invariants and these must be of the same type. Such cases are then checked individually, and in all cases occurring it is easy to prove that the corresponding algebras are isomorphic or nonisomorphic, as the case may be.

3. ISOMORPHISM CLASSES AND INVARIANTS

We use the usual physical basis for the algebra of the Poincaré group, i.e., the rotation generators L_i, the boosts K_i, and the translations P_μ ($i=1,2,3$, $\mu=0,1,2,3$). We write the commutation relations in the form

$$\begin{aligned} &[L_i, L_k] = \epsilon_{ikl} L_l, \quad && [L_i, K_k] = \epsilon_{ikl} K_l, \\ &[K_i, K_k] = -\epsilon_{ikl} L_l, \quad && [L_i, P_k] = \epsilon_{ikl} P_l, \\ &[K_i, P_k] = \delta_{ik} P_0, \quad && [K_i, P_0] = P_i, \\ &[P_\mu, P_\nu] = 0, \quad && [L_i, P_0] = 0. \end{aligned} \tag{16}$$

TABLE III. Three-dimensional subalgebras.

Type	Notation	Generators	Range of parameters under P_0	Range of parameters under P_0	Invariants
Abelian $3A_1$	$P_{10,4}$	$L_2+K_1, L_1-K_2, P_0-P_3$;			all generators
	$P_{12,5}$	L_3, P_0, P_3;			"
	$P_{13,6}$	K_3, P_1, P_2;			"
	$P_{14,4}$	L_2+K_1, P_0-P_3, P_2;			"
	$P_{15,2}$	P_0-P_3, P_1, P_2;			"
	$P_{15,3}$	P_1, P_2, P_3;			"
	$P_{15,4}$	P_0, P_1, P_2;			"
	$\widetilde{P}_{10,11}$	$L_2+K_1, L_1-K_2+P_2, P_0-P_3$;			"
	$\widetilde{P}_{14,13}$	$L_2+K_1-\frac{1}{2}(P_0+P_3), P_0-P_3, P_2$;			"
$A_2 \oplus A_1$	$P_{8,8}$	$(K_3; L_2+K_1) \oplus (P_2)$			P_2
	$P_{9,5}$	$(K_3; P_0-P_3) \oplus (L_3)$			L_3
	$P_{13,5}$	$(K_3; P_0-P_3) \oplus (P_2)$			P_2
	$\widetilde{P}_{13,11}$	$(K_3+aP_2; P_0-P_3) \oplus (P_1)$	$a>0$	$a>0$	P_1
$A_{3,1}$ (Weyl algebra)	$P_{14,5}$	$L_2+K_1, P_1; P_0-P_3$			P_0-P_3
	$P_{14,6}$	$L_2+K_1, P_2+bP_1; P_0-P_3$	$b\neq 0$	$b>0$	P_0-P_3
	$\widetilde{P}_{10,12}$ and $\widetilde{P}_{10,13}$	$L_2+K_1-\epsilon P_2, L_1-K_2+bP_2-\epsilon P_1; P_0-P_3$	$b>0,\ \epsilon=\pm 1$	$b>0,\ \epsilon=1$	P_0-P_3
	$\widetilde{P}_{10,14}$ and $\widetilde{P}_{10,15}$	$L_2+K_1-\epsilon P_2, L_1-K_2-\epsilon P_1; P_0-P_3$	$\epsilon=\pm 1$	$\epsilon=1$	P_0-P_3
	$\widetilde{P}_{14,14}$	$L_2+K_1-\frac{1}{2}(P_0+P_3), P_1; P_0-P_3$			P_0-P_3
	$\widetilde{P}_{14,15}$ and $\widetilde{P}_{14,16}$	$L_2+K_1-\epsilon P_2, P_1; P_0-P_3$	$\epsilon=\pm 1$	$\epsilon=1$	P_0-P_3
	$\widetilde{P}_{14,17}$	$L_2+K_1-\frac{1}{2}(P_0+P_3), P_2-bP_1; P_0-P_3$	$b\neq 0$	$b>1$	P_0-P_3
	$\widetilde{P}_{14,18}$ and $\widetilde{P}_{14,19}$	$L_2+K_1-\epsilon P_2, P_2-bP_1; P_0-P_3$	$b\neq 0,\ \epsilon=\pm 1$	$b>0,\ \epsilon=1$	P_0-P_3
$A_{3,2}$	$\widetilde{P}_{8,14}$	$K_3+aP_1; L_2+K_1, P_0-P_3$	$a>0$	$a>0$	$(P_0-P_3)\exp\left(-\frac{L_2+K_1}{a(P_0-P_3)}\right)$
	$\widetilde{P}_{8,16}$	$K_3-aP_2+bP_1; L_2+K_1, P_0-P_3$	$a>0,\ b\neq 0$	$a>0,\ b>0$	$(P_0-P_3)\exp\left(-\frac{L_2+K_1}{b(P_0-P_3)}\right)$
$A_{3,3}$ ($D \square T_2$)	$P_{7,5}$	$K_3; L_2+K_1, L_1-K_2$			$\frac{L_1-K_2}{L_2+K_1}$
	$P_{8,7}$	$K_3; L_2+K_1, P_0-P_3$			$\frac{P_0-P_3}{L_2+K_1}$
	$\widetilde{P}_{8,15}$	$K_3+aP_2; L_2+K_1, P_0-P_3$	$a>0$	$a>0$	$\frac{P_0-P_3}{L_2+K_1}$
$A_{3,4}$ (E(1,1))	$P_{11,4}$	$\cos cL_3+\sin cK_3; P_0, P_3$	$0<c<\pi, c\neq\pi/2$	$0<c<\pi/2$	$P_0^2-P_3^2$
	$P_{13,4}$	$K_3; P_0, P_3$			$P_0^2-P_3^2$
	$\widetilde{P}_{13,12}$	$K_3+aP_2; P_0, P_3$	$a>0$	$a>0$	$P_0^2-P_3^2$
$A_{3,6}$ (E(2))	$P_{6,4}$	$L_3; L_2+K_1, L_1-K_2$			$(L_2+K_1)^2+(L_1-K_2)^2$
	$P_{11,3}$	$\cos cL_3+\sin cK_3; P_1, P_2$	$0<c<\pi,\ c\neq\pi/2$	$0<c<\pi/2$	$P_1^2+P_2^2$
	$P_{12,6}$	$L_3; P_1, P_2$			$P_1^2+P_2^2$
	$\widetilde{P}_{6,9}$ and $\widetilde{P}_{6,10}$	$L_3+\epsilon(P_0-P_3); L_2+K_1, L_1-K_2$	$\epsilon=\pm 1$	$\epsilon=1$	$(L_2+K_1)^2+(L_1-K_2)^2$
	$\widetilde{P}_{12,15}$ and $\widetilde{P}_{12,16}$	$L_3-\epsilon(P_0+P_3); P_1, P_2$	$\epsilon=\pm 1$	$\epsilon=1$	$P_1^2+P_2^2$
	$\widetilde{P}_{12,17}$	$L_3+aP_0; P_1, P_2$	$a>0$	$a>0$	$P_1^2+P_2^2$
	$\widetilde{P}_{12,18}$	$L_3+aP_3; P_1, P_2$	$a\neq 0$	$a>0$	$P_1^2+P_2^2$
$A_{3,7}^p$ (S(3)) $p=\tan c>0$	$P_{5,4}$	$\cos cL_3+\sin cK_3; L_2+K_1,$ L_1-K_2	$0<c<\pi,$ $c\neq\pi/2$	$0<c<\pi/2$	$[(L_1-K_2)^2+(L_2+K_1)^2]$ $\times\left(\frac{(L_1-K_2)+i(L_2+K_1)}{L_1-K_2-i(L_2+K_1)}\right)^{i\tan c}$
$A_{3,8}$ SU(1,1)	$P_{4,4}$	$; L_3, K_1, K_2$			$L_3^2-K_1^2-K_2^2$
$A_{3,9}$ SU(2)	$P_{3,4}$	$; L_1, L_2, L_3$			$L_1^2+L_2^2+L_3^2$

The basis used in I was:

$$B_1=2L_3, \quad B_2=-2K_3, \quad B_3=-L_2-K_1,$$
$$B_4=L_1-K_2, \quad B_5=L_2-K_1, \quad B_6=L_1+K_2,$$
$$X_1=\tfrac{1}{2}(P_0-P_3), \quad X_2=P_2, \quad X_3=-P_1, \quad X_4=\tfrac{1}{2}(P_0+P_3). \tag{17}$$

Under parity Π and time reversal T we have

$$\Pi P_i=-P_i, \quad \Pi P_0=P_0, \quad \Pi K_i=-K_i, \quad \Pi L_i=L_i, \tag{18}$$
$$TP_i=-P_i, \quad TP_0=P_0, \quad TK_i=K_i \quad TL_i=-L_i. \tag{19}$$

We shall also have the opportunity to use a dilatation operator D, satisfying

TABLE IV. Four-dimensional subalgebras.

Type	Notation	Generators	Range of parameters under $P_0^\dagger$	Range of parameters under P	Invariants
$4A_1$	$P_{15,1}$	P_0, P_1, P_2, P_3;			P_0, P_1, P_2, P_3
$A_2 \oplus 2A_1$	$P_{13,2}$	$(K_3; P_0 - P_3) \oplus (P_1) \oplus (P_2)$			P_1, P_2
$A_{3,1} \oplus A_1$	$P_{10,3}$	$(L_1 - K_2, P_2; P_0 - P_3) \oplus (L_2 + K_1)$			$L_2 + K_1, P_0 - P_3$
	$P_{14,2}$	$(L_2 + K_1, P_1; P_0 - P_3) \oplus (P_2)$			$P_2, P_0 - P_3$
	$\tilde{P}_{10,9}$ and $\tilde{P}_{10,10}$	$(L_1 - K_2 - \epsilon P_1, P_2; P_0 - P_3) \oplus (L_2 + K_1 + \epsilon P_2)$	$\epsilon = \pm 1$	$\epsilon = 1$	$L_2 + K_1 + \epsilon P_2, P_0 - P_3$
	$\tilde{P}_{14,10}$	$(L_2 + K_1 - \frac{1}{2}(P_0 + P_3), P_1; P_0 - P_3) \oplus (P_2)$			$P_2, P_0 - P_3$
$A_{3,2} \oplus A_1$	$\tilde{P}_{8,11}$	$(2K_3 + aP_1; L_2 + K_1, P_0 - P_3) \oplus (P_2)$	$a > 0$	$a > 0$	$P_2, (P_0 - P_3)^a \exp\left[-2\frac{L_2 + K_1}{P_0 - P_3}\right]$
$A_{3,3} \oplus A_1$	$P_{8,4}$	$(K_3; L_2 + K_1, P_0 - P_3) \oplus (P_2)$			$P_2, \frac{L_2 + K_1}{P_0 - P_3}$
$A_{3,4} \oplus A_1$	$P_{9,4}$	$(K_3; P_0, P_3) \oplus (L_3)$			$L_3, P_0^2 - P_3^2$
	$P_{13,3}$	$(K_3; P_0, P_3) \oplus (P_1)$			$P_1, P_0^2 - P_3^2$
	$\tilde{P}_{13,10}$	$(K_3 + aP_2; P_0, P_3) \oplus (P_1)$	$a > 0$	$a > 0$	$P_1, P_0^2 - P_3^2$
$A_{3,6} \oplus A_1$	$P_{6,3}$	$(L_3; L_1 - K_2, L_2 + K_1) \oplus (P_0 - P_3)$			$P_0 - P_3, (L_1 - K_2)^2 + (L_2 + K_1)^2$
	$P_{9,3}$	$(L_3; P_1, P_2) \oplus (K_3)$			$K_3, P_1^2 + P_2^2$
	$P_{12,2}$	$(L_3; P_1, P_2) \oplus (P_0 - P_3)$			$P_0 - P_3, P_1^2 + P_2^2$
	$P_{12,3}$	$(L_3; P_1, P_2) \oplus (P_3)$			$P_3, P_1^2 + P_2^2$
	$P_{12,4}$	$(L_3; P_1, P_2) \oplus (P_0)$			$P_0, P_1^2 + P_2^2$
	$\tilde{P}_{12,11}$ and $\tilde{P}_{12,12}$	$(L_3 + \epsilon(P_0 + P_3); P_1, P_2) \oplus (P_0 - P_3)$	$\epsilon = \pm 1$	$\epsilon = 1$	$P_0 - P_3, P_1^2 + P_2^2$
	$\tilde{P}_{12,13}$	$(L_3 + aP_0; P_1, P_2) \oplus (P_3)$	$a > 0$	$a > 0$	$P_3, P_1^2 + P_2^2$
	$\tilde{P}_{12,14}$	$(L_3 + aP_3; P_1, P_2) \oplus (P_0)$	$a \neq 0$	$a > 0$	$P_0, P_1^2 + P_2^2$
$A_{3,8} \oplus A_1$	$P_{4,3}$	$(K_1, K_2, L_3) \oplus (P_3)$			$P_3, K_1^2 + K_2^2 - L_3^2$
$A_{3,9} \oplus A_1$	$P_{3,3}$	$(L_1, L_2, L_3) \oplus (P_0)$			$P_0, L_1^2 + L_2^2 + L_3^2$
$A_{4,1}$	$P_{14,3}$	$(L_2 + K_1, P_0 + P_3; P_0 - P_3, P_1)$			$P_0 - P_3, P_0^2 - P_1^2 - P_3^2$
	$\tilde{P}_{10,7}$	$L_2 + K_1 - \frac{1}{2}(P_0 + P_3), L_1 - K_2 + aP_1$; $P_0 - P_3, P_2$	$a \neq 0$	$a > 0$	$P_0 - P_3, P_2^2 + P_3^2 - P_0^2 + 2(P_0 - P_3) \times (L_2 + K_1 - aP_2)$
	$\tilde{P}_{10,8}$	$L_2 + K_1 - \frac{1}{2}(P_0 + P_3), L_1 - K_2$; $P_0 - P_3, P_2$			$P_0 - P_3, P_2^2 + P_3^2 - P_0^2 + 2(P_0 - P_3)(L_2 + K_1)$
	$\tilde{P}_{14,11}$ and $\tilde{P}_{14,12}$	$L_2 + K_1 - \epsilon P_2, P_0 + P_3; P_1, P_0 - P_3$	$\epsilon = \pm 1$	$\epsilon = 1$	$P_0 - P_3, P_0^2 - P_1^2 - P_3^2$
$A_{4,2}^h$, $h = 1$	$\tilde{P}_{7,7}$	$K_3 + aP_1; L_2 + K_1, L_1 - K_2, P_0 - P_3$	$a > 0$	$a > 0$	$\frac{L_1 - K_2}{P_0 - P_3}, (P_0 - P_3)^a \times \exp\left[-\frac{L_2 + K_1}{P_0 - P_3}\right]$
$A_{4,5}^{a,b}$, $a = b = 1$	$P_{7,4}$	$K_3; L_1 - K_2, L_2 + K_1, P_0 - P_3$			$\frac{L_1 - K_2}{P_0 - P_3}, \frac{L_2 + K_1}{P_0 - P_3}$
$A_{4,6}^{a,b}$, $a = b = \tan c$	$P_{5,3}$	$L_3 - \tan c K_3; L_1 - K_2, L_2 + K_1, P_0 - P_3$	$0 < c < \pi$, $c \neq \pi/2$	$0 < c < \pi/2$	$\frac{(P_0 - P_3)^2}{(L_1 - K_2)^2 + (L_2 + K_1)^2}$, $[(L_1 - K_2)^2 + (L_2 + K_1)^2] \times \left(\frac{(L_1 - K_2) - i(L_2 + K_1)}{(L_1 - K_2) + i(L_2 + K_1)}\right)^{i \tan c}$
$a = -\tan c$, $b = 0$	$P_{11,2}$	$L_3 - \tan c K_3; P_0 - P_3, P_1, P_2$	$0 < c < \pi$, $c \neq \pi/2$	$0 < c < \pi/2$	$P_1^2 + P_2^2$, $(P_0 - P_3)^2 \left[\frac{P_1 - iP_2}{P_1 + iP_2}\right]^{i \tan c}$
$A_{4,9}^h$, $h = 0$	$P_{8,5}$	$K_3, P_1; P_0 - P_3, L_2 + K_1$			none
	$P_{8,6}$	$K_3, P_1 + bP_2; P_0 - P_3, L_2 + K_1$	$b \neq 0$	$b > 0$	none
	$\tilde{P}_{8,12}$	$K_3 + aP_2, P_1; P_0 - P_3, L_2 + K_1$	$a > 0$	$a > 0$	none
	$\tilde{P}_{8,13}$	$K_3 + aP_2, P_1 + bP_2; P_0 - P_3, L_2 + K_1$	$a > 0$, $b \neq 0$	$a > 0$, $b > 0$	none
$A_{4,10}$	$\tilde{P}_{6,7}$ and $\tilde{P}_{6,8}$	$L_3; L_2 + K_1 - \epsilon P_2, L_1 - K_2 - \epsilon P_1$, $P_0 - P_3$	$\epsilon = \pm 1$	$\epsilon = 1$	$P_0 - P_3$, $4\epsilon L_3(P_0 - P_3) + (L_2 + K_1 - \epsilon P_2)^2 + (L_1 - K_2 - \epsilon P_1)^2$
$A_{4,12}$	$P_{2,4}$	$L_3, K_3; L_2 + K_1, L_1 - K_2$			none

$$[D,L_i]=[D,K_i]=0,\quad [D,P_\mu]=-P_\mu. \tag{20}$$

The invariants of the Poincaré group are, of course, well known. Within the enveloping algebras there are just two, determining the particle's mass and spin:

$$m^2=P_0^2-P_1^2-P_2^2-P_3^2, \tag{21}$$

$$W^2=W_\mu W^\mu, \tag{22}$$

where $W_\mu=\epsilon_{\mu\nu\lambda\delta}M_{\nu\lambda}P_\delta$ is the Pauli–Lubanski spin operator and $M_{0i}=K_i$, $M_{ik}=\epsilon_{ikl}L_l$.

Let us now proceed to describe the results summarized in Tables I–VII. In all tables the notation $P_{j,k}$ refers to one of the splitting subalgebras of Table III of I and $\hat{P}_{j,k}$ refers to one of the non-splitting subalgebras of Table IV of I. When listing generators of a subalgebra, we use a semicolon to indicate that all operators to the right of the semicolon belong to the derived algebra. All parameters denoted by a can be collapsed by dilatations into $a=1$ ($a=-1$) if they are positive

TABLE V. Five-dimensional subalgebras.

Type	Notation	Generators	Range of parameters under P_0'	under P_0	Invariants
$A_{3,4}\oplus 2A_1$	$P_{13,1}$	$(K_3;P_0,P_3)\oplus(P_1)\oplus(P_2)$			$P_0^2-P_3^2,P_1,P_2$
$A_{3,6}\oplus 2A_1$	$P_{12,1}$	$(L_3;P_1,P_2)\oplus(P_0)\oplus(P_3)$			$P_1^2+P_2^2,P_0,P_3$
$A_{3,6}\oplus A_2$	$P_{9,2}$	$(L_3;P_1,P_2)\oplus(K_3;P_0-P_3)$			$P_1^2+P_2^2$
$A_{4,1}\oplus A_1$	$P_{14,1}$	$(L_2+K_1,P_0-P_3;P_0+P_3,P_1)\oplus(P_2)$			$P_0^2-P_1^2-P_3^2;P_0-P_3,P_2$
$A_{4,9}^h\oplus A_1$ $h=0$	$P_{8,2}$	$(K_3,P_1;L_2+K_1,P_0-P_3)\oplus(P_2)$			P_2
$A_{5,4}$	$P_{10,2}$	$(L_2+K_1,L_1-K_2,P_1,P_2;P_0-P_3)$			P_0-P_3
$A_{5,5}$	$\tilde{P}_{10,6}$	$L_3+K_1-\frac{1}{2}(P_0+P_3),L_1-K_2,P_1;P_0-P_3,P_2$			P_0-P_3
$A_{5,13}^{apq}$ $a=-1$	$P_{11,1}$	$L_3+\cot cK_3;P_0,P_1,P_2,P_3$	$0<c<\pi$ $c\neq\pi/2$	$0<c<\pi/2$	$m^2,P_0^2-P_3^2,$
$p=0$ $q=\cot c$					$(P_0-P_3)^{2\cot c}\left(\frac{P_1-iP_2}{P_1+iP_2}\right)^i$
$A_{5,19}^{ab}$ $a=b=1$	$P_{7,3}$	$K_3,P_2;L_2+K_1,L_1-K_2,P_0-P_3$			$\frac{L_2+K_1}{P_0-P_3}$
$A_{5,20}^h$ $h=1$	$\tilde{P}_{7,6}$	$K_3+aP_1,P_2;L_2+K_1,L_1-K_2,P_0-P_3$	$a>0$	$a>0$	$(P_0-P_3)^{-a}\exp\left(\frac{L_2+K_1}{P_0-P_3}\right)$
$A_{5,30}^h$ $h=0$	$P_{8,3}$	$K_3;L_2+K_1,P_0,P_1,P_3$			$P_0^2-P_1^2-P_3^2$
	$\tilde{P}_{8,10}$	$K_3+aP_2;L_2+K_1,P_0,P_1,P_3$	$a>0$	$a>0$	$P_0^2-P_1^2-P_3^2$
$A_{5,35}^{ab}$ $a=0,\ b=1$	$P_{2,3}$	$L_3,K_3;L_2+K_1,L_1-K_2,P_0-P_3$			$\frac{(P_0-P_3)^2}{(L_2+K_1)^2+(L_1-K_2)^2}$

TABLE VI. Six-dimensional subalgebras.

dimL'	Notation	Generators	Range of parameters under P_0'	under P_0	Invariants
6	$P_{1,2}$	$;L_1,L_2,L_3,K_1,K_2,K_3$			$\mathbf{L}^2-\mathbf{K}^2,\mathbf{L}\cdot\mathbf{K}$
6	$P_{3,2}$	$;L_1,L_2,L_3,P_1,P_2,P_3$			$\mathbf{L}\cdot\mathbf{P},\mathbf{P}^2$
6	$P_{4,2}$	$;K_1,K_2,L_3,P_1,P_2,P_0$			$L_3P_0+K_2P_1-K_1P_2,$ $P_0^2-P_1^2-P_2^2$
5	$P_{5,2}$	$\cos cL_3+\sin cK_3;L_2+K_1,L_1-K_2,P_0-P_3,P_1,P_2$	$0<c<\pi$ $c\neq\pi/2$	$0<c<\pi/2$	none
5	$P_{6,2}$	$L_3;L_2+K_1,L_1-K_2,P_0-P_3,P_1,P_2$			$P_0-P_3;(P_0-P_3)L_3-P_2(L_2+K_1)-P_1(L_1-K_2)$
5	$\tilde{P}_{6,5}$ and $\tilde{P}_{6,6}$	$4L_3+\epsilon(P_0+P_3);L_2+K_1,L_1-K_2,P_0-P_3,P_1,P_2$	$\epsilon=\pm1$	$\epsilon=1$	$P_0-P_3,m^2+4\epsilon(-\mathbf{P}\cdot\mathbf{L}+P_0L_3-P_2K_1+P_1K_2)$
4	$P_{8,1}$	$(K_3;L_2+K_1,P_0,P_1,P_3)\oplus(P_2)$			m^2,P_2
4	$P_{9,1}$	$(L_3;P_1,P_2)\oplus(K_3,P_0,P_3)$			$P_1^2+P_2^2,P_0^2-P_3^2$
3	$P_{7,2}$	$K_3,P_1,P_2;L_2+K_1,L_1-K_2,P_0-P_3$			none
3	$P_{10,1}$	$L_2+K_1,L_1-K_2,P_0+P_3;P_1,P_2,P_0-P_3$			m^2,P_0-P_3

TABLE VII. Subalgebras of the Poincaré algebra of dimension d with $7 \le d \le 10$.

dim$L$	dimL'	Notation	Generators	Invariants
7	6	$P_{3,1}$	$(L_1, L_2, L_3, P_1, P_2, P_3) \oplus (P_0)$	$\mathbf{P}^2, \mathbf{LP}, P_0$
	6	$P_{4,1}$	$(K_1, K_2, L_3, P_1, P_2, P_0) \oplus (P_3)$	$P_0^2 - P_1^2 - P_2^2, L_3P_0 + K_2P_1 - K_1P_2, P_3$
	6	$P_{5,1}$	$\cos cL_3 + \sin cK_3; L_2 + K_1, L_1 - K_2, P_0, P_1, P_2, P_3$ $0 < c < \pi$, $c \neq \pi/2$ in $P_0^\uparrow$, $0 < c < \pi/2$ in P	m^2
	6	$P_{7,1}$	$K_3; L_2 + K_1, L_1 - K_2, P_0, P_1, P_2, P_3$	m^2
	5	$P_{2,2}$	$L_3, K_3; L_2 + K_1, L_1 - K_2, P_0 - P_3, P_1, P_2$	$L_3 - \frac{P_2}{P_0 - P_3}(L_2 + K_1) - \frac{P_1}{P_0 - P_3}(L_1 - K_2)$
	5	$P_{6,1}$	$L_3, P_0 + P_3; L_2 + K_1, L_1 - K_2, P_0 - P_3, P_1, P_2$	$m^2, P_0 - P_3,$ $-\mathbf{P} \cdot \mathbf{L} - K_1P_2 + K_2P_1 + L_3P_0$
8	6	$P_{2,1}$	$L_3, K_3; L_2 + K_1, L_1 - K_2, P_0, P_1, P_2, P_3$	$m^2, L_3 - \frac{P_2}{P_0 - P_3}(L_2 + K_1) - \frac{P_1}{P_0 - P_3}(L_1 - K_2)$
9			none	
10	10	$P_{1,1}$	$L_1, L_2, L_3, K_1, K_2, K_3, P_0, P_1, P_2, P_3$	m^2, W^2

(negative), without changing the ranges of the other parameters (in all tables).

All one-dimensional subalgebras of the Poincaré algebras are summarized in Table I. The connected part of the Poincaré group is denoted by $P_0^\uparrow$ (the proper orthochronous Poincaré group); the extended group, including Π, T, and ΠT is denoted by P. Some of the algebras in Table I will be mutually conjugated under the conformal group (e.g., $L_2 + K_1$ and P_3); however, we shall not go into this here.

All two-dimensional subalgebras are summarized in Table II. The generators of A_2 are written as $X; Y$ with $[X, Y] = -Y$.

All three-dimensional subalgebras are summarized in Table III. The symbols $A_{3,k}$ $(k = 1, \ldots, 9)$ of column 1 correspond to the classification of algebras referred to earlier.[10,16] Thus, $A_{3,1}$ is the Weyl algebra (isomorphic to the algebra generated by a linear momentum p_x, a coordinate x and a constant), $A_{3,3}$ is the semidirect sum of a dilatation and two translations, $A_{3,4}$ is the algebra of the pseudo-Euclidean group E(1,1), $A_{3,6}$ the algebra of the Euclidean group E(2). Further, $A_{3,7}^p$ generates the "screw group" S(3) (see I) and $A_{3,8}$ and $A_{3,9}$ are the simple algebras of SU(1,1) and SU(2).

The four-dimensional subalgebras are summarized in Table IV. According to the classification we use[10] twelve type of indecomposable four-dimensional real Lie algebras $A_{4,1}, \ldots, A_{4,12}$ exist, some of them depending on one or two parameters. We shall not give their commutation relations here, since they can be read off from column 3 and the relations (16).

The five dimensional Lie subalgebras are summarized in Table V. We again make use of an existing classification, originally due to Mukarakzyanov,[16] discussed in our earlier article.[10]

Table VI presents all six-dimensional subalgebras. To our knowledge, no complete classification of real six-dimensional Lie algebras exists. All such nilpotent algebras were classified by Morozov[17] and some of the solvable ones have been listed.[16] We do not, however, make use of this partial classification. In the first column of the table we give the dimension of the derived algebra. Algebras $P_{1,2}$, $P_{3,2}$, and $P_{4,2}$ are all perfect. They are respectively the algebras of the Lorentz group O(3,1), the Euclidean group E(3), and the pseudo-Euclidean group E(2,1). Clearly none of these are mutually isomorphic. The algebras $P_{5,2}$ for $0 < c < \pi/2$ are all different, since the three-dimensional factor algebras $\{\cos cL_3 + \sin cK_3, L_2 + K_1, L_1 - K_2\}$ for different values of c are never mutually isomorphic. Algebras $\tilde{P}_{6,5}$ and $\tilde{P}_{6,6}$ are isomorphic and conjugate to each other under ΠT reflection. It is easy to verify that $\tilde{P}_{6,5}$ (or $\tilde{P}_{6,6}$) and $P_{6,2}$ are not isomorphic. The two subalgebras with dim$L' = 4$, $P_{8,1}$ and $P_{9,1}$ are both separable and are clearly not isomorphic. For dim$L' = 3$ we have $P_{7,2}$ and $P_{10,1}$. These are not isomorphic, since $P_{10,1}$ has two invariants while $P_{7,2}$ has none.

All subalgebras of dimension 7, . . . ,10 are summarized in Table VII. Notice that $P_{3,1}$ is the direct sum of the algebra of E(3) with time translations and that $P_{4,1}$ is the direct sum of the algebra of E(2,1) with the complementary space translations.

4. CONCLUSIONS

Many of the subgroups and their invariants discussed above already have most interesting applications in physics. Thus the eight-dimensional algebra $P_{2,1}$ figures prominently in calculations performed in the "infinite momentum frame,"[18,19] in Dirac's "front form" of dynamics[20] and in research on "Galileian subdynamics."[21,22] Notice that the invariants of this group are the

mass squared m^2 and a generalization of the helicity operator

$$\frac{W_0 - W_3}{P_0 - P_3} = L_3 - \frac{P_2}{P_0 - P_3}(L_2 + K_1) - \frac{P_1}{P_0 - P_3}(L_1 - K_2) \quad (23)$$

that has been called "lightlike helicity" (or "light plane helicity").[23,24] For mass zero particles with discrete spin (photons, neutrinos, etc.) the operators $L_2 + K_1$ and $L_1 - K_2$ are represented by zero; hence (23) reduces to L_3.

The seven-dimensional Lie algebra $P_{2,2}$ plays an important role in studies of the dynamical properties of currents on lightlike (rather than spacelike) planes and of the relation between current and constituent quarks.[23–28]

The six-dimensional subgroups $P_{9,1}$ and $P_{10,1}$ have been used in a study of charged systems in a constant and uniform electromagnetic field.[29] It should be mentioned here that independent classifications of the subgroups of the Poincaré group have been provided by other authors.[30,31]

We would like to stress that the invariants of the Lie algebras found in this article should play an important role in any application of the corresponding algebras. In all cases where nonpolynomial invariants arise, these involve mutually commuting operators (e.g., the ratio of two mutually commuting polynomials). Thus, we can consider bases for irreducible representations, in which the corresponding operators are all simultaneously diagonal. In particular, representations can be so realized that the linear operators (polynomials in the generators) figuring in the general invariants are represented by operators of multiplication by a function, rather than by differential operators. Essentially arbitrary functions of these generators, occurring as invariants, can thus be given a mathematical and physical meaning.

To illustrate this point, let us consider as an example[32] the algebras $P_{5,4}$, $P_{6,4}$, and $P_{1,5}$ which can all be written as

$$\{\mathrm{cosc}L_3 + \mathrm{sinc}K_3; L_2 + K_1, L_1 - K_2\} \quad (24)$$

with $0 < c < \pi/2$, $c = 0$ or $c = \pi/2$, respectively. Following the method of induced representations,[33] for the group G generated by (24) we start out with the group H of translations of a plane (a horosphere) generated by $L_2 + K_1$ and $L_1 - K_2$. Next we look for orbits of the group G in $\mathring{H}$, where $\mathring{H}$ is the dual of H, i.e., the space of characters of H. In the case $c = 0$ [the Euclidean group E(2)] these orbits are circles, characterized by a radius δ where δ^2 is the eigenvalue of the Casimir operator $(L_2 + K_1)^2 + (L_1 - K_2)^2$. For $c = \pi/2$ (the group $D \square T_2$ of dilatations and translations of a Euclidean plane) these orbits are straight lines intersecting at the origin, characterized by an angle ϕ, where $\arctan\phi$ is the eigenvalue of the rational invariant $(L_1 - K_2)/(L_2 + K_1)$. Finally, for $0 < c < \pi/2$ [the group S(3)] the orbits are spirals, characterized say, by the distance d between the point $x = 1$, $y = 0$ and the closest to the right intersection (of each spiral with the x axis). This distance can be directly related to the eigenvalue of the invariant operator

$$[(L_1 - K_2)^2 + (L_2 + K_1)^2]\left\{\frac{(L_1 - K_2) + i(L_2 + K_1)}{(L_1 - K_2) - i(L_2 + K_1)}\right\}^{t\tan c}$$

The applications of general invariants of Lie algebras in representation theory and in physics will be further pursued elsewhere. In particular, we are interested in the representation theory of all subgroups of the Poincaré group, in harmonic analysis on these groups, on the special function aspects of these groups and in applications to the theory of invariant equations.

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[1] J. Patera, P. Winternitz and H. Zassenhaus, J. Math. Phys. **16**, 1597 (1975).
[2] J. Patera, P. Winternitz and H. Zassenhaus, J. Math. Phys. **16**, 1615 (1975).
[3] J. Patera, P. Winternitz and H. Zassenhaus, J. Math. Phys. **15**, 1378 (1974).
[4] J. Patera, P. Winternitz and H. Zassenhaus, J. Math. Phys. **15**, 1932 (1974).
[5] J. Patera, P. Winternitz and H. Zassenhaus, J. Math. Phys. **17**, 717 (1976).
[6] J. Patera, R.T. Sharp, P. Winternitz, and H. Zassenhaus, Can. J. Phys. (to be published).
[7] I.M. Gel'fand and A.A. Kirillov, Dokl ANSSR **167**, 503 (1966) [Sov. Math. **7**, 407 (1966)].
[8] Y. Chow, J. Math. Phys. **10**, 975 (1969).
[9] V.P. Maslov, *Operatornye metody* [Operator Methods] (Nauka, Moscow, 1973).
[10] J. Patera, R.T. Sharp, P. Winternitz, and H. Zassenhaus, J. Math. Phys. **17**, 986 (1976).
[11] E.G. Beltrametti and A. Blasi, Phys. Lett. **20**, 62 (1966).
[12] M. Pauri and G.M. Prosperi, Nuovo Cimento **43**, 533 (1966).
[13] M.E. Angelopoulos, C.R. Acad. Sci. Paris **264**, 585 (1967).
[14] R. Mirman, J. Math. Phys. **9**, 47 (1968).
[15] L. Abellanas and L. Martinez Alonso, J. Math. Phys. **16**, 1580 (1975).
[16] G.M. Mubarakzyanov, Izv. Vysshikh Uchebn. Zavedenii Mat.: No. 1 (32), 114; No. 3 (34), 99; No. 4 (35), 104 (1963).
[17] V.V. Morozov, Izv. Vysshikh Uchebn. Zavedenii Mat. No. 4 (5), 161 (1958).
[18] J. Kogut and L Susskind, Phys. Rep. **8**, 75 (1973).
[19] H. Bacry and N.P. Chang, Ann. Phys. (N.Y.) **47**, 407 (1968).
[20] P.A.M. Dirac, Rev. Mod. Phys. **21**, 392 (1949).
[21] P.A.M. Dirac, Proc. Roy. Soc. Lond. A **322**, 435 (1971); A **328**, 1 (1972).
[22] L.C. Biedenharn and H. Van Dam, Phys. Rev. D **9**, 471 (1974).
[23] S.P. de Alwis and J. Stern, Nucl. Phys. B **77**, 509 (1974).
[24] H. Leutwyler and J. Stern, Nucl. Phys. B **20**, 77 (1970).
[25] H. Leutwyler, Acta Physica Austriaca, Suppl. V, 320 (1968).
[26] J. Jersak and J. Stern, Nucl. Phys. B **7**, 413 (1968); Nuovo Cimento **59**, 315 (1969).
[27] H.J. Melosh, Phys. Rev. D **9**, 1095 (1974).
[28] S.P. de Alwis, Nucl. Phys. B **55**, 427 (1973).
[29] H. Bacry, Ph. Combe, and J.L. Richard, Nuovo Cimento A **67**, 267 (1970).

[30]W. Lassner, "Die Zusammenhängenden Untergruppen der Poincarégruppe", preprint, Leipzig, 1970.
[31]H. Bacry, Ph. Combe, and P. Sorba, Rep. Math. Phys. **5**, 145, 361 (1974).
[32]We are indebted to W. Miller, Jr. and M. Perroud for discussion and private communications on these points. All details and a discussion of the representation theory of all continuous subgroups of SL(2, *C*) will be contained in their forthcoming paper.
[33]G. W. Mackey, *Induced Representations of Groups in Quantum Mechanics* (Benjamin, New York, 1968).

Invariants of real low dimension Lie algebras*

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All invariant functions of the group generators (generalized Casimir operators) are found for all real algebras of dimension up to five and for all real nilpotent algebras of dimension six.

I. INTRODUCTION

An important problem arising in the representation theory of a Lie group or Lie algebra, and especially in physical applications, is the determination of the invariant functions of its generators, i.e., of functions of the generators, commuting with all generators.

From the mathematical point of view their importance is due to the following circumstances. They can be used to label irreducible representations of a given Lie group or Lie algebra and to split reducible representations into irreducible ones. Further, basis functions for irreducible representations of a Lie group can be constructed so as to correspond to the reduction of the group to a given chain of subgroups. The basis functions in such a case will be the common eigenfunctions of the invariant operators of all the groups in the chain. Invariant operators also play a crucial role in special function theory. Indeed the entire theory of special functions can be based on group representation theory[1-3] and different special functions occur as the eigenfunctions of different sets of invariant operators.

In physics, invariant operators of the symmetry group of a physical system and of its subgroups provide quantum numbers. Indeed, the eigenvalues of the invariant operators of the entire symmetry group will be the quantum numbers, characterizing the system as such (e.g., the particle mass and spin in the case of the Poincaré group). The invariant operators of subgroups will then characterize states of the system (its energy, linear or angular momentum, etc.).[4]

In other applications, invariant operators of dynamical groups provide mass formulas,[5,6] energy spectra,[7,8] and in general characterize specific properties of physical systems.

Another application is related to possible symmetry breakings in nature. Thus, in an idealized situation a physical quantity may be characterized by the invariants of some group. When further interactions, breaking the idealized symmetry are considered, the same quantity may also depend on the invariants of a subgroup or subgroups.

For further discussion of the applications of invariant operators we refer to recent literature on the subject.[9-14] Let us stress here that in this context the concept of an invariant need not mean a Casimir operator. Indeed, the problem of finding invariants will be reduced to that of solving a certain set of linear first order partial differential equations. These may have polynomial solutions, giving rise to Casimir operators (lying in the enveloping algebra of the corresponding Lie algebra). They may also have rational solutions, giving rise to rational invariants (ratios of two polynomials, both contained in the enveloping algebra), lying in the quotient field of the enveloping algebra. Finally, the equations may have more general solutions, including transcendental functions of various types, leading to general invariants. Moreover, for some Lie algebras the equations have no solution and the corresponding group has no invariant.

The invariants of semisimple groups were determined long ago[15]; their number is l, the rank of the group, and they may be chosen to be homogeneous symmetric polynomials in the generators.

Invariants have been determined only for a small number of nonsemisimple groups. For such groups as the Poincaré group,[16] the Euclidean group $E(3)$, or the Galilei group,[17] they are well known. Roman, Aghassi, and Huddleston[12] have given the invariants for a number of groups containing the Poincaré group; Abellanas and Alonso[13] have corrected some of their results and have determined the invariants for similar groups related to the Galilei group. Recently, all subgroups of the Poincaré and similitude groups of four-dimensional[18,19] and three-dimensional[20] Minkowski space have been found (the similitude group is the Poincaré group extended by dilations) and also all the subgroups of the $O(4, 1)$ de Sitter group.[21] Their invariants have been determined and the physical meaning of these invariants has been discussed.[14,20,21]

In this paper we give the invariants of all real Lie algebras of dimension less than or equal to five, and of all real nilpotent algebras of dimension six. A complete list of algebras of dimension up to five is given by Mubarakzyanov[22]; nilpotent algebras of dimension six are listed by Morozov.[23]

Section II describes the method used to find the invariants; although well known, it has never been applied systematically to low-dimension Lie algebras. In Sec. III we give the invariants of all algebras of dimension up to four; in Sec. IV algebras of dimension five are treated; Sec. VI gives invariants of all nilpotent algebras of dimension six. Section VII contains a discussion of the results and the future outlook.

II. METHOD FOR CALCULATING INVARIANTS

From now on we speak of real algebras rather than groups; the elements of the algebra are just the group generators X_i and the invariants we seek are those functions $F(X)$ which commute with all X's:

$$[X_i, F(X)] = 0, \quad i = 1, \ldots, r. \tag{1}$$

The commutation rules of the X's are known:

$$[X_i, X_j] = \sum_k X_k C_{ij}^k. \tag{2}$$

Many authors[9-11,13,14] have discussed the device, which we adopt, of replacing the X's by c-number differential operators

$$X_i \to \chi_i = \sum_{jk} x_k C_{ij}^k \partial_{x_j}, \tag{3}$$

which have the same commutation rules and act on a space of continuously differentiable functions of r real variables. The commutation relations (1) are replaced by the set of partial differential equations

$$\chi_i F(x) = 0 \tag{4}$$

which, one hopes, can be solved by standard methods. Then the solutions of (1) are obtained from those of (4) by the replacements $x_i \to X_i$ provided that the factors X_i in $F(X)$ can be ordered so that (4) implies (1).

The solutions of (4) encountered in this paper are all of the form

$$F(x) = \exp\left(\frac{u_{n+1}}{u_n}\right) \prod_{i=1}^{n} u_i^{a_i}, \tag{5}$$

where the u_i are homogeneous polynomials, relatively prime except possibly for u_{n+1} which may however be considered relatively prime to u_n; the a_i are (possibly complex) constants. Then (4) implies that

$$\frac{\chi_i u_{n+1}}{u_n} - \frac{u_{n+1}\chi_i u_n}{u_n^2} + \sum_{j=1}^{n} \frac{a_j \chi_i u_j}{u_j} = 0. \tag{6}$$

Now $\chi_i u_j$, for $1 \leq j \leq n$ is a polynomial of the same degree as u_j, which according to (6), contains u_j as a factor. Hence it is a constant multiple of u_j:

$$\chi_i u_j = \alpha_{ij} u_j, \quad 1 \leq j \leq n. \tag{7}$$

It then follows from (6) that u_n, u_{n+1} have the same degree and that

$$\chi_i u_{n+1} = \alpha_{in} u_{n+1} - \left(\sum_{j=1}^{n} \alpha_{ij} a_j\right) u_n. \tag{8}$$

Now we assert that to get an $F(X)$ which satisfies (1), it is only necessary to replace each polynomial $u_i(x)$ in $F(x)$, Eq. (5), by the corresponding polynomial $U_i(X)$, where each term in $U_i(X)$ is completely symmetrized as to order:

$$x_1 x_2 \cdots x_m \to (m!)^{-1} \sum_P X_{i_1} X_{i_2} \cdots X_{i_m}. \tag{9}$$

The sum is over all permutations $i_1 i_2 \cdots i_m$ of the integers $1, 2, \cdots, m$; the X_i need not be distinct.

Because commutation with X_j does not spoil the symmetrization, it follows that

$$\chi_i u = v \Rightarrow [X_i, U] = V, \tag{10}$$

where the arrow means that the equation on the left implies the one on the right. Here u, v are polynomials in the x's and U, V the corresponding symmetrized polynomials in the X's.

We make the reasonable *Ansatz* that if $[X_i, W]$ commutes with W, then for any complex number a,

$$[X_i, W^a] = aW^{a-1}[X_i, W] \tag{11a}$$

and

$$[X_i, \exp W] = [X_i, W] \exp W \tag{11b}$$

In (11a), W will be U_j, $1 \leq j \leq v$; and in (11b), W will be U_{n+1}/U_n.

Taking the commutator $[X_i, F(X)]$ and making use of (7), (8), (10), and (11), we see that $F(X)$ satisfies (1) and hence is an invariant. Our proof is a generalization of that given for rational functions by Abellanos and Alonso.[13]

We do not have an algorithm for the complete solution of the simultaneous partial differential equations (4). However a single equation of the form (4) with χ_i given by (3) may always be solved. We are led to consider the total differential equations

$$dx_j \Big/ \sum_k x_k C_{ij}^k = \text{independent of } j. \tag{12}$$

Ince[24] suggests replacing the left-hand side of (12) by new ratios whose numerators and denominators are appropriate linear combinations of the old ones

$$\sum_j dx_j\, \mu_{jl} \Big/ \sum_{jk} x_k C_{ij}^k \mu_{jl} = \text{independent of } l, \tag{13}$$

with the μ_{jl} chosen so that

$$\sum_j C_{ij}^k \mu_{jl} = \lambda_l \mu_{kl}, \tag{14}$$

i.e., μ_{kl} is an eigenvector of the matrix C_{ij}^k belonging to the eigenvalue λ_l (we suppress the dependence of μ_{jl} and λ_l on i). Then we have

$$\frac{dx_l'}{\lambda_l x_l'} = \text{independent of } l, \tag{15}$$

where $x_l' = \sum_j x_j \mu_{jl}$. Provided the eigenvectors are complete we get the complete solution of the single equation (4):

$$F(x) = \phi\left(\frac{x_2'^{\lambda_1}}{x_1'^{\lambda_2}}, \frac{x_3'^{\lambda_1}}{x_1'^{\lambda_3}}, \frac{x_4'^{\lambda_1}}{x_1'^{\lambda_4}}, \cdots\right). \tag{16}$$

We note that Ince's solution (16) may be generalized to include the case where the eigenvectors of C_{ij}^k are not complete. We augment them by the generalized eigenvectors $\mu_{jl}^{(h)}$ which satisfy

$$\sum_j C_{ij}^k \mu_{jl}^{(h)} = \lambda_l \mu_{kl}^{(h)} + \mu_{kl}^{(h-1)}. \tag{17}$$

Here $\mu_{kl}^{(0)} \equiv 0$ and $\mu_{kl}^{(1)}$ is an ordinary eigenvector. Choosing $x_l^{(h)} = \sum_j x_j \mu_{jl}^{(h)}$ as independent variables (i.e., casting the matrix C_{ij}^k in the Jordan normal form), we get (12) in the form

$$\frac{dx_l^{(h)}}{\lambda_l x_l^{(h)} + x_l^{(h-1)}} = \text{independent of } l, h, \tag{18}$$

which may be integrated straightforwardly. An example is worked out in Sec. V.

We conclude this section by referring to some simple properties of the invariants, pointed out by Abellanos and Alonso.[13] The invariants found in the subsequent sections of this paper, of course, have these properties: (a) The number of independent invariants is r-R, where r is the dimension of the algebra (order of the group) and R is the rank of the commutator table, considered as a matrix; for the purpose of computing this rank, the generators X_i are regarded as independent c-number variables. (b) Since an antisymmetric matrix has even rank the number of independent invariants is equal to the dimension of the algebra, modulo 2. (c) The invariants of semisimple and nilpotent algebras may be chosen as homogeneous polynomials, i.e., Casimir operators.

Note that a direct integration of equations of the type (15) or (18) will always lead to a set of independent invariants that is complete in the sense that all invariants can be expressed as functions of these. However, we have often found it convenient to replace these (r-R) invariants by a different set of (r-R) invariants. Indeed, taking appropriate functions of the obtained invariants, we can often obtain simpler invariant operators and can, in particular, require that these be hermitian (or at least symmetric) operators.

III. REAL LIE ALGEBRAS OF DIMENSION UP TO FOUR

In this and Secs. IV and V we ignore algebras which are the algebraic sums of algebras of lower dimension; their invariants are just those of the subalgebras of which they are the algebraic sum.

The algebra $A^a_{r,j}$ means simply the jth algebra of dimension r. The superscript(s), if any, give the value(s) of the continuous parameter(s) on which the algebra depends. Restrictions on the range of the parameters are to avoid double counting and algebraic sums of lower algebras and in a few cases, to single out special well-known algebras. Our list is based on that of Mubarakzyanov.[22]

There is just one real algebra $A_{1,1}$ of dimension one; it has one invariant, a Casimir operator, which is its

TABLE I. Real Lie algebras of dimensions three and four.

Name	Nonzero commutation relations	Invariants	Comments
$A_{3,1}$	$[e_2e_3]=e_1$	e_1	nilpotent (Algebra of Weyl group)
$A_{3,2}$	$[e_1e_3]=e_1,\ [e_2e_3]=e_1+e_2$	$e_1\exp[-e_2/e_1]$	solvable
$A_{3,3}$	$[e_1e_3]=e_1,\ [e_2e_3]=e_2$	e_2/e_1	solvable, $D\,\textcircled{+}\,T_2$
$A_{3,4}$	$[e_1e_3]=e_1,\ [e_2e_3]=-e_2$	e_1e_2	solvable, $E(1,1)$
$A^a_{3,5}$	$[e_1e_3]=e_1,\ [e_2e_3]=ae_2\ \ (0<\lvert a\rvert<1)$	$e_2e_1^{-a}$	solvable
$A_{3,6}$	$[e_1e_3]=-e_2,\ [e_2e_3]=e_1$	$e_1^2+e_2^2$	solvable, $E(2)$
$A^a_{3,7}$	$[e_1e_3]=ae_1-e_2,\ [e_2e_3]=e_1+ae_2\ \ (a>0)$	$(e_1^2+e_2^2)[(e_1+ie_2)/(e_1-ie_2)]^{ia}$	solvable
$A_{3,8}$	$[e_1e_3]=-2e_2,\ [e_1e_2]=e_1,\ [e_2e_3]=e_3$	$2e_2^2+e_1e_3+e_3e_1$	semisimple, SU(1,1)
$A_{3,9}$	$[e_1e_2]=e_3,\ [e_2e_3]=e_1,\ [e_3e_1]=e_2$	$e_1^2+e_2^2+e_3^2$	semisimple, SU(2)
$A_{4,1}$	$[e_2e_4]=e_1,\ [e_3e_4]=e_2$	$e_1,\ e_2^2-2e_1e_3$	nilpotent
$A^a_{4,2}$	$[e_1e_4]=ae_1,\ [e_2e_4]=e_2,\ [e_3e_4]=e_2+e_3\ \ (a\neq 0)$	$e_2\exp(-e_3/e_2),\ e_2^a/e_1$	solvable, derived algebra $\sim 3A_1$
$A_{4,3}$	$[e_1e_4]=e_1,\ [e_3e_4]=e_2$	$e_1\exp(-e_3/e_2),\ e_2$	solvable, derived algebra $\sim 3A_1$
$A_{4,4}$	$[e_1e_4]=e_1,\ [e_2e_4]=e_1+e_2,\ [e_3e_4]=e_2+e_3$	$e_1\exp\left(-\frac{e_2}{e_1}\right),\ \frac{2e_1e_3-e_2^2}{e_1^2}$	solvable, derived algebra $\sim 3A_1$
$A^{ab}_{4,5}$	$[e_1e_4]=e_1,\ [e_2e_4]=ae_2,\ [e_3e_4]=be_3$ $(ab\neq 0,\ -1\leq a\leq b\leq 1)$	$e_1^a/e_2,\ e_1^b/e_3$	solvable, derived algebra $\sim 3A_1$
$A^{ab}_{4,6}$	$[e_1e_4]=ae_1,\ [e_2e_4]=be_2-e_3,\ [e_3e_4]=e_2+be_3$ $(a\neq 0,\ b\geq 0)$	$\frac{e_1^{2b/a}}{e_2^2+e_3^2},\ (e_2^2+e_3^2)\left(\frac{e_2+ie_3}{e_2-ie_3}\right)^{ib}$	solvable, derived algebra $\sim 3A_1$
$A_{4,7}$	$[e_2e_3]=e_1,\ [e_1e_4]=2e_1,\ [e_2e_4]=e_2,\ [e_3e_4]=e_2+e_3$	none	solvable, derived algebra $\sim A_{3,1}$
$A_{4,8}$	$[e_2e_3]=e_1,\ [e_2e_4]=e_2,\ [e_3e_4]=-e_3$	$e_1,\ e_2e_3+e_3e_2-2e_1e_4$	solvable, derived algebra $\sim A_{3,1}$
$A^b_{4,9}$	$[e_2e_3]=e_1,\ [e_1e_4]=(1+b)e_1,\ [e_2e_4]=e_2,\ [e_3e_4]=be_3$ $(-1<b\leq 1)$	none	solvable, derived algebra $\sim A_{3,1}$ or $2A_1$ (for $b=0$)
$A_{4,10}$	$[e_2e_3]=e_1,\ [e_2e_4]=-e_3,\ [e_3e_4]=e_2$	$e_1,\ 2e_1e_4+e_2^2+e_3^2$	solvable, derived algebra $\sim A_{3,1}$
$A^a_{4,11}$	$[e_2e_3]=e_1,\ [e_1e_4]=2ae_1,\ [e_2e_4]=ae_2-e_3,\ [e_3e_4]=e_2+ae_3\ \ (a>0)$	none	solvable, derived algebra $\sim A_{3,1}$
$A_{4,12}$	$[e_1e_3]=e_1,\ [e_2e_3]=e_2,\ [e_1e_4]=-e_2,\ [e_2e_4]=e_1$	none	solvable, derived algebra $\sim 2A_1$

single element. There is one real algebra $A_{2,1}$ of dimension two. The commutation rule is $[e_1e_2]=e_2$; it is solvable. It has no invariant.

There are nine real algebras of dimension three, two of which depend on parameters and hence constitute continua of algebras and there are 12 real algebras of dimension four, five of which depend on parameters. In Table I are given the invariants of all three and four dimensional real algebras, and since Mubarakzyanov's work is relatively inaccessible, we also give in Table I the nonzero commutators of the elements.

TABLE II. Real Lie algebras of dimension five.

Name	Nonzero commutation relations	Invariants	Comments
$A_{5,1}$	$[e_3e_5]=e_1,\ [e_4e_5]=e_2$	$e_1,\ e_2,\ e_2e_3-e_1e_4$	nilpotent
$A_{5,2}$	$[e_2e_5]=e_1,\ [e_3e_5]=e_2,\ [e_4e_5]=e_3$	$e_1,\ e_2^2-2e_1e_3,\ e_2^3+3e_1^2e_4-3e_1e_2e_3$	nilpotent
$A_{5,3}$	$[e_3e_4]=e_2,\ [e_3e_5]=e_1,\ [e_4e_5]=e_3$	$e_1,\ e_2,\ e_3^2+2e_2e_5-2e_1e_4$	nilpotent
$A_{5,4}$	$[e_2e_4]=e_1,\ [e_3e_5]=e_1$	e_1	nilpotent
$A_{5,5}$	$[e_3e_4]=e_1,\ [e_2e_5]=e_1,\ [e_3e_5]=e_2$	e_1	nilpotent
$A_{5,6}$	$[e_3e_4]=e_1,\ [e_2e_5]=e_1,\ [e_3e_5]=e_2,\ [e_4e_5]=e_3$	e_1	nilpotent
$A_{5,7}^{abc}$	$[e_1e_5]=e_1,\ [e_2e_5]=ae_2,\ [e_3e_5]=be_3,$ $[e_4e_5]=ce_4\ (abc\neq 0,\ -1\leq c\leq b\leq a\leq 1)$	$e_1^a/e_2,\ e_1^b/e_3,\ e_1^c/e_4$	solvable
$A_{5,8}^{c}$	$[e_2e_5]=e_1,\ [e_3e_5]=e_3,\ [e_4e_5]=ce_4\ (0<\lvert c\rvert\leq 1)$ $[e_4e_5]=ce_4\ (0\neq c\leq b)$	$e_1,\ e_3^c/e_4,\ e_3\exp(-e_2/e_1)$	solvable
$A_{5,9}^{bc}$	$[e_1e_5]=e_1,\ [e_2e_5]=e_1+e_2,\ [e_3e_5]=be_3,$ $[e_4e_5]=ce_4\ (0\neq c\leq b)$	$e_1^b/e_3,\ e_1^c/e_4,\ e_1\exp(-e_2/e_1)$	solvable
$A_{5,10}$	$[e_2e_5]=e_1,\ [e_3e_5]=e_2,\ [e_4e_5]=e_4$	$e_1,\ e_2^2-2e_1e_3,\ e_4\exp(-e_2/e_1)$	solvable
$A_{5,11}^{c}$	$[e_1e_5]=e_1,\ [e_2e_5]=e_1+e_2,\ [e_3e_5]=e_2+e_3,$ $[e_4e_5]=ce_4\ (c\neq 0)$	$\frac{e_1^c}{e_4},\ e_1\exp\left(-\frac{e_2}{e_1}\right),\ \frac{2e_3}{e_1}-\frac{e_2^2}{e_1^2}$	solvable
$A_{5,12}$	$[e_1e_5]=e_1,\ [e_2e_5]=e_1+e_2,\ [e_3e_5]=e_2+e_3,$ $[e_4e_5]=e_3+e_4$	$e_1\exp\left(-\frac{e_2}{e_1}\right),\ \frac{2e_3}{e_1}-\frac{e_2^2}{e_1^2},$ $\frac{3e_4}{e_1}-\frac{3e_2e_3}{e_1^2}+\frac{e_2^3}{e_1^3}$	solvable
$A_{5,13}^{apq}$	$[e_1e_5]=e_1,\ [e_2e_5]=ae_2,\ [e_3e_5]=pe_3-qe_4,$ $[e_4e_5]=qe_3+pe_4\ (aq\neq 0,\ \lvert a\rvert\leq 1)$	$\frac{e_1^a}{e_2},\ \frac{e_1^{2p}}{e_3^2+e_4^2},\ e_1^{2q}\left(\frac{e_3+ie_4}{e_3-ie_4}\right)^t$	solvable
$A_{5,14}^{p}$	$[e_2e_5]=e_1,\ [e_3e_5]=pe_3-e_4,\ [e_4e_5]=e_3+pe_4$	$e_1,\ (e_3^2+e_4^2)\left(\frac{e_3+ie_4}{e_3-ie_4}\right)^{tp},$ $(e_3^2+e_4^2)\exp\left(-2p\frac{e_2}{e_1}\right)$	solvable
$A_{5,15}^{a}$	$[e_1e_5]=e_1,\ [e_2e_5]=e_1+e_2,\ [e_3e_5]=ae_3,$ $[e_4e_5]=e_3+ae_4\ (\lvert a\rvert\leq 1)$	$\frac{e_1^a}{e_3},\ e_1\exp\left(-\frac{e_2}{e_1}\right),\ e_3\exp\left(-\frac{e_4}{e_3}\right)$	solvable
$A_{5,16}^{pq}$	$[e_1e_5]=e_1,\ [e_2e_5]=e_1+e_2,\ [e_3e_5]=pe_3-qe_4,$ $[e_4e_5]=qe_3+pe_4\ (q\neq 0)$	$\frac{e_1^{2p}}{e_3^2+e_4^2},\ e_1^{2q}\left(\frac{e_3-ie_4}{e_3+ie_4}\right),\ e_1\exp\left(-\frac{e_2}{e_1}\right)$	solvable
$A_{5,17}^{spq}$	$[e_1e_5]=pe_1-e_2,\ [e_2e_5]=e_1+pe_2,\ [e_3e_5]=qe_3-se_4,$ $[e_4e_5]=se_3+qe_4\ (s\neq 0)$	$\frac{(e_1^2+e_2^2)^q}{(e_3^2+e_4^2)^p},\ (e_1^2+e_2^2)\left(\frac{e_1+ie_2}{e_1-ie_2}\right)^{tp},$ $(e_3^2+e_4^2)\left(\frac{e_3+ie_4}{e_3-ie_4}\right)^{tq/s}$	solvable
$A_{5,18}^{p}$	$[e_1e_5]=pe_1-e_2,\ [e_2e_5]=e_1+pe_2,$ $[e_3e_5]=e_1+pe_3-e_4,\ [e_4e_5]=e_2+e_3+pe_4\ (p\geq 0)$	$\frac{e_1e_4-e_2e_3}{e_1^2+e_2^2},\ (e_1^2+e_2^2)\left(\frac{e_1+ie_2}{e_1-ie_2}\right)^{tp},$ $(e_1^2+e_2^2)\exp\left(-2p\frac{e_1e_3+e_2e_4}{e_1^2+e_2^2}\right)$	solvable
$A_{5,19}^{ab}$	$[e_2e_3]=e_1,\ [e_1e_5]=ae_1,\ [e_2e_5]=e_2,$ $[e_3e_5]=(a-1)e_3,\ [e_4e_5]=be_4\ (b\neq 0)$	e_1^b/e_4^a	solvable
$A_{5,20}^{a}$	$[e_2e_3]=e_1,\ [e_1e_5]=ae_1,\ [e_2e_5]=e_2,$ $[e_3e_5]=(a-1)e_3,\ [e_4e_5]=e_1+ae_4$	$e_1\exp[-a(e_4/e_1)]$	solvable
$A_{5,21}$	$[e_2e_3]=e_1,\ [e_1e_5]=2e_1,\ [e_2e_5]=e_2+e_3$ $[e_3e_5]=e_3+e_4,\ [e_4e_5]=e_4$	e_4^2/e_1	solvable

TABLE II (*Continued*)

$A_{5,22}$	$[e_2e_3]=e_1,\ [e_2e_5]=e_3,\ [e_4e_5]=e_4$	e_1	solvable
$A^b_{5,23}$	$[e_2e_3]=e_1,\ [e_1e_5]=2e_1,\ [e_2e_5]=e_2+e_3,$ $[e_3e_5]=e_3,\ [e_4e_5]=be_4\ (b\neq 0)$	e_1^b/e_4^2	solvable
$A^\epsilon_{5,24}$	$[e_2e_3]=e_1,\ [e_1e_5]=2e_1,\ [e_2e_5]=e_2+e_3,$ $[e_3e_5]=e_3,\ [e_4e_5]=\epsilon e_1+2e_4\ (\epsilon=\pm 1)$	$e_1\exp[-2\epsilon(e_4/e_1)]$	solvable
$A^{bp}_{5,25}$	$[e_2e_3]=e_1,\ [e_1e_5]=2pe_1,\ [e_2e_5]=pe_2+e_3,$ $[e_3e_5]=pe_3-e_2,\ [e_4e_5]=be_4\ (b\neq 0)$	e_1^b/e_4^{2p}	solvable
$A^{p\epsilon}_{5,26}$	$[e_2e_3]=e_1,\ [e_1e_5]=2pe_1,\ [e_2e_5]=pe_2+e_3,$ $[e_3e_5]=pe_3-e_2,\ [e_4e_5]=\epsilon e_1+2pe_4\ (\epsilon=\pm 1)$	$e_1\exp[-2\epsilon p(e_4/e_1)]$	solvable
$A_{5,27}$	$[e_2e_3]=e_1,\ [e_1e_5]=e_1,\ [e_3e_5]=e_3+e_4,$ $[e_4e_5]=e_1+e_4$	$e_1\exp(-e_4/e_1)$	solvable
$A^a_{5,28}$	$[e_2e_3]=e_1,\ [e_1e_5]=ae_1,\ [e_2e_5]=(a-1)e_2,$ $[e_3e_5]=e_3+e_4,\ [e_4e_5]=e_4$	e_4^a/e_1	solvable
$A_{5,29}$	$[e_2e_4]=e_1,\ [e_1e_5]=e_1,\ [e_2e_5]=e_2,\ [e_4e_5]=e_3$	e_3	solvable
$A_{5,30}$	$[e_2e_4]=e_1,\ [e_3e_4]=e_2,\ [e_1e_5]=(a+1)e_1,$ $[e_2e_5]=ae_2,\ [e_3e_5]=(a-1)e_3,\ [e_4e_5]=e_4$	$(e_2^2-2e_1e_3)^{a+1}/e_1^{2a}$	solvable
$A_{5,31}$	$[e_2e_4]=e_1,\ [e_3e_4]=e_2,\ [e_1e_5]=3e_1,$ $[e_2e_5]=2e_2,\ [e_3e_5]=e_3,\ [e_4e_5]=e_3+e_4$	$(e_2^2-2e_1e_3)^3/e_1^4$	solvable
$A^a_{5,32}$	$[e_2e_4]=e_1,\ [e_3e_4]=e_2,\ [e_1e_5]=e_1,$ $[e_2e_5]=e_2,\ [e_3e_5]=ae_1+e_3$	$e_1^{2a}\exp[(e_2^2-2e_1e_3)/e_1^2]$	solvable
$A^{ab}_{5,33}$	$[e_1e_4]=e_1,\ [e_3e_4]=be_3,\ [e_2e_5]=e_2,$ $[e_3e_5]=ae_3\ (a^2+b^2\neq 0)$	$e_1^be_2^a/e_3$	solvable
$A^a_{5,34}$	$[e_1e_4]=ae_1,\ [e_2e_4]=e_2,\ [e_3e_4]=e_3,$ $[e_1e_5]=e_1,\ [e_3e_5]=e_2$	$(e_2^a/e_1)\exp(e_3/e_2)$	solvable solvable
$A^{ab}_{5,35}$	$[e_1e_4]=be_1,\ [e_2e_4]=e_2,\ [e_3e_4]=e_3,$ $[e_1e_5]=ae_1,\ [e_2e_5]=-e_3,\ [e_3e_5]=e_2\ (a^2+b^2\neq 0)$	$\frac{e_1^2}{(e_2^2+e_3^2)^b}\left(\frac{e_2+ie_3}{e_2-ie_3}\right)^{ia}$	solvable
$A_{5,36}$	$[e_2e_3]=e_1,\ [e_1e_4]=e_1,\ [e_2e_4]=e_2,$ $[e_2e_5]=-e_2,\ [e_3e_5]=e_3$	$(e_2e_3+e_3e_2+2e_1e_5)/e_1$	solvable
$A_{5,37}$	$[e_2e_3]=e_1,\ [e_1e_4]=2e_1,\ [e_2e_4]=e_2,$ $[e_3e_4]=e_3,\ [e_2e_5]=-e_3,\ [e_3e_5]=e_2$	$(e_2^2+e_3^2+2e_1e_5)/e_1$	solvable
$A_{5,38}$	$[e_1e_4]=e_1,\ [e_2e_5]=e_2,\ [e_4e_5]=e_3$	e_3	solvable
$A_{5,39}$	$[e_1e_4]=e_1,\ [e_2e_4]=e_2,\ [e_1e_5]=-e_2,$ $[e_2e_5]=e_1,\ [e_4e_5]=e_3$	e_3	solvable
$A_{5,40}$	$[e_1e_2]=2e_1,\ [e_1e_3]=-e_2,\ [e_2e_3]=2e_3,$ $[e_1e_4]=e_5,\ [e_2e_4]=e_4,\ [e_2e_5]=-e_5,\ [e_3e_5]=e_4$	$\{e_1e_4^2-e_2e_4e_5-e_3e_5^2\}_{\text{symmetrized}}$	solvable

IV. REAL ALGEBRAS OF DIMENSION FIVE

There are 40 algebras of dimension five[22]; 18 of them depend on one or more continuous parameters. Their commutation rules and invariants are presented in Table II.

We give here the solution of Eq. (4) for the algebra $A^p_{5,18}$, which illustrates some of the points discussed in Sec. II. The condition $\chi_i F(e)=0$ for $i=1, 2, 3, 4$ merely states that F is independent of e_5. The equation $\chi_5 F(e)=0$ reads

$$[(pe_1-e_2)\partial_{e_1}+(e_1+pe_2)\partial_{e_2}+(e_1+pe_3-e_4)\partial_{e_3}+(e_2+e_3+pe_4)\partial_{e_4}]F(e_1,e_2,e_3,e_4)=0. \tag{19}$$

The subsidiary equations for (19) [see Eq. (12)] are

$$\frac{de_1}{pe_1-e_2}=\frac{de_2}{e_1+pe_2}=\frac{de_3}{e_1+pe_3-e_4}=\frac{de_4}{e_2+e_3+pe_4}. \tag{20}$$

The matrix

$$C^k_{5j}=\begin{pmatrix} p & 1 & 1 & 0\\ -1 & p & 0 & 1\\ 0 & 0 & p & 1\\ 0 & 0 & -1 & p\end{pmatrix} \tag{21}$$

has two eigenvalues $p\pm i$. The new independent variables which correspond to its two eigenvectors are

$$e_\pm^{(1)}=e_1\pm ie_2, \tag{22}$$

while those which correspond to the two generalized eigenvectors are

$$e_\pm^{(2)}=e_3\pm ie_4. \tag{23}$$

Now Eqs. (20) are replaced by

$$\frac{de_+^{(1)}}{(p+i)e_+^{(1)}}=\frac{de_-^{(1)}}{(p-i)e_-^{(1)}}=\frac{de_+^{(2)}}{(p+i)e_+^{(2)}+e_+^{(1)}}$$
$$=\frac{de_-^{(2)}}{(p-i)e_-^{(2)}+e_-^{(1)}}. \tag{24}$$

From the equality of the first two ratios we get the invariant

$$(e_1^2+e_2^2)[(e_1+ie_2)/(e_1-ie_2)]^{ip}=C_1. \tag{25}$$

The equality of the first and third ratios, and of the second and fourth give two more invariants

$$C_\pm=e_\pm^{(1)}\exp[-(p\pm i)[e_\pm^{(2)}/e_\pm^{(1)}]]. \tag{26}$$

Instead of $C_\pm$ we use

$$C_2=\frac{1}{2(1+p^2)}\ln\frac{C_+^{1+ip}C_-^{1-ip}}{C_1}=\frac{e_1e_4-e_2e_3}{e_1^2+e_2^2} \tag{27}$$

and

$$C_3=C_+C_-\exp 2C_2=(e_1^2+e_2^2)\exp\left\{-2p\frac{e_1e_3+e_2e_4}{e_1^2+e_2^2}\right\}. \tag{28}$$

V. REAL NILPOTENT ALGEBRAS OF DIMENSION SIX

Morozov[23] has listed all real nilpotent algebras of dimension six. Their commutation rules and invariants are given in Table III. The invariants, of course, are all polynomials.

It is interesting that, contrary to the semisimple case, one cannot always find a functionally independent set of invariants for a nilpotent algebra which is also an integrity basis in the sense that any polynomial invariant can be expressed as a polynomial in them. For example $A_{6,1}$ has an invariant

$$C=e_4e_5^2-2e_3e_5e_6+2e_2e_6^2, \tag{29}$$

which, in terms of the polynomial invariants given in Table II, must be written

$$C=[(e_3e_6-e_4e_5)^2+e_6^2(2e_2e_4-e_3^2)]/e_4. \tag{30}$$

Similarly $A_{6,2}$ has an invariant

$$C=9e_3^2e_6^2-3e_4^2e_5^2-18e_3e_4e_5e_6+6e_3e_5^3+8e_4^3e_6, \tag{31}$$

TABLE III. Nilpotent algebras of dimension six.

Name	Nonzero commutation relations	Invariants
$A_{6,1}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_5]=e_6$	$e_4,\ e_6,\ e_3e_6-e_4e_5,\ 2e_2e_4-e_3^2$
$A_{6,2}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_4]=e_5,\ [e_1e_5]=e_6$	$e_6,\ 2e_4e_6-e_5^2,\ 2e_2e_6-2e_3e_5+e_4^2,$ $3e_3e_6^2-3e_4e_5e_6+e_5^3$
$A_{6,3}$	$[e_1e_2]=e_6,\ [e_1e_3]=e_4,\ [e_2e_3]=e_5$	$e_4,\ e_5,\ e_6,\ e_1e_5+e_3e_6-e_2e_4$
$A_{6,4}$	$[e_1e_2]=e_5,\ [e_1e_3]=e_6,\ [e_2e_4]=e_6$	$e_5,\ e_6$
$A_{6,5}^a$	$[e_1e_3]=e_5,\ [e_1e_4]=e_6,\ [e_2e_3]=ae_6,\ [e_2e_4]=e_5\ (a\neq 0)$	$e_5,\ e_6$
$A_{6,6}$	$[e_1e_2]=e_6,\ [e_1e_3]=e_4,\ [e_1e_4]=e_5,\ [e_2e_3]=e_5$	$e_5,\ e_6$
$A_{6,7}$	$[e_1e_3]=e_4,\ [e_1e_4]=e_5,\ [e_2e_3]=e_6$	$e_5,\ e_6$
$A_{6,8}$	$[e_1e_2]=e_3+e_5,\ [e_1e_3]=e_4,\ [e_2e_5]=e_6$	$e_4,\ e_6$
$A_{6,9}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_5]=e_6,\ [e_2e_3]=e_6$	$e_4,\ e_6$
$A_{6,10}^a$	$[e_1e_2]=e_3,\ [e_1e_3]=e_5,\ [e_1e_4]=e_6,$ $[e_2e_3]=ae_6,\ [e_2e_4]=e_5\ (a\neq 0)$	$e_5,\ e_6$
$A_{6,11}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_4]=e_5,\ [e_2e_3]=e_6$	$e_5,\ e_6$
$A_{6,12}$	$[e_1e_3]=e_4,\ [e_1e_4]=e_6,\ [e_2e_5]=e_6$	$e_6,\ 2e_3e_6-e_4^2$
$A_{6,13}$	$[e_1e_2]=e_5,\ [e_1e_3]=e_4,\ [e_1e_4]=e_6,\ [e_2e_5]=e_6$	$e_6,\ 2e_3e_6-e_4^2$
$A_{6,14}^a$	$[e_1e_3]=e_4,\ [e_1e_4]=e_6,\ [e_2e_3]=e_5,\ [e_2e_5]=ae_6\ (a\neq 0)$	$e_6,\ e_5^2+ae_4^2-2ae_3e_6$
$A_{6,15}$	$[e_1e_2]=e_3+e_5,\ [e_1e_3]=e_4,\ [e_1e_4]=e_6,\ [e_2e_5]=e_6$	$e_6,\ e_4^2-2e_3e_6$
$A_{6,16}$	$[e_1e_3]=e_4,\ [e_1e_4]=e_5,\ [e_1e_5]=e_6,$ $[e_2e_3]=e_5,\ [e_2e_4]=e_6$	$e_6,\ 3e_3e_6^2+e_5^3-3e_4e_5e_6$
$A_{6,17}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_4]=e_6,\ [e_2e_5]=e_6$	$e_6,\ e_4^2-2e_3e_6$
$A_{6,18}^a$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_4]=e_6,$ $[e_2e_3]=e_5,\ [e_2e_5]=ae_6\ (a\neq 0)$	$e_6,\ e_5^2+ae_4^2-2ae_3e_6$
$A_{6,19}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_4]=e_5,$ $[e_1e_5]=e_6,\ [e_2e_3]=e_6$	$e_6,\ e_5^2-2e_4e_6$
$A_{6,20}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_4,\ [e_1e_4]=e_5,$ $[e_1e_5]=e_6,\ [e_2e_3]=e_5,\ [e_2e_4]=e_6$	$e_6,\ e_5^3+3e_3e_6^2-3e_4e_5e_6$
$A_{6,21}$	$[e_1e_2]=e_3,\ [e_1e_5]=e_6,\ [e_2e_3]=e_4,$ $[e_2e_4]=e_5,\ [e_3e_4]=e_6$	$e_6,\ e_4^2+2e_2e_6-2e_3e_5$
$A_{6,22}$	$[e_1e_2]=e_3,\ [e_1e_3]=e_5,\ [e_1e_5]=e_6,$ $[e_2e_3]=e_4,\ [e_2e_4]=e_5,\ [e_3e_4]=e_6$	$e_6,\ 2e_5^3+3e_4^2e_6+6e_2e_6^2-6e_3e_5e_6$

which may be expressed as

$$C=[(2e_4e_6-e_5^2)^3+(3e_3e_6^2-3e_4e_5e_6+e_5^3)^2]/e_6^2. \tag{32}$$

VI. CONCLUSIONS

We have examined all existing real Lie algebras of dimension $r\leq 5$ and all real nilpotent Lie algebras of dimension $r=6$. For each algebra we have found all independent invariant functions $F(X_1,\ldots,X_r)$ of the generators. The invariants obtained as well as the classification of Lie algebras that we use, are summarized in Tables I–III. The tables include only algebraically indecomposable Lie algebras, i.e., those that cannot be written as algebraic sums of lower dimension Lie algebras (the invariants of an algebraic sum of Lie algebras are simply the invariants of the individual algebras in the sum).

Only one indecomposable real Lie algebra of dimension $r=2$ exists. It has no invariant. A glance at Table I shows nine types of three-dimensional algebras, two of which $A_{3,5}^a$ and $A_{3,7}^a$ are actually infinite one parameter families of algebras. These algebras have one invariant each. The 12 types of indecomposable four-dimensional algebras, each having either two invariants or none are listed with their invariants in the same table. The 40 types of five-dimensional algebras and their invariants are listed in Table II, the 22 types of nilpotent six-dimensional algebras in Table III.

Let us make a few comments on the results of this paper.

(i) General invariants, rational invariants, and Casimir operators all appear on the same footing, as solutions of the differential equations (4). Indeed, all invariants obtained can be written in the form

$$F(X_i)=\left[\prod_{k=1}^{n}U_k^{a_k}(X_i)\right]\exp\frac{U_{n+1}(X_i)}{U_n(X_i)}, \tag{33}$$

where $U_k(X_i)$ are homogeneous polynomials in the generators X_i, such that each term is symmetric with respect to permutations of the order of the generators. The a_k are constants, in some cases negative or complex ones. Clearly, if $U_{n+1}(X_i)\equiv 0$ and the numbers a_i are all mutually rational and of the same sign, then $F(X_i)$ defines a Casimir operator. If $U_{n+1}(X_i)\equiv 0$ and the numbers a_i are all mutually rational but not all of the same sign, then $F(X_i)$ defines a rational invariant. Otherwise $F(X_i)$ is a general invariant.

(ii) The generalization from polynomial invariants to all invariants seems to be a very natural one. Indeed, when an algebra depends on a parameter (or parameters), the parameter may figure in the expression for the invariant. For certain values of the parameter a general invariant may go over into a rational or polynomial one. Many such examples are found in our tables. Specifically, consider the algebras $A_{3,5}^a$ and $A_{3,7}^a$. The Lie group generated by $A_{3,5}^a$ is a subgroup of the similitude group of the pseudo-Euclidean plane. Indeed, consider the plane (x,t) with the metric $ds^2=dx^2-dt^2$. The similitude group in this case is generated by the dilations D, the proper Lorentz transformations K_1 and the time and space translations P_0 and P_1. Consider the three-dimensional subalgebra

$$S\equiv\frac{1}{2\cosh b}(e^bD+e^{-b}K_1),P_0,P_1\ ,\quad -\infty<b<\infty,\quad b\neq 0. \tag{34}$$

It is isomorphic to $A_{3,5}^a$ with $a=\tanh b$ and its invariant is

$$F=(P_0+P_1)^{\tanh b}/(P_0-P_1). \tag{35}$$

For $-\infty<b<\infty$ the expression $\tanh b$ runs through all (infinitely many) negative and positive rational numbers and in each of these cases the general invariant F will reduce to a rational or polynomial one.

The situation is similar for the algebra $A_{3,7}^a$. The corresponding Lie group is a subgroup of the similitude group of a Euclidean plane. Consider now the plane (x,y) with the metric $ds^2=dx^2+dy^2$. The similitude group is generated by the dilation D, the rotation L_3 and the translations P_1 and P_2. A subgroup isomorphic to $A_{3,7}^a$ is generated by

$$L_3+aD,\quad P_1,P_2,\quad 0<a<\infty, \tag{36}$$

and its invariant is

$$(P_1^2+P_2^2)[(P_1+iP_1)/(P_1-iP_2)]^{i/a}. \tag{37}$$

The invariant reduces to a Casimir operator or rational invariant in the limits $a\to 0$ or $a\to\infty$, respectively (the algebras $A_{3,6}$ and $A_{3,3}$).

(iii) From the physical point of view one can imagine a situation in which an algebra like (34) or (36) generates the symmetry group of a problem. An infinitesimally small change in the conditions of the system under study could change the value of say the parameter a characterizing the symmetry group and thus change a Casimir operator into a general invariant or vice versa.

(iv) The above arguments make it extremely plausible that general invariants should play the same role in representation theory and physical and other applications of group theory, as Casimir operators do. Indeed, consider the group generated by the algebra (36), but include the limiting cases $a\to 0$ and $a\to\infty$. The theory of induced representations[25] can be used to induce representations of the group from representations of the subgroup of translations. The problem then arises of classifying points in the space of characters of the representations of the translation group into orbits[26] under the action of the factor group generated by L_3+aD. For $a=0$ these orbits are circles, characterized by a radius p, where p^2 is a value of the invariant $P_1^2+P_2^2$. For $a\to\infty$ the orbits are straight lines intersecting at the origin, characterized by an angle ϕ, where ϕ is the inverse tangent of a value of the ratio P_2/P_1, figuring in the invariant $(P_1+iP_2)^i/(P_1-iP_2)^i$. For $0<a<\infty$ the orbits are spirals passing through the origin, characterized by a value of the invariant (37). It seems to us that all types of invariants thus partially or completely characterize the irreducible representations of the algebras considered.

(v) In order to use the invariants of an algebra it is necessary to give them a clear mathematical meaning. For all cases encountered in this paper this is facilitated by the fact that the individual "constituents" of the invariants (33) always commute. Thus, a rational in-

variant always occurs as the ratio of two commuting polynomials. The polynomials $U_{n+1}(X_i)$ and $U_n(X_i)$ in the exponential commute with each other and with the polynomials multiplying the exponential. Thus, it is always possible to choose a basis in which all of these mutually commuting operators are diagonal. The invariant $F(X_i)$ then simply reduces to a number that indeed characterizes a representation.

On the other hand, we are free to choose other bases for representations. Then $F(X_i)$ can be interpreted, e.g., as an integral operator.

(vi) In the case of semisimple algebras all invariants can be written as functions of l polynomial invariants, where l is the rank of the algebra. These l basic invariants (Casimir operators) form an integrity basis, i.e., any polynomial invariant can be written as a polynomial in the basic invariants.

(vii) In the case of nilpotent algebras all invariants can again be written as functions of r-R polynomial invariants (r is the dimension of the algebra, R the rank of the matrix of the commutation table). However, in this case the "basic invariants" do not necessarily form an integrity basis. Thus, higher-order polynomial invariants may exist, that are functions of the lower ones, but not polynomials in them. Examples were discussed in Sec. V.

(viii) The low-dimensional Lie algebras studied in this article should play a role in many applications. Indeed, very many of them occur as subalgebras of the fundamental groups of physics, such as the Poincaré group, Galilei group, de Sitter groups, conformal group etc.

Finally, let us note that many further questions, both conceptual and technical ones, remain open. Let us just mention a few of them.

(a) It would be desirable to obtain general formulas for the number of independent polynomial and rational invariants for an arbitrary algebra ($N = r - R$ is the number of all independent invariants). It would also be desirable to obtain general statements about the degree of the independent Casimir operators, to find out when they do form an integrity basis for all polynomial invariants, etc.

(b) The problem of finding all invariants has been reduced to that of solving a system of first-order linear differential equations. While we have provided a method for solving any one of the equations it would be useful to have an algorithm for finding the general solution of the entire system of equations.

(c) For physical applications it would be of interest to classify all real Lie algebras of higher dimensions (at least upto dimension $r = 10$) into equivalence classes and to find their invariants (since such algebras occur as subalgebras of, e.g., the conformal group of space time).

(d) Throughout this paper we have restricted ourselves to invariants that are obtained by solving certain differential equations. The solutions were assumed to be ordinary functions that are at least once continuously differentiable. Other solutions can exist in different spaces, in particular distribution type solutions can be of considerable interest. For example, the Poincaré group (inhomogeneous Lorentz group) has two Casimir operators m^2 and W^2 (mass squared and spin squared), which could be found using the methods of this paper. However, for $m^2 \geq 0$ a further invariant exists, namely, sign p_0, the sign of the energy. This quantity can be expressed as a distribution, e.g., in terms of a step function $\theta(p_0)$. A systematic approach to such "non functional" invariants should be provided.

(e) A rigorous and complete study of the representation theory of groups with nonpolynomial invariants should be provided. *Inter alia* this should establish whether the invariants suffice to label representations completely or whether further characteristics are necessary. This also raises the problem of finding the spectra of the invariants, of providing them with a rigorous meaning in each case, etc.

(f) Many problems related to physical applications of the invariants remain unsolved, in particular their relation to observable quantities.

We plan to return to the above problems in the near future.

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[1]N. Ya. Vilenkin, *Special Functions and the Theory of Group Representations* (Am. Math. Soc., Providence, R.I., 1968).
[2]W. Miller, Jr, *Lie Theory and Special Functions* (Academic, New York, 1968).
[3]J. D. Talman, *Special Functions. A Group Theoretic Approach* (Benjamin, New York, 1968).
[4]E. P. Wigner, Ann. Math. 40, 149 (1939).
[5]M. Gell-Mann, Phys. Rev. 125, 1067 (1962).
[6]S. Okubo, Prog. Theor. Phys. 16, 686 (1962).
[7]V. Bargmann, Z. Phys. 99, 576 (1936).
[8]M. J. Engelfield, *Group Theory and the Coulomb Problem* (Wiley, New York, 1972).
[9]E. G. Beltrametti and A. Blasi, Phys. Lett. 20, 62 (1966).
[10]M. Pauri and G. M. Prosperi, Nuovo Cimento 43, 533 (1966).
[11]R. Mirman, J. Math. Phys. 9, 47 (1968); M. E. Angelopoulos, C. R. Acad. Sci. Paris 264, 585 (1967).
[12]P. Roman, J. J. Aghassi, and P. L. Huddleston, J. Math. Phys. 13, 1852 (1972).

[13]L. Abellanos and L. M. Alonso, J. Math. Phys. **16**, 1580 (1975).
[14]J. Patera, R. T. Sharp, P. Winternitz, and H. Zassenhaus, J. Math. Phys. **17**, 977 (1976).
[15]G. Racah, Rend. Licei 8, 108 (1950).
[16]E. P. Wigner, Ann. Math. **40**, 149 (1939).
[17]J. M. Levy-Leblond, in *Group Theory and its Applications*, edited by E. M. Loebl (Academic, New York, 1972).
[18]J. Patera, P. Winternitz, and H. Zassenhaus, J. Math. Phys. **16**, 1597 (1975).
[19]J. Patera, P. Winternitz, and H. Zassenhaus, J. Math. Phys. **16**, 1615 (1975).
[20]J. Patera, R. T. Sharp, P. Winternitz, and H. Zassenhaus, Can. J. Phys. (to be published).
[21]J. Patera, P. Winternitz, and H. Zassenhaus, J. Math. Phys. **17**, 717 (1976).
[22]G. M. Mubarakzyanov, Izv. Vysshikh Uchebn. Zavedenii Mat. No. 1 (32), 114; No. 3 (34), 99; No. 4 (35), 104 (1963).
[23]V. V. Morozov, Izv. Vysshikh Uchebn. Zavedenii Mat. No. 4 (5) 161 (1958).
[24]R. L. Ince, *Ordinary Differential Equations* (Dover, New York, 1944).
[25]G. W. Mackey, *Induced Representations of Groups and Quantum Mechanics* (Benjamin, New York, 1968).
[26]W. Miller, Jr. and M. Perroud (private communications).

Coulombian asymptotic states

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We define and study Coulombian asymptotic states, denoted by $|\mathbf{k}\,\infty\rangle$, which are useful and important for stationary Coulombian scattering theory. Using these asymptotic states, we are able to derive from the off-shell T matrix the physical on-shell T matrix for Coulomb plus short-range potentials. This function is proportional to the physical scattering amplitude. A generalized Lippmann–Schwinger equation and related equations are derived. Many other applications of the asymptotic states exist. We show the precise connection of $|\mathbf{k}\,\infty\rangle$ with the time-dependent Coulomb scattering theory.

I. INTRODUCTION

The (nonrelativistic two-body) stationary scattering theory for short-range potentials [loosely speaking: $V(r)=O(r^{-\alpha})$, $\alpha>1$, $r\to\infty$] is well founded. If the potential is Coulomb-like, there appear difficulties that stem from the long range (in fact, infinite range) of the potential. Two main problems can be discerned: (i) the scattering amplitude is singular in the forward direction, such that it is not an integrable function there; (ii) the scattering states do not approach free states asymptotically (i.e., when $r\to\infty$) and, related to this fact, the T matrix in momentum representation has no half-shell and/or on-shell limit.

To solve problem (i), Herbst[1] and Taylor[2] independently introduced certain distributions (somewhat different from each other) which are suitable to handle the divergencies occurring in the forward direction.

In the present paper we define and study so-called Coulombian asymptotic states, in momentum representation denoted by $\langle\mathbf{p}\,|\mathbf{k}\,\infty\rangle$, which are suitable to solve problem (ii). They can be thought of as generalized distributions. The phrase "asymptotic state" is an abbreviation of "asymptotically Coulomb-modified improper free state." To be precise, in this paper we consider the *pure* Coulomb potential only. In a forthcoming paper, many applications of $|\mathbf{k}\,\infty\rangle$ will be reported, also to Coulomb plus short-range potential scattering formulas.

We note that the closed formula for $\langle\mathbf{p}\,|\mathbf{k}\,\infty\rangle$ [see Eqs. (3) and (4)] is not essentially new. Nutt[3] introduced these asymptotic states for the first time, although he defined them inaccurately. To our knowledge, the states have not been used or even mentioned afterwards, up until now. Presumably because an accurate definition and a clear interpretation of these asymptotic states were missing, their importance and usefulness have not been recognized.

In Sec. II we give the exact definition of the asymptotic states and of the class of "test functions" on which they are defined. In Sec. III we derive a generalized Lippmann-Schwinger equation and related equations. We introduce the so-called physical half-shell and on-shell T matrices and we show that the Coulomb scattering amplitude is $-2\pi^2$ times the physical on-shell Coulomb T matrix. In standard scattering theory this relation is well known (the adjective "physical" is then superfluous).

In Sec. IV we investigate the relation between the asymptotic states $\langle\mathbf{p}\,|\mathbf{k}\,\infty\rangle$ and certain formulas playing a basic role in the time-dependent Coulomb scattering theory. The connection we find there, yields a clear indication for the interpretation of the asymptotic states. Finally, Sec. V contains the summary and discussion.

II. DEFINITION OF THE ASYMPTOTIC STATES $|k\,\infty\rangle$

Already in 1951, Guth and Mullin[4] published an expression for $\langle\mathbf{p}\,|\mathbf{k}+\rangle_C$, the Coulomb scattering wave function in momentum representation at energy $k^2>0$. We are going to show now that from that expression $\langle\mathbf{p}\,|\mathbf{k}\,\infty\rangle$ can easily be obtained.

As usual we take $\hbar=2m=1$ (m is the reduced mass) and denote the Coulomb potential by $V_C(r)=2k\gamma/r$. In Sec. IV it will appear preferable to use the k-independent strength parameter $s\equiv-k\gamma$. Throughout this paper we shall be concerned mostly with pure Coulomb formulas. With a few exceptions, the subscript C will be suppressed. We adopt the following normalization:

$$\langle\mathbf{k}'+|\mathbf{k}+\rangle=\delta(\mathbf{k}'-\mathbf{k}),$$

which differs from the one in Refs. 3 and 4. According to Guth and Mullin[4] one has, with the usual convention $\epsilon\downarrow 0$,

$$\langle\mathbf{p}\,|V|\mathbf{k}+\rangle = \exp(-\pi\gamma/2)\,\Gamma(1+i\gamma)\,\frac{k\gamma}{\pi^2}\,\frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{(|\mathbf{p}-\mathbf{k}|^2+\epsilon^2)^{1+i\gamma}}, \tag{1}$$

$$\langle\mathbf{p}|\mathbf{k}+\rangle=\frac{-1}{2k\gamma}\,\frac{d}{d\epsilon}\,\langle\mathbf{p}\,|V|\mathbf{k}+\rangle. \tag{2}$$

The differentiation with respect to ϵ yields two terms. One of these is

$$\langle\mathbf{p}\,|\mathbf{k}_\epsilon\rangle\equiv\exp(-\pi\gamma/2)\,\Gamma(2+i\gamma)\,\frac{\epsilon}{\pi^2}\,\frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{2+i\gamma}}, \tag{3}$$

where the left-hand side is defined by the right-hand side. We introduce the notation

$$\langle\mathbf{p}\,|\mathbf{k}\,\infty\rangle\equiv\lim_{\epsilon\downarrow0}\langle\mathbf{p}\,|\mathbf{k}_\epsilon\rangle. \tag{4}$$

This is the "plus" state $\langle\mathbf{p}\,|\mathbf{k}\,\infty+\rangle$. The + sign will mostly be suppressed. The "minus" state is defined by

$$\langle\mathbf{p}\,|\mathbf{k}_\epsilon-\rangle\equiv\langle\mathbf{p}\,|\mathbf{k}_\epsilon\rangle^*, \tag{5}$$

$$\langle\mathbf{p}\,|\mathbf{k}\,\infty-\rangle\equiv\lim_{\epsilon\downarrow0}\langle\mathbf{p}\,|\mathbf{k}_\epsilon-\rangle. \tag{6}$$

Note that this definition is in analogy to the complete physical scattering state $|\mathbf{k}-\rangle$, for which we have

$$\langle \mathbf{p}|\mathbf{k}-\rangle = \langle \mathbf{p}|\mathbf{k}+\rangle^*.$$

We call $|\mathbf{k}_\epsilon \pm\rangle$ and $|\mathbf{k}\,\infty\pm\rangle$ "Coulombian asymptotic states." The limit $\epsilon \downarrow 0$ in Eqs. (1)–(6) should be carefully defined. We give a precise definition of the asymptotic states in the following theorem. The object h_ϵ appearing in the theorem plays the role of the Coulomb T matrix, as will be shown later on.

Theorem. Let $k \equiv |\mathbf{k}| > 0$ and

$$\langle h_\epsilon|\mathbf{p}\rangle \equiv (p-k-i\epsilon)^{i\gamma} f(\mathbf{p}), \tag{7}$$

with $f \in \mathfrak{L}_\infty(\mathbb{R}^3)$ and $f(\mathbf{p})$ continuous at $\mathbf{p}=\mathbf{k}$. Further let $\langle h_\epsilon|\mathbf{k}_\epsilon\rangle$ mean

$$\langle h_\epsilon|\mathbf{k}_\epsilon\rangle \equiv \int_{\mathbb{R}^3} d\mathbf{p}\,\langle h_\epsilon|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{k}_\epsilon\rangle,$$

where $\langle \mathbf{p}|\mathbf{k}_\epsilon\rangle$ has been defined in Eq. (3). Then

$$\lim_{\epsilon\downarrow 0}\langle h_\epsilon|\mathbf{k}_\epsilon\rangle = f(\mathbf{k})[(2k)^{-i\gamma}\exp(-\pi\gamma/2)\,\Gamma(1-i\gamma)]^{-1}. \tag{8}$$

Proof. The proof is essentially a generalization of Simon's "δ-function computation," see Ref. 5: $\lim_{\epsilon\downarrow 0}\epsilon(x^2+\epsilon^2)^{-1} = \pi\delta(x)$. Using Eqs. (3) and (7) and writing $f(\mathbf{p}) = f(\mathbf{p}) - f(\mathbf{k}) + f(\mathbf{k})$, we see that the proof of Eq. (8) is complete once we have proved the following two equations:

$$\text{(i)}\quad \lim_{\epsilon\downarrow 0}\epsilon \int d\mathbf{p}[f(\mathbf{p})-f(\mathbf{k})](p-k-i\epsilon)^{i\gamma} \times \frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{2+i\gamma}} = 0. \tag{9}$$

$$\text{(ii)}\quad \lim_{\epsilon\downarrow 0}\frac{\epsilon}{\pi^2}\exp(-\pi\gamma/2)\,\Gamma(2+i\gamma)\int d\mathbf{p}(p-k-i\epsilon)^{i\gamma} \times \frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{2+i\gamma}} = \frac{(2k)^{i\gamma}\exp(\pi\gamma/2)}{\Gamma(1-i\gamma)}. \tag{10}$$

(i) The integral in Eq. (9) exists when $\epsilon > 0$ and it is absolutely dominated by

$$\exp(2\pi|\gamma|)\int d\mathbf{p}\,|f(\mathbf{p})-f(\mathbf{k})|\{|\mathbf{p}-\mathbf{k}|^2+\epsilon^2\}^{-2}.$$

Replace the integration variable $\mathbf{p}$ by $\mathbf{q}=\mathbf{p}-\mathbf{k}$ and define the function $g(\cdot)$ by

$$g(q) \equiv \int d\hat{\mathbf{q}}\,|f(\mathbf{q}+\mathbf{k})-f(\mathbf{k})|. \tag{11}$$

Here $\hat{\mathbf{q}}$ denotes the unit vector in the direction of $\mathbf{q}$, and the domain of integration is the unit sphere. Then $g(\cdot)$ is measurable and essentially bounded, so $g \in \mathfrak{L}_\infty$. Furthermore, $g(0)=0$ and $g(q)$ is continuous at $q=0$. It is now sufficient to prove

$$\lim_{\epsilon\downarrow 0}\epsilon\int_0^\infty dq\,\frac{g(q)\,q^2}{(q^2+\epsilon^2)^2} = 0. \tag{12}$$

Take $q \to z = q/\epsilon$, then Eq. (12) becomes

$$\lim_{\epsilon\downarrow 0}\int_0^\infty \frac{dz\,g(\epsilon z)\,z^2}{(z^2+1)^2} = 0.$$

The integrand in this integral converges pointwise to zero and is essentially bounded by $\|g\|_\infty z^2/(z^2+1)^2$, which is integrable, so the integral has zero limit. This proves Eq. (9).

(ii) The integration over the angles in Eq. (10) is easily performed. We have to prove then

$$\lim_{\epsilon\downarrow 0}\epsilon\int_0^\infty \frac{dp\,p}{k(p-k-i\epsilon)^{i\gamma}}[p^2-(k+i\epsilon)^2]^{i\gamma}\{[(p-k)^2+\epsilon^2]^{-1-i\gamma} - [(p+k)^2+\epsilon^2]^{-1-i\gamma}\} = \pi\exp(\pi\gamma)(2k)^{i\gamma}|\Gamma(1+i\gamma)|^{-2}. \tag{13}$$

The integral here exists when $\epsilon > 0$. If one excludes any neighborhood of $p=k$, the integral exists also when $\epsilon = 0$. Consequently, the interval of integration $(0,\infty)$ may be replaced by an arbitrary neighborhood of the point $p=k$. This in turn implies that one may in Eq. (13) replace p/k by 1, $(p+k+i\epsilon)^{i\gamma}$ by $(2k)^{i\gamma}$, and neglect the term containing $[(p+k)^2+\epsilon^2]^{-1-i\gamma}$. Finally, one can simplify the integrand by dropping the factor $(p-k-i\epsilon)^{i\gamma}(p-k-i\epsilon)^{-i\gamma}=1$. All this means that it remains to be proved:

$$\lim_{\epsilon\downarrow 0}\int_0^\infty \frac{\epsilon\,dp}{(p-k)^2+\epsilon^2}\frac{(p-k-i\epsilon)^{i\gamma}}{(p-k+i\epsilon)^{i\gamma}} = \pi\exp(\pi\gamma)|\Gamma(1+i\gamma)|^{-2}. \tag{14}$$

The indefinite integral of the integrand in Eq. (14) is easily found, yielding for the left-hand side,

$$\lim_{\epsilon\downarrow 0} -\frac{1}{2\gamma}\frac{(p-k-i\epsilon)^{i\gamma}}{(p-k+i\epsilon)^{i\gamma}}\Big|_{p=0}^{p=\infty} = -\frac{1}{2\gamma}\left(1-\frac{\exp(\pi\gamma)}{\exp(-\pi\gamma)}\right).$$

Utilizing the well-known equality

$$\Gamma(1+i\gamma)\,\Gamma(1-i\gamma) = \pi\gamma/\sinh\pi\gamma,$$

we find that Eq. (14) is valid, so Eq. (19) has been proved. This completes the proof of the theorem.

Reviewing the above theorem and its proof, we find that the domain of integration $\mathbb{R}^3$, implicitly understood in Eq. (8), can be replaced by any neighborhood $\mathcal{N}(\mathbf{k})$ of the point $\mathbf{p}=\mathbf{k}$. In other words: The asymptotic state $\langle \mathbf{p}|\mathbf{k}\,\infty\rangle$ has *support* $\{\mathbf{k}\}$. We deduce from this that the class of "test functions" h_ϵ can be enlarged by relaxing the restrictions. It is sufficient to require only:

$$\begin{aligned} &f(\mathbf{p}) \text{ continuous at } \mathbf{p}=\mathbf{k} \text{ and } f \in \mathfrak{L}_\infty \text{ in some neighborhood } \mathcal{N}(\mathbf{k}),\\ &\langle h_\epsilon|\mathbf{k}_\epsilon\rangle \text{ well defined for all } \epsilon : \epsilon_0 > \epsilon > 0, \text{ some } \epsilon_0 > 0. \end{aligned} \tag{15}$$

Let the symbol $\mathcal{D}_{h_\epsilon}$ mean: in the sense of "generalized distributions" with the above defined "test functions" $\langle h_\epsilon|\mathbf{p}\rangle \equiv (p-k-i\epsilon)^{i\gamma} f(\mathbf{p})$. Then we have, in a formal compact notation, the *extended theorem*:

$$\langle \mathbf{p}|\mathbf{k}\,\infty\rangle = \delta(\mathbf{p}-\mathbf{k})\lim_{\epsilon\downarrow 0}[(p-k-i\epsilon)^{i\gamma}(2k)^{-i\gamma} \times \exp(-\pi\gamma/2)\,\Gamma(1-i\gamma)]^{-1},\ \mathcal{D}_{h_\epsilon}. \tag{16}$$

III. SOME STATIONARY SCATTERING FORMULAS

In Secs. III A–III C we shall derive the following three formulas:

$$|\mathbf{k}+\rangle = |\mathbf{k}\,\infty\rangle + G_0 V|\mathbf{k}+\rangle, \tag{17}$$

$$|\mathbf{k}+\rangle = |\mathbf{k}\,\infty\rangle + G_0 T|\mathbf{k}\,\infty\rangle, \tag{18}$$

$$\langle \mathbf{k}'\infty - |T|\mathbf{k}\,\infty\rangle = \langle \mathbf{k}'\,\infty - |V|\mathbf{k}+\rangle = \frac{-f^C(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')}{2\pi^2},\quad \hat{\mathbf{k}}' \neq \hat{\mathbf{k}},\quad k' = k \in \mathbb{R}^+. \tag{19}$$

Because of the well-known operator equality $G_0 T = GV$, Eq. (18) implies

$$|\mathbf{k}+\rangle = (\mathbb{1} + GV)|\mathbf{k}\,\infty\rangle. \tag{20}$$

The operators G, G_0, and T are supposed to have argument $(k+i\epsilon)^2$, $\epsilon \downarrow 0$, and f^C is the Coulomb scattering amplitude,

$$f^C(x) = -\frac{\gamma}{2k}\exp(2i\sigma_0)\left(\frac{1-x}{2}\right)^{-1-i\gamma} \tag{21}$$

Note that Eqs. (17)–(20) reduce to well-known equations of standard short-range potential scattering theory if one replaces $|\mathbf{k}\,\infty\rangle$ by the free state $|\mathbf{k}\rangle$. Then Eq. (17) is known as the Lippmann-Schwinger equation and Eq. (19) expresses that the on-shell T matrix is proportional to the amplitude. We call $\langle \mathbf{p}|T|\mathbf{k}\,\infty\rangle$ the physical half-shell T matrix and $\langle \mathbf{k}'\,\infty - |T|\mathbf{k}\,\infty\rangle$ the physical on-shell T matrix $(k'=k)$.

A. Proof of Eq. (17)

In order to derive Eq. (17), we perform the differentiation with respect to ϵ in Eqs. (1) and (2). This gives, at once,

$$\langle \mathbf{p}|\mathbf{k}+\rangle = \lim_{\epsilon\downarrow 0}\langle \mathbf{p}|\mathbf{k}_\epsilon\rangle - \lim_{\epsilon\downarrow 0}\frac{1}{p^2-(k+i\epsilon)^2} \times \exp(-\pi\gamma/2)\,\Gamma(1+i\gamma)\,\frac{k\gamma}{\pi^2}\,\frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{1+i\gamma}}. \tag{22}$$

The second term on the right-hand side is just $\langle \mathbf{p}|G_0V|\mathbf{k}+\rangle$, as can be seen by inspection. Equation (17) is the formal expression of Eq. (22).

B. Proof of Eq. (18)

Secondly, we have to derive Eq. (18). To this end, we prove that $T|\mathbf{k}\,\infty\rangle = V|\mathbf{k}+\rangle$, i.e.,

$$\lim_{\epsilon\downarrow 0}\langle \mathbf{p}|T((k+i\epsilon)^2)|\mathbf{k}_\epsilon\rangle = \langle \mathbf{p}|V|\mathbf{k}+\rangle, \quad \hat{\mathbf{p}}\neq\hat{\mathbf{k}}, \tag{23}$$

where the right-hand side is given by Eq. (1) and $\lim_{\epsilon\downarrow 0}$ is understood. Recalling the theorem, it is clear that we need the behavior of the off-shell Coulomb T matrix $\langle \mathbf{p}|T((k+i\epsilon)^2)|\mathbf{p}'\rangle$ at $p'=k$. For this purpose we consider Eqs. (13)–(18) of Ref. 6. The limit $p'\to k$ means in those equations: $x\to -1$, $y\to 0$. Furthermore, $1+I(y)/x \to (-y)^{i\gamma}\,\Gamma(1+i\gamma)\Gamma(1-i\gamma)$ and $y\to (p^2-k^2)(p'^2-k^2)/(4k^2q^2)$. Assuming $\hat{\mathbf{p}}\neq\hat{\mathbf{p}}'$, we derive from Eqs. (16) and (18) of Ref. 6,

$$\langle \mathbf{p}|T(k^2)|\mathbf{p}'\rangle = k\gamma(\pi q)^{-2}\,\Gamma(1+i\gamma)\,\Gamma(1-i\gamma) \times\left(\frac{(p^2-k^2)(k^2-p'^2)}{4k^2q^2}\right)^{i\gamma} f(p,p';k), \tag{24}$$

where the function f has pleasant properties. Besides on p, p', and k it depends on $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$, but these variables, being unimportant for the discussion, have been suppressed. The variable k is here supposed to be complex, with $\mathrm{Re}k>0$, $\mathrm{Im}k>0$. We let k approach the positive real axis from above. Then f becomes a function of the real positive variables p, p', and k, and this function is continuous at $p=k$ and/or at $p'=k$. Moreover,

$$f(p,k;k)\equiv f(k,p';k)\equiv f(k,k;k)\equiv 1, \tag{25}$$

and this equation is valid for all $\hat{\mathbf{p}}, \hat{\mathbf{p}}'$, provided only that $\hat{\mathbf{p}}\neq\hat{\mathbf{p}}'$. With the above formulas we can derive the physical half-shell limit and, in Sec III C, the physical on-shell limit of the Coulomb T matrix.

Since we wish to apply the theorem to Eq. (24), it is natural to replace k by $k+i\epsilon$ with k real positive. Now let p be fixed with $p\neq k$, and consider the expression between braces in Eq. (24). From the equality

$$[p^2-(k+i\epsilon)^2][(k+i\epsilon)^2-p'^2](k+i\epsilon)^{-2}(k^2+\epsilon^2)^2 = -2ik\epsilon[(k^2+\epsilon^2)^2-p^2p'^2]+(p^2-k^2+\epsilon^2) \times[(k^2+\epsilon^2)^2-p^2p'^2]+p'^2[(p^2-k^2+\epsilon^2)^2+4k^2\epsilon^2], \tag{26}$$

we see that

$$\{[p^2-(k+i\epsilon)^2][(k+i\epsilon)^2-p'^2](k+i\epsilon)^{-2}\}^{i\gamma} \to \exp(-\pi\gamma)\,k^{-2i\gamma}[p^2-(k+i\epsilon)^2]^{i\gamma}[p'^2-(k+i\epsilon)^2]^{i\gamma}, \tag{27}$$

when $p'\to k$, $\epsilon\downarrow 0$. Here γ may be taken real although it depends on $k+i\epsilon$, strictly speaking. We denote now $\mathbf{p}-\mathbf{k}$ by $\mathbf{q}$, which is consistent with the notation $\mathbf{q}=\mathbf{p}-\mathbf{p}'$ of Ref. 6 since $\mathbf{p}'\to\mathbf{k}$. Application of the theorem, in particular Eq. (16), to Eqs. (24) and (27) yields

$$\langle \mathbf{p}|T|\mathbf{k}\,\infty\rangle = \lim_{\epsilon\downarrow 0} k\gamma\pi^{-2} \times\exp(-\pi\gamma/2)\,\Gamma(1+i\gamma)\,q^{-2-2i\gamma}[p^2-(k+i\epsilon)^2]^{i\gamma}. \tag{28}$$

This expression may be identified with $\langle \mathbf{p}|V|\mathbf{k}+\rangle$ because of $\hat{\mathbf{p}}\neq\hat{\mathbf{k}}$ and the proof of Eq. (18) is complete.

We like to point out that Eq. (27) does not hold, in general. The left-hand side of Eq. (27) has its origin in the expression $(-y)^{i\gamma}$ in Eq. (18) of Ref. 6. Because of the logarithmic cut, running along the negative real axis, $(-y)^{i\gamma}$ cannot be replaced by $\exp(-\pi\gamma)\,y^{i\gamma}$, nor by $\exp(\pi\gamma)\,y^{i\gamma}$. In fact, y *can* become real negative, whereas y *cannot* become real positive, if $q>0$ and $\mathrm{Im}k\neq 0$. This can be seen as follows. Owing to $y=(x+1)/(x-1)$, we have $x=(y+1)/(y-1)$ and the assumption $0\leq y\leq 1$ implies $-\infty\leq x\leq -1$, so $x^2\geq 1$. With the help of Eq. (26), where now either $\epsilon>0$ or $\epsilon<0$, this leads indeed to a contradiction.

In this context it is interesting to note the related fact that $\langle \mathbf{p}'|T(k^2)|\mathbf{p}\rangle$ is a meromorphic function in the complex k plane, cut along the real k axis, and with an arbitrary neighborhood of the origin excluded. See Ref. 6, Eqs. (16)–(18) and also (24), where $T_l(k^2)$ has been expressed in terms of Legendre's second function $\mathfrak{Q}_l$. The branch cut of $\mathfrak{Q}_l$ there is just avoided when $\mathrm{Im}k\neq 0$ and $p'\neq p$, as can be shown with the help of Eq. (26).

C. Proof of Eq. (19)

In order to derive Eq. (19), we can apply the theorem at once to Eq. (28). Taking the epsilons in Eqs. (3) and (28) equal, we get

$$\langle \mathbf{k}'_\epsilon - |T|\mathbf{k}\,\infty\rangle_{k'=k} \xrightarrow[\epsilon\downarrow 0]{} \frac{-f^C(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')}{2\pi^2}.$$

However, we arrived at this equation in two successive steps. First the physical half-shell limit has been de-

termined and afterwards the physical on-shell limit. The *direct* physical on-shell limit is

$$\lim_{\epsilon\downarrow 0}\langle \mathbf{k}'_\epsilon - |T((k+i\epsilon)^2)|\mathbf{k}_\epsilon\rangle = \frac{-f^C(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')}{2\pi^2}, \quad k'=k\in\mathbb{R}^+. \tag{29}$$

We like to prove this equation in a direct way. Note that the theorem cannot be applied now. However, the following proof of Eq. (29) is very much like the proof of the theorem.

Insert Eqs. (3) and (24) into the expression

$$\lim_{\epsilon\downarrow 0}\int\int d\mathbf{p}\,d\mathbf{p}'\,\langle \mathbf{k}'_\epsilon - |\mathbf{p}'\rangle\langle \mathbf{p}'|T((k+i\epsilon)^2)|\mathbf{p}\rangle$$
$$\times\langle \mathbf{p}|\mathbf{k}_\epsilon\rangle, \quad k'=k\in\mathbb{R}^+. \tag{30}$$

The asymptotic states have support $\{\mathbf{k}'\}$ and $\{\mathbf{k}\}$, respectively, so we may replace q^2 by $2k^2(1-\hat{\mathbf{k}}\circ\hat{\mathbf{k}}')$ and the function f in Eq. (24) by one, according to Eq. (25). The integrations $\int d\hat{\mathbf{p}}$ and $\int d\hat{\mathbf{p}}'$ are now easily evaluated. Consider further

$$i\,\mathrm{Im}[(p-k-i\epsilon)(k+i\epsilon-p')(k+i\epsilon)^{-1}(k^2+\epsilon^2)]$$
$$= -i\epsilon(k^2+\epsilon^2-pp'),$$

and compare this with Eq. (26). Then it turns out that Eq. (30) can be expressed as

$$\frac{\gamma}{4\pi^2 k}\left(\frac{1-\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'}{2}\right)^{-1-i\gamma}\Gamma^3(1+i\gamma)\,\Gamma(1-i\gamma)\exp(-\pi\gamma)\,L, \tag{31}$$

with

$$L=\lim_{\epsilon\downarrow 0}\left(\frac{\epsilon}{\pi}\right)^2\int_0^\infty dp\int_0^\infty dp'\,\frac{(p-k+i\epsilon)^{-i\gamma}}{(p-k)^2+\epsilon^2}\,\frac{(p'-k+i\epsilon)^{-i\gamma}}{(p'-k)^2+\epsilon^2}$$
$$\times[(p-k-i\epsilon)(k+i\epsilon-p')]^{i\gamma}. \tag{32}$$

Changing variables according to $p-k=\epsilon z$, $p'-k=\epsilon z'$, we get

$$L=\pi^{-2}\int_{-\infty}^\infty\int_{-\infty}^\infty dz\,dz'\,\frac{(z+i)^{-i\gamma}}{z^2+1}\,\frac{(z'+i)^{-i\gamma}}{z'^2+1}$$
$$\times[(z-i)(i-z')]^{i\gamma}. \tag{33}$$

The order of integration is unimportant. Now we have $(z, z'\in\mathbb{R})$

$$\ln(z+i)=\tfrac{1}{2}\ln(z^2+1)+i\,\mathrm{arccot}z$$

and

$$\ln[(z-i)(i-z')]=\tfrac{1}{2}\ln[(z^2+1)(z'^2+1)]$$
$$+i\,\mathrm{arctan}z+i\,\mathrm{arctan}z',$$

where the inverse trigonometric functions are determined by their principal values

$$-\tfrac{1}{2}\pi<\mathrm{arctan}z<\tfrac{1}{2}\pi, \quad 0<\mathrm{arccot}z<\pi.$$

Using these equations we get

$$L=\pi^{-2}\int_{-\infty}^\infty\int_{-\infty}^\infty dz\,dz'\,(z^2+1)^{-1}(z'^2+1)^{-1}$$
$$\times\exp[\gamma(\mathrm{arccot}z-\mathrm{arctan}z+\mathrm{arccot}z'-\mathrm{arctan}z')].$$

This double integral is evaluated by standard means, yielding

$$L=(2\pi\gamma)^{-2}(\exp(-\pi\gamma/2)-\exp(3\pi\gamma/2))^2$$
$$=(\pi\gamma)^{-2}\exp(\pi\gamma)\sinh^2\pi\gamma=\exp(\pi\gamma)\,|\Gamma(1+i\gamma)|^{-4}. \tag{34}$$

Insertion of Eq. (34) into Eq. (31) proves Eq. (29), of which Eq. (19) is the formal expression.

In Sec. IV a different but closely related procedure to obtain the physical on-shell T matrix will be given, see Eq. (51).

Remark. As we said in Sec. I, the asymptotic states defined in the theorem are essentially the asymptotic states introduced by Nutt, see Eq. (15) of Ref. 3. However, Nutt's definition of these states and of the limits $\epsilon\downarrow 0$ is less careful than ours. Also his "minus" state differs from our state $|\mathbf{k}\infty-\rangle$. Probably because of these facts, he finds a different result for the Coulomb scattering amplitude. It contains in particular a factor $(2k/\epsilon^2)^{-2i\gamma}$, having no limit when $\epsilon\downarrow 0$.

IV. CONNECTION WITH TIME-DEPENDENT COULOMB SCATTERING

In the time-dependent scattering theory a basic role is played by Møller's wave operators $\Omega_\pm$, defined by

$$\Omega_\pm = s\text{-}\lim_{t\to\mp\infty}\Omega(t), \tag{35}$$

$$\Omega(t)\equiv\exp(iHt)\exp(-iH_0t), \tag{36}$$

where H is the Hamiltonian $H=H_0+V$. The strong limits in Eq. (35) exist when V has short range, but they do not exist when V is the Coulomb potential. According to Dollard,[7] the following modification has to be made. Define

$$\Omega^C(t)\equiv\exp(iHt)\exp(-iH_0t)\exp[-iA(t)], \tag{37}$$

where H is now the Coulomb Hamiltonian, and the "anomalous" operator $A(t)$ is defined by

$$A(t)\equiv -sH_0^{-1/2}\,\mathrm{sgn}(t)\ln(4H_0|t|), \quad t\neq 0. \tag{38}$$

$\mathrm{sgn}(t)$ denotes the sign of the time t and s is the potential strength, $V(r)=-2s/r$. In Sec. II we chose the notation $V(r)=2k\gamma/r$, but use of the constant s is here preferable. Because $A(t)$ is a function of H_0, Eq. (37) is equivalent to

$$\Omega^C(t)\equiv\exp(iHt)\exp[(-iH_0t)-iA(t)].$$

Dollard[7] proved that the strong limits of $\Omega^C(t)$ exist,

$$\Omega^C_\pm = s\text{-}\lim_{t\to\mp\infty}\Omega^C(t), \tag{39}$$

and that $\Omega^C_\pm$ can be correctly interpreted as the Coulomb wave operators.[8] For example, the improper stationary Coulomb scattering states may be written formally as

$$|\mathbf{k}\pm\rangle=\Omega^C_\pm|\mathbf{k}\rangle. \tag{40}$$

It is customary to introduce ϵ'-dependent wave operators $\Omega_{\epsilon'\pm}$ by means of the Bochner integrals (e.g., Prugovečki,[9] pp. 436 and 456),

$$\Omega_{\epsilon'\pm}\equiv\mp\epsilon'\int_0^{\mp\infty}dt\exp(\pm\epsilon' t)\,\Omega(t), \quad \epsilon'>0. \tag{41}$$

[Here we use ϵ' in order to avoid confusion. Indeed the operators G_0, G, and T turn out to have argument $k^2+i\epsilon'$. For example, Eqs. (36) and (41) yield formally

$$\Omega_{\epsilon'}|\mathbf{k}\rangle = i\epsilon' G(k^2 + i\epsilon')|\mathbf{k}\rangle. \tag{41'}$$

However, in the preceding sections we preferred to take the argument $(k+i\epsilon)^2$. To first order in ϵ we have $\epsilon' = 2k\epsilon$.] For a short-range potential one has (e.g., Ref. 9, p. 437)

$$\Omega_{\pm} = s\text{-}\lim_{\epsilon' \downarrow 0} \Omega_{\epsilon'\pm}. \tag{42}$$

In the case of the Coulomb potential, Eq. (42) has to be modified also. From the paper by Zorbas[10] (see, p. 122: Lemma) it follows that it should be replaced by

$$\Omega_{\pm}^{C} = s\text{-}\lim_{\epsilon' \downarrow 0} \Omega_{\epsilon'\pm} A_{\epsilon'\pm}^{-1}. \tag{43}$$

Here $\Omega_{\epsilon'\pm}$ are the Møller wave operators for the Coulomb potential, defined by Eqs. (36) and (41), and we have introduced the operators $A_{\epsilon'\pm}^{-1}$ which are defined by[11]

$$A_{\epsilon'\pm} \equiv \mp \epsilon' \int_0^{\mp\infty} dt \exp(\pm \epsilon' t) \exp[iA(t)], \quad \epsilon' > 0. \tag{44}$$

Upon substitution of Eq. (38) for $A(t)$, these integrals become essentially gamma-function integrals. Zorbas obtained the following explicit expressions [Ref. 10, Eq. (13), in different notation and with opposite sign convention, cf. Ref. 8],

$$A_{\epsilon'\pm} = \Gamma(1 \pm isH_0^{-1/2})(4H_0/\epsilon')^{\pm isH_0^{-1/2}}. \tag{45}$$

After this survey of the necessary formulas, we are now in a position to make the final step, and to show explicitly the connection with our asymptotic states. The operators $A_{\epsilon'\pm}$, being functions of H_0, are diagonal in momentum representation. From Eq. (45) we get (recall $\epsilon' \to 2k\epsilon$)

$$\langle \mathbf{p}|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = \delta(\mathbf{p}-\mathbf{k})[(2k/\epsilon)^{-i\gamma}\Gamma(1-i\gamma)]^{-1} \tag{46}$$

and

$$\langle \mathbf{p}|A_{2k\epsilon-}^{-1}|\mathbf{k}\rangle = \langle \mathbf{p}|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle^*. \tag{47}$$

Here we have turned back to the Sommerfeld parameter $\gamma \equiv -s/k$, and the + subscript has been suppressed. Note that Eq. (47) can also be obtained from the equality $A_{\epsilon'}^{\dagger} = A_{\epsilon'-}$, which is a consequence of the definition of $A_{\epsilon'\pm}$ [Eq. (44)] and of the equalities [cf. Eq. (38)],

$$A^{\dagger}(t) = A(t) = \mathrm{sgn}(t)\, A(|t|). \tag{48}$$

Now let h_ϵ be a "test function" as defined in Eq. (7),

$$\langle h_\epsilon|\mathbf{p}\rangle \equiv (p - k - i\epsilon)^{i\gamma} f(\mathbf{p}).$$

Then Eq. (46) at once yields

$$\langle h_\epsilon|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = f(\mathbf{k})[(2k)^{-i\gamma}\exp(-\pi\gamma/2)\,\Gamma(1-i\gamma)]^{-1}. \tag{49}$$

Comparison of Eq. (49) with Eq. (8) gives

$$\langle h_\epsilon|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = \lim_{\epsilon \downarrow 0} \langle h_\epsilon|\mathbf{k}_\epsilon\rangle, \tag{50}$$

which we denote formally by [cf. Eq. (16)]

$$|\mathbf{k}\,\infty\rangle \equiv \lim_{\epsilon \downarrow 0} |\mathbf{k}_\epsilon\rangle = \lim_{\epsilon \downarrow 0} A_{2k\epsilon}^{-1}|\mathbf{k}\rangle, \; \mathcal{D}_{h_\epsilon}. \tag{50'}$$

Furthermore, from Eqs. (46), (47), and (24), (25) we obtain

$$\lim_{\epsilon \downarrow 0} \langle \mathbf{k}'|A_{2k\epsilon-}^{\dagger -1}\, T((k+i\epsilon)^2) A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = -f^{C}(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')/(2\pi^2), \quad k' = k, \tag{51}$$

which should be compared with Eqs. (19) and (29). In the three final equations we have the desired connection of the Coulombian asymptotic states with the time-dependent Coulomb scattering formulas in explicit form.

Eventually two remarks are in order.

(i) The "plus" stationary scattering state $|\mathbf{k}+\rangle$ is connected with the limit $t \to -\infty$; the "minus" state $|\mathbf{k}-\rangle$ with $t \to +\infty$. So if we want to interpret the asymptotic states $|\mathbf{k}\,\infty\pm\rangle$ in analogy to $|\mathbf{k}\pm\rangle$, it follows from Eq. (47) that we should have

$$\langle \mathbf{p}|\mathbf{k}\,\infty-\rangle = \langle \mathbf{p}|\mathbf{k}\,\infty\rangle^*,$$

which agrees with the *definition* of $\langle \mathbf{p}|\mathbf{k}\,\infty-\rangle$, see Eqs. (4)–(6).

(ii) It is important to realize that $|\mathbf{k}_\epsilon\rangle$ and $A_{2k\epsilon}^{-1}|\mathbf{k}\rangle$ are objects, stemming from quite different starting points. Their equality in the sense $\mathcal{D}_{h_\epsilon}$ [see Eq. (50')] is very satisfactory, for this shows the way how to interpret $|\mathbf{k}_\epsilon\rangle$ in the time-dependent picture.

V. SUMMARY AND DISCUSSION

In Sec. II we defined asymptotic states $|\mathbf{k}\,\infty\pm\rangle \equiv \lim_{\epsilon \downarrow 0} |\mathbf{k}_\epsilon\pm\rangle$. According to the theorem proved there, these states can be considered as "generalized distributions" defined on a certain class of ϵ-dependent "test functions," see Eq. (16). We showed that the Coulomb T matrix in momentum representation belongs to this class of "test functions." This is an important result since it solves the half-shell and on-shell problems of the Coulomb T matrix. In Sec. III we derived some stationary scattering formulas in which the asymptotic states are applied, see Eqs. (17)–(20). In Sec. IV the connection of our asymptotic states with Dollard's[7] time-dependent formulation and Zorbas's[10] time-independent formulation of Coulomb scattering has been investigated. The main result is here expressed in Eqs. (50) and (51). The approach of this paper differs from the ordinary "screening" approach. With a screened Coulomb potential one gets the ordinary Lippmann-Schwinger equation in place of Eq. (17).

From the time-dependent theory (Sec. IV) it follows that the actual scattering of a particle (occurring at $t \approx 0$, say) should be considered *with respect to its behavior at* $t \to \pm\infty$. The movement of the particle (i.e., the time evolution of the scattering state in Hilbert space) is, at large times, not governed by the usual operator $\exp(-iH_0 t)$, but instead by $\exp[-iH_0 t - iA(t)]$, see Dollard.[7] The time dependence is translated into the ϵ'- dependence with the help of Eqs. (41) and (44). In this way Zorbas[10] obtained "anomalous" operators which we denote by $A_{\epsilon'\pm}$. In the time-independent picture, the improper free state $|\mathbf{k}\rangle$ has to be replaced by $A_{2k\epsilon}^{-1}|\mathbf{k}\rangle$. One can therefore (small ϵ meaning large times) interpret

$$-2\pi^2 \langle \mathbf{k}'|A_{2k\epsilon-}^{\dagger -1}\, T((k+i\epsilon)^2) A_{2k\epsilon}^{-1}|\mathbf{k}\rangle,$$

with $k' = k$ as the amplitude for the probability, to begin with the distorted free state $A_{2k\epsilon}^{-1}|\mathbf{k}\rangle$ and to find, after the scattering has taken place, the distorted free state denoted by $\langle \mathbf{k}'|A_{2k\epsilon-}^{\dagger -1}$. In the same way we interpret

$\langle \mathbf{k}'_\epsilon - | T((k+i\epsilon)^2) | \mathbf{k}_\epsilon \rangle$,

with $k' = k$ as the physical amplitude for an initial distorted free state $|\mathbf{k}_\epsilon\rangle$ and a final distorted free state $\langle \mathbf{k}'_\epsilon - |$. Translating back to the time-dependent picture, we get the correct description of the physical scattering process.

In conclusion we can say that the approaches with our asymptotic states $|\mathbf{k}_\epsilon \pm\rangle$ on the one hand, and with the operators $A^{-1}_{2k\epsilon\pm}$ which follow from the paper by Zorbas on the other hand, are equivalent in the sense of Eqs. (50) and (51).

The ideas concerning a "renormalization procedure," as the application of Eq. (16), or something like it, has been called sometimes, have been living in the literature since a long time. A list containing all relevant papers by other authors on this subject would become rather extensive.

The present paper clarifies some obscure points, it shows precisely *how* the asymptotic states can be applied, and, in particular from the connection with the time-dependent theory, it makes clear *why* just the "renormalization procedure" of Eq. (16) should be applied. In general, our asymptotic states restore the analogy of the stationary two-body Coulomb-like potential scattering formulae with the standard scattering formulae. This will be worked out in a subsequent paper, where we shall also have occasion to discuss the approaches by other authors.

From the theorem and Eqs. (16)–(20) it can be seen that $|\mathbf{k}^\infty\rangle$ is particularly suited to the two-body Coulomb T operator at energy $k^2 > 0$. Furthermore, we can show by means of explicit formulas that exactly the same asymptotic states can be applied to the total T operator when a short-range potential is added to the Coulomb potential. Because the two-body T operator is the basic object in N-body stationary scattering theory, we hope that the approach of this paper can be extended to multiparticle stationary scattering theory involving charged particles.

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[1] I. W. Herbst, Commun. Math. Phys. 35, 181 (1974).
[2] J. R. Taylor, Nuovo Cimento 23 B, 313 (1974).
[3] G. L. Nutt, J. Math. Phys. 9, 796 (1968).
[4] E. Guth and C. J. Mullin, Phys. Rev. 83, 667 (1951).
[5] B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms* (Princeton U. P., New York, 1971), p. 128.
[6] H. van Haeringen and R. van Wageningen, J. Math. Phys. 16, 1441 (1975).
[7] J. D. Dollard, J. Math. Phys. 5, 729 (1964).
[8] Note that our $\Omega^C_\pm$ is Dollard's Ω^τ_C.
[9] E. Prugovečki, *Quantum Mechanics in Hilbert Space* (Academic, New York, 1971).
[10] J. Zorbas, Lett. Nuovo Cimento 10, 121 (1974).
[11] The notation here is not standard. With the usual notation $\Omega_{\pm\epsilon'}$, $A_{\pm\epsilon'}$ one might be tempted to put $\epsilon' \to -\epsilon'$, $A_{\epsilon'} \to A_{-\epsilon'}$, which is obviously incorrect.

A characterization of the Einstein tensor in terms of spinors

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All tensors of contravariant rank two which are divergence-free on one index, concomitants of a spinor field $\sigma_{iAX'}$ together with its first two partial derivatives, and scalars under spin transformations are constructed. The Einstein and metric tensors are the only candidates.

1. INTRODUCTION

It is usually assumed that the field equations governing the interaction of the gravitational field with any other field (the latter having associated with it an energy–momentum tensor T^{ij}) are of the form

$$A^{ij} = T^{ij}, \tag{1.1}$$

where A^{ij} are the components of a type (2,0) tensor which is constructed only from those field variables characterizing the gravitational field. Furthermore, it is customary to demand that the choice of A^{ij} be restricted by the *identity*

$$A^{ij}{}_{|j} = 0, \tag{1.2}$$

in order that, as a consequence of (1.1), we have

$$T^{ij}{}_{|j} = 0.$$

Typically, if it is assumed that

(i) the gravitational field is characterized by a symmetric metric tensor g_{ab}, and

(ii) the quantities A^{ij} are constructed from g_{ab} and its first two partial derivatives, i.e.,

$$A^{ij} = A^{ij}(g_{ab}; g_{ab,c}; g_{ab,cd}), \tag{1.3}$$

then it is known that,[1] in a four-dimensional space, (1.2) and (1.3) imply that

$$A^{ij} = aG^{ij} + bg^{ij}, \tag{1.4}$$

where a, b are constants, and G^{ij} is the Einstein tensor. In this case (1.4) and (1.1) give rise to the usual Einstein field equations, where T^{ij} now satisfy

$$T^{ij} = T^{ji}. \tag{1.5}$$

However, it has been claimed by some,[2,3] that T^{ij} should be nonsymmetric, in which case, as has been pointed out by Ehlers,[4] in order to accommodate this possibility, the assumptions (i) and (ii) would have to be changed. The purpose of this note is to discuss the consequence of adopting one possible alternative to (i) and (ii).

It is known that the gravitational field can be characterized in terms of a spinor field $\sigma_{iAX'}$ or a tetrad field $\underset{(\alpha)}{h}{}^{i}$ $(\alpha = 1, \ldots, 4)$, these two characterizations being equivalent by virtue of the relations

$$\sigma_{iAX'} = \underset{(\alpha)}{h}{}^{i}\, \sigma_{\alpha AX'},$$

the $\sigma_{\alpha AX'}$ being the conventional Pauli spin matrices. These quantities are related to the metric by

$$g_{ij} = \sigma_{iAX'}\sigma_{jBY'}\epsilon^{AB}\epsilon^{X'Y'} = \sigma_{iAX'}\sigma_{j}^{AX'}. \tag{1.6}$$

Guided by these observations, and (1.3), *we shall therefore seek all tensors* A^{ij} *satisfying* (1.2) *and for which*

$$A^{ij} = A^{ij}(\sigma_{aAX'}; \sigma_{aAX',b}; \sigma_{aAX',bc}), \tag{1.7}$$

where A^{ij} *are also assumed to be invariant under arbitrary (unimodular) spin transformations.*

This problem is equivalent to finding all tensors A^{ij} satisfying (1.2) and

$$A^{ij} = A^{ij}(\underset{(\alpha)}{h}{}^{a}; \underset{(\alpha)}{h}{}^{a}{}_{,b}; \underset{(\alpha)}{h}{}^{a}{}_{,bc}), \tag{1.8}$$

where A^{ij} are scalars under arbitrary proper Lorentz transformations. Skew-symmetric tensors satisfying (1.2) and (1.8) are known;[5] however they are not scalars under arbitrary proper Lorentz transformations.

It is clear from (1.6) that every spin–tensor which is a concomitant of g_{ij} and its partial derivatives is always a concomitant of $\sigma_{iAX'}$ and its partial derivatives. If the converse to this were valid, then the above problem, viz. (1.2) and (1.7) would immediately reduce to (1.2) and (1.3), and so, without further calculation (1.4) would follow. Unfortunately a proof of the converse does not seem to exist in the literature.

The spinor notation which we adopt here is essentially that of Pirani.[6] From (1.6) it can be shown that the following is an identity (Schmutzer[7]):

$$\sigma^{aAY'}\sigma^{b}{}_{BY'}\sigma^{cBX'} = \tfrac{1}{2}(g^{ab}\sigma^{cAX'} + g^{bc}\sigma^{aAX'} - g^{ac}\sigma^{bAX'} + i\epsilon^{abcd}\sigma_{d}{}^{AX'}). \tag{1.9}$$

If we define $S^{ab}{}_{A}{}^{B}$ and $S^{ab}{}_{X'}{}^{Y'}$ by

$$S^{ab}{}_{A}{}^{B} = \sigma^{a}{}_{AX'}\sigma^{bBX'} - \sigma^{b}{}_{AX'}\sigma^{aBX'}, \tag{1.10}$$

$$S^{ab}{}_{X'}{}^{Y'} = \sigma^{a}{}_{AX'}\sigma^{bAY'} - \sigma^{b}{}_{AX'}\sigma^{aAY'}, \tag{1.11}$$

then repeated application of (1.9) gives rise to

$$\sigma_{t_{BX'}} S^{ab}{}_{A}{}^{B} + \sigma_{t_{AY'}} S^{ab}{}_{X'}{}^{Y'} = 2(\delta^{a}_{t}\sigma^{a}{}_{AX'} - \delta^{a}_{t}\sigma^{b}{}_{AX'}). \quad (1.12)$$

2. CHARACTERIZATION OF A^{rs}

Because the A^{ij} are assumed to satisfy (1.7) and to be the components of a type (2,0) tensor under arbitrary coordinate transformations, certain invariance identities[8] must be satisfied, one of which is

$$A^{rs;aAX',bc} + A^{rs;cAX',ab} + A^{rs;bAX',ca} = 0, \quad (2.1)$$

where $A^{rs;aAX',bc} = \partial A^{rs}/\partial \sigma_{aAX',bc}$ is a spin–tensor symmetric in bc.

The invariance of A^{ij} under spinor transformations also gives rise to invariance identities,[8] two of which are

$$A^{rs;tAX',cd}\sigma_{tBX'} = \tfrac{1}{2}\delta^{A}_{B}A^{rs;tCX',cd}\sigma_{tCX'}, \quad (2.2)$$

and

$$A^{rs;tAX',cd}\sigma_{tAY'} = \tfrac{1}{2}\delta^{X'}_{Y'}A^{rs;tAZ',cd}\sigma_{tAZ'}. \quad (2.3)$$

If we define the spin–tensor $A^{rs;ab,cd}$ by

$$A^{rs;ab,cd} = A^{rs;aAX',cd}\sigma^{b}{}_{AX'}, \quad (2.4)$$

then (2.1) gives rise to

$$A^{rs;ab,cd} + A^{rs;db,ac} + A^{rs;cb,da} = 0. \quad (2.5)$$

If we multiply (2.2) by $S^{ab}{}_{A}{}^{B}$, (2.3) by $S^{ab}{}_{X'}{}^{Y'}$ and add the resulting equations we find, by virtue of (1.12),

$$A^{rs;ab,cd} = A^{rs;ba,cd}. \quad (2.6)$$

From (2.5) and (2.6) it is easily seen that

$$A^{rs;ab,cd} = A^{rs;cd,ab}. \quad (2.7)$$

Up to the present, no use has been made of (1.2), which in view of (1.7) can be expressed in the form

$$A^{rs;aAX',cd}\sigma_{aAX',cds} + O^{r}(\sigma_{aAX'};\sigma_{aAX',b};\sigma_{aAX',bc}) = 0. \quad (2.8)$$

Differentiation of (2.8) with respect to $\sigma_{aAX',cds}$ thus yields

$$A^{rs;aAX',cd} + A^{rd;aAX',sc} + A^{rc;aAX',ds} = 0,$$

which, by (2.4), is equivalent to

$$A^{rs;ab,cd} + A^{rd;ab,sc} + A^{rc;ab,ds} = 0. \quad (2.9)$$

If we define $A^{rs;ab,cd;ij,kl}$ by

$$A^{rs;ab,cd;ij,kl} = (\partial A^{rs;ab,cd}/\partial \sigma_{iBY',kl})\sigma^{j}{}_{BY'}, \quad (2.10)$$

and note (2.4), we see that

$$A^{rs;ab,cd;ij,kl} = A^{rs;ij,kl;ab,cd}. \quad (2.11)$$

Elsewhere[1] it has been shown that, in a four-dimensional space, if $A^{rs;ab,cd;ij,kl}$ is any quantity which has the properties (2.5), (2.6), (2.7), (2.9), and (2.11) then

$$A^{rs;ab,cd;ij,kl} = 0. \quad (2.12)$$

[An alternative proof of (2.12), which readily suggests generalizations to higher dimensional spaces, is presented in the Appendix.]

A comparison of (2.12) and (2.10) establishes that $A^{ij;ab,cd}$ is independent of $\sigma_{iBY',kl}$, which, in turn, implies that $A^{ij;ab,cd}$ is also independent of $\sigma_{iBY',k}$,[9] i.e.,

$$A^{rs;ab,cd} = B^{rsabcd}(\sigma_{iAX'}), \quad (2.13)$$

where B^{rsabcd} is a spin–tensor with the same symmetry properties as $A^{rs;ab,cd}$, viz. (2.5), (2.6), (2.7), and (2.9).

From (2.4) and (2.13) we thus find

$$A^{rs;aAX',cd} = B^{rsabcd}\sigma_{b}{}^{AX'},$$

which, upon integration, yields

$$A^{rs} = B^{rsabcd}\sigma_{b}{}^{AX'}\sigma_{aAX',cd} + C^{rs}(\sigma_{aAX'};\sigma_{aAX',b}). \quad (2.14)$$

From (1.6) we see that

$$g_{ab,cd} = \sigma_{aAX',cd}\sigma_{b}{}^{AX'} + \sigma_{a}{}^{AX'}\sigma_{bAX',cd} + O_{abcd}(\sigma_{iAX'};\sigma_{iAX',j}).$$

When this is taken together with (2.14), it gives rise to

$$A^{rs} = \tfrac{1}{2}B^{rsabcd}g_{ab,cd} + D^{rs}(\sigma_{aAX'};\sigma_{aAX',b}),$$

which can be reexpressed[10] in the form

$$A^{rs} = \tfrac{1}{3}B^{rsabcd}R_{cabd} + B^{rs}(\sigma_{aAX'};\sigma_{aAX',b})$$

where B^{rs} is now a spin–tensor, which is therefore independent of $\sigma_{aAX',b}$, i.e.,

$$A^{rs} = \tfrac{1}{3}B^{rsabcd}R_{cabd} + B^{rs}(\sigma_{aAX'}). \quad (2.15)$$

All spin–tensors $B^{rs} = B^{rs}(\sigma_{aAX'})$ have been constructed[9] the result being

$$B^{rs} = bg^{rs}, \quad (2.16)$$

where b is a real constant.

Consequently, the problem of determining A^{rs} has reduced to the evaluation of the spin–tensor B^{rsabcd} where $B^{rsabcd} = B^{rsabcd}(\sigma_{iAX'})$ and where B^{rsabcd} satisfies (2.5), (2.6), (2.7), and (2.9). To do this we proceed somewhat indirectly, as follows.

It is easily seen that, because of the symmetry properties of B^{rsabcd},

$$B^{rtaicj}\delta^{sbd}_{tij} = 2(B^{rsabcd} + B^{rbadcs} + B^{rdascb}),$$

from which we obtain

$$B^{rtaicj}\delta^{sbd}_{tij} + B^{rtbicj}\delta^{sad}_{tij} + B^{rtaidj}\delta^{sbc}_{tij} + B^{rtbidj}\delta^{sac}_{tij} = 12B^{rsabcd}. \quad (2.17)$$

If we define

$$\beta^{ra}{}_{l}{}^{c} = -\tfrac{1}{12}\epsilon_{tijl}B^{rtaicj}, \quad (2.18)$$

and recall that

$$\delta^{sbd}_{tij} = -\epsilon^{sbdl}\epsilon_{tijl},$$

we see that (2.17) reads

$$B^{rsabcd} = \epsilon^{sbdl}\beta^{ra}{}_{l}{}^{c} + \epsilon^{sadl}\beta^{rb}{}_{l}{}^{c} + \epsilon^{sbcl}\beta^{ra}{}_{l}{}^{d} + \epsilon^{sacl}\beta^{rb}{}_{l}{}^{d}. \quad (2.19)$$

Consequently a knowledge of $\beta^{ra}{}_{l}{}^{c}$ determines B^{rsabcd}.

From (2.18) we note that

$$\beta^{ra}{}_{l}{}^{c} = \beta^{ra}{}_{l}{}^{c}(\sigma_{iAX'}) \quad (2.20)$$

and

$$\beta^{ra}{}_{l}{}^{c} = -\beta^{rc}{}_{l}{}^{a} \quad (2.21)$$

$$\beta^{ra}{}_{l}{}^{l} = 0. \quad (2.22)$$

We now define

$$\beta_{ABCDX'Y'Z'W'} = \sigma_{rAX'}\sigma_{aBY'}\sigma_{cCZ'}\sigma^{l}{}_{DW'}\beta^{ra}{}_{l}{}^{c}, \tag{2.23}$$

in which case (2.21) and (2.22) imply

$$\beta_{ABCDX'Y'Z'W'} = -\beta_{ACBDX'Z'Y'W'}, \tag{2.24}$$

and

$$\epsilon^{BD}\epsilon^{Y'W'}\beta_{ABCDX'Y'Z'W'} = 0, \tag{2.25}$$

respectively. From arguments similar to those presented in Lemma A3 of Ref. 9, we find by virtue of (2.24) and (2.25)

$$\beta_{ABCDX'Y'Z'W'} = ic[\epsilon_{BC}\epsilon_{AD}(\epsilon_{X'Y'}\epsilon_{Z'W'} + \epsilon_{X'Z'}\epsilon_{Y'W'}) - \epsilon_{Y'Z'}\epsilon_{X'W'}(\epsilon_{AB}\epsilon_{CD} + \epsilon_{AC}\epsilon_{BD})],$$

where c is a real constant. The latter is substituted in (2.23) which is then solved for $\beta^{ra}{}_{l}{}^{c}$, (1.9) being used repeatedly in the process, this giving rise to

$$\beta^{ra}{}_{l}{}^{c} = \tfrac{1}{3}a\epsilon^{racm}g_{lm}, \tag{2.26}$$

where a is a real constant. Equations (2.16), (2.19), and (2.26) are now substituted in (2.15) to yield

$$A^{rs} = aG^{rs} + bg^{rs}.$$

We thus have the following theorem.

Theorem: *If* $A^{rs} = A^{rs}(\sigma_{aAX'};\sigma_{aAX',b};\sigma_{aAX',bc})$ *is a spin–tensor and*

$$A^{rr}{}_{;s} = 0,$$

then

$$A^{rs} = aG^{rs} + bg^{rs}$$

where a, b *are constants*.

Consequently, we see that, even in this case, the symmetry of A^{rs} [and hence of T^{rs} by (1.1)] is again an inevitable consequence.

APPENDIX

The purpose of this appendix is to outline an alternative derivation of Eq. (2.12) which explicitly exhibits the role played by the dimensionality of the space. We begin by introducing quantities α_{ab} and β_{ij} which are both assumed to be symmetric in their indices but are otherwise arbitrary, and consider the expression

$$A^{ri_1;ai_2;ci_3;ii_4;hi_5}\delta^{s\ b\ d\ j\ h}_{i_1i_2i_3i_4i_5}\alpha_{ab}\alpha_{cd}\beta_{ij}\beta_{hk}.$$

By expanding the Kronecker delta and by repeatedly invoking the symmetries of $A^{rsi;ab,cd;ij,hk}$, viz. (2.5), (2.6), (2.7), and (2.9), as well as the symmetries induced by the expression $\alpha_{ab}\alpha_{cd}\beta_{ij}\beta_{hk}$ a lengthy, but nevertheless straightforward calculation, shows that

$$A^{ri_1;ai_2;ci_3;ii_4;hi_5}\delta^{s\ b\ d\ j\ h}_{i_1i_2i_3i_4i_5}\alpha_{ab}\alpha_{cd}\beta_{ij}\beta_{hk} = \tfrac{9}{2}[4A^{rsi;ab,cd;ij,hk} + A^{rsi;ab,ij;cd,hk}]\alpha_{ab}\alpha_{cd}\beta_{ij}\beta_{hk}. \tag{A1}$$

This equation holds irrespective of the dimension of the underlying space. However, for $n=4$, the left-hand side of (A1) vanishes identically in which case it is easily seen, on account of the arbitrary nature of the α_{ab} and β_{ij}, that

$$8A^{rsi;ab,cd;ij,hk} + A^{rsi;ab,ij;hk,cd} + A^{rsi;ab,hk;cd,ij} = 0. \tag{A2}$$

By successively interchanging the pairs (cd), (ij), and (hk) in (A2), it thus follows that

$$A^{rsi;ab,cd;ij,hk} = 0$$

as required.

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[1]D. Lovelock, J. Math. Phys. **13**, 874 (1972).
[2]O. Costa de Beauregard, "Translational Inertial Spin Effect," in *Perspectives in Geometry and Relativity*, *Hlavaty Festschrift* (University of Indiana Press, Bloomington, 1966), p. 44.
[3]D.W. Sciama, Proc. Cambridge Philos. Soc. **54**, 72 (1958).
[4]J. Ehlers, *Survey of General Relativity Theory. Relativity*, *Astrophysics and Cosmology* (Reidel, Holland, 1973), p. 1.
[5]B.O.J. Tupper, Can. Math. Bull. **16**, 111 (1972).
[6]F.A.E. Pirani, in *Lectures on General Relativity*, Summer Institute in Theoretical Physics, Brandeis (Prentice-Hall, Englewood Cliffs, N.J., 1965), Vol. 1, p. 249.
E. Schmutzer, *Relativistische Physik* (Akademische Verlaggesellschaft, Leipzig, 1968).
[8]J. Wainwright, Tensor **19**, 217 (1968).
[9]I.M. Anderson, Gen. Rel. Grav. **6**, 621 (1974).
[10]D. Lovelock and H. Rund, *Tensors, Differential Forms and Variational Principles* (Wiley-Interscience, New York, 1975).

Consequences of scaling in nonlinear partial differential equations*

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Scaling of the form $x = ax'$, $t = a^h t'$, $q = a^m Q$ of a nonlinear partial differential equation for q is connected with the form of the auxiliary functions in an inverse scattering method (AKNS scheme). Solvability of an equation by this scheme is treated. It is shown that only equations with $m = 2$ are solvable by using the method of inverse scattering in conjunction with the Schrödinger eigenvalue equation. The criterion $m = 2$ restricts the form of the terms in these equations. The terms, powers of q and its derivatives, can be found by inspection. A separate problem, the decay of a single soliton in the Korteweg–de Vries equation with damping, is solved using only scaling properties.

1. INTRODUCTION

Many nonlinear partial differential equations are invariant under scaling. An example is the Korteweg–de Vries equation[1] (KdV)

$$q_t + 12qq_x + q_{xxx} = 0. \tag{1.1}$$

The scaling

$$x' = ax, \quad t' = a^h t, \quad q(x,t) = a^m Q(x',t'), \tag{1.2}$$

with the choice

$$h = 3, \quad m = 2,$$

leaves (1.1) invariant. The scaling has been used to find polynomial conservation laws.[2,3]

Here we will give some other consequences of this scaling invariance, and give some examples. In Sec. 2 scaling in the formulation of Ablowitz *et al.*[4] (AKNS scheme for short) is treated. Assuming a scalable equation, it is shown that only terms of a certain type can occur in the various auxiliary polynomials. It should be stated here that some nonscalable equations are exactly solvable in the AKNS scheme. Such equations are not treated. A restriction is found for solvability of a scalable equation. In Sec. 3 we prove that a scaling invariant equation can only be solved by an inverse scattering method on the Schrödinger equation when $m = 2$ in (1.2). This determines the type of terms in that equation. It is expected that possible higher order inverse scattering schemes have similar properties. Nonlinear partial differential equations often describe some physical situation to a first order approximation in some small parameter. Dissipation of energy (damping) can be an important higher order correction to the equation. As an example, the KdV equation with damping is treated in Sec. 4. The functional form of the time dependence of a single soliton is shown to depend only on the power in the damping law. Only the scaling properties are used in the derivation.

2. SCALING IN THE AKNS SCHEME

Some nonlinear partial differential equations can be solved exactly by an inverse scattering method with the set of linear equations[4]

$$v_{1x} + i\zeta v_1 = qv_2, \quad v_{2x} - i\zeta v_2 = rv_1, \tag{2.1}$$

where

$$v_{1t} = Av_1 + Bv_2, \quad v_{2t} = Cv_1 - Av_2. \tag{2.2}$$

For equations invariant to a shift in x and t the functions A, B, C, and r are functions of x and t as functionals of $q, q_x, \cdots$. They can also be functions of the parameter ζ. The nonlinear equation of interest is one of the consistency conditions of (2.1) and (2.2), obtained by cross differentiation

$$q_t - 2Aq - B_x - 2i\zeta B = 0. \tag{2.3}$$

Two other conditions are

$$A_x = qC - rB, \tag{2.4a}$$

$$C_x = r_t + 2Ar + 2i\zeta C. \tag{2.4b}$$

For A, B, C, and r we choose polynomials in q, q_x, . . . , and ζ. In addition, the equation for r, (2.4b), has to be consistent with (2.3).

The scaling (1.2) leads to restrictions on the type of terms we can have in these polynomials. Without loss of generality we can take for the scaling of the new quantities in (2.1),

$$\begin{aligned} &v_1 = a^j V_1(x',t'), \quad v_2 = V_2(x',t'), \\ &\zeta = aZ, \quad r = a^n R(x',t'). \end{aligned} \tag{2.5}$$

Equation (2.1) is invariant if we choose for j and n

$$j = m - 1, \quad n = 2 - m. \tag{2.6}$$

Equation (2.2) is also invariant, and A, B, and C scale as

$$\begin{aligned} &A = a^h A'(Q(x',t'), Q'_x, \ldots, Z), \\ &B = a^{h+j} B'(Q', Q'_x, \ldots, Z), \\ &C = a^{h-j} C'(Q', Q'_x, \ldots, Z). \end{aligned} \tag{2.7}$$

A, B, and C are homogeneous functions of a. Often A, B, and C are polynomials in q, the derivatives q_x, q_{xx}, . . . , and ζ. In this case each term in the polynomial must have the same scaling power as the polynomial itself. This determines the type of terms that can occur in this polynomial. The terms in polymial conservation laws can be found this way.

As an example, consider the KdV equation, for which $m = 2$ and $h = 3$. It follows that $j = 1$,

$$A = a_1\zeta^3 + a_2\zeta q + a_3 q_x,$$
$$B = b_1\zeta^4 + b_2\zeta^2 q + b_3\zeta q_x + b_4 q_{xx} + b_5 q^2, \tag{2.8}$$
$$C = c_1\zeta^2 + c_2 q,$$

and r is constant, as its power $n=0$. These are indeed the terms that appear. The complex coefficients $a_1, \ldots, c_2$ can easily be calculated.

For the nonlinear Schrödinger equation [Eq. (2.14) with $s=2$], $m=1$ and $h=2$. We find for A

$$A = a_1\zeta^2 + a_2\zeta q + a_3\zeta q^* + a_4 q q^* + a_5 q_x + a_6 q_x^*. \tag{2.9}$$

B and C contain the same terms, as the parameter $j=0$. For r, with parameter $n=1$, we have

$$r = d_1\zeta + d_2 q + d_3 q^*. \tag{2.10}$$

Not all terms actually appear, as (2.3) and (2.4) give additional restrictions. The MKdV equation [Eq. (2.12) with $s=2$] also has the forms (2.9) and (2.10).

The different terms in the equation for $u = v_1/v_2$, can be obtained. However, not all terms have the same invariance properties under the transformation $(u,\zeta) \to (\pm u, \pm\zeta^*)$ used in the derivation of Bäcklund transformations,[5] so the Bäcklund transformation cannot be found by inspection. If it exists, it has the right scaling properties (compare the explicit forms in Ref. 5). This scaling of the Bäcklund transformation was known earlier for the sin-Gordon equation.[6]

The homogeneity of A, B, and C has another consequence. Successive partial differentiations of for example A, with respect to the continuous parameter a (Q, x', t' and Z fixed) at $a=1$ (Euler's theorem) gives

$$\zeta\frac{\partial A}{\partial\zeta} + mq\frac{\partial A}{\partial q} + (m+1)q_x\frac{\partial A}{\partial q_x} + \cdots = hA,$$
$$\zeta^2\frac{\partial^2 A}{\partial\zeta^2} + 2m\zeta q\frac{\partial^2 A}{\partial\zeta\partial q} + m^2q^2\frac{\partial^2 A}{\partial q^2} + 2m(m+1)qq_x\frac{\partial^2 A}{\partial q\partial q_x} + \cdots = h(h-1)A, \tag{2.11}$$

For h positive and integral the rhs is zero after h differentiations. For positive integer m this can only happen if each of the partial derivatives is zero. Thus A, B, and C are polynomials in $q, q_x, \ldots$, and ζ. If $m=0$, all terms except the ones with q have to be zero. A can then be an arbitrary function of q, times a function of $q_x, \ldots$, and ζ. This is the case for the sin-Gordon equation.[4,7] For $m=-1$ we have the same property with q_x.

The above can decide whether a given equation fits the AKNS scheme. For example, for a generalized KdV equation

$$q_t + 2(s+1)(s+2)/s^2 q^s q_x + q_{xxx} = 0, \tag{2.12}$$

with $s=\frac{1}{2}$,[8] the parameter $m=4$. With (2.6) we have $j=3$ and $n=-2$. B is of the sixth order in a, and has to contain a term $q^{3/2}$. This gives the term $q^{1/2}q_x$ in (2.12). But then the sixth partial derivative with respect to q does not give zero, (2.11) is violated, and we conclude that (2.12) does not fit in the AKNS scheme.

If the order s in (2.12) is greater than 2, we have the noninteger scaling

$$ms = h-1 = 2, \quad m = 2/s. \tag{2.13}$$

Similarly, the equations with $s>2$ do not fit the AKNS scheme. B is of order $2+2/s$ in q, and contains a term q^{s+1}. The rhs has noninteger power, and does not vanish after $s+1$ differentiations. This excludes a polynomial for B. The same is true for higher order nonlinear Schrödinger equations

$$iq_t + q_{xx} + 2(s+2)/s^2|q|^s q = 0. \tag{2.14}$$

Here A has a term $|q|^s$, giving $|q|^s q$ in the equation. After h differentiations the lhs still contains a term q^{s-h}, and (2.11) is violated.

Another way to decide whether a given equation fits the AKNS scheme uses the conservation laws. An equation that fits the AKNS scheme has an infinite number of these.[7] It is easily verified that there is one for each scaling power,

$$I_n(q) = a^n I_n'(Q). \tag{2.15}$$

Some way be trivial, for example, the even ones for the KdV equation.

Conversely, an equation that does not have the sequence (2.15) does not fit in the AKNS scheme. It is relatively straightforward to find a nontrivial conservation law with a given scaling, if it exists. By verifying the first few conservation laws we can see easily if a given equation fits the AKNS scheme. As an example, for the generalized KdV equation (2.12) we find conservation laws of power $2/s-1$ and $4/s-1$,

$$\frac{\partial}{\partial t} I_{2/s-1} = \frac{\partial}{\partial t}\int q\, dx = 0, \tag{2.15a}$$

$$\frac{\partial}{\partial t} I_{4/s-1} = \frac{\partial}{\partial t}\int q^2\, dx = 0, \tag{2.15b}$$

but a conservation law with power 1,

$$\frac{\partial}{\partial t}\int q^s\, dx = -\frac{s(s-1)(s-2)}{2}\int q^{s-3}q_x^3\, dx, \tag{2.15c}$$

only exists for $s=1$ and $s=2$. As seen above, (2.12) for $s=1/2$ or $s>2$ does not fit the AKNS scheme.

3. EQUATIONS SOLVABLE BY THE INVERSE SCATTERING METHOD FOR THE SCHRÖDINGER EQUATION

From (2.1) we have

$$v_{2xx} + (\zeta^2 - rq)v_2 + r_x v_1 = 0. \tag{3.1}$$

This is the Schrödinger equation for an inverse scattering method, with rq as potential, if r_x is zero.

Then the parameter n is zero, and we have with (2.6)

$$n=0, \quad m=2, \quad j=1. \tag{3.2}$$

So only equations with scaling parameter $m=2$ can be solved by inverse scattering on the Schrödinger equation. The parameter h is not determined by this argument. The terms in the equation for q are now completely determined for given h. As the first example, for $h=3$ we find the terms of the KdV equation (1.1).

For $h=5$ we have the form

$$q_t + P_1 q^2 q_x + (P_2 q q_{xxx} + P_3 q_x q_{xx}) + q_{xxxxx} = 0, \tag{3.3}$$

where terms transformable into one another have been grouped together with parentheses. We can establish the terms in A, B, and C, as done above, and calculate the constants p with (2.3) and (2.4). This gives

$$P_1 = 3rP_2, \quad P_3 = 2P_2. \tag{3.4}$$

Equation (3.3) is identical to the one given by Gardner *et al.*[1] (p. 132), after an independent scaling of q and t to change the coefficients. The next one, for $h=7$, is obtained in a similar way. With $r=-1$ we find

$$q_t + 110q^3q_x + 70(q^2q_{xxx} + 4qq_xq_{xx} + q_x{}^3) + 14(qq_{\mathrm{V}} + 3q_xq_{\mathrm{IV}} + 5q_{xx}q_{xxx}) + q_{\mathrm{VII}} = 0. \tag{3.5}$$

(The roman subscripts denote the number of x derivatives.) Existence of these equations is not guaranteed by scaling alone, as the recursion relations for the coefficients of the terms in A, B, and C which follow from (2.3) and (2.4) are overdetermined.

Another way of calculating the coefficients in (3.3) is with the conservation laws. The terms in the conservation laws only depend on m, but the coefficients can differ with the different equations. As we want (3.3) to be exactly solvable we can assume the same conservation laws as for the KdV equation. From (2.15b) we find the last ratio of (3.4), and from the next conservation law

$$I_5 = \int (q^3 + bq_x^2)\,dx, \qquad P_1 = -(3/2b)P_2, \quad P_2 = -15/3b. \tag{3.6}$$

With the coefficient $b=-\frac{1}{2}$ as for the KdV equation we have the first ratio of (3.4), with $r=-1$ and $P_2=10$. The coefficients in (3.5) could be found similarly. We then have to use I_7 also.

4. DAMPING IN THE KdV EQUATION

The KdV equation with damping will be treated in this section, as a different application of the scaling properties. Energy dissipation, accounted for by damping, is an important higher order effect in some physical applications of the KdV equation.[10] If the damping is weak it can be taken into account by damping each Fourier mode separately.[11] Our example, the KdV equation with damping, is

$$q_t + 12qq_x + q_{xxx} + \mathrm{FT}^{-1}[\gamma(k)q(k)] = 0. \tag{4.1}$$

FT denotes Fourier transformation, $\gamma(k)$ is the damping, and $q(k)$ is the Fourier transform of $q(x,t)$. A stationary soliton solution of the equation without damping will now decay slowly. We will show, by a simple scaling argument, that the time dependence of the decay only depends on the power d in the damping law

$$\gamma(k) = \epsilon |k|^d, \quad \epsilon \ll 1. \tag{4.2}$$

The soliton balances nonlinearity and dispersion. As these are the dominant effects, we expect the soliton to keep its functional form

$$Q = \frac{1}{\cosh^2(x-4t)} + O(\epsilon). \tag{4.3}$$

We assume[10,11] that the weak damping slowly changes the scale a, $a=a(t)$, of the scaling (1.2). The decay of the soliton can then be found by[12] the equation for the energy of the soliton part,

$$\frac{\partial}{\partial t}\int q^2\,dx + 4\pi \int \gamma_k(k)|q(k)|^2\,dk = 0. \tag{4.4}$$

The calculations are now simple. For the Fourier transform $q(k)$ of q we have the scaling, with (1.2) and $m=2$

$$q(k) = a^{m-1}Q(k') = \frac{1}{2\pi}\int q(x)\exp(-ikx)\,dx, \tag{4.5}$$

$$k' = k/a.$$

Then an equation for $a(t)$ follows, using the scaling (1.2) and (4.5),

$$\frac{\partial a}{\partial t} = -\frac{B\epsilon}{A(2m-1)}a^{d+1}, \tag{4.6}$$

where A and B are the constants

$$A = \int Q^2\,dx' = 4\pi\int_0^\infty |Q(k')|^2\,dk',$$

$$B = 4\pi\int_0^\infty |k'|^d |Q(k')|^2\,dk'. \tag{4.7}$$

The solution of (4.6) is

$$a = \frac{a(0)}{(1+\epsilon\nu t)^{1/d}}, \tag{4.8}$$

$$\nu = \frac{a^{d-1}(0)}{(2m-1)}\frac{B}{A}d,$$

together with the limiting case of exponential decay when $d=0$. The manner of decay is only determined by the power d in the damping law, and not by the various parameters in the undamped equation, or by the initial condition. These enter only in the constants.

The constant B/A can be calculated by taking the Fourier transform of (4.3). It follows that

$$\frac{B}{A} = \frac{\Gamma(d+3)\zeta(d+2)}{\Gamma(3)\zeta(2)\pi^d} \tag{4.9}$$

where ζ is the Riemann zeta function. The result (4.8), with the constant (4.9) and $m=2$ contains the four cases treated before.[11]

The calculation proceeds in the same way for other nonlinear equations with damping (or growth) terms. Examples are the generalized KdV equation (2.12), for $s \neq 4$, and the nonlinear Schrödinger equation.

CONCLUSIONS

Some implications of the scaling (1.2) have been treated. Scaling both explains the form of the various auxiliary functions in the AKNS scheme, and yields the various equations solvable by the inverse scattering method using the Schrödinger equation. Possibilities for their terms can be found by a simple inspection. Solvability of an equation in the AKNS scheme is restricted by the scaling properties. In a separate application of the scaling properties we have shown that the time dependence of the decay of a single soliton in the KdV equation follows from scaling only.

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[1]C.S. Gardner, J.M. Greene, M.D. Kruskal, and R.M. Miura, Commun. Pure Appl. Math. **27**, 97 (1974).
[2]R.M. Miura, C.S. Gardner, and M.D. Kruskal, J. Math. Phys. **9**, 1204 (1968); M.D. Kruskal, R.M. Miura, C.S. Gardner, and N.J. Zabusky, J. Math. Phys. **11**, 952 (1970).
[3]H. Steudel, Ann. Phys. **32**, 205 (1975).
[4]M.J. Ablowitz, D.J. Kaup, A.C. Newell, and H. Segur, Phys. Rev. Lett. **31**, 125 (1973); V.E. Zakharov and A.B. Shabat, Zh. Eksp. Teor. Fiz. **61**, 118 (1971) [Sov. Phys. JETP **34**, 62 (1972)].
[5]H.H. Chen, Phys. Rev. Lett. **33**, 925 (1974).
[6]L.P. Eisenhart, *A treatise on the differential geometry of curves and surfaces* (Dover, New York, 1960), pp. 280ff.
[7]M. Wadati, H. Sanuki, and K. Konno, Prog. Theor. Phys. **53**, 419 (1975).
[8]H. Schamel, J. Plasma Phys. **9**, 377 (1973).
[9]G.L. Lamb, J. Math. Phys. **15**, 2157 (1974).
[10]E. Ott and R.N. Sudan, Phys. Fluids **12**, 2388 (1969).
[11]E. Ott and R.N. Sudan, Phys. Fluids **13**, 1432 (1970).
[12]E. Ott, Phys. Fluids **14**, 748 (1971).

On the Schrödinger equation in fluid-dynamical form*

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The fluid-dynamical form of the Schrödinger equations is studied to examine the nature of the quantum forces arising from the quantum potential of Madelung and Bohm. It is found that they are in the form of a stress tensor having diagonal and nondiagonal components. Future studies of these quantum stress tensors in a many-body system may shed some light on the mechanism of spontaneous symmetry breaking and the generation of vorticity in many nuclear systems.

I. INTRODUCTION

It is well known that the time-dependent Schrödinger equation can be written as an equation of continuity and another equation analogous to the Euler equation in fluid dynamics, as was first pointed out by Madelung[1] in 1926. Recently, there is considerable interest in studying the dynamics of nonrelativistic single-particle[2] and many-body[3,4] systems by making use of such an analogy. It can be shown[3,4] that starting with the time-dependent Hartree—Fock formulation of the many-body problem, one can again obtain conservation laws of the classical type for the macroscopic density field $n(\mathbf{r}, t)$ and the velocity field $\mathbf{u}(\mathbf{r}, t)$, the difference being the presence of force terms of quantum origin. In this note, we wish to examine these forces arising from the quantum potential of Madelung[1] and Bohm[5] and show that they are in the form of a stress tensor having diagonal and nondiagonal components. Such an understanding will provide some help in formulating a macroscopic theory of a many-body quantum system.

II. TIME-DEPENDENT SCHRÖDINGER EQUATION IN FLUID DYNAMICAL FORM

The results of Madelung can be breifly stated. The time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}, t) + V(\mathbf{r}, t)\psi(\mathbf{r}, t) \tag{1}$$

is equivalent to the following set of equations:

$$\psi(\mathbf{r}, t) = \phi(\mathbf{r}, t)\exp[imS(\mathbf{r}, t)/\hbar - i\Omega(t)], \tag{2}$$

$$\frac{\partial}{\partial t}\phi^2 + \nabla\cdot(\phi^2\nabla S) = 0, \tag{3}$$

and

$$\frac{\partial}{\partial t}\nabla S + (\nabla S\cdot\nabla)\nabla S = -\frac{1}{m}\left(\nabla\frac{-(\hbar^2/2m)\nabla^2\phi}{\phi} + \nabla V\right), \tag{4}$$

where without loss of generality, the functions ϕ, S, and Ω can all be taken to be real functions. Here and henceforth, for conciseness of notation, the independent variables $\mathbf{r} = (x_1, x_2, x_3)$ and t are suppressed unless indicated otherwise. The factor $-(\hbar^2/2m)\nabla^2\phi/\phi$ which appears on the righthand side of Eq. (4) is known as the Bohm potential in the theory of hidden variables.[6]

Starting with Eq. (4) and with the help of Eq. (3), we get

$$\frac{\partial}{\partial t}(\phi^2\nabla_i S) + \sum_j \nabla_j(\phi^2\nabla_i S\nabla_j S) = -\frac{1}{m}\left(\phi^2\nabla_i\frac{-(\hbar^2/2m)\nabla^2\phi}{\phi} + \phi^2\nabla_i V\right), \tag{5}$$

where ∇_i is the gradient operator in the x_i direction. It can be shown easily that

$$\phi^2\nabla_i\left(\frac{\nabla^2\phi}{\phi}\right) = \nabla_i(\tfrac{1}{2}\nabla^2\phi^2) - 2\sum_j \nabla_j(\nabla_i\phi\nabla_j\phi). \tag{6}$$

In consequence, Eq. (5) becomes

$$m\frac{\partial}{\partial t}(\phi^2\nabla_i S) + \sum_j \nabla_j(m\phi^2\nabla_i S\nabla_j S + p_{ij}^{(q)}) = -\phi^2\nabla_i V, \tag{7}$$

where

$$p_{ij}^{(q)} = -(\hbar^2/4m)\nabla^2\phi^2\delta_{ij} + (\hbar^2/m)\nabla_i\phi\nabla_j\phi. \tag{8}$$

If we interpret $\phi^2 = n$ as the density field, ∇S as the velocity field, then one recognizes Eq. (3) as the equation of continuity and Eq. (7) as analogous to the Euler equation in fluid dynamics. The superscript q in the stress tensor $p_{ij}^{(q)}$ indicates that this is a stress tensor of quantum origin (being proportional to $\hbar^2$), and we shall call it the quantum stress tensor. Each diagonal component of the quantum stress tensor consists of two terms, one proportional to the Laplacian of the single-particle density, and the other to the square of the gradient of the wavefunction. The nondiagonal components of the stress tensor are proportional to the product of their respective directional gradients of the wavefunction and are, in general, nonzero.

It is of interest to examine the effects of the quantum stress on the density distribution. The diagonal elements $p_{11}^{(q)}$, $p_{22}^{(q)}$, and $p_{33}^{(q)}$ are the quantum pressure in different directions, and they need not be equal. In addition, it is generally nonuniform spatially. The nondiagonal components are shear stresses, and they tend to create vorticity if they are not balanced. A stationary state is obtained when the pressure and the shear stress are counterbalanced by the force $\phi^2\nabla V$ arising from the potential V. In this case, the cancellation of the shear stress is due mainly to the nonuniformity in ϕ^2 which produces large force density gradients.

III. APPLICATION OF THE FLUID-DYNAMICAL FORM OF THE SCHRÖDINGER EQUATION

We shall discuss below the application of the fluid-dynamical form of the Schrödinger equation in a many-body fermion system in the Hartree—Fock approxima-

tion. The case of a more general treatment of the many-body problem will be discussed elsewhere.

In the time-dependent Hartree—Fock approximation, a many-body fermion system consists of a collection of particles occupying single-particle states whose wavefunctions $\psi_\alpha(\mathbf{r}, t)$ satisfy the equation[7]

$$i\hbar\frac{\partial}{\partial t}\psi_\alpha(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi_\alpha(\mathbf{r}, t) + V_\alpha(\mathbf{r}, t)\psi_\alpha(\mathbf{r}, t), \tag{9}$$

where

$$V_\alpha(\mathbf{r}, t) = \int d^3r_2\left[\sum_\beta \psi_\beta(\mathbf{r}_2, t)\psi_\beta^*(\mathbf{r}_2, t)v(\mathbf{r}, \mathbf{r}_2) - \sum_\beta \psi_\beta^*(\mathbf{r}_2, t)\psi_\beta(\mathbf{r}, t)v(\mathbf{r}, \mathbf{r}_2)\psi_\alpha(\mathbf{r}_2, t)/\psi_\alpha(\mathbf{r}, t)\right]. \tag{10}$$

In Eq. (10), $v(\mathbf{r}, \mathbf{r}_2)$ is the two-body interaction and the summation is over the set of occupied states. Equation (9) is in the same form as Eq. (1) with the exception that because $\psi_\alpha(\mathbf{r}, t)$ is, in general, complex, V_α of Eq. (9) has both real and imaginary parts. One can follow the same procedure outlined in Sec. I by writing the wavefunction in terms of the amplitude and phase factors:

$$\psi_\alpha(\mathbf{r}, t) = \phi_\alpha(\mathbf{r}, t)\exp[im S_\alpha(\mathbf{r}, t)/\hbar - i\Omega_\alpha(t)]. \tag{11}$$

After substituting Eq. (11) into (9) and separating the resultant equation into real and imaginary parts, one obtains equations analogous to Eqs. (3) and (4):

$$\frac{\partial\phi_\alpha^2}{\partial t} + \nabla\cdot(\phi_\alpha^2\nabla S_\alpha) = \frac{2}{\hbar}\phi_\alpha^2 \mathrm{Im}V_\alpha \tag{12}$$

$$\frac{\partial}{\partial t}\nabla S_\alpha + (\nabla S_\alpha\cdot\nabla)\nabla S_\alpha = -\frac{1}{m}\left(\nabla\frac{\phi_\alpha[-(\hbar^2/2m)\nabla^2\phi_\alpha]}{\phi_\alpha^2} + \nabla \mathrm{Re}V_\alpha\right). \tag{13}$$

Combining Eqs. (12) and (13), one obtains the analog of Eq. (5)

$$\frac{\partial}{\partial t}(\phi_\alpha^2\nabla S_\alpha) + \nabla\cdot(\phi_\alpha^2\nabla S_\alpha\nabla S_\alpha) = -\frac{1}{m}\phi_\alpha^2\left\{\nabla\frac{\phi_\alpha[-(\hbar^2/2m)\nabla^2\phi_\alpha]}{\phi_\alpha^2} + \nabla \mathrm{Re}V_\alpha\right\} + \frac{2}{\hbar}\phi_\alpha^2\nabla S_\alpha\,\mathrm{Im}V_\alpha. \tag{14}$$

After summing Eqs. (12) and (14) over all the occupied single-particle states, we get

$$\frac{\partial}{\partial t}\sum_\alpha\phi_\alpha^2 + \nabla\cdot\sum_\alpha\phi_\alpha^2\nabla S_\alpha = 0 \tag{15}$$

and

$$\frac{\partial}{\partial t}\sum_\alpha\phi_\alpha^2\nabla S_\alpha + \nabla\cdot\sum_\alpha\phi_\alpha^2\nabla S_\alpha\nabla S_\alpha = -\frac{1}{m}\left\{\sum_\alpha\phi_\alpha^2\nabla\frac{\tau_\alpha}{\phi_\alpha^2} + \left[\sum_\alpha\phi_\alpha^2(\mathbf{r})\right]\int d^3r_2\nabla_r v(\mathbf{r}, \mathbf{r}_2)\sum_{\alpha'}\phi_{\alpha'}^2(\mathbf{r}_2) - \int d^3r_2[\nabla_r v(\mathbf{r}, \mathbf{r}_2)]\left|\sum_\alpha\psi_\alpha(\mathbf{r})\psi_\alpha^*(\mathbf{r}_2)\right|^2\right\}, \tag{16}$$

where $\tau_\alpha = [-(\hbar^2/2m)\nabla^2\phi_\alpha]\varphi_\alpha$. Upon introducing the density function

$$n(\mathbf{r}, t) = \sum_\alpha\phi_\alpha^2(\mathbf{r}, t), \tag{17}$$

and the average velocity $\mathbf{u}$

$$\mathbf{u}(r, t) = \sum_\alpha\phi_\alpha^2(\mathbf{r}, t)\nabla S_\alpha(\mathbf{r}, t)/\sum_\alpha\phi_\alpha^2(\mathbf{r}, t), \tag{18}$$

we get the equation of continuity

$$\frac{\partial n}{\partial t} + \nabla\cdot n\mathbf{u} = 0. \tag{19}$$

We introduce the Dirac one-body density matrix $\mathcal{N}^{(1)}(\mathbf{r}, \mathbf{r}_2)$

$$\mathcal{N}^{(1)}(\mathbf{r}, \mathbf{r}_2) = \sum_\alpha\psi_\alpha(\mathbf{r}, t)\psi_\alpha^*(\mathbf{r}_2, t). \tag{20}$$

Then Eq. (16) can be written as

$$\frac{\partial}{\partial t}\sum_\alpha\phi_\alpha^2\nabla S_\alpha + \nabla\cdot\sum_\alpha\phi_\alpha^2\nabla S_\alpha\nabla S_\alpha = -\frac{1}{m}\left(\sum_\alpha\phi_\alpha^2\nabla\frac{\tau_\alpha}{\phi_\alpha^2} + n\int d^3r_2 n(r_2)\nabla_r v(\mathbf{r}, \mathbf{r}_2) - \int d^3r_2|\mathcal{N}^{(1)}(\mathbf{r}, \mathbf{r}_2)|^2\nabla_r v(\mathbf{r}, \mathbf{r}_2)\right). \tag{21}$$

Equations (19) and (21) are the same as what we derived from time-dependent Hartree—Fock equations in density matrix form.[3]

We note that

$$\sum_\alpha\phi_\alpha^2\frac{\partial S_\alpha}{\partial x_i}\frac{\partial S_\alpha}{\partial x_j} = nu_iu_j + \sum_\alpha\phi_\alpha^2\left(\frac{\partial S_\alpha}{\partial x_i} - u_i\right)\left(\frac{\partial S_\alpha}{\partial x_j} - u_j\right). \tag{22}$$

Equation (21) can therefore be written as

$$\frac{\partial}{\partial t}nu_i + \sum_{j=1}^3\frac{\partial}{\partial x_j}nu_iu_j = -\frac{1}{m}\sum_{j=1}^3\frac{\partial}{\partial x_j}(p_{ij}^{(t)} + p_{ij}^{(q)}) - \frac{n}{m}\int d^3r_2 n(\mathbf{r}_2)\frac{\partial}{\partial x_i}v(\mathbf{r}, \mathbf{r}_2) + \frac{n}{m}\int d^3r_2|\mathcal{N}^{(1)}(\mathbf{r}, \mathbf{r}_2)|^2\frac{\partial}{\partial x_i}v(\mathbf{r}, \mathbf{r}_2), \tag{23}$$

where we introduce the thermal stress tensor $p_{ij}^{(t)}$ in analogy with the kinetic theory of gases [as suggested by Eq. (22)]

$$p_{ij}^{(t)} = m\sum_\alpha\phi_\alpha^2\left(\frac{\partial S_\alpha}{\partial x_i} - u_i\right)\left(\frac{\partial S_\alpha}{\partial x_j} - u_j\right), \tag{24}$$

and also the total quantum stress tensor $p_{ij}^{(q)}$

$$p_{ij}^{(q)} = -\frac{\hbar^2}{4m}\delta_{ij}\nabla^2 n + \frac{\hbar^2}{m}\sum_\alpha(\nabla_i\phi_\alpha)(\nabla_j\phi_\alpha). \tag{25}$$

The analogy between Eq. (23) for the many-body system and the classical Euler equation is now clear.

We note in passing that the quantum stress tensor can also be given in two other different forms:

$$p_{ij}^{(q)} = \frac{\hbar^2}{4m}\delta_{ij}\nabla^2 n - \frac{\hbar^2}{m}\sum_\alpha\varphi_\alpha\nabla_i\nabla_j\varphi_\alpha, \tag{26}$$

and

$$p_{ij}^{(q)} = -\frac{\hbar^2}{2m}\sum_\alpha\varphi_\alpha\nabla_i\nabla_j\varphi_\alpha + \frac{\hbar^2}{2m}\sum_\alpha(\nabla_i\varphi_\alpha)(\nabla_j\varphi_\alpha). \tag{27}$$

IV. DISCUSSION

From the fluid-dynamical form of the Schrödinger equation we obtain a simple description of a many-body quantum system in terms of the macroscopic density field $n(\mathbf{r}, t)$, the velocity field $\mathbf{u}(\mathbf{r}, t)$ and the coupling between the macroscopic and the microscopic degrees of freedom. A complete macroscopic description can be made by examining $p_{ij}^{(t)}$, $p_{ij}^{(q)}$, and the exchange term and finding plausible approximations for these quantities.[3] Such a description has its application in studying the dynamics of two heavy nuclei in collision.

On the other hand, the description in terms of both microscopic and macroscopic variables as is expressed in Eq. (23) can be of some help in other types of problems. For example, as is well known, many nuclei in their ground state have nonspherical density distributions (spontaneous symmetry breaking). In this static case, the left-hand side and $p_{ij}^{(t)}$ in Eq. (23) are zero and the equilibrium density distribution is obtained by balancing the forces due to the quantum stress tensor $p_{ij}^{(q)}$ and the internucleonic forces. One may wish to investigate whether indeed for these nuclei the quantum pressure is so anisotropic and nonuniform as to distort the system to its nonspherical ground state.[8] The possibility of a strongly anisotropic and nonuniform quantum pressure also makes it interesting to study the density distributions of liquid ^{3}He at low temperature in small assemblies.

The nondiagonal components of the quantum stress has its effect in those nonequilibrium phenomena in which the quantum shear stress cannot be completely counterbalanced by the force density $n\nabla V$. In consequence, vorticity may be created. Such an effect has been studied in great detail by Kan and Griffin[2] for a single-particle Schrödinger fluid. Future investigations on the formation of vorticity along the lines of Kan and Griffin for a many-body system will be of great interest.

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[1]E. Madelung, Z. Phys. **40**, 332 (1926).
[2]J.J. Griffin and K.K. Kan, *Proceedings of the Third International Symposium on the Chemistry and Physics of Fission*, Rochester, N.Y., 1973, SM-174/58 (IAEA, Vienna, 1974); also K.K. Kan, Ph.D. thesis, University of Maryland, June 1975.
[3]C.Y. Wong, J.A. Maruhn, and T.A. Welton, Nucl. Phys. A **253**, 469 (1975).
[4]S.E. Koonin and A.K. Kerman (to be published); also, S.E. Koonin, Ph.D. thesis, M.I.T., June 1975.
[5]D. Bohm, Phys.Rev. **85**, 180 (1952).
[6]L.E. Belinfante, *Survey of Hidden Variables Theory*, Natural Philosophy Monographs, Vol. 55 (Pergamon, New York, 1973).
[7]See, for example, G.E. Brown, *Unified Theory of Nuclear Models* (Interscience, New York, 1964).
[8]See, for example, M. Brack, J. Damgaard, A.S. Jensen, H.C. Pauli, V.M. Strutinsky, and C.Y. Wong, Rev. Mod. Phys. **44**, 320 (1972).

Nonlinear differential–difference equations and Fourier analysis

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The conceptual analogy between Fourier analysis and the exact solution to a class of nonlinear differential–difference equations is discussed in detail. We find that the dispersion relation of the associated linearized equation is prominent in developing a systematic procedure for isolating and solving the equation. As examples, a number of new equations are presented. The method of solution makes use of the techniques of inverse scattering. Soliton solutions and conserved quantities are worked out.

I. INTRODUCTION

Many interesting physical phenomena, such as ladder type electric circuits,[1] vibration of particles,[2] collapse of Langmuir waves in plasma physics,[3] to cite a few, can be modeled by nonlinear differential-difference equations. Unfortunately, due to the inherent difficulties of nonlinear problems, most methods of solution apply only in special circumstances. The usual techniques of investigation are to make use of a small parameter in a perturbation analysis, or else to linearize the problem completely. In either case, certain important features of the full nonlinear problem are lost. For a class of physically interesting nonlinear problems this difference can be remedied by an exact method which makes use of the technique of inverse scattering first discovered by Gardner, Greene, Kruskal, and Miura[4,5] in their now classic work on the Korteweg–de Vries equation (KdV). They showed that a key step in developing the exact method of solution was the intimate relationship between the KdV equation and a linear scattering problem, the Schrödinger eigenvalue equation.

The work of Zakharov and Shabat[6] definitely showed that the method developed for KdV was indeed no fluke. Employing techniques due to Lax,[7] they showed that the physically interesting nonlinear Schrödinger evolution equation was associated with a new eigenvalue problem. They were then able to solve the evolution equation by inverse scattering. Subsequently, Ablowitz, Kaup, Newell, and Segur[8] discovered a scheme which both isolates and solves a class of nonlinear partial differential equations. Included in this class are the nonlinear Schrödinger, KdV, modified KdV, and Sine–Gordon equations. In Ref. 8 the important role of the dispersion relation of the associated problem is discussed.

It is significant that these ideas apply to certain types of discrete evolution equations. Flaschka[9] has shown that the Toda lattice equation[2] is related to a discretized Schrödinger eigenvalue problem. By employing an inverse scattering analysis similar to that of Case and Kac[10] and Case,[11] he was able to solve the equation. Similar results were also found by Manakov.[12] Motivated by these results, Ablowitz and Ladik[13] proposed a new discrete eigenvalue problem, an appropriate generalization of a discretized version of the eigenvalue problem of Zakharov and Shabat, as a basis for generating solvable discrete equations. They found that the nonlinear self-dual network and Toda lattice equations were the important equations. These equations are second order in time systems. In this paper we will work with the same eigenvalue problem as in Ref. 13. However, we find that in addition to a class of second order in time systems there is also a class of solvable first order in time systems. Included in this category are discrete (differential–difference) versions of the nonlinear Schrödinger, KdV, modified KdV, and "sine–Gordon" equations. In addition, the inverse scattering analysis presented in Ref. 13 must be suitably modified to handle these first order in time systems effectively. We explain how to accomplish this, present the soliton solutions, and discuss how one can use the scattering equations to obtain an infinite number of conserved quantities.

Beyond this, however, we wish to convince the reader that the procedure is, in essence, analogous to discrete Fourier analysis. Let us begin this task by writing down a general linear differential–difference equation,

$$U_{n_t} = -i\omega(E)U_n, \tag{1.1}$$

where E is the shift operator $EU_n = U_{n+1}$. Hence if we take $\omega(E) = (E + E^{-1} - 2)$, (1.1) is equivalent to

$$iU_{n_t} = U_{n+1} + U_{n-1} - 2U_n. \tag{1.2}$$

[(1.2) is an equation which we shall discuss in detail later in this paper, as it is the linear portion of the discrete nonlinear Schrödinger equation.] We will refer to $\omega(E)$ as the dispersion relation.

The exact solution of (1.1) is obtained by discrete Fourier analysis. Defining the transform pair

$$U(n,t)=\frac{1}{2\pi i}\oint b(z,t)z^{n-1}\,dz, \tag{1.3a}$$

$$b(z,t)=\sum_{-\infty}^{\infty}U(n,t)z^{-n}, \tag{1.3b}$$

where the loop integral in (1.3a) is around the unit circle, the reader can verify that $b(z,t)$ satisfies

$$b(z,t)=b(z,0)\exp[-i\omega(z)t]. \tag{1.4}$$

Hence we have a quadrature solution to the initial value problem [$U(n,0)$ is assumed to decay sufficiently rapidly as $|n|\to\infty$]. Conceptually, the steps in the solution process can be summarized as follows. At $t=0$ we are given $U(n,0)$. We then find the Fourier transform at the initial instant, $b(z,0)$. For all later times Eq. (1.1) yields the simple relation (1.4) for $b(z,t)$, whereupon the exact solution $U(n,t)$ is given by (1.3a). Schematically we have

$$U(n,0)\to b(z,0)\overset{\omega}{\to}b(z,t)\to U(n,t).$$

In the nonlinear case the key step is to first make an association between the evolution equation and a linear-eigenvalue (scattering) problem. In this paper the evolution equations are all related to the following scattering problem[13]:

$$\begin{aligned}V_{1_{n+1}}&=zV_{1_n}+Q_n(t)V_{2_n}+S_n(t)V_{2_{n+1}},\\ V_{2_{n+1}}&=(1/z)V_{2_n}+R_n(t)V_{1_n}+T_n(t)V_{1_{n+1}}.\end{aligned} \tag{1.5}$$

The various equations are distinguished by the associated time dependence,

$$\begin{aligned}V_{1_{n_t}}&=A_nV_{1_n}+B_nV_{2_n},\\ V_{2_{n_t}}&=C_nV_{1_n}+D_nV_{2_n}.\end{aligned} \tag{1.6}$$

Corresponding to each nonlinear evolution equation $U_{n_t}=N(U_n)$ is a set of functions $A_n,\ldots,D_n$ (depending in general on Q_n, R_n, S_n, T_n) with $\partial z/\partial t=0$, such that (1.5) and (1.6) have as their integrability condition $U_{n_t}=N(U_n)$. Typical, is the differential–difference nonlinear Schrödinger equation,

$$iU_{n_t}=U_{n+1}+U_{n-1}-2U_n\pm U_n^*U_n(U_{n+1}+U_{n-1}), \tag{1.7}$$

where U_n^* is the complex conjugate of U_n. In the derivation of (1.7) $R_n=U_n=\mp Q_n^*$, $S_n=T_n=0$. In general the potentials Q_n, R_n, S_n, T_n appear in the evolution equation as dependent variables. We shall present a method of finding the $A_n,\ldots,D_n$ corresponding to each evolution equation. The crucial quantity which makes the isolation of each equation both natural and straight forward is the *dispersion relation of the associated linearized problem*. For example, the linearized form of (1.7) is (1.2). In Sec. II we shall show how the linear dispersion relation $\omega(z)=z+1/z-2$ is used to enable us to deduce (1.7).

The solution procedure is as follows. At $t=0$ we are given the initial conditions for the evolution equation, in this case $U_n(0)$. The scattering problem is then solved for the "scattering data" at the initial instant: $S(z,0)$ (the discrete eigenvalues, the "reflection coefficient," and bound state normalization constants). For later times even though the potentials evolve according to nonlinear differential–difference equations, the scattering data satisfies very simple relations. In particular, the discrete eigenvalues are time independent and the time dependence of the other portion is proportional to $\exp[-i\omega(z^2)t]$. Thus we find the time dependence of the scattering data $S(z,t)$ is related to the dispersion relation of the linearized problem. Then, given $S(z,t)$, one recovers the solution of the evolution equation by mapping back to physical space via the inverse scattering equations. Schematically for $U_n(t)$ the process can be summarized as follows:

$$U_n(0)\to S(z,0)\overset{\omega}{\to}S(z,t)\to U_n(t).$$

The procedure is analogous to Fourier analysis. Here the scattering data plays the role of the Fourier transform (1.3b) and the inverse scattering equations play the role of (1.3a).

In Sec. II we show how to isolate the various interesting equations. We go through the example problem (1.7) in detail, and simply list the others. For algebraic ease we will take $S_n=0$, $T_n=0$. This results in first order in time evolution equations.

In Sec. III we discuss the inverse scattering problem and the simplifications $S_n=0$, $T_n=0$ yield. In Sec. IV soliton solutions and conserved quantities are found.

II. EVOLUTION EQUATIONS

The method of isolating solvable evolution equations requires us to first find equations for A_n, B_n, C_n, D_n in (1.6). For simplicity in this presentation, we shall take $S_n=0$, $T_n=0$, and work out one specific example in detail, namely (1.7). When the procedures are understood, they can be carried out for the more general case, S_n, $T_n\neq 0$. In addition, (1.7) is in a class of first order in time systems which was not discussed in Ref. 13 whereas the more general case was considered for second order in time systems.

The $A_n,\ldots,D_n$ equations are obtained by setting $(\partial/\partial t)(EV_{i_n})=E(V_{i_{n_t}})$, $i=1,2$, where E is the shift operator, and requiring the eigenvalue z to be time invariant, $\partial z/\partial t=0$. We find

$$z\Delta_nA_n+R_nB_{n+1}-Q_nC_n=0, \tag{2.1a}$$

$$1/zB_{n+1}-zB_n+Q_n(A_{n+1}-D_n)=Q_{n_t}, \tag{2.1b}$$

$$zC_{n+1}-1/zC_n-R_n(A_n-D_{n+1})=R_{n_t}, \tag{2.1c}$$

$$1/z\Delta_nD_n+Q_nC_{n+1}-R_nB_n=0, \tag{2.1d}$$

where $\Delta_nA_n=A_{n+1}-A_n$, etc. We now wish to solve the system (2.1). In general the nonlinear evolution equation is the integrability condition necessary for (2.1) to have a solution. However, corresponding to each evolution equation is a set of $A_n,\ldots,D_n$. The question, then, is how do we go about isolating a particular evolution equation. This is where the dispersion relation of the

associated linearized problem is useful. In Sec. III we show that, in the case where Q_n, $R_n \to 0$ (and also S_n, T_n in the more general case) as $|n| \to \infty$, then $\lim_{n\to\infty}(A_n - D_n) = -i\omega(z^2)$. In the case of the nonlinear Schrödinger equation (1.7), its linearized version (1.2) has the dispersion relation $\omega(z^2) = z^2 + 1/z^2 - 2$. This suggests using the following finite expansions in z for $A_n, \ldots, D_n$:

$$A_n = A_n^{(2)}z^2 + A_n^{(0)}, \quad B_n = B_n^{(1)}z + B_n^{(-1)}/z,$$

$$C_n = C_n^{(1)}z + C_n^{(-1)}/z, \quad D_n = D_n^{(0)} + D_n^{(-2)}/z^2.$$

The reader should note that the parity of the functions $A_n, \ldots, D_n$ are consistent with Eqs. (2.1). Substituting these expansions into (2.1) and equating powers of z yields a system of twelve equations in eight unknowns $(A_n^{(2)}, \ldots, D_n^{(-2)})$. We have found it easiest to solve for the coefficients of the highest and lowest powers of z first.

The coefficient of z^3 in (2.1a) yields $\Delta_n A_n^{(-2)} = 0$, whereas the coefficient of z^{-3} in (2.1d) yields $\Delta_n D_n^{(-2)} = 0$. The solutions are $A_n^{(2)} = A_-^{(2)} = \text{const}$ and $D_n^{(-2)} = D_-^{(-2)} = \text{const}$. Continuing to z^2, we find $B_n^{(1)} = Q_n A_-^{(2)}$ from (2.1b), $C_n^{(1)} = R_{n+1}A_-^{(2)}$ from (2.1c); for z^{-2} we have $B_n^{(-1)} = Q_{n-1}D_-^{(-2)}$ from (2.1b), and $C_n^{(-1)} = R_n D_-^{(-2)}$ from (2.1c). At z (2.1a) yields

$$\Delta_n A_n^{(0)} = (Q_n R_{n-1} - R_n Q_{n+1})A_-^{(2)} = \Delta_n(-R_{n-1}Q_n A_-^{(2)})$$

and (2.1d) is *identically* satisfied. Similarly, the coefficient of z^{-1} in (2.1a) is identically satisfied while from (2.1d) we have

$$\Delta_n D_n^{(0)} = (R_n Q_{n-1} - Q_n R_{n+1})D_n^{(-2)} = \Delta_n(-Q_{n-1}R_n D_-^{(-2)}).$$

Solving the above equations for $A_n^{(0)}$ and $D_n^{(0)}$, we find

$$\begin{aligned} A_n^{(0)} &= -R_{n-1}Q_n A_-^{(2)} + A_-^{(0)}, \\ D_n^{(0)} &= -Q_{n-1}R_n D_-^{(-2)} + D_-^{(0)}, \end{aligned} \tag{2.2}$$

where $A_-^{(0)}$ and $D_-^{(0)}$ are constants. The two remaining equations (coefficients of z^0) are evolution equations. (2.1b), (2.1c) require Q_n, R_n to satisfy,

$$R_{n_t} = (1 - R_nQ_n)(R_{n+1}D_-^{(-2)} - R_{n-1}A_-^{(2)}) - R_n(A_-^{(0)} - D_-^{(0)}), \tag{2.3a}$$

$$Q_{n_t} = (1 - R_nQ_n)(Q_{n+1}A_-^{(2)} - Q_{n-1}D_-^{(-2)}) + Q_n(A_-^{(0)} - D_-^{(0)}). \tag{2.3b}$$

Thus, we have solved (2.1) using the expansions $A_n, \ldots, D_n$ as suggested by $\omega(z^2)$. The twelve equations determine the eight unknowns $A_n^{(2)}, \ldots, D_n^{(-2)}$, and leave four integrability conditions. Two are trivially satisfied, and the other two are the evolution equations (2.3); the solutions for $A_n, \ldots, D_n$ are summarized below:

$$\begin{aligned} A_n &= A_-^{(2)}(z^2 - R_{n-1}Q_n) + A_-^{(0)}, \\ B_n &= A_-^{(2)}Q_n z + D_-^{(-2)}Q_{n-1}\frac{1}{z}, \\ C_n &= A_-^{(2)}R_{n-1}z + D_-^{(-2)}R_n\frac{1}{z}, \\ D_n &= D_-^{(0)} + D_-^{(-2)}\left(\frac{1}{z^2} - Q_{n-1}R_n\right). \end{aligned} \tag{2.4}$$

The nonlinear Schrödinger equation is obtained by taking $A_-^{(2)} = D_-^{(-2)*} = -i$, $A_-^{(0)} = D_-^{(0)*} = i$, and requiring $R_n = \mp Q_n^*$. Then the coupled system (2.3a, b) are mutually consistent, and we have

$$iQ_{n_t} = Q_{n+1} + Q_{n-1} - 2Q_n \pm Q_nQ_n^*(Q_{n+1} + Q_{n-1}). \tag{2.5}$$

We also point out that the dispersion relation $\omega(z^2)$ satisfies the following relationship with A_n, D_n:

$$\lim_{n\to\infty}(A_n - D_n) = -i(z^2 + 1/z^2 - 2) = -i\omega(z^2),$$

subject to $\lim_{|n|\to\infty} Q_n = 0$.

A second interesting evolution equation can be immediately obtained from the previous results. It is related to the modified Korteweg–de Vries (MKdV) equation, and its dispersion relation is given by $\omega(z^2) = i(z^2 - 1/z^2)$. Taking $A_-^{(2)} = D_-^{(-2)} = 1$, $A_-^{(0)} = D_-^{(0)} = 0$ and $R_n = \mp Q_n$, (2.3) yields

$$Q_{n_t} = (1 \pm Q_n^2)(Q_{n+1} - Q_{n-1}). \tag{2.6}$$

The reader again can see that $\lim_{n\to\infty}(A_n - D_n) = -i\omega(z)^2$ is satisfied. The continuum limit of (2.6) is related to MKdV by setting $Q_n = \Delta x\bar{Q}_n$ and expanding $Q_{n+1} = Q \pm \Delta xQ_x + (\Delta x^2/2)Q_{xx} \pm (\Delta x^3/6)Q_{xxx} + \cdots$. We find,

$$\bar{Q}_t = (1 \pm \Delta x^2\bar{Q}^2)[2\Delta x\bar{Q}_x + (\Delta x^3/6)\bar{Q}_{xxx} + \cdots]. \tag{2.7}$$

$\bar{Q}$ has an asymptotic solution of the form $\bar{Q} \sim f(y, \Upsilon)$, where $y = x + 2\Delta xt$, $\Upsilon = (\Delta x^3/3)t$; $f(y, \Upsilon)$ satisfies

$$f_\Upsilon = f_{yyy} \pm 6f^2 f_y. \tag{2.8}$$

An even more closely related equation is obtained by expanding A_n in powers of z^4, z^2, z^0. Corresponding to the linear dispersion relation $\omega(z^2) = z^4/2 - z^2 + 1/z^2 - 1/(2z^4)$, we find,

$$\begin{aligned} Q_{n_t} = (1 \pm Q_n^2)[&Q_{n-1} - Q_{n+1} + \tfrac{1}{2}Q_{n+2}(1 \pm Q_{n+1}^2) - \tfrac{1}{2}Q_{n-2}(1 \pm Q_{n-1}^2) \\ &\pm \tfrac{1}{2}Q_n(Q_{n+1}^2 - Q_{n-1}^2)]. \end{aligned} \tag{2.9}$$

If we scale $Q_n = \Delta x\bar{Q}_n$, then $\bar{Q} \sim \Delta xf(x, \Upsilon)$, where $\Upsilon = \Delta x^3 t$ and (2.9) is directly reducable to MKdV.

Another first order in time equation we have found is related to the sine–Gordon equation in characteristic coordinates, $U_{xt} = \sin U$. Its dispersion relation is given by $\omega(z^2) = 2i\sigma/(z^2 - 1/z^2)$. The corresponding evolution equation is given by

$$\begin{aligned} &2\sigma Q_n + Q_{n-1_t}(1 - Q_n^2) - Q_{n+1_t}(1 + Q_n^2) - Q_{n+1}(Q_n^2)_t \\ &- [Q_{n+1}(1 + Q_n^2) + Q_{n-1}(1 - Q_n^2)]\sum_{k=-\infty}^{n-1}\frac{(Q_k^2)_t}{1 + Q_k^2} \\ &= 2Q_n\sum_{k=-\infty}^{n-1}\left[Q_k\left(Q_{k+1}\frac{(Q_k^2)_t}{1 + Q_k^2} + Q_{k+1_t} + Q_{k-1_t}\right)\right]. \end{aligned} \tag{2.10}$$

It should be noted that the expansion procedure is carried out by first scaling $A_n, \ldots, D_n$ by $A_n = \bar{A}_n/(z^2 - 1/z^2), \ldots, D_n = \bar{D}_n/(z^2 - 1/z^2)$. The continuum limit requires us to take $\sigma = \Delta x$, $Q_n = \Delta x\bar{Q}_n$. Then (2.10) yields

$$\bar{Q} - \bar{Q}_{xt} - 4\bar{Q}\int_{-\infty}^{x}\bar{Q}\bar{Q}_t\,dx' \sim 0. \tag{2.11}$$

(This is basically what is found in the continuous case.[8]) Letting $Q = \frac{1}{2}U_x$ shows that (2.11) is reducible to $U_{xt} = \sin U$ under the condition $U(-\infty) = 0 \pmod{2\pi}$.

In addition to the above equations are both (i) second order in time equations and (ii) a class of equations related to a discretized Schrödinger equation. In Ref. 13 we have shown that by using the eigenvalue problem (1.5), in conjunction with (1.6), a set of equations for A_n, B_n, C_n, D_n [which reduce to (2.1) when $S_n = T_n = 0$] is obtained. Expanding A_n as $A_n = A_n^{(1)} z + A_n^{(0)}$ etc. yields the self-dual network,

$$I_{n_t} = (1 \pm I_n^2)(\tilde{V}_{n-1} - \tilde{V}_n),$$
$$\tilde{V}_{n_t} = (1 \pm \tilde{V}_n^2)(I_n - I_{n+1}), \tag{2.12}$$

where $R_n = \mp Q_n = I_n$, $T_n = \mp S_n = \tilde{V}_n$ are the relations for the potentials in (1.5). The dispersion relation of (2.12) is obtained by looking for special solutions $I_n = z^{2n} \times \exp(-i\omega t)$, $\tilde{V}_n = z^{2n} \exp(-i\omega t)$ in the linearized form of (2.12). We find $\omega = \pm i(z - 1/z)$. This function naturally suggests the correct expansions for $A_n, \ldots, D_n$ used in Ref. 13.

If we choose the potentials to satisfy $R_n = 0$, $T_n = 1$, $Q_n = -\beta_n$, $S_n = 1 - \alpha_n$, then the eigenvalue problem (1.5) is reducible to a discretized Schrödinger equation,

$$\alpha_n V_{2n+1} + V_{2n-1} + \beta_n V_{2n} = \lambda V_{2n}, \tag{2.13}$$

where $\lambda = z + 1/z$. The same expansion in powers of z that gives (2.12) now yields the Toda lattice equation,

$$\tilde{Q}_{n_{tt}} = \exp[-(\tilde{Q}_n - \tilde{Q}_{n-1})] - \exp[-(\tilde{Q}_{n+1} - \tilde{Q}_n)], \tag{2.14}$$

where $Q_n = \tilde{Q}_{n_t}$, $S_n = 1 - \exp[-(\tilde{Q}_{n+1} - \tilde{Q}_n)]$. The reader can verify that the dispersion relation of the linearized form of (2.14) also is $\omega = \pm i(z - 1/z)$ as in the self-dual network. The difference is that the choice of potentials, hence the eigenvalue problem, is different. Similarly, if we expand in powers of z beginning at z^2 with the choice of potentials $R_n = 0$, $Q_n = 0$, $T_n = 1$, $S_n = 1 - \exp(-u_n)$ we find the evolution equation

$$u_{n_t} = \exp(-u_{n-1}) - \exp(-u_{n+1}). \tag{2.15}$$

(2.15) has a linearized dispersion relation given by $\omega = i(z^2 - 1/z^2)$. (2.15) has also been discussed by Manakov[12] and Kac and van Moerbeke.[14] It can be verified that if we let $u \sim \Delta x^2 f(\chi, \Upsilon)$, where $\chi = x + 2\Delta x t$, $\Upsilon = \frac{1}{3}\Delta x^3 t$, then in the continuum limit (2.15) is the KdV equation

$$f_\Upsilon = f\chi\chi\chi - 6ff\chi. \tag{2.16}$$

Thus (2.15) is analogous to (2.6), and it is intimately related to the discrete Schrödinger eigenvalue problem (2.13). In a similar sense there is an equation, analogous to (2.9), corresponding to the higher order dispersion relation $\omega = z^4/2 - z^2 + 1/z^2 - 1/(2z^4)$ which reduces directly to KdV. Expansion of A_n, etc., to powers of z^4, etc., and choosing the arbitrary constants appropriately yields

$$\begin{aligned} u_{n_t} = {} & 3[\exp(u_{n+1}) - \exp(-u_{n-1})] + \tfrac{1}{2}\exp(-u_{n-1}) \\ & \times [\exp(-u_{n-1}) + \exp(-u_{n+2})] + \tfrac{1}{2}\exp(-u_n) \\ & \times [\exp(-u_{n-1}) - \exp(-u_{n+1})] - \tfrac{1}{2}\exp(-u_{n+1}) \\ & \times [\exp(-u_{n+1}) + \exp(-u_{n+2})], \end{aligned} \tag{2.17}$$

which reduces to (2.16) if we take $u \sim \Delta x^2 f(x, \Upsilon)$, $\Upsilon = \Delta x^3 t$ in the continuum limit.

Finally, we point out that the evolution equations (2.14), (2.15), and (2.17) can be deduced directly from the discrete Schrödinger equation (2.13). They are found by using (2.13) in conjunction with an assumed time dependence of the form $V_{n_t} = A_n V_{n+1} + B_n V_n$ and expanding in powers of λ. In Ref. 13 this procedure is discussed and (2.14) is deduced. If we take $\beta_n = 0$ in (2.13), this procedure yields (2.15) when we terminate at λ (i.e., $A_n = A_n^{(1)}\lambda + A_n^{(0)}$, etc.), and (2.17) when we terminate at λ^3. In any event the method of solution for these equations differ from (2.5), (2.6), (2.9), and (2.12) as the inverse scattering is different for the different eigenvalue problems.

III. METHOD OF SOLUTION

In this section we shall discuss the inverse scattering of the eigenvalue problem (1.5) in the case where Q_n, R_n, S_n, $T_n \to 0$ as $|n| \to \infty$. Hence, this method is not applicable to the evolution equations (2.14), (2.15), and (2.17) for which the discrete Schrödinger equation applies. However, the methods of Case and Kac[10] and Case[11] are applicable in these cases. We also wish to note that the inverse scattering of (1.5) was considered by Ablowitz and Ladik.[13] However, the special case when $S_n = T_n = 0$ [corresponding to Eqs. (2.5), (2.6), (2.9) and (2.10)] allows certain important modifications which were not previously presented. It is via the theory of inverse scattering that the solutions to the nonlinear evolution equations can be found. The basic steps for carrying out the solution process have been discussed in Sec. I. Here we will elaborate on these steps as they apply to the eigenvalue problem (1.5) and time dependence (1.6).

For convenience it will be assumed that the potentials are on compact support; that is, Q_n, R_n, S_n, T_n vanish for $|n| \geq N_0$. Let us define the time independent eigenfunctions $\bar{\phi}_n$, ϕ_n, $\bar{\psi}_n$, ψ_n of (1.5) as

$$\begin{aligned} & n \to -\infty\colon \phi_n \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} z^n, \quad \bar{\phi}_n \sim \begin{pmatrix} 0 \\ -1 \end{pmatrix} z^{-n}, \\ & n \to +\infty\colon \psi_n \sim \begin{pmatrix} 0 \\ 1 \end{pmatrix} z^{-n}, \quad \bar{\psi}_n \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} z^n. \end{aligned} \tag{3.1}$$

The scattering coefficients a, $\bar{a}$, b, $\bar{b}$ associated with the eigenvalue problem are defined by the relations

$$\begin{aligned} \phi_n &= a(z,t)\bar{\psi}_n + b(z,t)\psi_n, \\ \bar{\phi}_n &= -\bar{a}(z,t)\psi_n + \bar{b}(z,t)\bar{\psi}_n. \end{aligned} \tag{3.2}$$

It is assumed that $\bar{a}(z)$ (we will not write the t dependence explicitly in what follows) and $a(z)$ have a finite number of simple zeros inside and outside the unit circle, respectively. The zeros of $\bar{a}$, denoted by $\bar{z}_k$, and the zeros of a, denoted by z_k, turn out to be the discrete eigenvalues of (1.5). The remaining elements of the scattering data are as follows: the "reflection coefficients" are given by the ratios b/a and $\bar{b}/\bar{a}$, and the bound state normalization constants are

$$C_k = \left(b(z) \Big/ \frac{da(z)}{dz}\right)_{z=z_k}, \quad \bar{C}_k = \left(\bar{b}(z) \Big/ \frac{d\bar{a}(z)}{dz}\right)_{z=\bar{z}_k}. \tag{3.3}$$

In the important special cases of $R_n = \mp Q_n^*$, $S_n = \mp T_n^*$ the barred and unbarred quantites are related by

$$\bar{z}_k = 1/z_k^*, \quad \bar{b} = \pm b^*, \qquad \bar{a} = a^*, \quad \bar{C}_k = \pm (1/z_k^{*2}) C_k^*. \tag{3.4}$$

The first step in obtaining the solution is to obtain the scattering data at $t = 0$. We are given Q_n, R_n, S_n, T_n at $t = 0$; hence we must solve the eigenvalue problem at $t = 0$ for ψ_n, $\bar{\psi}_n$, ϕ_n, $\bar{\phi}_n$. With the potentials on compact support this is accomplished most readily by putting (1.5) into the two explicit forms

$$V_{1_{n+1}} = [(z + R_n S_n) V_{1_n} + (Q_n + S_n/z) V_{2_n}]/(1 - S_n T_n),$$
$$V_{2_{n+1}} = [(z T_n + R_n) V_{1_n} + (T_n Q_n + 1/z) V_{2_n}]/(1 - S_n T_n), \tag{3.5}$$

and

$$V_{1_n} = [(1/z + T_n Q_n) V_{1_{n+1}} - (S_n/z + Q_n) V_{2_{n+1}}]/(1 - R_n Q_n),$$
$$V_{2_n} = [-(z T_n + R_n) V_{1_{n+1}} + (z + R_n S_n) V_{2_{n+1}}]/(1 - R_n Q_n), \tag{3.6}$$

and iterating from $n = -N_0$ and $n = N_0$, respectively. Once this has been done, Eqs. (3.2) can be used to determine $\bar{z}_k$, $\bar{b}_0/\bar{a}_0$ [i.e., $\bar{b}(z, 0)/\bar{a}(z, 0)$], and $\bar{C}_{k,0}$ in terms of the initial data $Q_n(0)$, $T_n(0)$.

At this point it is important to note that there is a degree of degeneracy in determining the scattering data corresponding to the special case of $S_n = T_n = 0$. Assuming R_n and Q_n are on compact support, an induction argument based on iterating (3.5) and (3.6) shows that $a(z)$, $\bar{a}(z)$ are polynomials in z of even degree. Similarly it is found that $b(z)$, $\bar{b}(z)$ are polynomials of odd degree; hence $\bar{a}$ is an even function and $\bar{b}$ is an odd function. The parity of $\bar{a}$ and $\bar{b}$ implies that eigenvalues of (1.5), if they exist, occur in positive—negative pairs and

$$\bar{C}_k(\bar{z}_+) = C_k(\bar{z}_- = -\bar{z}_+), \quad C_k(z_+) = C_k(z_-).$$

At this stage the initial conditions have been mapped into the scattering data at $t = 0$. Next the time evolution of the scattering data must be found. The remarkable feature of this method, similar to that of Fourier analysis, is the separation of the spatial variable from the time variable. This allows the computation of the time evolution of the scattering data from (1.6) using the asymptotic forms of A_n, D_n. Since ϕ, $\bar{\phi}$, ψ, $\bar{\psi}$ have time independent boundary conditions (3.1), they do not satisfy (1.6). We therefore define eigenfunctions $\phi^{(t)}$, $\bar{\phi}^{(t)}$, $\psi^{(t)}$, $\bar{\psi}^{(t)}$, which satisfy both (1.5) and (1.6). From (2.1) as $|n| \to \infty$, B_n $C_n \to 0$, and A_n, $D_n \to$ constants. Then, in order to satisfy both (1.5) and (1.6), we define these new eigenfunctions by

$$\phi_n^{(t)} = \phi_n \exp\left[\left(\lim_{n\to\infty} A_n\right) t\right],$$
$$\bar{\phi}_n^{(t)} = \bar{\phi}_n \exp\left[\left(\lim_{n\to\infty} D_n\right) t\right],$$
$$\psi_n^{(t)} = \psi_n \exp\left[\left(\lim_{n\to\infty} D_n\right) t\right], \tag{3.7}$$
$$\bar{\psi}_n^{(t)} = \bar{\psi}_n \exp\left[\left(\lim_{n\to\infty} A_n\right) t\right].$$

Since these functions are linearly independent, we may write

$$\phi_n^{(t)} = a_0 \bar{\psi}_n^{(t)} + b_0 \psi_n^{(t)},$$
$$\bar{\phi}_n^{(t)} = -\bar{a}_0 \psi_n^{(t)} + \bar{b}_0 \bar{\psi}_n^{(t)}. \tag{3.8}$$

Susbstitution of (3.7) into (3.8) and comparison with (3.2) yields

$$\bar{a} = \bar{a}_0 \exp[(D_+ - D_-)t], \quad \frac{\bar{b}}{\bar{a}} = \frac{\bar{b}_0}{\bar{a}_0} \exp[(A_+ - D_+)t] \tag{3.9}$$

and by analytic continuation

$$\bar{C}_k = \bar{C}_{k,0} \exp[(A_+ - D_+)t], \tag{3.10}$$

where in the above $A_+ \equiv \lim_{n\to\infty} A_n$, etc. [For example, (2.4) gives $(A_+ - D_+) = -i(z^2 + 1/z^2 - 2)$.]

At this point in the solution process, all the necessary data needed to reconstruct the potentials have been found. As in the case of Fourier analysis, we need to go from "scattering space" to physical space, i.e., we wish to reconstruct $U(x, t)$. The theory of inverse scattering tells us how this is accomplished. In Ref. 13 the details are worked out. Here we will present the results and add some simplifications when $S_n = T_n = 0$.

From Ref. 13, when $S_n = \mp T_n^*$, $R_n = \mp Q_n^*$ the inversion is begun by computing

$$F(m + n; t) = \frac{1}{2\pi i} \oint \frac{\bar{b}}{\bar{a}}(z, t) z^{m+n-1}\, dz - \sum_{k=1}^{N} \bar{C}_k(t) \bar{z}_k^{\,m+n-1}. \tag{3.11}$$

The integral and summation terms correspond to the contributions of the continuous and discrete spectra, respectively, of the eigenvalue problem (1.5). $F(m + n; t)$ bears a strong resemblance to Eq. (1.3a) of the linear theory, the difference being the discrete term (which gives rise to the important soliton solutions). Next we solve the coupled summation equation

$$K_1(n, m; t) - F(m + n; t) - \sum_{n'=n+1}^{\infty} K_2^*(n, n'; t) F(m + n'; t) = 0,$$
$$K_2(n, m; t) \pm \sum_{n=n+1}^{\infty} K_1^*(n, n'; t) F(m + n; t) = 0. \tag{3.12}$$

The solutions allow us to reconstruct the potentials by

$$Q_n(t) = -K_1(n, n + 1; t), \tag{3.13a}$$

and if $T_n \neq 0$,

$$T_n(t) = \pm \frac{1}{[1 \pm Q_n(t) Q_n^*(t)]} \times [K_1^*(n, n + 2; t) - K_1^*(n, n + 1; t) K_2^*(n, n + 1; t)]. \tag{3.13b}$$

In the case when $S_n = T_n = 0$ there are significant simplifications. As discussed earlier, it can be shown that $(\bar{b}_0/\bar{a}_0)(z)$ is an odd function of z, $(A_+ - D_+)$ is even in z, the eigenvalues occur in positive—negative pairs, and for each such pair there is one $\bar{C}_{k,0}$ of the same sign. These symmetry properties mean that (3.11) may be written in the form ($p \geq 1$)

$$F(n+m;t)=\begin{Bmatrix} 2F_R(n+m;t) & m=n+2p-1 \\ 0 & m=n+2p \end{Bmatrix}, \quad (3.14)$$

where

$$F_R(n+m;t)=\frac{1}{2\pi i}\oint_{C_R}\frac{\bar{b}}{\bar{a}}(z,t)z^{n+m-1}\,dz-\sum_{k=1}^{N/2}\bar{C}_k(t)\bar{z}^{m+n-1}, \quad (3.15)$$

and $\oint_{c_R}$ denotes the integral along the right portion of the unit circle only. This means that Eq. (3.12) also separates. We find ($p \geq 1$)

$$K_1(n,m;t)=\begin{Bmatrix} K_{1_R}(n,m;t) & m=n+2p-1 \\ 0 & m=n+2p \end{Bmatrix} \quad (3.16a)$$

and

$$K_2(n,m;t)=\begin{Bmatrix} K_{2_R}(n,m;t) & m=n+2p \\ 0 & m=n+2p-1 \end{Bmatrix}. \quad (3.16b)$$

Thus, Eq. (3.13) is identically satisfied (as it must), and an alternative form for (3.12) and (3.13a) is

$$K_{1_R}(n,m;t)-2F_R(n+m;t)\pm 4\sum_{n'}^{\infty}\sum_{n''}^{\infty}K_{1_R}(n,n'';t)F_R^*(n'+n'',t)F_R(n'+m;t)=0, \quad (3.17)$$

($n'=n+2,n+4,\ldots,\infty;\ n''=n+1,n+3,\ldots,\infty$), where $Q_n(t)$ is recovered from the relation

$$Q_n(t)=-K_{1_R}(n,n+1;t). \quad (3.18)$$

The continuum limit to the partial differential case is now direct.

Finally we point out how $A_+ - D_+$ is related to the dispersion relation. It is clear from (3.17) and (3.18) that for sufficiently large $n \to \infty$

$$Q_n(t) \sim -2F_R(2n+1;t). \quad (3.19)$$

Thus in these regions the solution approximately satisfies the linearized equation. Thus by using (1.3)—(1.4) and (3.9)—(3.11), the time dependence in $F_R(2n+1;t)$ must obey the condition

$$-i\omega(z^2)=\lim_{n\to\infty}(A_n-D_n)=(A_+-D_+). \quad (3.20)$$

To summarize, we have found the following:

(i) Given the initial data [$Q_n(0)$, etc.] we solve the direct scattering problem (1.5) for the initial scattering data,

$$S(z,0):\{\bar{z}_1,\ldots,\bar{z}_N,\bar{b}(z,0)/\bar{a}(z,0),\bar{C}_{k,0}\}.$$

(ii) We find from (1.6) the scattering data for all time,

$$S(z,t):\{\bar{z}_1,\ldots,\bar{z}_N,(\bar{b}_0/\bar{a}_0)\exp(-i\omega t),\ \bar{C}_{k,0}\exp(-i\omega t)\}.$$

(iii) Given $S(z,t)$, we solve a linear summation equation [either (3.12) or (3.17)] and recover the potentials [via (3.13) or (3.18) depending on whether or not $T_n = \mp S_n^*$ is zero] from this solution. The dispersion relation is a crucial conceptual quantity in this theory. First of all, it suggests how to isolate and characterize a given evolution equation, and second it is the distinguishing function in the time dependence of the scattering data $S(z,t)$. For the above reasons we consider this procedure a natural extension of discrete Fourier analysis to nonlinear differential—difference equations. We term the inverse process as "the inverse scattering transform."

IV. SOLITONS AND CONSERVATION LAWS

In this section we will present important special solutions of the evolution equations. These solutions are termed solitons,[15] because the nonlinear interactions are elastic. We shall see that the existence of soliton modes is due entirely to the discrete spectrum. In this section the discussion of these solutions will be restricted to the evolution equations obtained by letting $R_n = -Q_n^*$ $S_n = -T_n^*$.

The first case to be considered is the first order in time equations corresponding to $S_n = T_n = 0$. As was mentioned in Sec. III when S_n and T_n both vanish the eigenvalues, if they exist, occur in positive—negative pairs. In this case a pair of eigenvalues gives rise to a single soliton. For this situation $F_R(n+m;t)$ in (3.15) is given by

$$F_R(n+m;t)=-\bar{C}_1\bar{z}_1^{\,m+n-1}. \quad (4.1)$$

The solution to (3.17) can be found by making use of the contraction

$$\tilde{K}_1(n)=\sum_m K_{1_R}(n,m)\bar{z}^{*m},\quad (m=n+1,n+3,\ldots,\infty). \quad (4.2)$$

By following the technique of Ref. 13, $\tilde{K}_1(n)$ is given by

$$\tilde{K}_1(n)=\frac{-2\bar{C}_1\bar{z}_1^{\,n-1}(\bar{z}_1\bar{z}_1^*)^{n+1}}{[1+4\bar{C}_1\bar{C}_1^*(\bar{z}_1\bar{z}_1^*)^{2n+2}/[1-(\bar{z}_1\bar{z}_1^*)^2]^2][1-(\bar{z}_1\bar{z}^*)^2]}, \quad (4.3)$$

and $K_{1_R}(n,m)$ is found to be

$$K_{1_R}(n,m)=\frac{-2\bar{C}_1\bar{z}_1^{\,m+n-1}}{1+4\bar{C}_1\bar{C}_1^*(\bar{z}_1\bar{z}_1^*)^{2n+2}/(1-(\bar{z}_1\bar{z}_1^*)^2)^2}, \quad (4.4)$$

$m=n+2p-1$.

From (3.18) the general soliton solution for $\bar{z}_1 = \exp(-w+ie)$ ($w>0$), $\bar{C}_k=\bar{C}_{k,0}\exp[-i\omega(\bar{z}_1^{\,2})t]$ in terms of the dispersion relation is given by

$$Q_n=\left(\frac{\bar{C}_{1,0}}{\bar{C}_{1,0}^*}\right)^{1/2}\exp(-(i/2)\{\omega(\bar{z}_1^{\,2})+[\omega(\bar{z}_1^{\,2})]^*\}t+2in\theta)$$
$$\times\sinh 2w\,\mathrm{sech}(2nw-(i/2)\{[\omega(z_1^2)]^*-\omega(\bar{z}_1^{\,2})\}t+\bar{\phi}_0), \quad (4.5)$$

where $\bar{\phi}_0=-\ln(|\bar{C}_{1,0}|/\sinh 2w)$. For the case of the nonlinear Schrödinger equation (2.5) ($Q_n=-R_n^*$) using the dispersion relation $\omega(z^2)=z^2+1/z^2-2$ in (4.5) yields

$$Q_n=\exp[i(2n\theta-2\cosh 2w\cos 2\theta t+2t+\theta_0)]$$
$$\times\sinh 2w\,\mathrm{sech}(2nw+2\sin 2\theta\sinh 2wt+\phi_0) \quad (4.6)$$

where θ_0 is defined by $\bar{C}_{1,0}=|\bar{C}_{1,0}|\exp(i\theta_0)$.

The second case is the second order in time systems corresponding to keeping all four potentials. Unlike the preceeding first order equations where a pair of eigenvalue gives rise to one soliton, here one eigenvalue gives rise to one soliton. For this solution mode

$F(n+m;t)$ is given by

$$F(n+m;t) = -\bar{C}_1 \bar{z}_1^{\,m+n-1}. \tag{4.7}$$

For this case, in order to determine the solutions, the solution to (3.12) must be found. By quoting the results of Ref. 13, $K_1(n, m; t)$ and $K_2(n, m; t)$ are given by

$$K_1(n, m; t) = \frac{-\bar{C}_1 \bar{z}_1^{\,m+n-1}}{1+\bar{C}_1\bar{C}_1^*(\bar{z}_1\bar{z}_1^*)^{2n+1}/(1-\bar{z}_1\bar{z}_1^*)^2} \tag{4.8}$$

and

$$K_2(n, m; t) = \frac{-\bar{C}_1\bar{C}_1^*(\bar{z}_1\bar{z}_1^*)\bar{z}_1^{\,n}\bar{z}_1^{\,m}}{[1+\bar{C}_1\bar{C}_1^*(\bar{z}_1\bar{z}_1^*)^{2n+1}/(1-\bar{z}_1\bar{z}_1^*)](1-\bar{z}_1\bar{z}_1^*)}. \tag{4.9}$$

Using the appropriate values of $K_1(n, m; t)$ and $K_2(n, m; t)$ in (3.13), the general soliton solution for $z_1 = \exp(-w + i\theta)$ $(w > 0)$, $\bar{C}_1 = \bar{C}_{1,0}\exp[-i\omega(\bar{z}_1^2)t]$ is given in terms of the dispersion relation by

$$Q_n = \left(\frac{\bar{C}_{1,0}}{\bar{C}_{1,0}^*}\right)^{1/2} \exp(-(i/2)\{\omega(\bar{z}_1^2) + [\omega(\bar{z}_1^2)]^*\}t + i2n\theta)$$
$$\times \sinh w \operatorname{sech}(2nw - (i/2)\{[\omega(\bar{z}_1^2)]^* - \omega(\bar{z}_1^2)\}t + \phi_0), \tag{4.10}$$

$$T_n = -1\left(\frac{\bar{C}_{1,0}^*}{\bar{C}_{1,0}}\right)^{1/2} \exp(-(i/2)\{\omega(\bar{z}_1^2) - [\omega(\bar{z}_1^2)]^*\}t - i(2n+1)\theta)$$
$$\times \sinh w \operatorname{sech}(2nw - (i/2)([\omega(\bar{z}_1^2)]^* - \omega(\bar{z}_1^2))t + \phi_0 + w),$$

where $\phi_0 = -\ln(|\bar{C}_{1,0}|/(2\sinh w))$. In the case of the self-dual network,[13] the dispersion relation is given by $\omega(z^2) = \pm i(z - 1/z)$, and the results of (4.10) can be simplified to yield

$$Q_n = \operatorname{sgn}(\bar{C}_{1,0}) \sinh w \operatorname{sech}(2nw \pm 2\sinh wt + \phi_0),$$
$$T_n = \mp \operatorname{sgn}(C_{1,0}) \sinh w \operatorname{sech}(2nw \pm 2\sinh wt + \phi_0 + w). \tag{4.11}$$

Connected with the class of solvable evolution equations derived in Sec. II is an infinite sequence of conservation laws. Following Zahharov and Shabat,[6] these laws can be constructed systematically from the scattering problem by considering asymptotic expansions of $\bar{a}(z)$. The details of the derivation of the conserved quantities will be enumerated for the case of $S_n = T_n = 0$. The same procedure can be followed when $S_n \neq 0$, $T_n \neq 0$; hence we will only list the first few conservation laws.

The asymptotic form of $\bar{a}(z)$ as $n \to -\infty$ can be obtained by solving equation (3.2) for $\bar{a}(z)$ and applying the boundary conditions (3.1); thus

$$\bar{a}(z) \sim -\bar{\phi}_{2_n} z^n. \tag{4.12}$$

From the eigenvalue problem (1.5) we eliminate $\bar{\phi}_{1_n}$ and obtain a difference equation for the expression $\bar{\phi}_{2_n} z^n$, which is given by

$$\Delta_n\left(\frac{\Delta_n(z^n\bar{\phi}_{2_n})}{z^{2n+1}R_n}\right) = Q_n z^{2n-1}(z^n\bar{\phi}_{2_n}). \tag{4.13}$$

By defining

$$-\bar{\phi}_{2_n} z^n = \prod_{k=-\infty}^{\infty} g_k, \tag{4.14}$$

Eq. (4.13) takes the form

$$g_{n+1}(g_{n+2} - 1) - z^2\frac{R_{n+1}}{R_n}(g_{n+1} - 1) = z^2 R_{n+1} Q_n. \tag{4.15}$$

An asymptotic expansion for g_n in powers of z^2 is obtained by substituting the expression

$$g_n = g_n^{(0)} + g_n^{(1)} z^2 + g_n^{(2)} z^4 + \cdots \tag{4.16}$$

into (4.15) and solving for the coefficients in a recursive manner. Thus g_n is given by

$$g_n = 1 + z^2 R_{n-1} Q_{n-2} + z^4 R_{n-1} Q_{n-3}(1 - R_{n-2}Q_{n-2}) + \cdots. \tag{4.17}$$

Taking the logarithm of (4.14), we obtain

$$\log[\bar{a}(z)] = \sum_{-\infty}^{\infty} \log(1 + z^2 R_{n-1} Q_{n-2}$$
$$+ z^4 R_{n-1} Q_{n-3}(1 - R_{n-2}Q_{n-2}) + \cdots), \tag{4.18}$$

which can be expressed as

$$\log[\bar{a}(z)] = \sum_{-\infty}^{\infty} \{z^2 R_{n-1} Q_{n-2}$$
$$+ z^4[R_{n-1}Q_{n-3}(1 - R_{n-2}Q_{n-2}) - \tfrac{1}{2}R_{n-1}^2 Q_{n-2}^2] + \cdots\}; \tag{4.19}$$

since $\bar{a}(z)$ is time independent, each of the coefficients C_i in the asymptotic expansion

$$\log[\bar{a}(z)] = \sum_{i=0}^{\infty} C_i z^{2i} \tag{4.20}$$

is constant. The $\{C_i\}$, $i = 1, 2, \cdots$, are our infinite number of conserved quantities. The first two are found to be

$$C_1 = \sum_{k=-\infty}^{\infty} R_k Q_{k-1}, \tag{4.21a}$$

$$C_2 = \sum_{k=-\infty}^{\infty} [R_k Q_{k-2}(1 - R_{k-1}Q_{k-1}) - \tfrac{1}{2}R_k^2 Q_{k-1}^2]. \tag{4.21b}$$

In the general case when $S_n \neq 0$, $T_n \neq 0$, a similar procedure applies. However, here it is the quantity $\bar{a}(z)\prod_{-\infty}^{\infty}(1 - S_k T_k)$ that is constant. We list the first two:

$$C_1 = \sum_{k=-\infty}^{\infty} (S_{k-1}R_k + T_k Q_k), \tag{4.22a}$$

$$C_2 = \sum_{k=-\infty}^{\infty} [S_{k-1}T_k + R_k Q_{k-1}(1 - S_{k-1}T_{k-1})$$
$$- \tfrac{1}{2}(S_{k-1}R_k + T_k Q_k)^2]. \tag{4.22b}$$

In addition to these there is an additional conserved quantity to the above. This is

$$C_0 = \prod_{-\infty}^{\infty}\left(\frac{1 - R_k Q_k}{1 - S_k T_k}\right),$$

which is found from the Wronskian (see Ref. 13). This quantity is always positive when $Q_k = -R_k^*$, $T_k = -S_k^*$. This is a nice feature to maintain in any (numerical) difference scheme.[16]

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[1]R. Hirota, J. Phys. Soc. Japan **35**, 289 (1973).
[2]M. Toda, Prog. Theor. Phys. Suppl. **45**, 1974 (1970).
[3]V. Zakharov, S. Musher, and A. Rubenshik, Zh. Eksp. Teor. Fiz. Pis. Red. **19**, 249 (1974) [Sov. Phys. JETP Lett. **19**, 151 (1974)].
[4]C. Gardner, J. Greene, M. Kruskal, and R. Miura, Phys. Rev. Lett. **19**, 1095 (1967).
[5]C. Gardner, J. Greene, M. Kruskal, and R. Miura, Comm. Pure Appl. Math. **21**, 167 (1968).
[6]V. Zakharov and A. Shabat, Zh. Eksp. Teor. Fiz. **61**, 118 (1971) [Sov. Phys. JETP **34**, 62 (1972)].
[7]P. Lax, Comm. Pure Appl. Math. **21**, 167 (1968).
[8]M. Ablowitz, D. Kaup, A. Newell, and H. Segur, Stud. Appl. Math. **53**, 255 (1974).
[9]H. Flaschka, Prog. Theor. Phys. **51**, 703 (1974).
[10]K. Case and M. Kac, J. Math. Phys. **14**, 594 (1973).
[11]K. Case, J. Math. Phys. **14**, 916 (1973).
[12]S. Manakov, Zh. Eksp. Teor. Fiz. **67**, 543 (1974) [Sov. Phys. JETP **40**, 269 (1975)].
[13]M. Ablowitz and J. Ladik, J. Math. Phys. **16**, 598 (1975).
[14]M. Kac and P. van Moerbeke, Proc. Natl. Acad. Sci. USA **72**, 1627 (1975).
[15]N. Zabusky and M. Kruskal, Phys. Rev. Lett. **15**, 86 (1965).
[16]M. Ablowitz and J. Ladik, Stud. Appl. Math. (to be published).

Bivariational bounds in a complex Hilbert space, and correction terms for Padé approximants*

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Let A be a closed linear transformation from a complex Hilbert space $\mathfrak{H}$ into itself, with $D(A)$, the domain of the operator, dense in $\mathfrak{H}$. Suppose that A satisfies $\langle A\phi, A\phi\rangle \geq a^2\langle\phi,\phi\rangle$ for all $\phi \in D(A)$, where a is a positive constant. Then for the case where the equation $A\phi = f$, with $f \in \mathfrak{H}$ given, possesses a solution $\phi \in D(A)$, bivariational functionals are presented which yield upper and lower bounds for both the real and imaginary parts of $\langle g,\phi\rangle$ for any given $g \in \mathfrak{H}$. The case $A = (1+zK)$ with z a complex parameter is then considered. With appropriate choices for the trial functions involved, the functionals yield the $[N+J-1/N-J]$ Padé approximants ($J = 0, 1, \cdots, N$; $N = 1,2,\cdots,$) to $F(z) = \langle g,\phi\rangle$ together with correction terms such that bounds on $F(z)$ ensue. Finally, an arbitrary analytic function $G(z)$, regular within a closed contour C and continuous within and on C, is considered. The above theory leads to bounds on $G(z)$ in the form of $[N+J-1/N-J]$ Padé approximants together with correction terms. The results are then generalized for arbitrary $[L/M]$ Padé approximants to $G(z)$ with the aid of the Hermite error formula.

I INTRODUCTION

One of the major problems in approximation theory in general, and in Padé approximation theory in particular, is the assessment of the accuracy of the approximation. Generally speaking, for a well-constructed approximation, additional information is required beyond that used to construct the approximant. For example, if it is known that an analytic function belongs to a particular class, such as series of Stieltjes, then inclusion regions can be constructed directly from the Padé approximants for the value of the function. If in addition the radius of convergence of the series is known, the inclusion regions can be tightened. In this paper we consider approximations to the solutions of functional equations and approximations to analytic functions. We will show how certain additional quantitative information, which may well be available in some practical situations, can be used to construct inclusion regions from our approximants. Since the true value lies in the intersection of all such inclusion regions, and since our inclusion regions do not seem to possess a nesting property, it turns out to be useful to compute all of the inclusion regions. We will first treat the functional equation and later as an application, as well as by an independent method, treat analytic functions.

Let $\mathfrak{H}$ be a complex Hilbert space with inner product $\langle\ ,\ \rangle$. Let A be a closed linear transformation from $\mathfrak{H}$ into itself, with domain $D(A)$ dense in $\mathfrak{H}$, and suppose that it is possible to find a positive constant a such that

$$\langle A\Phi, A\Phi\rangle \geq a^2\langle\Phi,\Phi\rangle \quad \text{for all } \Phi \in D(A). \tag{1.1}$$

Let $f \in \mathfrak{H}$ be given such that the problem

$$A\phi = f \tag{1.2}$$

possesses a solution $\phi \in D(A)$. Then we begin in Sec. II by showing how bivariational upper and lower bounds can be imposed on both the real and imaginary parts of the quantity

$$\langle g,\phi\rangle \quad \text{for any given } g \in \mathfrak{H}. \tag{1.3}$$

In previous work[1-3] similar bivariational bounds have been established for the case where the Hilbert space is real. These bounds have lent themselves to a variety of applications including the determination of pointwise bounds for the solutions of two-point boundary-value problems[4] and one-electron Schrödinger equations.[5] Of special interest, for the situation where the operator A in (1.2) is positive and self-adjoint, it has been shown[6] how bivariational functionals lead to Padé approximants plus *correction terms* such that bounds are obtained for functions of the form

$$\tilde{F}(x) = \int_0^\infty \frac{d\mathring{\phi}(u)}{1+ux}, \quad x > 0, \tag{1.4}$$

where $\mathring{\phi}(u)$ is of bounded variation on $0 \leq u < \infty$ and $\tilde{F}(x)$ is a generalization of a series of Stieltjes.

In Sec. III we consider the application of the bivariational bounds, developed in Sec. II, to the case $A = (1 + zK)$, where z is a complex variable and the domain of the linear operator K is the whole of $\mathfrak{H}$. With appropriate choices for the trial functions involved, the bivariational functionals are shown to yield the $[N+J-1/N-J]$ Padé approximants ($J = 0, 1, \ldots, N; N = 1, 2, \ldots$) to

$$F(z) = \langle g, (1+zK)^{-1}f\rangle \tag{1.5}$$

together with correction terms such that bounds on the real and imaginary parts of $F(z)$ ensue. These correction terms involve similar information to that required for the construction of the Padé approximants, and they can often be evaluated explicitly. An understanding of the structure and formation of such cor-

rection terms is important because Padé approximants are now often used to approximate physical functions of the form (1.5) (see, for example, the applications given in Refs. 7 and 8 and also Refs. 9 and 10). With the aid of correction terms each Padé approximant leads to rigorous information about $F(z)$. Bounds associated with one approximant can supply useful information about $F(z)$ where another approximant with different pole locations leads to wide bounds, and vice versa. By forming a variety of different Padé approximants plus correction terms one should be able to obtain good bounds on $F(z)$ throughout various regions in the complex plane.

Finally, in Sec. IV we consider an arbitrary analytic function $G(z)$ which is regular within a closed contour C, and continuous within and on C. The above theory leads to bounds on $G(z)$ in the form of $[N+J-1/N-J]$ Padé approximants together with correction terms. The results are then generalized for arbitrary $[L/M]$ Padé approximants with the aid of the Hermite error formula. Given an appropriate set of information about $G(z)$, a "Padé Table" of upper and lower bounds on $G(z)$ can be constructed straightforwardly. Seen as a whole, this table supplies useful information about $G(z)$ for all z lying within C.

II. BIVARIATIONAL BOUNDS IN A COMPLEX HILBERT SPACE

We will suppose in all that follows that A is a closed linear transformation from a complex Hilbert space $\mathfrak{H}$ into itself, with $D(A)$ dense in $\mathfrak{H}$. We will suppose that A has the property (1.1), and that $f\in\mathfrak{H}$ has been given such that (1.2) possesses a solution $\phi\in D(A)$. We note that (1.1) ensures that ϕ is unique.

Since $D(A)$ is dense in $\mathfrak{H}$, A uniquely defines its adjoint A^*,[11] and we have

$$\langle\xi, A\eta\rangle = \langle A^*\xi, \eta\rangle \quad \text{for all } \eta\in D(A),\quad \xi\in D(A^*). \tag{2.1}$$

A^* is also a closed linear transformation from $\mathfrak{H}$ into itself, and $D(A^*)$ is dense in $\mathfrak{H}$. Since A is closed we have[12]

$$(A^*)^* = A. \tag{2.2}$$

Now let $g\in\mathfrak{H}$ be given. Then in order to derive bivariational bounds for $\langle g,\phi\rangle$ we must introduce the auxiliary equation

$$A^*\psi = g, \tag{2.3}$$

for which we have the following lemma:

Lemma: The equation $A^*\psi = g$ has at least one solution ψ for any $g\in\mathfrak{H}$.

Proof. A^*A is a positive self-adjoint operator in[11] $\mathfrak{H}$, and from (1.1) it follows that it is bounded below away from zero over its domain. Its inverse is thus a self-adjoint, bounded and therefore closed operator. As such its domain is necessarily the whole of $\mathfrak{H}$. Hence, the range of A^*A is the whole of $\mathfrak{H}$. Hence, the range of A^* is the whole of $\mathfrak{H}$, which proves the lemma.

In all that follows we shall use ψ to denote a solution of (2.3). In order to handle bounds on the real and imaginary parts of complex quantities succintly, we introduce the notation

$$z_1 \succcurlyeq z_2, \quad \text{or equivalently} \quad -z_1 \preccurlyeq -z_2, \tag{2.4}$$

whenever z_1 and z_2 are complex numbers such that

$$\mathrm{Re}z_1 \geqslant \mathrm{Re}z_2 \quad \text{and} \quad \mathrm{Im}z_1 \geqslant \mathrm{Im}z_2. \tag{2.5}$$

The following statements are immediate:

$$\text{if } z_1 \succcurlyeq z_2, \text{ and } c\geqslant 0, \Rightarrow cz_1 \succcurlyeq cz_2; \tag{2.6a}$$

$$\text{if } z_1 \succcurlyeq z_2, \Rightarrow -z_2 \succcurlyeq -z_1; \tag{2.6b}$$

$$\text{if } z_1 \succcurlyeq z_2, \text{ and } z_3 \succcurlyeq z_4, \Rightarrow z_1+z_3 \succcurlyeq z_2+z_4; \tag{2.6c}$$

$$\text{for all complex } z,\quad (1+i)|z| \succcurlyeq z \succcurlyeq -(1+i)|z|, \tag{2.6d}$$

where $|z| = \{z\bar{z}\}^{1/2}$, with $\bar{z}$ the complex conjugate of z.

We will write $\|\eta\| = \langle\eta,\eta\rangle^{1/2}$ to denote the usual Hilbert space norm of any vector $\eta\in\mathfrak{H}$. The central result of this paper can now be given.

Theorem. Bivariational upper and lower bounds on the real and imaginary parts of $\langle g,\phi\rangle$ for any $g\in\mathfrak{H}$ are supplied by the two functionals

$$\mathcal{J}_\pm(\Psi,\Phi) = -\langle\Psi, A\Phi\rangle + \langle\Psi, f\rangle + \langle g,\Phi\rangle \pm (1+i)a^{-1}\|A\Phi - f\|\cdot\|A^*\Psi - g\| \tag{2.7}$$

according to

$$\mathcal{J}_+(\Psi,\Phi) \succcurlyeq \langle g,\Phi\rangle \succcurlyeq \mathcal{J}_-(\Psi,\Phi) \tag{2.8}$$

for all $\Psi\in D(A^*)$ and $\Phi\in D(A)$. The bounds are attained whenever either $\Psi=\psi$ of (2.3) or $\Phi=\phi$ of (1.2).

Proof. It follows from the lemma that we can always write

$$\Psi = \psi + \delta\Psi, \tag{2.9}$$

with $\delta\Psi = (\Psi-\psi)\in D(A^*)$. Similarly, from the assumption that (1.2) possesses a solution $\phi\in D(A)$, we can write

$$\Phi = \phi + \delta\Phi, \tag{2.10}$$

with $\delta\Phi\in D(A)$. Hence

$$\mathcal{J}_\pm(\Psi,\Phi) = \langle g,\phi\rangle - \langle\delta\Psi, A\delta\Phi\rangle \pm (1+i)a^{-1}\|A\delta\Phi\|\cdot\|A^*\delta\Psi\|, \tag{2.11}$$

which establishes the bivariational nature of the two functionals since there are no first-order terms. To establish the bounding properties of the functionals we observe that

$$\begin{aligned}(1+i)a^{-1}\|A\delta\Phi\|\cdot\|A^*\delta\Psi\| &\succcurlyeq (1+i)\|\delta\Phi\|\cdot\|A^*\delta\Psi\| \quad \text{[using (1.1)]}\\ &\succcurlyeq (1+i)|\langle A^*\delta\Psi,\delta\Phi\rangle| \quad \text{(using Schwarz's inequality)}\\ &= (1+i)|\langle\delta\Psi, A\delta\Phi\rangle| \quad \text{[using (2.2)]}\\ &\succcurlyeq \langle\delta\Psi, A\delta\Phi\rangle \quad \text{[using (2.6d)]},\end{aligned} \tag{2.12}$$

and similarly

$$\langle\delta\Psi, A\delta\Phi\rangle \succcurlyeq -(1+i)a^{-1}\|A\delta\Phi\|\cdot\|A^*\delta\Psi\|. \tag{2.13}$$

On combining the observation (2.11) with the inequalities (2.12) and (2.13), the relation (2.8) is obtained. The last statement of the theorem is immediate from (2.11) with $\delta\Phi=0$ or $\delta\Psi=0$. This completes the proof of the theorem.

Let us write

$$\mathcal{J}_{\pm}(\Psi,\Phi)=\mathcal{J}(\Psi,\Phi)\pm C(\Psi,\Phi), \tag{2.14}$$

where

$$\mathcal{J}(\Psi,\Phi)=-\langle\Psi,A\Phi\rangle+\langle\Psi,f\rangle+\langle g,\Phi\rangle \tag{2.15}$$

and

$$C(\Psi,\Phi)=(1+i)a^{-1}\|A\Phi-f\|\cdot\|A^*\Psi-g\|. \tag{2.16}$$

Then $\mathcal{J}(\Psi,\Phi)=\langle g,\phi\rangle-\langle\delta\Psi,A\delta\Phi\rangle$ is itself a stationary approximation to the quantity of interest $\langle g,\phi\rangle$. This functional occurs in bivariational bounds associated with real Hilbert space,[1,2] and also arises as the basis of approximate methods in theoretical physics and chemistry (see, for example, Refs. 12 and 13). The purely second-order functional $C(\Psi,\Phi)$ supplies corrections to $\mathcal{J}(\Psi,\Phi)$, such that bounds for $\langle g,\phi\rangle$ ensue.

We consider briefly some methods for choosing "best" trial functions $\hat{\Psi}\in T_1$ and $\hat{\Phi}\in T_2$ from families of trial functions $T_1\subseteq D(A^*)$ and $T_2\subseteq D(A)$. Ideally one would choose two different pairs of trial functions to maximize the real and imaginary parts of $\mathcal{J}_-(\Phi,\Psi)$, and one would similarly have to minimize the real and imaginary parts of $\mathcal{J}_+(\Phi,\Psi)$. However, this optimization procedure is difficult even in the case of linearly variable trial functions. An alternative method is to choose $\hat{\Psi}$ and $\hat{\Phi}$ so as to minimize $\|A^*\Psi-f\|$, $\Psi\in T_1$ and $\|A\Phi-f\|$, $\Phi\in T_2$, respectively, for then $|\mathcal{J}_+(\hat{\Psi},\hat{\Phi})-\mathcal{J}_-(\hat{\Psi},\hat{\Phi})|$ is as small as possible. We note that one can sensibly choose $\hat{\Psi}$ and $\hat{\Phi}$ independently because of the last statement in the theorem. Another possibility is to choose $\hat{\Psi}$ and $\hat{\Phi}$ so as to make $\mathcal{J}(\Psi,\Phi)$ stationary with respect to variations in $\Psi\in T_1$ and $\Phi\in T_2$. In the case of linearly variable trial functions the latter procedure is attractive because the algebra is straightforward. Furthermore, by picking the underlying basis functions appropriately one can often arrange things so that $\mathcal{J}(\Psi,\Phi)$ is some *a priori* given approximation to $\langle g,\phi\rangle$, as we do in Sec. III.

III. PADE APPROXIMANTS AND CORRECTION TERMS WHEN $A=(1+zK)$

Here we suppose

$$A=(1+zK), \tag{3.1}$$

where z is a complex parameter and K is a closed linear transformation from $\mathfrak{H}$ into itself such that

$$D(K)=\mathfrak{H}. \tag{3.2}$$

In order that bivariational bounds shall apply to the operator A in (3.1), we must have available a positive constant a such that

$$\langle(1+zK)\Phi,(1+zK)\Phi\rangle\geq a^2\langle\Phi,\Phi\rangle \quad \text{for all } \Phi\in\mathfrak{H}. \tag{3.3}$$

Such a constant, depending on z, can readily be derived in terms of a positive constant c such that

$$\langle K\Phi,K\Phi\rangle=\langle\Phi,K^*K\Phi\rangle\leq c^2\langle\Phi,\Phi\rangle \quad \text{for all } \Phi\in\mathfrak{H}. \tag{3.4}$$

The existence of a finite value for c is assured by the Hellinger-Toepiltz theorem[11] since the domain of the positive self-adjoint operator K^*K is the whole of $\mathfrak{H}$. A suitable value for c^2 is any upper bound to the spectrum of K^*K. If we now set $z=|z|\exp(i\theta)$, we have

$$\begin{aligned}&\langle(1+zK)\Phi,(1+zK)\Phi\rangle\\&\quad=\langle\Phi,\Phi\rangle+2|z|\,\mathrm{Re}(\exp(i\theta)\langle\Phi,K\Phi\rangle)+|z|^2\langle K\Phi,K\Phi\rangle\\&\quad\geq(\langle\Phi,\Phi\rangle^{1/2}-|z|\langle K\Phi,K\Phi\rangle^{1/2})^2,\end{aligned} \tag{3.5}$$

where we have made use of the Schwarz-type inequality

$$\mathrm{Re}(\exp(i\theta)\langle\Phi,K\Phi\rangle)\geq-\langle\Phi,\Phi\rangle^{1/2}\langle K\Phi,K\Phi\rangle^{1/2}. \tag{3.6}$$

It follows from (3.4) and (3.5) that we can choose

$$a=(1-|z|c) \quad \text{whenever } |z|\leq 1/c. \tag{3.7}$$

Alternative expressions for a, with corresponding ranges of validity, can be derived in terms of upper and lower bounds for the self-adjoint operator (K^*+K).[2]

Given that there exists a positive constant a such that (3.3) is true, the condition that K is closed and defined throughout $\mathfrak{H}$ ensures that the equation

$$(1+zK)\phi=f \tag{3.8}$$

possesses a unique solution $\phi\in\mathfrak{H}$ for any $f\in\mathfrak{H}$ (the proof of this is similar to that of the lemma in Sec. II). Hence, the theorem of Sec. II supplies bivariational bounds for the real and imaginary parts of the function

$$F(z)=\langle g,\phi\rangle=\langle g,(1+zK)^{-1}f\rangle \tag{3.9}$$

for any f and g in $\mathfrak{H}$. For example, with the value for a in (3.7) we obtain

$$\begin{aligned}&\mathcal{J}(\Psi,\Phi)-(1+i)(1-|z|c)^{-1}\|(1+zK)\Phi-f\|\\&\qquad\times\|(1+\bar{z}K^*)\Psi-g\|\leq F(z)\\&\qquad\leq\mathcal{J}(\Psi,\Phi)+(1+i)(1-|z|c)^{-1}\|(1+zK)\Phi-f\|\\&\qquad\times\|(1+zK^*)\Psi-g\|\end{aligned} \tag{3.10}$$

for all complex z such that $|z|<1/c$, where now

$$\mathcal{J}(\Psi,\Phi)=-\langle\Psi,(1+zK)\Phi\rangle+\langle\Psi,f\rangle+\langle g,\Phi\rangle \tag{3.11}$$

and Ψ and Φ are arbitrary members of $\mathfrak{H}$.

We now show how bounds of the structure (3.10) can be made to yield $[N+J-1/N-J]$ Padé approximants to $F(z)(J=0,1,\ldots,N;\ N=1,2,\ldots)$ together with correction terms. Consider the linearly variable trial functions

$$\Psi=\sum_{j=0}^{J-1}(-\bar{z})^j(K^*)^jg+\sum_{j=J}^{N-1}a_j(K^*)^jg \tag{3.12}$$

and

$$\Phi=\sum_{j=0}^{J-1}(-z)^jK^jf+\sum_{j=J}^{N-1}b_jK^jf, \tag{3.13}$$

where $a_J, a_{J+1},\ldots,a_{N-1}$ and $b_J, b_{J+1},\ldots,b_{N-1}$ are complex numbers. Choosing the a_j's and b_j's so as to make $\mathcal{J}(\Psi,\Phi)$ stationary, it is found as in Ref. 6 that the resulting optimal trial vectors can be written

$$\hat{\Psi}=\sum_{j=0}^{J-1}(-\bar{z})^j(K^*)^j g-(-\bar{z})^J \frac{\begin{vmatrix} 0 & \bar{F}_{2J} & \bar{F}_{2J+1} & \cdots & \bar{F}_{J+N-1} \\ (K^*)^J g & (\bar{F}_{2J}+\overline{zF}_{2J+1}) & (\bar{F}_{2J+1}+\overline{zF}_{2J+2}) & \cdots & (\bar{F}_{J+N-1}+\overline{zF}_{J+N}) \\ (K^*)^{J+1} g & (\bar{F}_{2J+1}+\overline{zF}_{2J+2}) & (\bar{F}_{2J+2}+\overline{zF}_{2J+3}) & \cdots & (\bar{F}_{J+N}+\overline{zF}_{J+N+1}) \\ \vdots & \vdots & \vdots & & \vdots \\ (K^*)^{N-1} g & (\bar{F}_{J+N-1}+\overline{zF}_{J+N}) & (\bar{F}_{J+N}+\overline{zF}_{J+N+1}) & \cdots & (\bar{F}_{2N-2}+\overline{zF}_{2N-1}) \end{vmatrix}}{\begin{vmatrix} (\bar{F}_{2J}+\overline{zF}_{2J+1}) & (\bar{F}_{2J+1}+\overline{zF}_{2J+2}) & \cdots & (\bar{F}_{J+N-1}+\overline{zF}_{J+N}) \\ (\bar{F}_{2J+1}+\overline{zF}_{2+J2}) & (\bar{F}_{2J+2}+\overline{zF}_{2J+3}) & \cdots & (\bar{F}_{J+N}+\overline{zF}_{J+N+1}) \\ \vdots & \vdots & & \vdots \\ (\bar{F}_{J+N-1}+\overline{zF}_{J+N}) & (\bar{F}_{J+N}+\overline{zF}_{J+N+1}) & \cdots & (\bar{F}_{2N-2}+\overline{zF}_{2N-1}) \end{vmatrix}}, \tag{3.14}$$

and similarly

$$\hat{\Phi}=\sum_{j=0}^{J-1}(-z)^j K^j f-(-z)^J \frac{\begin{vmatrix} 0 & F_{2J} & \cdots & F_{J+N-1} \\ K^J f & (F_{2J}+zF_{2J+1}) & \cdots & (F_{J+N-1}+zF_{J+N}) \\ \vdots & \vdots & & \vdots \\ K^{N-1} f & (F_{J+N-1}+zF_{J+N}) & \cdots & (F_{2N-2}+zF_{2N-1}) \end{vmatrix}}{\begin{vmatrix} (F_{2J}+zF_{2J+1}) & \cdots & (F_{J+N-1}+zF_{J+N}) \\ \vdots & & \vdots \\ (F_{J+N-1}+zF_{J+N}) & \cdots & (F_{2N-2}+zF_{2N-1}) \end{vmatrix}}, \tag{3.15}$$

where

$$F_n=\langle g,K^n f\rangle, \quad n=0,1,\ldots,2N-1. \tag{3.16}$$

We note that the first column in the determinant occurring in the numerator of each of the expressions (3.14) and (3.15) consists of members of $\mathfrak{H}$, whereas the remaining elements are simply complex numbers. The numbers F_n in (3.16) correspond to the coefficients in the formal power series expansion of $F(z)$ about $z=0$,

$$F(z)=\langle g,(1+zK)^{-1}f\rangle=\sum_{n=0}^{\infty}F_n(-z)^n. \tag{3.17}$$

The stationary approximation to $F(z)$ corresponding to $\hat{\Psi}$ and $\hat{\Phi}$ is found to be

$$\mathcal{J}(\hat{\Psi},\hat{\Phi})=\sum_{j=0}^{2J-1}F_j(-z)^j-(z)^{2J} \frac{\begin{vmatrix} 0 & F_{2J} & \cdots & F_{J+N-1} \\ F_{2J} & (F_{2J}+zF_{2J+1}) & \cdots & (F_{J+N\,1}+zF_{J+N}) \\ \vdots & \vdots & & \vdots \\ F_{J+N-1} & (F_{J+N-1}+zF_{J+N}) & \cdots & (F_{2N-2}+zF_{2N-1}) \end{vmatrix}}{\begin{vmatrix} (F_{2J}+zF_{2J+1}) & \cdots & (F_{J+N-1}+zF_{J+N}) \\ \vdots & & \vdots \\ (F_{J+N-1}+zF_{J+N}) & \cdots & (F_{2N-2}+zF_{2N-1}) \end{vmatrix}}. \tag{3.18}$$

The latter is precisely *Nuttall's compact formula*[14] for the $[N+J-1/N-J]$ Padé approximant to the function represented by the power series on the right-hand side of (3.17).

We next evaluate the correction term

$$C(\hat{\Psi},\hat{\Phi})=(1+i)a^{-1}\|(1+zK)\hat{\Phi}-f\|\cdot\|(1+zK^*)\hat{\Psi}-g\| \tag{3.19}$$

corresponding to the approximation (3.18). Using straightforward algebra similar to that used in Ref. 6, we derive

$$(1+zK)\hat{\Phi}-f=-(z)^N\frac{\begin{vmatrix} K^Jf & F_{2J} & \cdots & F_{J+N-1} \\ K^{J+1}f & F_{2J+1} & \cdots & F_{J+N} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ K^Nf & F_{J+N} & \cdots & F_{2N-1} \end{vmatrix}}{\begin{vmatrix} (F_{2J}+zF_{2J+1}) & \cdots & (F_{J+N-1}+zF_{J+N}) \\ \cdot & & \circ \\ \cdot & & \circ \\ \cdot & & \circ \\ (F_{J+N1}+zF_{J+N}) & \cdots & (F_{2N-2}+zF_{2N-1}) \end{vmatrix}} \tag{3.20}$$

and

$$(1+zK^*)\hat{\Psi}-g=-(\bar{z})^N\frac{\begin{vmatrix} (K^*)^Jg & \bar{F}_{2J} & \cdots & \bar{F}_{J+N-1} \\ (K^*)^{J+1}g & \bar{F}_{2J+1} & \cdots & \bar{F}_{J+N} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ (K^*)^Ng & \bar{F}_{J+N} & \cdots & \bar{F}_{2N-1} \end{vmatrix}}{\begin{vmatrix} (\bar{F}_{2J}+\overline{zF}_{2J+1}) & & (\bar{F}_{J+N-1}+\overline{zF}_{J+N}) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ (\bar{F}_{J+N-1}+\overline{zF}_{J+N}) & \cdots & (\bar{F}_{2N-2}+\overline{zF}_{2N-1}) \end{vmatrix}}. \tag{3.21}$$

We note that the denominator of (3.20) is exactly the same as the denominator of the $[N+J-1/N-J]$ Padé approximant to $F(z)$ written in the form (3.18), whilst the denominator of (3.21) is its complex conjugate. The isolation of the z dependence in both of the above expressions is in line with the "accuracy-through-order" arguments used elsewhere.[15,16]

We now have

$$\|(1+zK)\hat{\Phi}-f\|=\Gamma_{N,J}|z|^N/|Q_{N-J}(z)|, \tag{3.22}$$

where $Q_{N-J}(z)$ is the polynomial of degree $N-J$ occurring in the denominator of (3.18), and where

$$\Gamma_{N,J}=\left\langle \begin{vmatrix} K^Jf & F_{2J} & \cdots & F_{J+N-1} \\ K^{J+1}f & F_{2J+1} & \cdots & F_{J+N} \\ \circ & \circ & & \circ \\ \circ & \circ & & \circ \\ \circ & \circ & & \circ \\ K^Nf & F_{J+N} & \cdots & F_{2N-1} \end{vmatrix}, \begin{vmatrix} K^Jf & F_{2J} & \cdots & F_{J+N-1} \\ K^{J+1}f & F_{2J+1} & \cdots & F_{J+N} \\ \circ & \circ & & \circ \\ \circ & \circ & & \circ \\ \circ & \circ & & \circ \\ K^Nf & F_{J+N} & \cdots & F_{2N-1} \end{vmatrix} \right\rangle^{1/2} \tag{3.23}$$

The latter is simply a positive constant which involves the numbers

$$F_n=\langle g,K^nf\rangle, \quad n=2J,2J+1,\ldots,2N-1 \tag{3.24}$$

already used in the construction of the Padé approximant, together with the numbers

$$\sigma_{l,m}=\langle K^lf,K^mf\rangle, \quad l,m=J,J+1,\ldots,N. \tag{3.35}$$

Writing $Q_{N-J}(z)$ in the form

$$Q_{N-J}(z)=\sum_{n=0}^{N-J}q_n(-z)^n, \tag{3.26}$$

one can show that (3.23) can be rewritten

$$\Gamma_{N,J}=\Big(\sum_{l=J}^{N}\sum_{m=J}^{N}\sigma_{l,m}\bar{q}_{N-l}q_{N-m}\Big)^{1/2}. \tag{3.27}$$

In a similar way we obtain

$$\|(1+\bar{z}K^*)\hat{\Psi}-g\|=S_{N,J}|z|^N/|Q_{N-J}(z)|, \tag{3.28}$$

where

$$S_{N,J}=\Big(\sum_{l=J}^{N}\sum_{m=J}^{N}\mu_{l,m}q_{N-l}\bar{q}_{N-m}\Big)^{1/2} \tag{3.29}$$

is a positive constant which involves the numbers

$$\mu_{l,m}=\langle (K^*)^l g,(K^*)^m g\rangle,\quad l,m=J,\ J+1,\cdots N \tag{3.30}$$

in addition to the F_n's.

Substituting (3.18), (3.22), and (3.28) into (3.10) with $\Psi=\hat{\Psi}$ and $\Phi=\hat{\Phi}$, we obtain

$$[N+J-1/N-J]-\frac{(1+i)\Gamma_{N,J}S_{N,J}|z|^{2N}}{|Q_{N-J}(z)|^2(1-|z|c)}\leq F(z)$$
$$\leq[N+J-1/N-J]+\frac{(1+i)\Gamma_{N,J}S_{N,J}|z|^{2N}}{|Q_{N-J}(z)|^2(1-|z|c)} \tag{3.31}$$

valid whenever $|z|<1/c$.

Expressions of the form (3.31) will be of practical use when bounds are sought for a physical function $F(z)$, known to be expressible in the form (3.9): provided that an appropriate set of F_n's, $\sigma_{l,m}$'s, and $\mu_{l,m}$'s can be obtained either from experimental measurements, or direct calculations, bounds on $F(z)$ will follow. This will certainly be the case where K is a known matrix, or else an integral operator with compact kernel such as can arise in a Fredholm integral equation, and the vectors f and g are known (see, for example, Ref. 17). We observe the similarity in character between the numbers $\sigma_{l,m}$ and $\mu_{l,m}$, and the numbers F_n which are needed for the formation of Padé approximants to $F(z)$. We speculate that in many of the cases where the Padé method is already used as an approximation technique there is already enough information available for the construction of correction terms.

IV. CORRECTION TERMS FOR PADÉ APPROXIMANTS TO ANALYTIC FUNCTIONS

Let $G(z)$ be any given analytic function which is regular within a smooth contour C, and continuous within and on C. Then Cauchy's theorem[18] tells us

$$G(z)=\frac{1}{2\pi i}\oint_C\frac{G(\xi)\,d\xi}{(\xi-z)} \tag{4.1}$$

for all points z interior to the contour. We suppose that the origin $z=0$ is interior to C, so that $G(z)$ possesses the Taylor series expansion

$$G(z)=\sum_{n=0}^{\infty}G_n z^n, \tag{4.2}$$

with

$$G_n=\frac{1}{n!}G^{(n)}(0)=\frac{1}{2\pi i}\oint_C\frac{G(\xi)\,d\xi}{\xi^{n+1}}. \tag{4.3}$$

In this section we consider the construction of correction terms for $[L/M]$ Padé approximants to $G(z)$, and their usage.

We begin by showing that by appropriately choosing a Hilbert space $\mathfrak{H}$, a linear operator K in $\mathfrak{H}$, and a pair of vectors f and g in $\mathfrak{H}$, $G(z)$ can be expressed in the form of $F(z)$ in (3.9). By following the theory of Sec. III we then obtain bounds on $G(z)$ in the form of $[N+J-1/N-J]$ Padé approximants together with correction terms. Guided by these results we then show how correction terms for arbitrary $[L/M]$ Padé approximants can be deduced directly from the Hermite error formula.

First, let us rewrite (4.1) as

$$G(z)=\oint_{\tilde{C}}\frac{H(\eta)\,d\eta}{(1+z\eta)}, \tag{4.4}$$

where $\tilde{C}$ is the image of C under the transformation

$$\xi=-1/\eta, \tag{4.5}$$

and where

$$H(\eta)=\frac{-G(-1/\eta)}{2\pi i\eta}. \tag{4.6}$$

Now introduce the Hilbert space of complex-valued functions on the contour $\tilde{C}$ according to $h=h(\eta)\in\mathfrak{H}$ if

$$\oint_{\tilde{C}}|h(\eta)|^2|d\eta|<\infty. \tag{4.7}$$

The inner product between any pair of elements $h_1\in\mathfrak{H}$ and $h_2\in\mathfrak{H}$ is defined by

$$\langle h_1,h_2\rangle=\oint_{\tilde{C}}\overline{h_1(\eta)}\,h_2(\eta)\,|d\eta|. \tag{4.8}$$

Define a linear operator K in $\mathfrak{H}$ by

$$Kh(\eta)=\eta h(\eta)\ \text{ for all } h\in\mathfrak{H}. \tag{4.9}$$

Then K is a closed linear transformation from $\mathfrak{H}$ into itself with domain the whole of $\mathfrak{H}$. The adjoint of K is K^* which acts according to

$$K^*h(\eta)=\bar{\eta}h(\eta)\ \text{ for all } h\in\mathfrak{H}. \tag{4.10}$$

We note that

$$\langle Kh,Kh\rangle=\oint_{\tilde{C}}|h(\eta)|^2\cdot|\eta|^2\cdot|d\eta|\leq\max\{|\eta|^2:\eta\in\tilde{C}\}\langle h,h\rangle \tag{4.11}$$

so that a suitable value for the constant c occurring in (3.4) is given by

$$c^2=\max\{|\eta|^2:\eta\in\tilde{C}\}=\max\{1/|\xi|^2:\xi\in\tilde{C}\}$$
$$=1/\min\{|\xi|^2:\xi\in C\}=1/d^2, \tag{4.12}$$

where d is the shortest distance from the origin to the contour C. Hence the theory of Sec. III applies with $\mathfrak{H}$ and K as defined here. In particular, the bounds (3.31) apply with

$$F(z)=\langle g,(1+zK)^{-1}f\rangle=\oint_{\tilde{C}}\frac{\overline{g(\eta)}f(\eta)\,|d\eta|}{1+z\eta}. \tag{4.13}$$

To obtain bounds on the given analytic function $G(z)$ we now choose f and g in $\mathfrak{H}$ such that

$$\overline{g(\eta)}h(\eta)=H(\eta)\exp[i\Theta(\eta)], \tag{4.14}$$

where $\Theta(\eta)$ is the angle between the tangent to $\tilde{C}$ at η and the x axis. Then we have

$$F(z)=\oint_{\tilde{C}}\frac{H(\eta)\exp[i\Theta(\eta)]\,|d\eta|}{1+z\eta}=\oint_{\tilde{C}}\frac{H(\eta)\,d\eta}{1+z\eta}=G(z). \tag{4.15}$$

The values for the constants F_n occurring in the formula (3.18) for the $[N+J-1/N-J]$ Padé approximant to $G(z)$ are simply

$$F_n=(-1)^nG_n,\quad n=0,1,\ldots,2N-1 \tag{4.16}$$

as can be seen by comparison of (3.17) and (4.2). In addition to the $F_{\cdot}$'s we also need to know the numbers $\sigma_{l,m}$ and $\mu_{l,m}$ $(l,m=J,J+1,\ldots,N)$ defined in (3.25) and (3.30). These quantities depend explicitly on the individual choices for $f(\eta)$ and $g(\eta)$ satisfying (4.14), and here we make the symmetrical choice

$$f(\eta)=g(\eta), \tag{4.17}$$

so that

$$\sigma_{l,m}=\langle K^l f, K^m f\rangle=\oint_{\tilde{C}}\bar{\eta}^l\eta^m|H(\eta)|\cdot|d\eta|$$
$$=\frac{(-1)^{l+m}}{2\pi}\oint_C\frac{|G(\xi)||d\xi|}{\bar{\xi}^l\xi^m|\xi|}=\mu_{m,l}, \tag{4.18}$$

for $l,m=J,\ J+1,\ \ldots,N$. Hence the constants $\sigma_{l,m}$ and $\mu_{l,m}$ depend upon the absolute value of the given analytic function $G(z)$ on the contour C. These constants can be thought of as certain moments of the function $G(z)$, and as such they are not so very different from the moments G_n $(n=0,1,\ldots,2N-1)$ required for the construction of the $[N+J-1/N-J]$ Padé approximant to $G(z)$. They differ from the G_n's in that their values depend strongly on the situation of the contour C, which is at our disposal in a given problem. We note that since $\sigma_{l,m}=\mu_{m,l}$ we have the correction constant

$$\Gamma_{N,J}S_{N,J}=\sum_{l=J}^{N}\sum_{m=J}^{N}\sigma_{l,m}\bar{q}_{N-l}q_{N-m}. \tag{4.19}$$

For the case where C is a circle of radius R centered at the origin we have

$$\sigma_{l,m}=\frac{(-1)^{l+m}}{2\pi R^{l+m}}\int_{-\pi}^{+\pi}\exp[i(l-m)\theta]|G(Re^{i\theta})|\,d\theta \tag{4.20}$$

for each l and m; and in this case,

$$c=1/R, \tag{4.21}$$

so that bounds will be obtained when $|z|<R$. If $G(z)$ is real on the real axis within C, then we see that the $[N+J-1/N-J]$ Padé approximant together with correction terms for $G(z)$ may be constructed provided that we know the numbers $G_n(n=0,1,\ldots,2N-1)$ together with the numbers

$$\mathcal{J}_k(R)=\frac{1}{2\pi}\int_{-\pi}^{+\pi}(\cos k\theta)|G(Re^{i\theta})|\,d\theta,\quad k=0,1,\ldots,N-J. \tag{4.22}$$

Alternative requisite sets of given information, involving, for example, moments of $|G(Re^{i\Theta})|^2$, may be derived by making choices other than (4.17) for the functions $f(\eta)$ and $g(\eta)$ satisfying (4.14).

We observe here, and prove later on, that $|G(\xi)|$ *in* (4.18) *may be replaced by* $|\tilde{G}(\xi)|$, *any real valued function of* $\xi\in C$ *such that*

$$|G(\xi)|\leq|\tilde{G}(\xi)|\quad\text{for all }\xi\in C, \tag{4.23}$$

without altering the validity of the resulting correction terms. This result is the analog of the replacement theorem proved in Ref. 6. One might be given, for example, that $|G(z)|\leq|e^z|$ on $|z|=R$ for some $R>0$, in which case the numbers $\mathcal{J}_k(R)$ could be replaced by the modified Bessel functions $I_k(R)$ $(k=0,\ 1,\ \ldots,\ N-J)$, tables of which are readily available.[19]

For the case $G(z)=e^z$, $R=3$, and $N=2$, we obtain for example the bounds

$$\frac{\frac{1}{2}+\frac{1}{6}z}{\frac{1}{2}-\frac{1}{3}z+\frac{1}{12}z^2}-\frac{(1+i)|z|^4[0.007\,987]}{[1-\frac{1}{3}|z|]|\frac{1}{2}-\frac{1}{3}z+\frac{1}{12}z^2|^2}\leq e^z$$
$$\leq\frac{\frac{1}{2}+\frac{1}{6}z}{\frac{1}{2}-\frac{1}{3}z+\frac{1}{12}z^2}+\frac{(1+i)|z|^4[0.007\,987]}{[1-\frac{1}{3}|z|]|\frac{1}{2}-\frac{1}{3}z+\frac{1}{12}z^2|^2}, \tag{4.24}$$

valid for all z such that $|z|<3$. At $z=(-1+i)$, this gives the bounds

$$[(0.2059)+(0.3235)i]\pm(0.1015)(1+i), \tag{4.25}$$

compared with the correct value

$$\exp(-1+i)=(0.19877)+(0.30956)i. \tag{4.26}$$

More generally, in the case of a given analytic function $G(z)$ it is possible to infer correction terms for arbitrary $[L/M]$ Padé approximants directly from the Hermite error formula.[20] Let us write

$$[L/M]=P_L(z)/Q_M(z) \tag{4.27}$$

in the usual way.[20] Then we have

$$Q_M(z)G(z)-P_L(z)=0(z^{L+M+1}), \tag{4.28}$$

so that if $R_M(z)$ is any polynomial of degree at most M,

$$R_M(z)Q_M(z)G(z)-R_M(z)P_L(z)=O(z^{L+M+1}). \tag{4.29}$$

But then from Cauchy's theorem it follows that

$$R_M(z)Q_M(z)G(z)-R_M(z)P_L(z)$$
$$=\frac{z^{L+M+1}}{2\pi i}\oint_C\frac{R_M(\xi)Q_M(\xi)G(\xi)\,d\xi}{(\xi-z)\xi^{L+M+1}} \tag{4.30}$$

for all z interior to C. [The term $R_M(\xi)P_L(\xi)$ has been omitted from the numerator in the integral because it is a polynomial of degree less than $(L+M+1)$ and hence makes no contribution.] Hence we have

$$|G(z)-[L/M]|\leq\frac{|z|^{L+M+1}}{2\pi|R_M(z)|\cdot|Q_M(z)|}$$
$$\times\left|\oint_C\frac{R_M(\xi)Q_M(\xi)G(\xi)\,d\xi}{(\xi-z)\xi^{L+M+1}}\right|. \tag{4.31}$$

Any upper bound $B_{[L/M]}(z)$ to the quantity on the right-hand side of (4.31) can be interpreted as a correction term to $[L/M]$ according to

$$[L/M]-(1+i)B_{[L/M]}(z)\leq G(z)\leq[L/M]+(1+i)B_{[L/M]}(z). \tag{4.32}$$

There is clearly a variety of ways for imposing upper bounds $B_{[L/M]}(z)$ on the right-hand side of (4.31). The method to be used depends on what additional information about $G(z)$ one is given, over and above the implicity assumed knowledge of the coefficients G_n, $n=0,1,\ldots,L+M$. Here we suppose that we know the numbers $\sigma_{l,m}$ and $\mu_{l,m}$ defined in (4.18), and accordingly choose

$$R_M(z)=Q_M(z)=\sum_{m=0}^{M}q_m(-z)^m. \tag{4.33}$$

If we suppose

$$L+M+1=2N, \tag{4.34}$$

where N is a positive integer then we have

$$\frac{1}{2\pi}\left|\oint_C \frac{R_M(\xi)Q_M(\xi)G(\xi)\,d\xi}{(\xi-z)\xi^{L+M+1}}\right| = \frac{1}{2\pi}\left|\oint_C \frac{Q_M(\xi)^2 G(\xi)\,d\xi}{(\xi-z)\xi^{2N}}\right| \le \frac{1}{2\pi}\oint_C \frac{|Q_M(\xi)|^2\cdot|G(\xi)|\,|d\xi|}{|1-z/\xi|\,|\xi|^{2N}\cdot|\xi|}$$

$$\le \frac{1}{1-|z|c}\sum_{l=0}^{M}\sum_{m=0}^{M}\left(\frac{(-1)^{l+m}}{2\pi}\oint_C \frac{|G(\xi)|\,|d\xi|}{\xi^{N-l}\xi^{N-m}|\xi|}\right)\bar{q}_l q_m$$

$$= \frac{1}{1-|z|c}\sum_{l'=N-M}^{N}\sum_{m'=N-M}^{N}\sigma_{l',m'}\bar{q}_{N-l'}q_{N-m'} \quad \text{for all } |z|<\frac{1}{c}. \tag{4.35}$$

Here c is the positive constant defined by (4.12), and the constants $\sigma_{l',m'}$, $(l',m'=N-M+1,\ldots,N)$ are the same as defined in (4.18) except that now we allow negative values for the indices where necessary. Similarly, if we suppose

$$L+M+1=2N+1, \tag{4.36}$$

where N may be zero or a positive integer, then we have

$$\frac{1}{2\pi}\left|\oint_C \frac{Q_M(\xi)^2 G(\xi)\,d\xi}{(\xi-z)\xi^{2N+1}}\right| \le \frac{c}{1-|z|c}\sum_{l=0}^{M}\sum_{m=0}^{M}\frac{(-1)^{l+m}}{2\pi}\oint_C \frac{|G(\xi)|\cdot|d\xi|}{\xi^{N-l}\xi^{N-m}|\xi|}\bar{q}_l q_m$$

$$= \frac{c}{1-|z|c}\sum_{l'=N-M}^{N}\sum_{m'=N-M}^{N}\sigma_{l',m'}\bar{q}_{N-l'}q_{N-m'} \quad \text{for } |z|<\frac{1}{c}. \tag{4.37}$$

Hence we have the correction terms

$$B_{[L/M]}(z)=\begin{cases}\dfrac{|z|^{2N}}{(1-|z|c)|Q_M(z)|^2}\displaystyle\sum_{l'=N-M}^{N}\sum_{m'=N-M}^{N}\sigma_{l',m'}\bar{q}_{N-l'}q_{N-m'} & (L+M+1=2N),\\[2ex] \dfrac{c|z|^{2N}}{(1-|z|c)|Q_M(z)|^2}\displaystyle\sum_{l'=N-M}^{N}\sum_{m'=N-M}^{N}\sigma_{l',m'}\bar{q}_{N-l'}q_{N-m'} & (L+M+1=2N+1),\end{cases} \tag{4.38}$$

which apply whenever $|z|<1/c$. Substituting (4.38) into (4.32) we obtain upper and lower bounds on $G(z)$ for all $|z|<1/c$. In the case of the $[N+J-1/N-J]$ Padé approximants these bounds are identical with the previous bounds, (3.31) wherein $\Gamma_N S_N$ is given by (4.19).

We see here that the quantities $\sigma_{l',m'}$ can be replaced throughout by the quantities

$$\sigma_{l',m'}=\frac{(-1)^{l'+m'}}{2\pi}\oint\frac{|\tilde{G}(\xi)|\,|d\xi|}{\bar{\xi}^{l'}\xi^{m'}|\xi|} \tag{4.39}$$

$(l',m'=N-M,\ N-M+1,\ldots,N)$, without altering the validity of the resulting upper and lower bounds on $G(z)$. $|\tilde{G}(\xi)|$ is any real valued function of $\xi\in C$ such that (4.23) holds. This result is immediate because $|G(\xi)|$ can be replaced by $|\tilde{G}(\xi)|$ in the sequences of inequalities (4.35) and (4.37). In particular, the assertion made around (4.23) is now proved.

Alternative correction terms $B_{[L/M]}$ of the same structure as those in (4.38), and still involving various of the numbers $\sigma_{l',m'}$, can be derived by replacing powers of $|\xi|$ by powers of $1/c$ at appropriate points in the inequalities (4.35) and (4.37). However, we prefer the $B_{[L/M]}(z)$'s defined in (4.38) since their derivation seems to be the most direct. Again, correction terms involving for example moments of $|G(\xi)|^2$ instead of moments of $|G(\xi)|$ can be evolved by introducing an appropriate Schwarz inequality as a preliminary step in the the imposition of upper bounds on the right-hand side of

TABLE I. Showing the various $[L/M]\pm(1+i)B_{[L/M]}(Z)$, which can be constructed using the information given in the example (see text). Bounds on both real and imaginary parts of $G(Z)$ are implied for $|Z|<3$.

L \ M	0	1	2
0	$\frac{1}{1}\pm\frac{(1+i)[1.62693]}{1-\frac{1}{3}\lvert Z\rvert}$	$\frac{1}{1-Z}\pm\frac{(1+i)\lvert Z\rvert^2[2.78752]}{(1-\frac{1}{3}\lvert Z\rvert)[1-Z]^2}$	$\frac{1}{1-Z+\frac{1}{2}Z^2}\pm\frac{(1+i)\lvert Z\rvert^2[1.38480]}{(1-\frac{1}{3}\lvert Z\rvert)\lvert 1-Z+\frac{1}{2}Z^2\rvert^2}$
1	$\frac{1+Z}{1}\pm\frac{(1+i)[0.542310]}{1-\frac{1}{3}\lvert Z\rvert}$	$\frac{1+\frac{1}{2}Z}{1-\frac{1}{2}Z}\pm\frac{(1+i)\lvert Z\rvert^2[0.148239]}{(1-\frac{1}{3}\lvert Z\rvert)\lvert 1-\frac{1}{2}Z\rvert^2}$	$\frac{1+\frac{1}{3}Z}{1-\frac{2}{3}Z+\frac{1}{6}Z\rvert^2}\pm\frac{(1+i)\lvert Z\rvert^4[0.0319467]}{(1-\frac{1}{3}\lvert Z\rvert)\lvert 1-\frac{2}{3}Z+\frac{1}{6}Z^2\rvert^2}$
2	$\frac{1+Z+\frac{1}{2}Z^2}{1}\pm\frac{(1+i)\lvert Z\rvert^2[0.180770]}{1-\frac{1}{3}\lvert Z\rvert}$	$\frac{1+\frac{2}{3}Z+\frac{1}{6}Z^2}{1-\frac{1}{3}Z}\pm\frac{(1+i)\lvert Z\rvert^4[0.0228993]}{(1-\frac{1}{3}\lvert Z\rvert)\lvert 1-\frac{1}{3}Z\rvert^2}$	...
3	$\frac{1+Z+\frac{1}{2}Z^2+\frac{1}{6}Z^3}{1}\pm\frac{(1+i)\lvert Z\rvert^4[0.0602567]}{1-\frac{1}{3}\lvert Z\rvert}$	...	...

TABLE II. "Padé table" of upper and lower bounds on $G(1)$, see example in text.

L \ M	0	1	2
0	3.4404 1.4404	$+\infty$ $-\infty$	10.3088 −6.3088
1	2.8135 1.1865	3.38894 2.1106	2.85836 2.47506
2	2.7711 2.2288	2.8273 2.6727	
3	2.7570 2.5763		

(4.31). Bounds obtained in this way can be shown in the case of $[N-1/N]$ to correspond to choosing $f(\eta)$ and $g(\eta)$ satisfying (4.14) distinct from the symmetrical choice (4.17). Finally, one can choose $R_M(z)$ different from $Q_M(z)$ in (4.31). In this case we have found that it is difficult to impose upper bounds on the right-hand side of (4.31) which are efficient and which at the same time require simple sets of given information about $G(z)$.

We consider the application of the bounds given by (4.38). Suppose for example we are given that a certain analytic function $G(z)$ is regular within and on the contour $|z|=R$, that $G(z)$ is real on the real axis within C, that we know the Taylor series coefficients G_n, $n=0, 1, \ldots, 2N-1$, and that we know the moments $\mathcal{J}_k(R)$ defined in (4.22), for $k=0,1,\ldots,K$, some integer $K\geq 0$.

TABLE III. Upper and lower bounds on $G(x)$ supplied by $[3/0] \pm B_{[L/M]}(x)$, $[2/1] \pm B_{[2/1]}(x)$, and $[1/2] \pm B_{[1/2]}(x)$ for various x such that $-3<x<+3$; see example in text. For each x the best bounds obtained are underlined.

	Bounds on $G(x)$ associated with		
x	[3/0]	[2/1]	[1/2]
−1.75	1.2444 −1.4683	0.4227 0.0115	0.2560 0.0553
−1.50	0.6726 −0.5476	0.3530 0.1469	0.2679 0.1531
−1.25	0.4579 −0.0464	0.3492 0.2537	0.3091 0.2481
−1.00	0.4237 0.2429	0.3943 0.3557	0.3779 0.3494
−0.75	0.4864 0.4355	0.4812 0.4688	0.4759 0.4653
−0.50	0.60869 0.59965	0.60841 0.60588	0.60733 0.60479
−0.25	0.77890 0.77839	0.77893 0.77876	0.77886 0.77866
+0.25	1.28411 1.28360	1.28421 1.28397	1.28414 1.28376
+0.50	1.6503 1.6413	1.6525 1.6475	1.6518 1.6423
+0.75	2.1270 2.0761	2.1422 2.1078	2.1435 2.0670
+1.25	3.6090 3.1046	3.8709 3.3076	4.0501 2.5840
+2.00	9.2256 3.4410	18.8925 −0.8925	18.8010 −8.8010

Then we have enough information for the construction of all $[L/M]$ Padé approximants to $G(z)$ complete with correction terms $B_{[L/M]}(z)$, where L and M are restricted by $L+M\leq 2N-1$ and $M\leq K$. Thus we can construct a corresponding "Padé table" of upper and lower bounds on $G(z)$, valid whenever $|z|<R$. Seen as a whole this table should supply useful information about $G(z)$ for all z such that $|z|<R$.

Example. Let $G(z)$ be known to be an analytic function, regular and real on the real axis when $|z|\leq 3$; and suppose we know

$$G_0=1,\quad G_1=1,\quad G_2=\tfrac{1}{2},\quad G_3=\tfrac{1}{6},\quad \mathcal{J}_0(3)=4.880\,792\,59,$$

$$\mathcal{J}_1(3)=3.953\,370\,22,\quad \text{and}\quad \mathcal{J}_2(3)=2.245\,212\,44.$$

Then in Table I we give the various Padé approximants to $G(z)$ together with associated correction terms which can be constructed using the above information. In Table II we give the corresponding upper and lower bounds on $G(1)$. The best upper and lower bounds here give

$$2.7570\geq G(1)\geq 2.6727;$$

the upper bound corresponds to $[3/0]$ and the lower bound corresponds to $[2/1]$. In Table III we compare the bounds associated with the three approximants $[3/0]$, $[2/1]$, and $[1/2]$, at various points along the real axis; for each x the best upper and the best lower bound is italicized. The advantage of considering the bounds associated with each of the three approximants is apparent. We note $G(z)$ *could* be e^z in this example.

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[1]M.F. Barnsley and P.D. Robinson, Proc. R. Soc. Lond. A **338**, 527 (1974).
[2]M.F. Barnsley and P.D. Robinson, Proc. Roy. Soc. Edinb. (to be published).
[3]A.M. Arthurs and M.E. Jones, J. Math. Anal. Appl. (to be published).
[4]M.F. Barnsley and P.D. Robinson, J. Math. Anal. Appl. (to be published).
[5]M.F. Barnsley, Phys. Lett. A 53, 124 (1975).
[6]M.F. Barnsley, J. Math. Phys. **16**, 918 (1975).
[7]*The Padé Approximant in Theoretical Physics*, edited by G.A. Baker, Jr. and G.L. Gammel (Academic, New York, 1970).
[8]*Padé Approximants and Their Applications*, edited by P.R. Graves-Morris (Academic, New York, 1973).
[9]E.J. Heller and W.P. Reinhardt, Phys. Rev. A 7, 365 (1973).
[10]E. Brändas and D.A. Micha, J. Math. Phys. **13**, 155 (1972).
[11]F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Ungar, New York, 1955).
[12]W.M. Stacey, Jr., *Variational Methods in Nuclear Reactor Physics* (Academic, New York, 1974).
[13]S.T. Epstein, *The Variational Method in Quantum Chemistry* (Academic, New York, 1974).
[14]J. Nuttall, Phys. Rev. **157**, 1312 (1967).
[15]S.T. Epstein, J. Chem. Phys. **48**, 4716 (1968).
[16]M.F. Barnsley and P.D. Robinson, J. Inst. Math. Appl. **14**, 229 (1974).
[17]J.S.R. Chisholm, in Ref. 7, pp. 171–82; G.A. Baker, Jr., J. Math. Phys. **16**, 813 (1975).
[18]E.T. Copson, *The Theory of Functions of a Complex Variable* (Oxford U.P., Oxford, 1935).
[19]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I.A. Segun (Dover, New York, 1965).
[20]G.A. Baker, Jr., *The Essentials of Padé Approximants* (Academic, New York, 1975).

The maximal solvable subalgebras of the real classical Lie algebras*

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The classification of the maximal solvable subalgebras of $sl(n,R)$, $su^*(n)$, $so^*(n)$, $sp(n,R)$ and $usp(p,q)$ is given, thus supplementing the cases $su(p,q)$ and $so(p,q)$ performed elsewhere.

I. INTRODUCTION

This article follows the task undertaken by Patera, Winternitz, and Zassenhaus[1,2] concerning the classification of the maximal solvable subalgebras of the real semisimple Lie algebras. The physical motivation to this study is the same; it was exposed at length in the two quoted articles, and therefore we do not reconsider it. Let us only point out that the symplectic groups, which are examined here among others, have their own importance in particular in the context of the linear canonical transformations in classical and quantum mechanics[3] and in some group theoretical models of nuclei.[4]

The method used is a specialization of the one developed by the above-mentioned authors.[1] However, to avoid a separate treatment of each algebra by means of its standard realization as a matrix algebra, we preferred to use some classical results on the real forms of the simple Lie algebras.[5] We recall them briefly in Sec. II in a form adapted to our further needs. Section III is devoted to the construction of a recursive method for finding the conjugacy classes of $sl(n,R)$, $su^*(n)$, $so(p,q)$, $so^*(n)$, $sp(n,R)$, and $usp(p,q)$ [the missing case $su(p,q)$ and the case $so(p,q)$ are already known[1,2]]. In Sec. IV we draw up a list of results by displaying a representative of each class in term of a matrix algebra; the cases $sl(3,R)$, $sp(4,R)$, and $usp(2,2)$ are constructed explicitly.

II. THE REAL FORMS OF THE CLASSICAL LIE ALGEBRAS

Let L be a Lie algebra over C. If $\mathcal{D}: L \to L$ is a conjugation of L (i.e., an involutary antilinear automorphism of L), the set

$$L_{\mathcal{D}} = \{x \in L; \mathcal{D}x = x\}$$

naturally provided with a real Lie algebra structure is called a real form of L. Two real forms $L\mathcal{D}_1$ and $L\mathcal{D}_2$ are said to be conjugate (or equivalent) if an automorphism ϕ of L exists such that $\phi \circ \mathcal{D}_1 = \mathcal{D}_2 \circ \phi$.

All the real classical Lie algebras are real forms of the complex classical Lie algebras. Actually

$$sl(n,C)_{\mathcal{D}_1} = sl(n,R), \quad n \geq 2,$$
$$sl(n,C)_{\mathcal{D}_2} = su(p,q), \quad p+q=n \geq 2,$$
$$sl(n,C)_{\mathcal{D}_3} = su^*(n), \quad n \text{ even} \geq 4,$$
$$so(n,C)_{\mathcal{D}_1} = so(p,q), \quad n \geq 2,$$
$$so(n,C)_{\mathcal{D}_2} = so^*(n), \quad n \text{ even} \geq 4,$$
$$sp(n,C)_{\mathcal{D}_1} = sp(n,R), \quad n \text{ even} \geq 2,$$
$$sp(n,C)_{\mathcal{D}_2} = usp(p,q), \quad p,q,n \text{ even}, \ p+q=n \geq 2,$$

where, since $su(p,q) \simeq su(q,p)$, $so(p,q) \simeq so(q,p)$, and $usp(p,q) \simeq usp(q,p)$, we restrict ourselves to the cases $p \geq q \geq 0$.

To describe the operators $\mathcal{D}_i$, we use a fundamental representation $\rho: L \to \mathrm{End}(V)$ $(V \simeq C^n)$, where L is one of the above-mentioned complex Lie algebras. With the exception of the case where $L = su(p,q)$, for each real form $L_{\mathcal{D}}$ there exists always an antilinear transformation $D: V \to V$ such that

$$\rho(\mathcal{D}x) = D\rho(x)D^{-1}, \quad \forall x \in L,$$
$$D^2 = \pm I.$$

In cases when D is an involution $(D^2 = I)$, the representation ρ is called virtually real by which we mean that it induces a (real) representation

$$\rho_{\mathcal{D}}: L \to \mathrm{End}(V_D),$$

where V_D is the real vector space $V_D = \{v \in V; Dv = v\}$ $(\dim_C V = \dim_R V_D)$. In cases when D is an antiinvolution $(D = -I)$, no such real vector space exists. The representation ρ is called antireal: It induces a "complex" representation

$$\rho_{\mathcal{D}}: L \to \mathrm{End}(V).$$

Through the representation ρ, each real form [except $su(p,q)$] can be characterized by an involution or antiinvolution antilinear operator D. The equivalence relation between real forms can be transferred to the set of these operators with the following results:

(A) $sl(n,R)$: Any D such that $D^2 = I$. (For example, if a basis $\{e_i\}_{i=1,\ldots,n}$ of V is given, D can be taken as the complex conjugation $K: K(\sum_i v_i e_i) = \sum_i \bar{v}_i e_i$.)

(B) $su^*(n)$: Any D such that $D^2 = -I$.

(C) $so(p,q)$: The representation ρ of $so(n,C)$ admits an invariant symmetric form $(\ ,\ ): V \times V \to C$. Any involution D such that the form $\langle u, v\rangle = (Du, v)$ is Hermitian with signature (p,q) [or equivalently such that the restriction to $V_D \times V_D$ of $\langle\ ,\ \rangle$ is symmetric with signature (p,q)]. If $\overline{(Du,v)} = (u, D^T v)$, it is always possible to take a D for which $D^T = D$.

(D) $so^*(n)$: Any anti-involution D such that the form $\langle u, v\rangle = (Du, v)$ is anti-Hermitian. It is always possible to take a D for which $D^T = -D$.

(E) $\mathrm{sp}(n,R)$: The representation ρ of $\mathrm{sp}(n,C)$ admits an invariant symplectic for $\mathrm{m}(\ ,\ ): V\times V\to C$. Any involution D such that the form $\langle u,v\rangle=(Du,v)$ is anti-Hermitian (or equivalently such that the restriction to $V_D\times V_D$ of $\langle\ ,\ \rangle$ is symplectic). D can be always chosen such that $D^T=-D$.

(F) $\mathrm{usp}(p,q)$: Any anti-involution D such that the form $\langle u,v\rangle=(Du,v)$ is Hermitian with signature (p,q). D also here can be chosen such that $D^T=-D$.

III. GENERAL PROPERTIES OF THE CONSIDERED MAXIMAL SOLVABLE SUBALGEBRAS

The whole argument is based on a Lie's theorem on solvable matrix algebras.[6] Let $S\subset L$ be a maximal solvable subalgebras; then its complexification $S'\subset L'_D=L$ is also solvable but not necessarily maximal. Consider then the representation $\rho: L\to \mathrm{End}(V)$ of the preceding section and exclude the special case $L_D=\mathrm{su}(p,q)$. Lie's theorem asserts that there exists a vector $v\in V$ $(v\neq 0)$ and a weight $\lambda: S'\to C$ such that

$$\rho(s')\,v=\lambda(s')v,\quad \forall s'\in S'.$$

Since $S\subset S'$ and $\rho(x)D=D\rho(x)$ for all $x\in L$, we have

$$\begin{aligned}&\rho(s)v=\lambda(s)v\\ &\rho(s)Dv=\overline{\lambda(s)}Dv\end{aligned}\quad,\quad s\in S. \tag{1}$$

The subspace $W=Cv+CDv$, of dimension one or two depending on whether v and Dv are or are not colinear, is invariant with respect to $\rho(S)$ and $\rho(S')$; in addition $D: W\to W$. Notice that the dimension of W is always equal to two if D is an anti-involution.

To continue, it is necessary to distinguish the cases where ρ does or does not admit an invariant bilinear form.

A. $L=\mathrm{sl}(n,C)$ $(n\geqslant 3)$

In fact we can trivially extend to $L=\mathrm{gl}(n,C)$.

Let us introduce the following two subalgebras:

$$N=\{n\in L;\ \rho(n): V\to V;\ \rho(n): W\to W\},$$
$$Z=\{z\in L;\ \rho(z): V\to W;\ \rho(z): W\to\{0\}\}.$$

Z clearly is an ideal of N and $S'\subset N$; since Z_D+S is solvable $(Z_D=Z\cap L_D)$, we have

$$Z_D\subset S\subset N_D \tag{2}$$

and S is maximal in $N_D=N\cap L_D$. By using the very definitions of L and Z, it is easy to verify that all the weight vectors of Z belong to W; from this property and the inclusion (2), it follows then that W contains all the weight vectors of S.

Let

$$\Delta_1: N\to\mathrm{gl}(W),\quad \Delta_2: N\to\mathrm{gl}(V/W)$$

be the injective homomorphisms defined naturally by ρ on the restriction W and the factor space V/W. The two antilinear operators $D_1: W\to W$ and $D_2: V/W\to V/W$ induced by D are involutions or anti-involutions together with D and define the two real forms $\Delta_i(N)_{D_i}$, $i=1,2$. It is clear that $\Delta_i(N_D)=\Delta_i(N)_{D_i}$. $\Delta_i(S)$ $(S\subset N)$ is therefore a maximal solvable subalgebra of $\Delta_i(N)_{D_i}$, where $\Delta_1(N)_{D_1}\simeq\mathrm{gl}(d,R)$ and $\Delta_2(N)_{D_2}\simeq\mathrm{gl}(n-d,R)$ $(d=\dim W)$.

Consider now the question of the equivalence of two maximal solvable subalgebras S_1 and S_2 under the inner automorphisms of L_D. Let W_1 and W_2 be their weight subspaces; a necessary condition for equivalence is of course that $\dim W_1=\dim W_2$. If this is the case, then there always exists a regular mapping T such that $T: W_1\to W_2$ and $DT=TD$. This latter equation means that T defines an inner automorphism of $\mathrm{gl}(n,C)$ and therefore $S_1\sim TS_2T^{-1}$; it is thus sufficient to examine the cases when $W_1=W_2=W$, which we shall now assume. The two subalgebras S_1 and S_2 have then the same ideal Z and $\Delta_1(S_1)$ is equivalent to $\Delta_1(S_2)$ since they act on the same maximal weight space. It follows then directly from these remarks that a necessary and sufficient condition for S_1 and S_2 to be equivalent is that $\Delta_2(S_1)$ and $\Delta_2(S_2)$ are equivalent.

With respect to a basis of V obtained by completion of a basis of weight vectors of W, the subalgebra S admits a matrix representation of the form

$$\rho(S)=\begin{pmatrix}R_1 & R_2\\ 0 & R_4\end{pmatrix}, \tag{3}$$

where $R_1=\Delta_1(S)$, $R_4=\Delta_2(S)$, and

$$\rho(Z_D)=\begin{pmatrix}0 & R_2\\ 0 & 0\end{pmatrix}.$$

The antilinear operator D can be put in the form

$$D=\begin{pmatrix}J_1 & 0\\ 0 & J_2\end{pmatrix}K,$$

where K is the complex conjugation and $J_i\bar{J}_i=\pm I$ $(D^2=\pm I)$, $i=1,2$.

B. $L=\mathrm{so}(n,C)$ or $\mathrm{sp}(n,C)$

Let us first suppose that no weight vector $v\in V$ exists such that $W=Cv+CDv$ is isotropic with respect to the invariant bilinear form. V therefore admits the direct decomposition

$$V=W_1\oplus W_2\oplus\cdots\oplus W_k,$$

where $W_i=Cv_i+CDv_i$, $i=1,\ldots,k$, is a nonisotropic weight space. This is due to the fact that V is always a direct sum $V=(W_1\oplus\cdots W_i)\oplus(W_1\oplus\cdots\oplus W_i)^{\perp}$ of two subspaces invariant with respect to $\rho(S')$. The subalgebra S is therefore Abelian and since it is maximal, it is a *compact Cartan subalgebra*. These subalgebras always exist except for $\mathrm{so}(p,q)$ when p and q are both odd numbers. The dimension of the W_i is always two if n is even. If n is odd, the dimension of one of the subspaces W_i is one, and that of the rest is again two.

Let us now suppose that at least one weight vector $v\in V$ exists, such that $W=Cv+CDv$ is isotropic (W is then in fact completely isotropic since $D^T=\pm D$). Let us introduce the two following subalgebras:

$$N=\{n\in L;\ \rho(n): V\to V;\ \rho(n): W^{\perp}\to W^{\perp};\ \rho(n): W\to W\},$$
$$Z=\{z\in L;\ \rho(z): V\to W^{\perp};\ \rho(z): W^{\perp}\to W;\ \rho(z): W\to\{0\}\},$$

where $W^\perp$ denotes the orthogonal complement of $W(W\subset W^\perp)$. [If $W=W^\perp$ (2 $\dim W=\dim V$), there is nothing more to add.]

As for the preceding case, we have

$$Z_D\subset S\subset N_D$$

from where it follows that S is maximal in N_D and that all the weight vectors belong to W.

Considering the three homomorphisms

$$\Delta_1: N\to \mathrm{gl}(W)$$
$$\Delta_2: N\to \mathrm{gl}(W^\perp/W)$$
$$\Delta_3: N\to \mathrm{gl}(V/W^\perp)$$

induced naturally by ρ on the restriction W and on the factor spaces $W^\perp/W$ and $V/W^\perp$, we see at once that Δ_1 and Δ_3 are surjective. We also see that $\Delta_2(N)$ is equal to the orthogonal or symplectic Lie algebra of the endomorphisms of $W^\perp/W$ with respect to the bilinear form induced by the bilinear form on $V\times V$. On the other hand, since $D: W\to W$ and $D: W^\perp\to W^\perp$, this operator induces the three antilinear operators $D_1: W\to W$, $D_2: W^\perp/W\to W^\perp/W$, $D_3: V/W^\perp\to V/W^\perp$, which are involution or anti-involution together with D. These three operators define three real forms $\Delta_i(N)_{D_i}$, $i=1,2,3$ and, of course, $\Delta_i(N)_{D_i}=\Delta_i(N_D)$. If $d=\dim W$, $\Delta_1(S)$ and $\Delta_3(S)$ are maximal solvable subalgebras of $\Delta_1(N)_{D_1}\simeq\Delta_3(N)_{D_3}\simeq \mathrm{gl}(d,R)$, while $\Delta_2(S)$ is a maximal solvable subalgebra of $\Delta_2(N)_{D_2}$; this latter is of the same type as L_D, that is, isomorphic to $\mathrm{so}^*(n-4)$ if $L_D=\mathrm{so}^*(n)$, to $\mathrm{so}(p-d,q-d)$ if $L_D=\mathrm{so}(p,q)$, to $\mathrm{sp}(n-2d,R)$ if $L_D=\mathrm{sp}(n,R)$, and to $\mathrm{usp}(p-2,q-2)$ if $L_D=\mathrm{usp}(p,q)$.

For the question of equivalence of two maximal solvable subalgebras S_1 and S_2 of L_D, it is easy to show, in the same way as for the preceding case, that a necessary and sufficient condition for S_1 and S_2 to be equivalent is that the dimension of their weight spaces be the same and that $\Delta_2(S_1)\sim\Delta_2(S_2)$.

With respect to a Witt decomposition of V, a maximal solvable subalgebra S which is not a compact Cartan subalgebra admits a matrix representation of the form

$$\rho(S)=\begin{pmatrix} R_1 & R_2 & R_3\\ 0 & R_5 & R_6\\ 0 & 0 & R_9\end{pmatrix}, \tag{4}$$

where $R_1=\Delta_1(S)$, $R_5=\Delta_2(S)$, $R_9=\Delta_3(S)$, and

$$\rho(Z_D)=\begin{pmatrix} 0 & R_2 & R_3\\ 0 & 0 & R_6\\ 0 & 0 & 0\end{pmatrix}.$$

The antilinear operator D can be put into the form

$$D=\begin{pmatrix} J_1 & & 0\\ & J_2 & \\ 0 & & J_3\end{pmatrix}K$$

with $J_i\bar{J}_i=\pm I(D^2=\pm I)$. For the matrix B associated with the bilinear form (,), we have

$$B=\begin{pmatrix} 0 & & B_3\\ & B_5 & \\ B_6 & & 0\end{pmatrix};$$

this matrix is symmetric or skew-symmetric depending on the symmetric or symplectic character of (,).

The above discussion makes it clearly that the problem of classifying the maximal solvable subalgebras of a classical real Lie algebra either is immediately solved (compact Cartan subalgebra) or can be reduced to the classification of the maximal solvable subalgebras of a Lie algebra $\Delta_2(N)_D$ of the same type as L_D but of lower dimension. We have thus provided a recursive procedure for constructing the required subalgebras.

IV. CLASSIFICATION AND EXAMPLES

For $\mathrm{su}(p,q)$ and $\mathrm{so}(p,q)$ we refer to the two quoted paper, Refs. 1 and 2. The remaining cases are considered in the order of increasing difficulty.

We symplify our notation in identifying S with its representative $\rho(S)$.

A. su* (2r) [$r\geqslant 2$, su* (2) $\simeq$ su (1, 1)]

$D^2=-I$; henceforth $\dim W=2$.

The recursive procedure just described allows us to represent each maximal solvable subalegra by a matrix

$$S=\begin{pmatrix} A_1 & & & *\\ & A_2 & & \\ 0 & & \ddots & \\ & & & A_r\end{pmatrix}$$

with

$$A_i=\begin{pmatrix}\lambda_i & 0\\ 0 & \bar{\lambda}_i\end{pmatrix},\quad \lambda_i\in C.$$

Hence there exists only *one conjugacy class of maximal solvable subalebras of* $su^*(2r)$.

By choosing

$$D=\begin{pmatrix} J & & 0\\ & \ddots & \\ 0 & & J\end{pmatrix}K \quad\text{with } J=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix},$$

the condition $DS=SD$ implies for the block decomposition

$$S=\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1r}\\ & A_{22} & \cdots & A_{2r}\\ & & \ddots & \vdots\\ 0 & & & A_{rr}\end{pmatrix}$$

the conditions

$$A_{ij}=\begin{pmatrix} a_{ij} & b_{ij}\\ -\bar{b}_{ij} & \bar{a}_{ij}\end{pmatrix}\ \text{if } i<j,\quad A_{ii}=\begin{pmatrix} a_{ii} & 0\\ 0 & \bar{a}_{ii}\end{pmatrix}$$

and [from tr(S)]

$$\sum_{i=1}^{r}(a_{ii}+\bar{a}_{ii})=0.$$

We notice that the 2×2 matrices A_{ij} are nothing else than standard realizations of the quaternionic numbers.

B. so* (2r) [$r\geq 2$, so* (2) $\simeq$ so (1, 1)]

$D^2=-I.$

A first conjugacy class is furnished by the *compact Cartan subalgebras*. With respect to a weight vectors basis, these latter are represented by

$$S=\begin{pmatrix} A_1 & & 0 \\ & \ddots & \\ 0 & & A_r \end{pmatrix} \quad \text{with } A_k=\begin{pmatrix} ia_k & 0 \\ 0 & -ia_k \end{pmatrix}, \quad a_k\in R$$

In this same basis, D can be chosen as

$$D=\begin{pmatrix} J & & 0 \\ & \ddots & \\ 0 & & J \end{pmatrix} K,$$

while the matrix associated with the symmetric form (,) would be

$$B=\begin{pmatrix} iK & & 0 \\ & \ddots & \\ 0 & & iK \end{pmatrix}, \quad K=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The other conjugacy classes contain subalgebras represented by matrices of the form

$$S=\begin{pmatrix} A_1 & & & & & & * \\ & \ddots & & & & & \\ & & A_s & & & & \\ & & & E & & & \\ & & & & C_s & & \\ & & & & & \ddots & \\ 0 & & & & & & C_1 \end{pmatrix},$$

$$1\leq s\leq \left[\frac{r}{2}\right] \quad ([x]=\text{entire part of } x)$$

where

$$A_k=\begin{pmatrix} \lambda_k & 0 \\ 0 & \bar{\lambda}_k \end{pmatrix}$$

and where E is either a compact Cartan subalgebra of so*$(2r-4s)$ or is $\emptyset$ (void) if $s=r/2$ (which implies r is even). Taking into account the conjugacy conditions just found, we see that the conjugacy classes are uniquely determined by the dimension of the Cartan subalgebra E. Hence there exist $[r/2]+1$ *conjugacy classes of maximal solvable subalgebras of so*$^*(2r)$.

By keeping the same matrix form for D, the matrix B becomes here

$$B=\begin{pmatrix} & & & & & iK \\ & & 0 & & \iddots & \\ & & & iK & & \\ & & \hat{B} & & & \\ & iK & & 0 & & \\ \iddots & & & & & \\ iK & & & & & \end{pmatrix}$$

with

$$\hat{B}=\begin{pmatrix} iK & & 0 \\ & \ddots & \\ 0 & & iK \end{pmatrix} \quad \text{or} \quad \emptyset,$$

which permits us, in particular, to verify that

$$C_k\begin{pmatrix} -\bar{\lambda}_k & 0 \\ 0 & -\lambda_k \end{pmatrix} \quad \text{if } A_k=\begin{pmatrix} \lambda_k & 0 \\ 0 & \bar{\lambda}_k \end{pmatrix}.$$

The other matrix elements of S are computed by means of the two conditions

$$DS=SD, \quad BS^T=-SB.$$

C. usp [2p, 2q) [$p+q=r>1$, usp (2, 0) $\simeq$ su(1, 1)]

$D^2=-I.$

Here also, a first conjugacy class is furnished by the *compact Cartan subalgebras*

$$S=\begin{pmatrix} A_1 & & 0 \\ & \ddots & \\ 0 & & A_r \end{pmatrix}, \quad A_k=\begin{pmatrix} ia_k & 0 \\ 0 & -ia_k \end{pmatrix}, \quad a_k\in R,$$

for which

$$D=\begin{pmatrix} J & & 0 \\ & \ddots & \\ 0 & & J \end{pmatrix} K,$$

$$B=\begin{pmatrix} J & & & & 0 & \left.\vphantom{\begin{matrix}a\\a\\a\end{matrix}}\right\}p \\ & \ddots & & & & \\ & & J & & & \\ & & & -J & & \left.\vphantom{\begin{matrix}a\\a\\a\end{matrix}}\right\}q \\ & & 0 & & \ddots & \\ & & & & & -J \end{pmatrix}$$

For the other conjugacy classes, a matrix representative is given by

$$S=\begin{pmatrix} A_1 & & & & & * \\ & \ddots & & & & \\ & & A_s & & & \\ & & & E & & \\ & & & & C_s & \\ & & & & & \ddots \\ 0 & & & & & C_1 \end{pmatrix}, \quad 1\leq s\leq q,$$

where

$$A_k=\begin{pmatrix} \lambda_k & 0 \\ 0 & \bar{\lambda}_k \end{pmatrix}$$

and where E is either a compact Cartan subalgebra of usp$(2p-2s, 2q-2s)$ or $\emptyset$ (which implies $p=q$). The situation is therefore the same as in the preceding case: The conjugacy classes are uniquely characterized by the dimension of the Cartan subalgebra E. Since $p\geq q$, this dimension varies between $2r-2q$ and $2r$ by steps of 2. There exist consequently $q+1$ *conjugacy classes of maximal solvable subalgebras of usp*(p,q).

Taking the same D as above, putting

$$B=\begin{pmatrix} 0 & & & & K \\ & \ddots & & \iddots & \\ & & \hat{B} & & \\ & \iddots & & \ddots & \\ -K & & & & 0 \end{pmatrix}$$

with $\hat{B}=\begin{pmatrix} J & & & & 0 \\ & \ddots & & & \\ & & J & & \\ & & & -J & \\ & & & & \ddots \\ 0 & & & & -J \end{pmatrix}$ $\begin{matrix} \\ \\ \\ \\ \\ \end{matrix}\!\!\begin{matrix} \} p-s \\ \\ \\ \\ \} q-s \end{matrix}$ or $\emptyset$,

and considering the conditions

$$DS=SD, \quad BS^T=-SB,$$

we can compute all the elements of S. In particular, we can verify that

$$C_k=\begin{pmatrix} -\bar{\lambda}_k & 0 \\ 0 & -\lambda_k \end{pmatrix} \text{ if } A_k=\begin{pmatrix} \lambda_k & 0 \\ 0 & \bar{\lambda}_k \end{pmatrix}.$$

Example: usp(2, 2): Since $q=1$, there exist two classes; with

$$D=\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} K$$

a representative of a compact Cartan subalgebra is

$$S_1=\begin{pmatrix} ia & 0 & 0 & 0 \\ 0 & -ia & 0 & 0 \\ 0 & 0 & ib & 0 \\ 0 & 0 & 0 & -ib \end{pmatrix}, \quad a,b\in R,$$

when

$$B=\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$

A representative of the other class is

$$S_2=\begin{pmatrix} \lambda & 0 & ia & 0 \\ 0 & \bar{\lambda} & 0 & -ia \\ 0 & 0 & -\bar{\lambda} & 0 \\ 0 & 0 & 0 & -\lambda \end{pmatrix}, \quad \lambda\in C,\ a\in R,$$

when

$$B=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.$$

Since usp(2, 2) $\simeq$ so(4, 1) we can compare these results with those obtained in Ref. 2.

D. sl (n, R)

$D^2=I$.

The maximal solvable subalgebras admit a matrix representation of the form

$$S=\begin{pmatrix} A_1 & & & * \\ & A_2 & & \\ & & \ddots & \\ 0 & & & A_s \end{pmatrix},$$

where

$$A_j=\begin{pmatrix} \lambda_j & 0 \\ 0 & \bar{\lambda}_j \end{pmatrix} \text{ or } A_j=(c_j), \quad \lambda_j\in C,\ c_j\in R.$$

Since D is here an involution, we have $\dim W=1$ or 2. With respect to a basis of vectors belonging to V_D, we should have

$$A_j=\begin{pmatrix} a_j & -b_j \\ b_j & a_j \end{pmatrix} \text{ or } A_j=(c_j), \quad a_j,b_j,c_j\in R$$

with a constraint on the a_j and c_j due to the zero trace condition. All the elements of the matrices S are real because $D=K$.

Each conjugacy class is therefore uniquely characterized by an ordered set of numbers $(\deg A_1, \deg A_2, \ldots, \deg A_s)$, where $\deg A_j=1$ or 2 and $\sum_{j=1}^{s} \deg A_j=n$. *The number N_n of conjugacy classes of maximal solvable subalgebras of $sl(n,R)$* satisfies, by virtue of the recursive procedure, the equation

$$N_n=N_{n-1}+N_{n-2};$$

since $N_1=1$ and $N_2=2$, N_n is simply the Fibonacci number[2]

$$N_n=F_n=\frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^n-\left(\frac{1-\sqrt{5}}{2}\right)^n\right].$$

Example: sl(3, R): There exist three conjugacy classes (1, 1, 1), (1, 2), (2, 1),

$$S_{(1,1,1)}=\begin{pmatrix} a & b & c \\ 0 & d & e \\ 0 & 0 & -a-d \end{pmatrix},$$

$$S_{(1,2)}=\begin{pmatrix} -2a & b & c \\ 0 & a & -d \\ 0 & d & a \end{pmatrix},$$

$$S_{(2,1)}=\begin{pmatrix} a & -b & c \\ b & a & d \\ 0 & 0 & -2a \end{pmatrix}.$$

[The classification of all subalgebras of sl(3, R) was performed by Nôno.[7]]

E. sp (2r, R) [$r\geqslant 2$, sp(2, $\mathbb{R}$) $\simeq$ sl(2, $\mathbb{R}$)]

$D^2=I$.

The conjugacy class of *compact Cartan subalgebras* is represented by

$$S=\begin{pmatrix} A_1 & & 0 \\ & \ddots & \\ 0 & & A_r \end{pmatrix}, \quad A_j=\begin{pmatrix} 0 & a_j \\ a_j & 0 \end{pmatrix}, \quad a_j\in R,$$

for which $D=K$ and

$$B=\begin{pmatrix} J & & 0 \\ & \ddots & \\ 0 & & J \end{pmatrix}.$$

The other conjugacy classes of maximal solvable subalgebras admit a representative of the form

$$S=\begin{pmatrix} A_1 & & & & & * \\ & \ddots & & & & \\ & & A_s & & & \\ & & & E & & \\ & & & & C_s & \\ & & & & & \ddots \\ 0 & & & & & & C_1 \end{pmatrix}, \quad 1\leq s\leq r,$$

with

$$A_j=\begin{pmatrix} a_j & -b_j \\ b_j & a_j \end{pmatrix} \quad \text{or} \quad A_j=(c_j), \quad a_j, b_j, c_j\in R,$$

and E either a compact Cartan subalgebra of $\mathrm{sp}(2r-4s,R)$ or $\emptyset$ (which here is always possible). We have here $D=K$ and

$$B=\begin{pmatrix} 0 & & & & & K \\ & \ddots & & & \iddots & \\ & & K & & & \\ & & & \hat{B} & & \\ & & & & -K & \\ & & & & \ddots & \\ -K & & & & & 0 \end{pmatrix}$$

with $\hat{B}=\begin{pmatrix} J & & 0 \\ & \ddots & \\ 0 & & J \end{pmatrix}$ or $\emptyset$.

From the conditions

$$\bar{S}=S \quad \text{and} \quad BS^T=-SB,$$

it is possible to compute the elements of the matrices S; in particular we have

$$C_j=\begin{pmatrix} -a_j & b_j \\ -b_j & -a_j \end{pmatrix} \quad \text{if } A_j=\begin{pmatrix} a_j & -b_j \\ b_j & a_j \end{pmatrix},$$
$$c_j=(-c_j) \qquad \text{if } A_j=(c_j).$$

Each conjugacy class is therefore uniquely characterized by an ordered set of numbers $(\deg A_1,\ldots,\deg A_s;\deg E)$, with $\deg A_i=1$ or 2,

$$0\leq \deg E\leq n \quad \text{and} \quad 2\sum_{i=1}^{s}\deg A_i+\deg E=2r.$$

The number N_r of conjugacy classes of maximal solvable subalgebras of $sp(2r,R)$ satisfies the recursive equation

$$N_r=1+N_{r-1}+N_{r-2} \quad \text{with } N_1=2 \text{ and } N_2=4.$$

Putting $M_r=N_r+1$, we obtain $M_r=M_{r-1}+M_{r-2}$ with $M_1=3$, $M_2=5$. Henceforth

$$M_r=F_{r+2} \quad \text{and} \quad N_r=F_{r+2}-1.$$

Example: $\mathrm{sp}(4,R)$: There exist four conjugacy classes: (6) (the compact one), (1,1;0), (1;2), and (2;0):

$$S_{(6)}=\begin{pmatrix} 0 & a & 0 & 0 \\ -a & 0 & 0 & 0 \\ 0 & 0 & 0 & b \\ 0 & 0 & -b & 0 \end{pmatrix}, \quad B=\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$

$$S_{(1,1;0)}=\begin{pmatrix} a & b & c & d \\ 0 & e & 0 & c \\ 0 & 0 & -e & -b \\ 0 & 0 & 0 & -a \end{pmatrix}, \quad B=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$S_{(1\,2)}=\begin{pmatrix} a & b & c & d \\ 0 & 0 & e & c \\ 0 & -e & 0 & -b \\ 0 & 0 & 0 & -a \end{pmatrix}, \quad B=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$S_{(2\ 0)}=\begin{pmatrix} a & b & c & d \\ -b & a & e & c \\ 0 & 0 & -a & -b \\ 0 & 0 & b & -a \end{pmatrix}, \quad B=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.$$

Since $\mathrm{sp}(4,R)\simeq \mathrm{so}(3,2)$, we are able to compare these results with those given in Ref. 2.

V. CONCLUSION

With this article, the classification of the maximal solvable subalgebras of the classical real algebras is completed. The real exceptional Lie algebras (E,F,G) may be treated in the same way, although some matrix manipulations become uncomfortable to handle. They may represent some physical interest in view of the recent renewal of interest in the exceptional Lie groups in elementary particle physics.

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[1]J. Patera, P. Winternitz, and H. Zassenhaus, J. Math. Phys. 15, 1378 (1974).
[2]J. Patera, P. Winternitz, and H. Zassenhaus, J. Math. Phys. 15, 1932 (1974).
[3]P. Kramer, M. Moshinsky, and T.H. Seligman, in *Group Theory and Its Applications*, edited by E.M. Loebl (Academic, New York, 1975), Vol. 3.
[4]B.H. Flowers, Proc. Roy. Soc. Lond. A 212, 248 (1952).
[5]J. Tits, *Tabellen zu den einfachen Lie Gruppen und ihren Darstellungen* (Springer, Berlin and New York, 1967).
[6]N. Jacobson, *Lie Algebras* (Interscience, New York, 1962).
[7]T. Nôno, J. Math. Anal. Appl. 24, 110 (1968).

Quantization as deformation theory

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We show that any rule for quantization of functions on the phase space of a dynamical system is equivalent to a deformation of the Poisson bracket, in the sense of Lie algebras. All Schrödinger-type quantizations are equivalent mathematically but not physically. We examine whether a quantization rule exists in which the Poisson bracket of the free Hamiltonian and any function not more than quadratic in momentum gets quantized into the commutator of the quantized versions of these two observables. We show that if the (Riemannian) configuration manifold is irreducible, this condition uniquely specifies the quantization of these functions, in the cases when it can be satisfied. However, it can only be satisfied for systems whose configuration manifolds are one-dimensional, or have vanishing Ricci tensor, or are spaces of constant curvature. Thus the condition will not serve as a general physical principle which could be invoked to fix a quantization rule.

1. NOTATION

M = Riemannian configuration manifold of a dynamical system, metric tensor g, local coordinates $q^1 \cdots q^n$. $T^{(s)}M$ = space of real C^∞ fully symmetric contravariant tensor fields S on M with valence $v(S) = s$. $C_s(S) = S^{i_1 \cdots i_s}(q) p_{i_1} p_{i_2} \cdots p_{i_s}$ = homogeneous function on phase space T^*M associated with S. $[S, T] \in T^{(s+t-1)}M$ = Schouten concomitant,[1] related to the Poisson bracket by

$$\{C_s(S), C_t(T)\} = -C_{s+t-1}([S, T]).$$

$A = \oplus_{s=0}^{\infty} T^{(s)}M$ = graded Lie algebra of sequences of symmetric tensor fields with Schouten concomitant as Lie product. This algebra is isomorphic to the Lie subalgebra of C^∞ functions on T^*M which are polynomial in the p's.[2] $H = L^2(M, \mathbb{C})$ with the measure given by g = Hilbert space of wavefunctions Ψ on M.

2. QUANTIZATION AND DEFORMATION THEORY

Any quantization scheme associates each classical observable $C_s(S)$ with a Hermitian operator $Q_s(S)$ on H.

If $\phi \in T^{(0)}M$ is a scalar field on M [so $\phi = C_0(\phi)$], then in the Schrödinger representation the associated quantum mechanical operator is given by

$$(Q_0(\phi)\Psi)(m) = \phi(m)\Psi(m), \quad m \in M. \tag{2.1}$$

If $X \in T^{(1)}M$ is a vector field on M [so that $C_1(X)(q, p) = X^i(q) p_i$] the corresponding quantum mechanical operator is given by (for example[3])

$$Q_1(X)\Psi = \tfrac{1}{2}(-i\hbar X^i \partial_i + \text{conjugate})\Psi = -i\hbar(X^i \partial_i \Psi + \tfrac{1}{2}(\text{div}X)\Psi). \tag{2.2}$$

With this quantization rule, the elements of the Lie subalgebra $A_1 = T^{(0)}M \oplus T^{(1)}M$ of A are quantized canonically, i.e.,

$$[Q(S), Q(T)] = -i\hbar Q([S, T]), \quad \forall\ S, T \in A_1.$$

For $U \in T^{(2)}M$,

$$Q_2(U)\Psi = \tfrac{1}{2}((-i\hbar)^2 U^{i_1 i_2} \nabla_{i_1} \nabla_{i_2} + \text{conjugate})\Psi + \hbar^4 \alpha(U)\Psi, \tag{2.3}$$

where ∇_i is the covariant derivative and $\alpha(U)$ is a scalar field which depends linearly on U and its covariant derivatives, but has no generally agreed form. Probably its form is determined by some physical principle. In this paper we rule out one possibility for this principle, which at first sight seemed attractive. Namely, we show that if $\alpha(U)(m)$ depends only on the zeroth, first, and second derivatives of U at m [see Eq. (3.3)], one cannot in a general manifold M choose $\alpha(U)$ so that the commutator of $Q_2(U)$ with the free Hamiltonian $Q_2(\frac{1}{2}g^{-1})$ is canonical, i.e.,

$$[Q_2(U), Q_2(\tfrac{1}{2}g^{-1})] = -i\hbar Q_3([U, \tfrac{1}{2}g^{-1}]), \quad \forall\ U \in T^{(2)}M$$

(although this is possible in some manifolds, which we enumerate).

To start, let us choose some particular quantization scheme, for example, for $S \in T^{(s)}M$,

$$Q_s(S)\Psi = \tfrac{1}{2}(-i\hbar)^s [S^{i_1 \cdots i_s} \nabla_{i_1} \cdots \nabla_{i_s} \Psi + \nabla_{i_1} \cdots \nabla_{i_s}(S^{i_1 \cdots i_s}\Psi)] \tag{2.4}$$

as a reference scheme. All other Schrödinger-type quantization schemes agree with this one to leading order. The scheme (2.4) leads to commutation relations of the form

$$[Q_s(S), Q_t(T)] = -i\hbar(Q_{s+t-1}([S, T]) + \hbar^2 Q_{s+t-3}(F_1(S, T)) + \hbar^4 Q_{s+t-5}(F_2(S, T)) + \cdots). \tag{2.5}$$

This commutator provides a new Lie product on A,

$$[S, T]' = [S, T] + \hbar^2 F_1(S, T) + \cdots,$$

which is a deformation[4] of the original Schouten concomitant or Poisson bracket algebra.

The map $F_1 : T^{(s)}M \times T^{(t)}M \to T^{(s+t-3)}M$ is a cocycle of order 2 in the Lie algebra cohomology of A, with the adjoint action.[5] If

$$\eta : T^{(s)}M \to T^{(s-2)}M, \quad \eta' : T^{(s)}M \to T^{(s-4)}M, \ \cdots \tag{2.6}$$

are cochains of order 1 in A, and we alter some given quantization scheme Q in (2.5) to another one, Q', related to Q by

$$Q'_s(S) = Q_s(S) + \hbar^2 Q_{s-2}(\eta(S)) + \hbar^4 Q_{s-4}(\eta'(S)) + \cdots, \tag{2.7}$$

then the new commutation relations are

$$[Q'_s(S), Q'_t(T)] = -i\hbar(Q'_{s+t-1}([S, T]) + \hbar^2 Q'_{s+t-3}((F_1 + d\eta)(S, T)) + \cdots), \tag{2.8}$$

where

$$d\eta(S, T) = [S, \eta(T)] - [T, \eta(S)] - \eta([S, T]) \tag{2.9}$$

is the usual exterior derivative.[5] We shall restrict ourselves throughout to quantization schemes of the form (2.7). Such schemes are essentially real in that the quantities $P'_s(S)$ given by

$$P'_s(S) = i^s Q'_s(S)$$

are (anti-) Hermitian if s is (odd) even and the commutators of the P's with each other involve no factors i.

It follows from Eqs. (2.8) and (2.9) that all quantization schemes in the Schrödinger representation lead one to the same element of $H_2(A, A)$ and in this sense are mathematically equivalent. However, commutation relations have physical significance, so that they are not physically equivalent. It may well be that if one chose a different polarization of T^*M (in the sense of Kostant[6]) for quantization, then one could be led to a different element of $H_2(A, A)$. Following the work of Godbillon and Vey[7,8] there has been considerable study of the relation between foliations and cohomology, but not in connection with quantization. Effort in this direction might be fruitful.

It is well known that F_1 is not exact for any configuration manifold; there is no quantization scheme in which all commutators are canonical. The problem is to find a criterion based on physical grounds which fixes the scheme uniquely. We present a candidate for such a criterion, together with its physical motivation in the next section.

3. TIME DEVELOPMENT

In classical mechanics, for a system with Hamiltonian $\frac{1}{2}g^{ij}(q)p_i p_j \equiv C_2(\frac{1}{2}g^{-1})$, the time development of the observable $C_s(S)$ is given by Hamilton's equation

$$\frac{d}{dt}C_s(S) = \{C_s(S), C_2(\tfrac{1}{2}g^{-1})\} = C_{s+1}([\tfrac{1}{2}g^{-1}, S]).$$

In quantum mechanics in the Heisenberg picture, the equation (2.5) is an equal time commutation relation for operators $Q_s(S)$ whose time development is given by the Heisenberg equation of motion

$$\frac{d}{dt}Q_s(S) = i[Q_2(\tfrac{1}{2}g^{-1}), Q_s(S)].$$

Tensors K which satisfy

$$[g^{-1}, K] = 0$$

are called Killing tensors[1]; for such a K, $C(K)$ is a constant of the classical motion.

In terms of components, if $S \in T^{(s)}M$,

$$[g^{-1}, S]^{i_1 \cdots i_{s+1}} = 2S^{(i_1 \cdots i_s; i_{s+1})},$$

where round brackets enclosing indices indicate that these are symmetrized. The set of Killing tensors is a Lie subalgebra of A. It is at first sight a natural desideratum that if K is a Killing tensor, then $Q(K)$ should commute with $Q(g^{-1})$, so that constants of the classical motion provide constants of the quantal motion under quantization. Such a condition cannot be sufficiently strong to specify a quantization scheme uniquely in all cases; most configuration manifolds possess no Killing fields whatever but have only locally defined constants of the classical motion.[9] In terms of cohomology, such a quantization scheme Q' will exist if, in the starting scheme Q, F_1 is exact when restricted to the arguments (g^{-1}, K). The manifolds with most Killing vectors are the spaces of constant curvature, and for these Underhill and Taraviras[10] have exhibited a quantization scheme in which classical constants give quantal constants.

In the rest of this paper we examine whether a scheme Q' exists in which one has a stronger condition, namely, that for all S

$$[Q'(g^{-1}), Q'(S)] = -i\hbar Q'([g^{-1}, S]), \tag{3.1}$$

that is to say, all commutators with the free Hamiltonian are canonical. In cohomology terms, F_1 must be exact when restricted to the arguments (g^{-1}, S), i.e.,

$$F_1(g^{-1}, S) = -d\eta(g^{-1}, S) \tag{3.2}$$

for some 1-cochain η. [If the configuration space is R^n with the Euclidean metric, the Weyl rule[11] satisfies condition (3.1) so we have nothing to prove in that case.]

Because it is difficult to do better, we restrict our consideration of Eq. (3.2) to tensors S of valence at most 2, and to cochains η given by the form, for $U \in T^{(2)}M$,

$$\eta(U) = \eta_{ab}U^{ab} + \eta_{abc}U^{ab;c} + \eta_{abcd}U^{ab;cd}. \tag{3.3}$$

Thus we assume that the value of the scalar field $\eta(U)$ at the point m of M depends only on the value and derivatives up to second order of U at M; we exclude nonlocal dependence.[12] In order that they be specified uniquely by the values $\eta(U)$, we require the tensor fields η to possess the symmetries

$$\eta_{ab} = \eta_{ba}, \quad \eta_{abc} = \eta_{bac}, \quad \eta_{abcd} = \eta_{bacd} = \eta_{abdc}.$$

In the quantization scheme (2.4) we already have condition (3.1) when S is a scalar field. [This condition is related to the expression for $Q(\phi X)$ in terms of $Q(\phi)$ and $Q(X)$. See Ref. 13 for details.]

In the next section we show that the equations

$$F_1(g^{-1}, X) = -d\eta(g^{-1}, X), \ \forall\ X \in T^{(1)}M, \tag{3.4}$$

$$F_1(g^{-1}, U) = -d\eta(g^{-1}, U), \ \forall\ U \in T^{(2)}M, \tag{3.5}$$

yield several conditions on the tensors η_{ab}, η_{abc}, and η_{abcd}. On the assumption that the configuration space is irreducible (that is to say,[14] it admits no parallel vector fields or equivalently its holonomy group at any point acts transitively on the unit tangent vectors there), these conditions can be satisfied only for spaces with vanishing Ricci tensor and spaces of constant curvature. In

these cases the solution η is unique. The uniqueness of a solution η to Eqs. (3.4) and (3.5) is unusual in cohomology theory and requires explanation. One can usually add to η a coboundary, $\eta \to \eta + d\theta$, at will. However, here the 1-cochain η has to map $T^{(s)}M$ into $T^{(s-2)}M$, and no exact 1-cochain has this property. An exact 1-cochain dT, $T \in A$, acts on $S \in A$ according to the rule

$$dT(S) = [S, T]$$

and increases the valence by $v(T) - 1$. The lowest value which this can take is -1.

4. CALCULATION

We first analyze the condition (3.4) that $F_1(g^{-1}, X)$ should be exact. With the scheme Q given by Eq. (2.4), it is straightforward to compute, for $X \in T^{(1)}M$, that

$$F_1(g^{-1}, X) = -\tfrac{1}{2}X^a{}_{;ab}{}^b + \tfrac{1}{2}(X^{a;b} + X^{b;a})_{;ab}. \tag{4.1}$$

We shall find the most general cochain η of the form (3.3) which satisfies (3.4). Substitution of Eqs. (3.3), (2.9), and (4.1) into (3.4) yields, for all vector fields X [note that $\eta(X) = 0$ since η lowers valence by two]

$$\begin{aligned} &X^a \eta^b{}_{b;a} + 2\eta_{ab}X^{a;b} + 2\eta_{abc}X^{a;bc} + 2\eta_{abcd}X^{a;bcd} \\ &\quad = -\tfrac{1}{2}X^a{}_{;ab}{}^b + \tfrac{1}{2}(X^{a;b} + X^{b;a})_{;ab} \\ &\quad = \tfrac{1}{2}(g_{ab}g_{cd}X^{a;bcd} + 2R_{ab}X^{a;b} + R_{;a}X^a). \end{aligned} \tag{4.2}$$

Here R_{ab} is the Ricci tensor and $R = R^a{}_a$ is the scalar curvature. Equating coefficients of the derivatives of X here requires care, as not all covariant derivatives are independent. Let us first solve a general problem of this type.

Suppose we have four tensor fields $\alpha_{i_1 i_2 \cdots i_n}$, $n = 1, \ldots, 4$ such that for all vector fields X,

$$\alpha_{a(bcd)}X^{a;bcd} + \alpha_{a(bc)}X^{a;bc} + \alpha_{ab}X^{a;b} + \alpha_a X^a = 0.$$

Then we may conclude that

$$\alpha_{a(bcd)} = \alpha_{a(bc)} = \alpha_{ab} = \alpha_a = 0,$$

since the tensors X^a, $X^{a;b}$, $X^{a;(bc)}$, $X^{a;(bcd)}$ may be chosen independently at any point. (Once those values have been fixed, so have all the second and third order nonsymmetrized derivatives.) If instead we are given that

$$\alpha_{abcd} = \alpha_{bacd} = \alpha_{abdc},$$

$$\alpha_{abc} = \alpha_{bac}, \quad \alpha_{ab} = \alpha_{ba}$$

and, for all X,

$$\alpha_{abcd}X^{a;bcd} + \alpha_{abc}X^{a;bc} + \alpha_{ab}X^{a;b} + \alpha_a X^a = 0,$$

then by writing the first two terms as symmetrized and antisymmetrized combinations, and reducing the antisymmetric derivatives of X to lower order by means of the curvature tensor, we may deduce the following:

(i) $\alpha_{a(bcd)} = 0$,

which implies, by simple algebra,

$$\alpha_{(abc)d} = 0 \quad \text{and} \quad \alpha_{abcd} = \alpha_{cdab}.$$

(ii) $\alpha_{a(bc)} = 0$,

which implies

$$\alpha_{abc} = 0.$$

(iii) $\alpha_{ab} = \tfrac{2}{3}\alpha_{ijka}R_b{}^{ijk}$,

which, since α_{ab} is symmetric in ab, implies

$$\alpha_{ijka}R_b{}^{ijk} = \alpha_{ijkb}R^{aijk}.$$

(iv) $\alpha_a = \tfrac{2}{3}\alpha_{ijkl}R_a{}^{ijk;l}$.

Applying these results to our Eq. (4.2) we find, from (i),

$$\tfrac{1}{2}g_{a(b}g_{cd)} = 2\eta_{a(bcd)}.$$

Let us define f_{abcd} by

$$\eta_{abcd} = \tfrac{1}{4}g_{ab}g_{cd} + f_{abcd}. \tag{4.3}$$

Then

$$f_{abcd} = f_{bacd} = f_{abdc} = f_{cdab} \tag{4.4}$$

and

$$f_{a(bcd)} = f_{(abc)d} = 0. \tag{4.5}$$

These symmetry conditions restrict f_{abcd} to having as many independent components as the curvature R_{abcd}. However, f_{abcd} obeys additional conditions besides these. We find from (ii) that

$$\eta_{abc} = 0,$$

from (iii) that

$$2\eta_{ab} - R_{ab} = \tfrac{4}{3}f_{ijka}R_b{}^{ijk} \tag{4.6}$$

and

$$f_{ijka}R_b{}^{ijk} = f_{ijkb}R_a{}^{ijk}, \tag{4.7}$$

and from (iv) that

$$\begin{aligned} \eta^b{}_{b;a} - \tfrac{1}{2}R_{;a} &= \tfrac{4}{3}f_{ijkl}R_a{}^{ijk;l} \\ &= \tfrac{2}{3}f_{ijkl}R^{lijk}{}_{;a}, \end{aligned} \tag{4.8}$$

where the last line follows from the symmetries of f_{ijkl} and the identities obeyed by the curvature tensor. Comparing (4.6) and (4.8), we see we may replace (4.8) by

$$f_{ijkl;a}R^{lijk} = 0. \tag{4.9}$$

In summary, we may regard (4.6) as an expression for η_{ab} in terms of f_{abcd}. The latter must possess the symmetry properties (4.4) and (4.5) and satisfy (4.7) and (4.9). Such tensors f_{abcd} exist; examples are constant multiples of the tensor

$$\overset{\circ}{f}_{abcd} \equiv \tfrac{1}{8}(2g_{ab}g_{cd} - g_{ac}g_{bd} - g_{ad}g_{bc}). \tag{4.10}$$

Hence it is possible to quantise in many ways so that

$$[Q(g^{-1}), Q(X)] = -iQ([g^{-1}, X]), \quad X \in T^{(1)}M.$$

We turn now to the condition (3.5) that $F_1(g^{-1}, U)$ be exact. The analysis is similar but more complicated. One may verify directly from the definitions (2.4), (2.5) that the vector field $F_1(g^{-1}, U)$ is

$$F_1(g^{-1}, U) = \xi(\tilde{U}) + \beta(U),$$

where

$$\tilde{U} = [g^{-1}, U],$$

$$\zeta(\tilde{U})^j = \tilde{U}^{jbc}{}_{;bc} + \tfrac{1}{4}(\tilde{U}^{bc}{}_c{}^{;j}{}_b - \tilde{U}^{jb}{}_b{}^{;c}{}_c),$$

and

$$\beta(U)^j = \tfrac{2}{3}(R^b{}_c U^{cj} - U^b{}_c R^{cj})_{;b} - U^{bc}{}_{;bc}{}^j.$$

Condition (3.5) thus states that, for all $U \in T^{(2)}M$,

$$\zeta(\tilde{U}) + \beta(U) + [g^{-1}, \eta(U)] - [U, \eta(g^{-1})] = \eta(\tilde{U}),$$

which in components is

$$\tfrac{2}{3}(R^b{}_c U^{cj} - U^b{}_c R^{cj})_{;b} - U^{bc}{}_{;bc}{}^j - 2U^{jb}\eta^a{}_{a;b}$$

$$+ 2(\eta_{ab}U^{ab} + \{\tfrac{1}{4}g_{ab}g_{cd} + f_{abcd}\}U^{ab;cd})^{;j} = (\eta - \zeta)(\tilde{U})^j. \quad (4.11)$$

Let us expand the right-hand side in covariant derivatives of $\tilde{U}$, as we did for $\eta(U)$ in (3.3):

$$(\eta - \zeta)(\tilde{U})^j = \omega^j{}_{abc}\tilde{U}^{abc} + \omega^j{}_{abc.d}\tilde{U}^{abc;d} + \omega^j{}_{abc.de}\tilde{U}^{abc;de}. \quad (4.12)$$

Equation (4.11) ensures that no higher terms exist. We suppose that the ω's are symmetric in abc, and that

$$\omega^j{}_{abc.de} = \omega^j{}_{abc.ed}$$

so that they are uniquely prescribed by (4.12).

The symmetrized derivatives U^{ab}, $U^{ab;c}$, $U^{ab;(cd)}$, $U^{ab;(cde)}$ are all independent, and

$$U^{ab;cde} = U^{ab;(cde)} + \text{terms in } U \text{ and } U',$$

$$U^{ab;cd} = U^{ab;(cd)} + \text{terms in } U,$$

where U, U' denote zero and first order derivatives. Hence we may at once equate the symmetrized coefficients of U'' and U'''. Noting that

$$\omega^j{}_{abc}\tilde{U}^{abc} = 2\omega^j{}_{abc}U^{ab;c},$$

we equate the symmetrized coefficients of U'' in Eq. (4.11) to obtain

$$f_{abcd}{}^{;j} = \omega^j{}_{ab(c.d)}$$

Equation (4.5) now implies that

$$\omega^j{}_{a(bc.d)} = 0$$

or

$$\omega_b + \omega_c + \omega_d = 0,$$

where ω_d stands for $\omega^j{}_{abc.d}$. Evidently this implies $\omega_d = 0$ and so f is a parallel tensor,[14]

$$f_{abcd}{}^{;j} = 0. \quad (4.13)$$

This condition contains (4.9) as a special case, and also implies (4.7).

Let us assume henceforth that the Riemannian manifold (M, g) is irreducible.[14] Then the only solution of Eq. (4.13) having the symmetries (4.4) and (4.5) is

$$f = \lambda \overset{\circ}{f}, \quad (4.14)$$

where λ is a constant and $\overset{\circ}{f}$ is given by Eq. (4.10). To see this,[15] we regard the tensor $f^{ab}{}_{cd}(m)$ as a map of the space $T^{(2)}M_m$ of symmetric contravariant second order tensors at m into $T^{(2)}M_m$. Equation (4.13) implies that this map commutes with parallel transport, and hence commutes with all members of the holonomy group. Since M is irreducible, the holonomy group is $SO(n)$. Now $T^{(2)}M_m$ reduces under the action of $SO(n)$ into the sum of the space of traceless tensors and the space of multiples of the inverse metric, which are irreducible under the action. Hence, by Schur's lemma,

$$f^{ab}{}_{cd} = \alpha(\delta^a{}_c\delta^b{}_d + \delta^a{}_d\delta^b{}_c) + \beta g^{ab}g_{cd}, \quad (4.15)$$

where the first term is the identity on $T^{(2)}M$, and the second is the projection operator onto the element g^{-1}. Equation (4.13) implies that α and β are constants. The symmetry condition (4.5) reduces (4.15) to (4.14). It follows from (4.14) and (4.6) that

$$\eta_{ab} = \tfrac{1}{2}R_{ab} + \tfrac{2}{3}f_{ijka}R_b{}^{ijk} = \tfrac{1}{4}(2 + \lambda)R_{ab}. \quad (4.16)$$

To obtain the coefficients of the U and U' terms in (4.11), we must compute the terms of those types which are left over after the cancellation of the symmetrized third order terms. Equation of the symmetrized U''' terms in (4.11) yields

$$-U_{bc}{}^{;(bcj)} + 2\eta_{abcd}U^{ab;(cdj)} = 2\omega^j{}_{abc.de}U^{ab;(cde)},$$

from which it follows that

$$\omega^j{}_{ab(c.de)} = 3v_{ab(cd}\delta^j{}_{e)} \equiv v^j{}_{ab.cde}, \quad (4.17)$$

where by (4.14)

$$3v_{abcd} = \tfrac{1}{4}(g_{ab}g_{cd} - g_{ac}g_{bd} - g_{ad}g_{bc}) + f_{abcd}$$

$$= \tfrac{1}{4}[(1 + \lambda)g_{ab}g_{cd} - (1 + \tfrac{1}{2}\lambda)(g_{ac}g_{bd} + g_{ad}g_{bc})].$$

We wish to solve (4.17) for the ω's in terms of the v's. Notice that there are as many equations as unknowns since the $v^j{}_{ab.cde}$ are symmetric in the first two and in the last three lower indices, whereas the $\omega^j{}_{abc.de}$ are the other way round. Determined inspection yields the solution

$$\omega^j{}_{abc.de} = v^j{}_{de.abc} + 3v^j{}_{(ab.c)de} - \tfrac{3}{2}(v^j{}_{d(a.bc)e} + v^j{}_{e(a.bc)d}), \quad (4.18)$$

which is easily shown to be unique. A direct but lengthy calculation yields that if ω is related to v by (4.17) and if $v_{abcd} = v_{bacd} = v_{abdc} = v_{cdab}$, then

$$\omega^j{}_{abc.de}U^{ab;cde} - 3v_{abcd}U^{ab;cdj} = R^j(v, U), \quad (4.19)$$

where

$$R^j(v, U)$$

$$= -2U^{j\alpha}v_{abcd}R^{bcda}{}_{;\alpha} + 2U^{\alpha\beta}v_{abc\alpha}(4R_\beta{}^{jbc;a} - R_\beta{}^{abc;j})$$

$$+ U^{j\alpha;\beta}(-6v_{abc\beta}R_\alpha{}^{abc} + 2v_{abc\alpha}R_\beta{}^{abc})$$

$$+ U^{\alpha\beta;\gamma}(9v_{\alpha ab\gamma}R^j{}_\beta{}^{ab} + 6v_{\alpha ab\gamma}R^{jba}{}_\beta$$

$$+ \tfrac{5}{2}v_{\alpha\beta ab}R^{aj}{}_\gamma{}^b + 3v_{ab\alpha\gamma}R^{ja}{}_\beta{}^b + v_{\alpha ab\beta}R^{ja}{}_\gamma{}^b). \quad (4.20)$$

Equations (4.11), (4.19), and (4.20) now give

$$\tfrac{1}{3}(R^b{}_c U^{cj} - U^b{}_c R^{cj})_{;b} + (\eta_{\alpha\beta}U^{\alpha\beta})^{;j} - \eta^a{}_{a;\alpha}U^{\alpha j} - R^j(v, U)$$

$$= \omega^j{}_{abc}U^{ab;c}, \quad (4.21)$$

where η_{ab} is given by (4.16).

Equating the symmetrized coefficients of U and U' gives, respectively,

$$(\lambda+1)R_{\alpha\beta;\gamma}=0 \tag{4.22}$$

and

$$X^j{}_{mnp} \equiv (3\lambda+4)R^j{}_{(mn)p} - 3(\lambda+1)g_{p(m}R^j{}_{n)}$$
$$= -3\omega^j{}_{mnp} - (\tfrac{9}{4}\lambda+\tfrac{21}{8})g_{(mn}R^j{}_{p)} + \tfrac{9}{4}(\lambda+2)R_{(mn}\delta^j{}_{p)}. \tag{4.23}$$

The right-hand side of Eq. (4.23) is fully symmetric in the suffices mnp. The left side, which we have denoted $X^j{}_{mnp}$, is, *a priori*, symmetric only in mn. In order that Eq. (4.23) can hold for some $\omega^j{}_{mnp}$, we evidently require that $X^j{}_{mnp}$ is also fully symmetric in mnp, i.e.,

$$X^j{}_{mnp} = X^j{}_{mpn},$$

which gives

$$(3\lambda+4)R^j{}_{mnp} = (\lambda+1)(g_{pm}R^j{}_n - g_{mn}R^j{}_p). \tag{4.24}$$

We now have to discuss cases.

(i) If $\dim M = 1$, then both sides of (4.24) vanish for all λ, and so λ is arbitrary. However, $\overset{\circ}{f}$ vanishes, so a unique solution η of the form (3.3) exists,

$$\eta(S) = \tfrac{1}{4}g_{11}g_{11}S^{11;11}.$$

(ii) If $\dim M > 1$ and $\lambda = -\frac{4}{3}$, then

$$g_{pm}R^j{}_n = g_{mn}R^j{}_p,$$

from which, by taking the trace, we see that the Ricci tensor vanishes. For curved spaces with vanishing Ricci tensor, again there is a unique solution η. (We have excluded flat spaces from consideration by our irreducibility hypothesis.)

(iii) If $\dim M > 1$ and the Ricci tensor does not vanish, then

$$R^j{}_{mnp} = \frac{\lambda+1}{3\lambda+4}(g_{pm}R^j{}_n - g_{mn}R^j{}_p),$$

that is, M must be a space of constant curvature and $\lambda = -(n+3)/(n+2)$, where $n = \dim M$. Again $\eta(S)$ is unique.

In each case, Eq. (4.22) is satisfied automatically. These are the only irreducible configuration manifolds which admit a Schrödinger-type quantization which gives canonical commutators of the free Hamiltonian with functions which are at most quadratic in momentum. Any other irreducible configuration manifold gives a counter example. Hence the hypothesis (3.1) is no use for fixing a general quantization rule.

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[1] P.D. Sommers, J. Math. Phys. **14**, 787 (1973).
[2] N.M.J. Woodhouse, Comm. Math. Phys. **44**, 9 (1975).
[3] R. Hermann, *Vector Bundles in Mathematical Physics*, II (Benjamin, New York, 1970), Eq. 5.22.
[4] M. Lévy-Nahas, J. Math. Phys. **8**, 1211 (1967).
[5] N. Jacobson, *Lie Algebras* (Interscience, New York 1962).
[6] B. Kostant, *Quantisation and Unitary Representations*, Lecture Notes in Mathematics Vol. **170** (Springer-Verlag, Berlin, 1970).
[7] C. Godbillon and J. Vey, C.R. Acad. Sci. A **273**, 92 (1971).
[8] S.G. Gindikin, A.A. Kirillov and D.B. Fuks, Russian Math. Surveys **29**, 5 (1974).
[9] L. Galgani and A. Scotti, Nuovo Cimento **2**, 189 (1972).
[10] J. Underhill and S. Taraviras, Proc. Fourth Int. Colloq. on Group Theoretical Methods in Physics, Nijmegen 1975.
[11] H. Weyl, *Theory of Groups and Quantum Mechanics* (Dover, New York, 1950), 2nd ed., p. 275.
[12] I.M. Gel'fand and D.B. Fuks have investigated the cohomologies of the related infinite-dimensional Lie algebra of vector fields on a manifold, using nonlocal cochains. See Ref. 8. In their language, F_1 and η are diagonal. However, F_1 and η take values in the adjoint representation, whereas most of the research to date has been on the trivial real representation.
[13] F.J. Bloore and I.R. Ghobrial, J. Phys. A **8**, 1863 (1975).
[14] S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry. I* (Interscience, New York, 1963).
[15] We thank Dr. Edwin Ihrig for this argument.

Quasiclassical scattering above barriers in one dimension

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The Schrödinger equation is studied at energy levels above the highest values of the potential for wavelengths smaller than the scale of the potential variations. The first approximation to the scattering matrix is then expressed in terms of a single parameter a_+ representable as, effectively, a Fourier transform. This is used to prove the transcendental property of reflection for smooth potentials and to obtain the precise, first approximation to the scattering matrix for a very large class of analytic potentials.

1. INTRODUCTION

One-dimensional scattering has been of considerable interest in quantum physics, and the case of central symmetry is formally reducible to it.[1] Many approximations have been tried for energies above the maximal potential value, where traditional WKB approaches are not applicable even in the quasiclassical limit. A family of explicit solutions of Schrödinger's equation are due to Epstein,[1] and a correct treatment of scattering has been given by Fedoryuk[2] for a class of meromorphic potentials with simple roots. The following reports a much simpler, and much more general, approach; it is based on a rigorous optical method,[3] but greatly simplifies the results there obtained.

The first step (Sec. 2) is to express the scattering matrix in terms of just two integrals, of which one is a mere phase correction and the other, a_+, akin to a Fourier integral. Admittedly, it is the transform of the main unknown function, but that does not preclude highly informative inferences, for instance, smooth potentials are seen to reflect but transcendentally[4]—which is the reason for the failure[5] of traditional WKB approaches.

A combination of contraction, turning point, and stationary phase arguments is used in Sec. 3 to calculate the explicit, first asymptotic approximation to the Fourier type transform a_+ for any potential $U(x)$ analytic near the real x axis and for which the first relevant breakdowns of analyticity, further from that axis, are due to singularities of reasonably common type.

The probability of reflection is then "exponentially small" in the quasiclassical parameter, but that need not[6] imply numerical smallness. In fact, as the simplicity of the following extends promise of generalizations, so its precision extends hope of some usefulness for scattering that is barely quasiclassical.

2. FORMULATION

We consider Schrödinger's equation

$$\frac{h^2}{2m}\frac{d^2\psi}{dx^2}+(E-U(x))\psi=0$$

at energy levels $E>\text{l. u. b. } U(x)$ at which the wavelength bound $2\pi h[2m(E-\text{l. u. b. } U)]^{-1/2}=2\pi\epsilon$ is fairly small [compared with g. l. b. $(U\,dx/dU)$]. The "particle" is then modulated by the potential $U(x)$. Schrödinger's equation may be rewritten as

$$\epsilon^2\frac{d^2\psi}{dx^2}+q^2\psi=0,\quad q^2=\frac{(E-U(x))}{(E-\text{l. u. b. } U)}\geq 1 \tag{1}$$

and a more natural independent variable is

$$\xi=\int_0^x q(x')\,dx' \tag{2}$$

in terms of which Schrödinger's equation becomes

$$\frac{d^2\psi}{d\xi^2}+\phi(\xi)\frac{d\psi}{d\xi}+\epsilon^{-2}\psi=0,\quad \phi(\xi)=\frac{1}{2q^2}\frac{dq}{dx}\,. \tag{3}$$

Since $E>U(x)$, there is no classical scattering. For simplicity in the definition of quantum scattering, it is assumed that $U-U_\pm=\text{const}$ as $x\to\pm\infty$, respectively[7]; the corresponding limits of q are $q_\pm$. Then[8] Schrödinger's equation has solutions $u_+(\xi)$, $v_+(\xi)$, $u_-(\xi)$, $v_-(\xi)$ with the property

$$\exp(-i\xi/\epsilon)u_\pm\to 1,\quad \exp(i\xi/\epsilon)v_\pm\to 1\ \text{ as } x\to\pm\infty \tag{4}$$

and the derivatives of these expressions tend to zero. Since u_-, v_- are a fundamental solution system of (1), u_+ and v_+ must be linear combinations

$$\begin{pmatrix}u_+\\ v_+\end{pmatrix}=\begin{pmatrix}s_{11}&s_{12}\\ s_{21}&s_{22}\end{pmatrix}\begin{pmatrix}u_-\\ v_-\end{pmatrix}\equiv S\begin{pmatrix}u_-\\ v_-\end{pmatrix} \tag{5}$$

of u_-, v_- with scattering matrix S, which the following aims to estimate.

From (1) and (4), since ϵ and q are real for real x, $v(\bar{x})=\bar{u}(x)$, where the bar denotes complex conjugation, and it follows from (5) that

$$s_{22}=\bar{s}_{11},\quad s_{21}=\bar{s}_{12}.$$

Since (1) has constant Wronskian $W_x(\psi,\bar{\psi})$, the matrix elements are further related by

$$q_+/q_-=|s_{11}|^2-|s_{12}|^2, \tag{6}$$

which expresses conservation of probability current. It may also be interpreted in terms of transmission and reflection coefficients t, r defined by the requirement that (1) have a solution

$$\psi(x)=tu_+=u_-+rv_-. \tag{7}$$

Then

$$t=s_{11}^{-1},\quad r=s_{12}/s_{11} \tag{8}$$

and (6) takes the form

$$(q_+/q_-)|t|^2+|r|^2=1. \tag{9}$$

For the determination of the scattering matrix, it is convenient to introduce also a solution representation

for (1) different from the familiar ["L–G" or WKB(J)"] representation (4). Substitution in (1) or (3) shows

$$w(x) = q^{-1/2} \exp(-i\xi/\epsilon)(1 - a(\xi)) \exp \int_\xi^\infty \phi(s)a(s)\,ds \tag{10}$$

to satisfy (1) if

$$\frac{da}{d\xi} = -2i\epsilon^{-1}a + (a^2 - 1)\phi. \tag{11}$$

For definiteness, let $a(\xi)$ denote a solution of (11) for which

$$a \to 0 \quad \text{as} \quad \xi \to -\infty. \tag{12}$$

On the hypothesis

$$\frac{dq}{dx} \in C(\mathbb{R}) \cap L(\mathbb{R}), \tag{13}$$

which implies the same property for $\phi(\xi)$, by (2) and (3), $a(\xi)$ exists for all real ξ and $|a(\xi)| < 1$, and (11), (12) may be rewritten as

$$a(\xi) \exp(-2i\xi/\epsilon) = \int_{-\infty}^{\xi} ([a(s)]^2 - 1)\phi(s) \exp(-2is/\epsilon)\,ds. \tag{14}$$

It follows that

$$a(\xi) \exp(-2i\xi/\epsilon) \to \int_{-\infty}^{\infty} (a^2 - 1)\phi \exp(-2is/\epsilon)\,ds = a_+ \quad \text{as } \xi \to \infty. \tag{15}$$

Since $q(x)$ is real, $\overline{w(x)}$ is another solution, and the Wronskian

$$\begin{aligned} W_x(w, \bar{w}) &= w\bar{w}' - w'\bar{w} \\ &= i\epsilon^{-1}q\,|w|^2(1 - |a|^2)/|1 - a|^2 \\ &= i\epsilon^{-1}|g|^2(1 - |a|^2) \neq 0 \end{aligned}$$

by (12). Therefore, the solution (7) is $c_1w_1 + c_2w_2$ and by (15) and (4), $c_1/c_2 = \bar{a}_+$ and $c_2(1 - |a_+|^2) = tq_+^{1/2}$, and since the constancy of the Wronskian implies

$$|g|^2 = 1 - |a_+|^2 \quad \text{for } g(\epsilon) = \exp \int_{-\infty}^{\infty} \phi(s)a(s)\,ds, \tag{16}$$

it is found from (4), (5), (7), and (8) that

$$s_{11} = t^{-1} = (q_+/q_-)^{1/2}\bar{g}(1 - |a_+|^2)^{-1} = (q_+/q_-)^{1/2}g^{-1} \tag{17}$$

$$s_{12}/s_{11} = r = \bar{a}_+ g/\bar{g}. \tag{18}$$

The scattering matrix is thus represented in terms of the integrals (15) and (16), of which the former will turn out to be the more important. It is closely akin to a Fourier integral with large parameter ϵ^{-1} in the exponent, because[3] $a(\xi) \to 0$ with ϵ uniformly in ξ on $\mathbb{R}$, if only $u'(x) \in L(\mathbb{R})$. It therefore yields to the asymptotic methods developed for Fourier transforms, and that implies a great deal of immediate information, even though (15) only represents a_+ as the transform of an unknown function. For instance, if the potential $U(x)$ is smooth, say, "gentle[9]" in the sense $U(x) \in C^\infty(\mathbb{R})$ with $d^nU/dx^n \in L(\mathbb{R})$ for every n, then (1), (2), (3), (11) show $\phi(\xi)$ and $a(\xi)$ to inherit this property and[10] (15) shows a_+ to be *transcendentally small* in ϵ. The converse holds equally[10]: transcendental smallness of a_+ requires gentleness of the potential. True *exponential* smallness of a_+ is seen from the Laplace integral theorem to require *analyticity* of $a(\xi)$, and hence also of the potential $U(x)$.

The converse is also known[3]: If $U(x)$ is analytic on a strip about the real x axis of positive minimal width, and $U'(x) \to 0$ as $|\mathrm{Re}x| \to \infty$ in this strip locally uniformly in $\mathrm{Im}x$, and $U'(x) \in L(-\infty, \infty)$ with respect to $\mathrm{Re}x$ at fixed negative

$$\mathrm{Im}\xi = \mathrm{Im} \int_0^x q(y)\,dy = -c,$$

then $d > 0$ exists such that

$$a_+ \exp(2c/\epsilon) \to 0 \quad \text{as } \epsilon \to 0 \quad \text{for } 0 \leq c < d. \tag{19}$$

Since l. u. b. $|a(\xi)| \to 0$ with ϵ,

$$g \to 1 \quad \text{as } \epsilon \to 0, \tag{20}$$

by (16), it follows that g contributes to the first approximation for the scattering matrix only the (small) phase of s_{11}; for completeness, it is given in the Appendix.

It is desirable, however, to mention the following implication of these simple results. The most common approach to quasiclassical scattering, by WKB or similar or equivalent procedures, can play no useful role at all in above-barrier scattering by potentials smooth enough to make the reflection (18) transcendental.[4] This is not only because those approaches can lead to approximations for reflection only by semifortuitous accident. Even the correct, asymptotic expansions for *transmission* obtained by these approaches are almost irrelevant under the circumstances envisaged, because (9), (18), (19) then show transmission to differ in magnitude only transcendentally from $[E - U(-\infty)/E - U(\infty)]^{1/2}$; all that can ever be achieved by the asymptotic expansions is a description of the small transmission phase correction caused by the barriers.

3. SCATTERING PARAMETER

We therefore focus attention now on the scattering parameter a_+, from which the scattering matrix can be computed by (17), (18) (except for small phase corrections), and on the plausible case of an analytically smooth potential $U(x)$. The estimate (19) then suggests that the amount of reflection is determined by the manner in which this analyticity breaks down with increasing distance from the real axis of the ξ plane. More precisely, by (15) and (11), the issue is the analyticity of the modulation function $\phi(\xi)$ defined by (1)–(3). The breakdown will be assumed due to roots or singular points of the potential U of a reasonably common type: $U(x)$ is assumed analytic on a neighborhood N of the real axis, except for a set S_* of "transition points" x_0 of type

$$U(x) = E - U_0(x - x_0)^\nu(1 + Q(x)) \tag{21}$$

with real ν, $U \neq 0$, $Q(x)$ analytic at x_0, and $Q(x_0) = 0$, such that S_* has no limit point,

$$0 < \text{g. l. b.}_{S_*} |\mathrm{Im}\xi| = m, \tag{22}$$

and no other boundary point of N has $|\mathrm{Im}\xi| = m$. For M independent of ϵ, moreover, $\phi(\xi) \in L(-\infty, -M) \cap L(M, \infty)$ with respect to $\mathrm{Re}\xi$ at $\mathrm{Im}\xi = -m$, and $U'(x) \to 0$ as $|\mathrm{Re}x| \to \infty$ uniformly in $|\mathrm{Im}x| < m/q_{+,-}$.

The class of potentials thus envisaged includes not only the polynomials and rational functions, but also the entire meromorphic functions of Fedoryuk[2] and the transcendental class of Epstein[1] and many more. Since branch points, even of infinite order, are admitted, it may be conjectured that the results below will be found

to extend also to logarithmic branch points when their turning point structure becomes known.

The asymptotics of the Fourier type transform (15) is discussed elsewhere[3] in detail and it will help to summarize here just the essence of the argument. If the path in (15) can be shifted from the real axis to a parallel line in the lower half-plane of ξ, then a constant, exponentially small factor $\exp(-\operatorname{Im}\xi/\epsilon)$ can be extracted from the integral, after which standard methods may suffice for its treatment. The best exponential factor is obtained by shift to the line L: $\operatorname{Im}\xi = -m$, but two obstacles are in the way: ϕ is (nonintegrably) singular at a transition point, and (15) indicates that $a(\xi)$ might itself contain exponential factors—which could spoil any benefits from the shift of path.

Envisage first the case of a single transition point, x_0, with image ξ_0 on L. The obstacles can then be overcome by a combination of a contraction mapping for the nonlinear integral equation (14), to the left of ξ_0, with turning point results[11] at ξ_0 and with another contraction for (14) to the right of ξ_0. This serves to establish

$$\text{l. u. b.}_{\operatorname{Re}\xi<\operatorname{Re}\xi_0-\sqrt{\epsilon}} |a(\xi)| \to 0 \quad \text{as } \epsilon \to 0, \tag{23}$$

$$\text{l. u. b.}_{\operatorname{Re}\xi>\operatorname{Re}\xi_0+\sqrt{\epsilon}} \left| a(\xi) - 2i\cos\left(\frac{\pi}{\nu+2}\right)\exp\frac{2i(\xi-\xi_0)}{\epsilon} \right| \to 0$$
$$\text{as } \epsilon \to 0 \tag{24}$$

on L and that the path in (15) can indeed be shifted to L. But then combination of (23), (24) with the Riemann—Lebesque lemma leads, as for a Fourier integral, to the principle of stationary phase[10] for the integral on L with (only dominant) critical point ξ_0, i. e.,

$$a_+ \sim \int_{\xi_0-\delta}^{\xi_0+\delta} (a^2-1)\phi \exp(-2i\xi/\epsilon)\,d\xi = I$$

for any $\delta > 0$. The Fourier type transform has now served its purpose; it was arrived by observing in (11) that $(a^2-1)\phi\exp(-2i\xi/\epsilon) = d(a\exp(-2i\xi/\epsilon))/d\xi$, whence

$$I = \lim_{(\xi-\xi_0)/\epsilon\to+\infty} a(\xi)\exp(-2i\xi/\epsilon) - \lim_{(\xi-\xi_0)/\epsilon\to-\infty} a(\xi)\exp(-2i\xi/\epsilon)$$

and so by (23), (24),

$$a_+ \sim 2i\cos\left(\frac{\pi}{\nu+2}\right)\exp(-2i\xi_0/\epsilon) \tag{25}$$

with ν defined by (21) and $\xi_0 = \int_0^{x_0} q(s)\,ds$ by (2).

For the case of several transition points $\xi_1, \ldots, \xi_k$ with $\operatorname{Im}\xi_j = -m$, the combination of contraction with turning point theory needs to be repeated for each and it is then found[3] that the shift of path in (15) remains justified and $a(\xi)\exp(-2i\xi/\epsilon)$ increases by (25) (with the appropriate values of ν and ξ_0) across each transition point. By the principle of stationary phase, therefore

$$a_+ \sim 2i\sum_{j=1}^{k}\cos\left(\frac{\pi}{\nu_j+2}\right)\exp(-2i\xi_j/\epsilon)$$
$$= 2i\exp(-2m/\epsilon)\sum_{1}^{k}\cos\left(\frac{\pi}{\nu_j+2}\right)\exp(-2i\operatorname{Re}\xi_j/\epsilon) \tag{26}$$

for any finite number of transition points.

This includes Fedoryuk's[2] result for a pair of simple turning points of a meromorphic function as a special case; the additive nature of the contributions of the individual transition points becomes more visible in the present formulation.

It is seen from (26) that circumstances can arise in various ways in which, for certain "resonant" values of the wavenumber ϵ^{-1}, the contributions of several transition points cancel out in a_+. This need not be limited to potentials $U(x)$ even in $\operatorname{Re}x$. In practice, however, the chance of encountering more than a pair [and these on account of evenness of $U(x)$] seems remote, and the resonant ϵ-sequence is then obvious from (26) and gives abnormally small reflection.

A somewhat similar effect arises even for a solitary transition point, if it be a singular transition point with a value of ν ($\leq -\frac{4}{3}$) in (21) for which $\cos[\pi/(\nu+2)]$ vanishes in (25). The probability of reflection is then abnormally small for all sufficiently small ϵ.

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APPENDIX

The phase correction is readily obtained by standard WKB or equivalent approaches without complex embedding. For instance, if $\phi(\xi)$ is to assumed to be of bounded variation, in addition to (13), then by the Riemann—Lebesgue lemma

$$\int_{-\infty}^{\infty} \phi(s)\exp(-2is/\epsilon) = \frac{i\epsilon}{2}\phi(\xi)\exp(-2i\xi/\epsilon) + o(\epsilon)$$

uniformly for $\xi \in \mathbf{R}$, and hence from (14),

$$a(\xi) = -(i\epsilon/2)\phi(\xi) + o(\epsilon)$$

whence from (16)

$$g(\epsilon) = \exp[-(i\epsilon/2)\int_{-\infty}^{\infty}\phi^2\,d\xi + o(\epsilon)]$$

in (17) and (18).

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[1]P. S. Epstein, Proc. Nat. Acad. Sci. U.S. 16, 627 (1930); L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, London, 1965), p. 79.
[2]M. V. Fedoryuk, Differ. Uravn. 1, 631, 1525 (1965) [Differ. Eqns. 1, 483, 1201 (1965)].
[3]R. E. Meyer, SIAM J. Appl. Math. 29, 481 (1975).
[4]In the small (wavelength) parameter ϵ of the quasiclassical approximation. That is, the reflection coefficient is "zero to all orders" (in the sense of asymptotic expansion in powers of ϵ), but not necessarily as small as $\exp(-\text{const}/\epsilon)$.
[5]J. J. Mahony, Q. Appl. Math. 25, 313 (1967).
[6]F. W. J. Olver, *Error bounds for asymptotic expansions, Asymptotic Solutions of Differential Equations and their Applications*, edited by C. H. Wilcox (Wiley, New York, 1964).
[7]How this, and the related asymptotic conditions on $U(x)$ introduced later, can be removed in a more abstract approach is sketched by R. E. Meyer and E. J. Guay, Z. Angew. Math. Phys. 25, 643 (1974).
[8]F. W. J. Olver, *Introduction to Asymptotics and Special Functions* (Academic, New York, 1975).
[9]J. E. Littlewood, Ann. Phys. 21, 233 (1963).
[10]D. S. Jones, J. Inst. Math. Its Appl. 2, 197 (1966).
[11]R. E. Langer, Trans. Am. Math. Soc. 34, 447 (1932).

Some new ensembles of random matrices*

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In this article, we introduce ensembles of random matrices in which not all of the matrix elements are functionally independent. The functional dependence is defined by restricting the class of unitary similarity transformations which will diagonalize a member of the ensemble. The statistical properties of the eigenvalues are then studied for some of these ensembles.

1. INTRODUCTION

Until recently, most of the work in the statistical theory of energy levels has been based on rotationally invariant ensembles of random matrices whose matrix elements are functionally independent.[1] Recent interest in ensembles which correspond to systems with a small term in their Hamiltonian that is not time reversal invariant has led to the study of ensembles which are not rotationally invariant. Unfortunately, for those ensembles which have been considered, when N (the dimensionality of the matrices) is arbitrary, it is difficult to study the statistical properties analytically.[2-7]

Further, recent work indicates that for many physical systems the assumption that the matrix elements are functionally independent may in fact be incorrect.[8-13] Thus, the question of how functional dependence among the matrix elements would show up in the statistical properties of the energy levels and the level widths is of current interest.

In this article we introduce some new ensembles, which contain matrices whose elements are functionally dependent. These ensembles are defined in such a way that the joint distribution for the eigenvalues and rotation parameters can be given explicitly for any N when the time-reversal—noninvariant term in the Hamiltonian is of arbitrary size. These ensembles have the added advantage that the number of off-diagonal elements which have nonzero imaginary parts can be specified. Thus, these ensembles offer the opportunity for the study of the effects on the statistical properties of the energy spectrum due to the dependence among matrix elements, the presence of a time-reversal—noninvariant term, and the variation of the number of nonzero imaginary parts.

In this article we study the level density and spacing distributions. It is shown that when the number of nonzero imaginary parts is small, the calculations can be carried out analytically for some ensembles. However, when the number is large it appears that one will have to resort to numerical calculations.

2. MATHEMATICAL DEFINITION OF ENSEMBLES

We shall denote by $\mathbf{H}$ the Hermitian matrix corresponding to the Hamiltonian of a system. These matrices will be assumed to be $N\times N$, where N is large. The real and imaginary parts will be denoted by $\mathbf{R}$ and $\mathbf{T}$, respectively. Since $\mathbf{H}$ is Hermitian,

$$R_{ij}=R_{ji}, \tag{2.1}$$

$$T_{ij}=-T_{ji}, \quad i\neq j, \tag{2.2}$$

and

$$T_{ii}=0. \tag{2.3}$$

The ensemble can be specified mathematically by the joint distribution, $P(\mathbf{H})$, for the N^2 variables, R_{ij}, $i\geq j$, and T_{ij}, $i>j$. Here we shall consider distributions of the form

$$P(\mathbf{H})\,d\mathbf{H}=\hat{P}(\mathrm{Tr}\mathbf{H}^n)\exp(-\gamma\textstyle\sum T_{ij}^2)\,\mu(\mathbf{H})\,d\mathbf{H}, \tag{2.4}$$

where

$$d\mathbf{H}=\prod_i dR_{ii}\prod_{k>j} dR_{jk}\,dT_{ik}, \tag{2.5}$$

and $\hat{P}$ is a function only of traces of various powers of $\mathbf{H}$ (i.e., $\hat{P}$ is rotationally invariant). The factor $\mu(\mathbf{H})$ specifies the functional dependence of the matrix elements, and can, at least in principle, be expressed using Dirac delta functions.

Note that the parameter γ affects the "size" of the time-reversal—noninvariant part of the Hamiltonian. For example, if $\mu(\mathbf{H})\equiv 1$, $\gamma\to 0^+$ and $\gamma\to+\infty$ correspond to the orthogonal and unitary cases, respectively.[14] It should be noted that by $\gamma\to+\infty$ we mean

$$\lim_{\gamma\to+\infty}\int_{-\infty}^{+\infty} dT_{12}\cdots\int_{-\infty}^{+\infty} dT_{N-1N}P(\mathbf{H})$$

$$=\int_{-\infty}^{+\infty} dT_{12}\cdots\int_{-\infty}^{+\infty} dT_{N-1N}\hat{P}(\mathrm{Tr}\mathbf{H}^n)\delta(\mathbf{T})$$

$$=\hat{P}(\mathrm{Tr}\mathbf{R}^n),$$

where

$$\delta(\mathbf{T})\equiv\prod_{i>j}\delta(T_{ij}).$$

Since $\mathbf{H}$ is Hermitian, there exists a unitary matrix $\mathbf{A}$ such that

$$\mathbf{H}=\mathbf{AEA}^\dagger, \tag{2.6}$$

where $E_{ij}=\delta_{ij}E_i$ and the E_i are the energy levels of the system. The ensembles considered below will be defined by (2.4) where $\mu(\mathbf{H})$ is such that for every $\mathbf{H}$ the corresponding $\mathbf{A}$ can be written in the form

$$A_{11}=e_1C_1, \tag{2.7}$$

$$A_{i1}=e_iC_i\prod_{r=1}^{i-1}S_r, \qquad N\geq i\geq 2, \tag{2.8}$$

$$A_{ii}=e_ie_{i-1}^*C_iC_{i-1}, \qquad N\geq i\geq 2, \tag{2.9}$$

$$A_{ij}=e_i e^*_{j-1}C_iC_{j-1}\prod_{r=j}^{i-1}S_r, \quad N\geq i>j\geq 2, \tag{2.10}$$

$$A_{i-1i}=-S_{i-1}, \quad N\geq i\geq 2, \tag{2.11}$$

$$A_{ij}=0, \quad j>i+1, \tag{2.12}$$

where

$$S_r\equiv \sin\phi_r, \tag{2.13}$$

$$C_r\equiv \cos\phi_r, \tag{2.14}$$

and

$$e_r\equiv \exp(i\psi_r). \tag{2.15}$$

The rotation parameters, ϕ_r and ψ_r, will be restricted such that

$$0\leq \phi_r\leq a_r\leq \pi/2 \tag{2.16}$$

and

$$0\leq \psi_r\leq b_r<2\pi, \tag{2.17}$$

when $r=1,2,\ldots,N-1$, and

$$\phi_N=\psi_N=0. \tag{2.18}$$

It should be noted that **A** as given by (2.7)—(2.18) is not the most general unitary matrix.[15] Also, this restriction on **A** does not define $\mu(\mathbf{H})$ uniquely. That is, the restrictions on **A** imply certain functional relationships among the matrix elements. If we let z_i denote those matrix elements which are taken to be dependent, then our ensembles will be defined by choosing $\mu(\mathbf{H})\equiv\sum_\nu\prod_i\delta[z_i - z_i^\nu(\mathbf{H})]$. The summation over ν is to allow for the fact (as is shown below) that the relationships between the matrix elements may not yield single-valued functions. The number of functions involved depends on the region considered in the matrix element space (i.e., the limits of integration on the independent variables). Since it is possible to select a different set of matrix elements to be the dependent variables, there is in general more than one ensemble [i.e., $\mu(\mathbf{H})$ corresponding to the given restrictions on **A**].

The connection between the matrix elements of **H** and the eigenvalues and rotation parameters is given by (2.6). For **A** as defined above it follows directly that

$$H_{ii}=C_i^2\Delta_i+E_{i+1}, \quad i=1,2,\ldots,N, \tag{2.19}$$

$$H_{ij}=e_ie_j^*C_iC_j\Delta_i\prod_{r=i}^{j-1}S_r, \quad j>i, \tag{2.20}$$

where

$$\Delta_i\equiv\sum_{j=1}^{i}P_{ij}\xi_j, \quad i=1,2,\ldots,N, \tag{2.21}$$

$$\begin{aligned} P_{ij}&\equiv\prod_{r=j}^{i-1}S_r^2, && i>j,\\ &\equiv 1, && i=j, \end{aligned} \tag{2.22}$$

$$\xi_j\equiv E_j-E_{j+1}, \quad j=1,\ldots,N, \tag{2.23}$$

and where $E_{N+1}\equiv 0$. These equations express the N^2 variables, R_{ij}, $j\geq i$, T_{ij}, $j>i$, in terms of the $3N-2$ variables E_i, $i=1,2,\ldots,N$, ϕ_r, ψ_r, $r=1,2,\ldots,N-1$. Thus at most $3N-2$ of the R_{ij} and T_{ij} can be chosen as independent variables.

It can be shown by direct calculation that

$$|J|=\left|J\begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix}\right|=\left|\left(\prod_{r=1}^{N-1}S_rC_r^3\Delta_r^2\right)/C_1^2\right|, \tag{2.24}$$

where J is the Jacobian and where

$$\mathbf{x}\equiv(R_{11},R_{22},\ldots,R_{NN},R_{12},R_{23},\ldots,R_{N-1,N}, T_{12},T_{23},\ldots,T_{N-1,N}) \tag{2.25}$$

and

$$\mathbf{y}=(E_1,E_2,\ldots,E_N,\phi_1,\phi_2,\ldots,\phi_{N-1},\psi_1,\psi_2,\ldots,\psi_{N-1}). \tag{2.26}$$

Thus, provided that the range of the y_i (or equivalently of the x_i) are restricted such that $J>0$ (or $J<0$) there is a 1—1 correspondence between the variables **x** and **y**. Thus, if no further restrictions are imposed on the ensemble, the x_i can be used as independent variables.

Let us now examine some of the obvious functional relationships between the matrix elements and the inverse relationships between **x** and **y**. It follows easily from (2.20) that

$$T_{ij}=R_{ij}\tan(\psi_i-\psi_j), \quad \forall j>i. \tag{2.27}$$

Thus, the ψ_i's determine the relative size of the imaginary parts of the off-diagonal elements. Note that by restricting the ψ_i we can specify the number of T_{ij} which are not identically zero. For example, if we impose the conditions $\psi_i\equiv 0$, $i=2,\ldots,N-1$, then $T_{ij}\equiv 0$, $\forall j>i>1$, but $T_{1j}\not\equiv 0$, $j>1$. If we also require $\psi_1\equiv 0$, we have an orthogonal ensemble.

If we set $j=i+1$ in (2.27), the resulting equations can be used to show that

$$\psi_i=\sum_{j=i}^{N-1}\tan^{-1}(T_{jj+1}/R_{jj+1}), \quad i=1,2,\ldots,N-1. \tag{2.28}$$

Insertion of (2.28) into (2.27) gives the T_{ij}/R_{ij}, $j\geq i+2$ as functions of the R_{ii+1} and T_{ii+1}. Note that this yields a total of $(N-1)(N-2)/2$ independent relationships connecting the matrix elements.

From (2.20) it can be shown that

$$|H_{ij}|^2C_k^2=|H_{ik}|^2C_j^2\prod_{r=k}^{j-1}S_r^2, \quad j>k>i. \tag{2.29}$$

It follows immediately that

$$|H_{ij}|^2/|H_{ik}|^2=|H_{i'j}|^2/|H_{i'k}|^2, \quad j>k>i \text{ and } k>i'. \tag{2.30}$$

There are $(N-2)(N-3)/2$ independent conditions on the matrix elements contained in (2.30). The total number of independent conditions in (2.27) and (2.30) is $(N-2)^2$. Thus, there are an additional $4(N+1)$ independent relationships. These appear to be of a nontrivial nature.

The ϕ_i, $i=2,3,\ldots,N-1$, can be expressed in terms of the H_{ij}, using (2.29). In particular, if we let $j=k+1$, Eq. (2.29) reduces to

$$|H_{ik+1}|^2C_k^2=|H_{ik}|^2C_{k+1}^2S_k^2. \tag{2.31}$$

Since $C_N\equiv 1$, for $k=N-1$ we have from (2.31)

$$\tan^2\phi_{N-1}=|H_{iN}|^2/|H_{iN-1}|^2. \tag{2.32}$$

The ϕ_i, $i=N-2, N-3, \ldots, 2$ can now be found by an iterative procedure using the recursion relation (2.31).

From (2.19) and (2.20) it follows that

$$E_{i+1}=H_{ii}+r_i, \quad i=1,\ldots,N-1, \tag{2.33}$$

where

$$r_i \equiv \pm \left|H_{ki}H_{ii+1}\right| / \left|H_{ki+1}\right|. \tag{2.34}$$

Inserting (2.33) into the equation $\sum_{i=1}^{N}(H_{ii}-E_i)=0$, we obtain

$$E_1=H_{NN}-\sum_{i=2}^{N-1} r_i. \tag{2.35}$$

Thus, aside from ϕ_1, the eigenvalues and rotation parameters can be found in terms of the matrix elements in a relatively straightforward manner.

3. ORTHOGONAL ENSEMBLES

In this section we consider ensembles in which every T_{ij} is identically zero (i.e., orthogonal ensembles). In particular, we define

$$\mu(\mathbf{H}) \equiv \prod_{j>i}\delta(T_{ij})\sum_{\nu}\prod_{j>i+1}\delta[R_{ij}-r_{ij}^{(\nu)}(\mathbf{R})], \tag{3.1}$$

where the $r_{ij}^{(\nu)}$ are functions of R_{ii} and R_{ii+1}, which are defined by the restriction that $\mathbf{H}$ can be diagonalized by an orthogonal matrix $\mathbf{A}$ of the form given by (2.7)–(2.12) with $\psi_r \equiv 0$, $r=1,\ldots,N-1$.

The joint distribution for the rotation parameters and eigenvalues, $p(\mathbf{E},\phi)$, is defined by

$$p_{\mathrm{ort}}(\mathbf{E},\phi)\,d\mathbf{E}\,d\phi \equiv P(R_{ii},R_{ii+1})\left|J\right|d\mathbf{E}\,d\phi, \tag{3.2}$$

where

$$d\mathbf{E} \equiv \prod dE_i, \tag{3.3}$$

$$d\phi \equiv \prod d\phi_r, \tag{3.4}$$

$$J \equiv J\begin{pmatrix} R_{ii}, & R_{ii+1} \\ E_j, & \phi_r \end{pmatrix}, \tag{3.5}$$

$$P(R_{ii},R_{ii+1}) \equiv \int_{V_R}\hat{P}\mu\,d\mathbf{H}' = \eta F(\mathbf{E}), \tag{3.6}$$

$$F(\mathbf{E})=\hat{P}(\mathrm{Tr}\mathbf{H}^n), \tag{3.7}$$

$$d\mathbf{H}' \equiv \prod_{j>i} dT_{ij}\prod_{j>i+1} dR_{ij}, \tag{3.8}$$

and η is a constant which depends on the region V_R. It follows directly from (2.19)–(2.22), with $\psi_r \equiv 0$, that

$$\left|J\right| = \left|\left(\prod_{r=1}^{N-1} C_r\Delta_r\right)\Big/ C_1\right|. \tag{3.9}$$

We shall define V_R by the conditions $0 \leq \phi_r \leq a_r \leq \pi/2$ and $E_r > E_{r+1}$, $r=1,2,\ldots,N-1$. Thus, the joint distribution for the ϕ_r and E_r can be written as

$$p_{\mathrm{ort}}(\mathbf{E},\phi)=\eta\left[\left(\prod_{r=1}^{N-1} C_r\Delta_r\right)\Big/ C_1\right]F(\mathbf{E}). \tag{3.10}$$

It follows from (2.21) and (2.22) that

$$\prod_{i=1}^{N-1}\Delta_i = \sum_{\mathbf{n}} b_{\mathbf{n}} w_{\mathbf{n}}(\phi)\,\hat{\Delta}_{\mathbf{n}}, \tag{3.11}$$

where

$$w_{\mathbf{n}}(\phi)=\prod_{r=1}^{N-2} S_r^{2g_r}, \tag{3.12}$$

$$\hat{\Delta}_{\mathbf{n}}=\prod_{r=1}^{N-1}\xi_r^{n_r}, \tag{3.13}$$

$$g_r = N-r-1-m_r, \tag{3.14}$$

$$m_r=\sum_{i=r+1}^{N-1} n_i, \quad r=0,1,\ldots,N-2, \qquad =0, \quad r=N-1, \tag{3.15}$$

and

$$b_{\mathbf{n}}=\prod_{r=1}^{N-1}\binom{g_r+1}{n_r}\delta_{m_0 N-1}. \tag{3.16}$$

It should be noted that $b_{\mathbf{n}}=0$ if any $n_r > g_r+1$. Thus, in (3.11) $n_r=0,1,\ldots,g_r+1$. Note also that we have adopted the convention $\binom{g}{0}=1$ if $g<0$.

Inserting (3.11) into (3.10), we obtain

$$p_{\mathrm{ort}}(\mathbf{E},\phi)=\eta\sum_{\mathbf{n}} B_{\mathbf{n}}\hat{w}_{\mathbf{n}}(\phi)f_{\mathbf{n}}(\mathbf{E})\delta_{m_0 N-1}, \tag{3.17}$$

where

$$\hat{w}_{\mathbf{n}}(\phi)=d_{\mathbf{n}}w_{\mathbf{n}}(\phi)\prod_{r=2}^{N-1} C_r \tag{3.18}$$

and

$$f_{\mathbf{n}}(\mathbf{E})=\hat{d}_{\mathbf{n}}\hat{\Delta}_{\mathbf{n}}F(\mathbf{E}).$$

The constants $\hat{d}_{\mathbf{n}}$, $d_{\mathbf{n}}$, and $B_{\mathbf{n}}$ are defined as

$$d_{\mathbf{n}}^{-1}=\int_0^{a_1} S_1^{2g_1}d\phi_1\prod_{r=2}^{N-2}(\sin a_r)^{2g_r+1}/(2g_r+1), \tag{3.19}$$

$$\hat{d}_{\mathbf{n}}^{-1}=\int d\mathbf{E}\,\hat{\Delta}_n F(\mathbf{E}), \tag{3.20}$$

and

$$B_{\mathbf{n}}=b_{\mathbf{n}}(d_{\mathbf{n}}\hat{d}_{\mathbf{n}})^{-1}, \tag{3.21}$$

respectively.

It follows immediately that

$$f_{\mathrm{ort}}(\mathbf{E})=\eta\sum_{\mathbf{n}} B_{\mathbf{n}}f_{\mathbf{n}}(\mathbf{E}), \tag{3.22}$$

where $f_{\mathrm{ort}}(\mathbf{E})$ is the joint distribution function for all of the eigenvalues. Equation (3.22) can be rewritten as

$$f_{\mathrm{ort}}(\mathbf{E})=g_{\mathrm{ort}}(\mathbf{E})F(\mathbf{E}), \tag{3.23}$$

where

$$g_{\mathrm{ort}}(\mathbf{E}) \equiv \eta\sum_{\mathbf{n}} b_{\mathbf{n}}d_{\mathbf{n}}^{-1}\hat{\Delta}_n. \tag{3.24}$$

Note that $g_{\mathrm{ort}}(\mathbf{E})$ is a polynomial function of the E_i of degree $N-1$.

Since the factor $g_{\mathrm{ort}}(\mathbf{E})$ originates from the Jacobian connecting the independent matrix elements with the eigenvalues and rotation parameters, and since the matrix elements are linear in the eigenvalues it is clear that the joint eigenvalue distribution derived from any orthogonal ensemble of the form (2.4) will be of the form (3.23) where $g_{\mathrm{ort}}(\mathbf{E})$ is a polynomial function of the E_i of degree less or equal to the total number of independent $R_{i,j}$, $j \geq i$. Further, since any polynomial func-

tion of the E_i can be written as a polynomial function in the ξ_i, the joint eigenvalue distribution can always be written as a linear combination of functions of the form $\prod_{i=1}^{N}\xi_i^{n_i}F(\mathbf{E})$. In general, one must treat the linear combination term by term.[16]

For definiteness, we shall consider only one specific case. However, it should be clear that any term of the form just noted can be treated in exactly the same way as this particular case.

In particular, we consider

$$f(\mathbf{E})=\lim_{a\to 0^+} f_{\mathrm{ort}}(\mathbf{E})=f_1(\mathbf{E}) =\eta\prod_{i=1}^{N-1}(E_i-E_{i+1})F(\mathbf{E}), \tag{3.25}$$

where η is the normalization constant, and where $\mathbf{n}=\mathbf{1}$ means that $n_r=1$, $r=1,2,\ldots,N-1$. This, of course, serves as the first approximation to $f_{\mathrm{ort}}(\mathbf{E})$ as given by (3.22) when the a_r are small. From (2.19) and (2.20) it can be seen that this corresponds to an ensemble where the off-diagonal elements are very small as compared with the diagonal elements.

Note that there is a repulsion effect present in (3.25). However, it involves only nearest neighbors. On the other hand, it is well known that if the matrix elements are all independent,

$$p_{\mathrm{ort}}(\mathbf{E})=\eta'\prod_{i>j}|E_i-E_j|F(\mathbf{E}), \tag{3.26}$$

where η' is the normalization constant.[17] That is, the repulsion effect involves all pairs of eigenvalues. One might expect that this difference will not show up in the level density and nearest neighbor spacing distribution as clearly as it will in the higher order spacing distributions, e.g., the next nearest spacing distribution.

For definiteness, let us now assume that

$$F(\mathbf{E})=N!\,\alpha^N\exp(-\alpha\textstyle\sum E_i), \tag{3.27}$$

so that

$$f(\mathbf{E})=N!\,(N-1)!\,\alpha^{2N-1}\prod(E_i-E_{i+1})\exp(-\alpha\textstyle\sum E_i), \tag{3.28}$$

where $E_1\geq E_2\geq E_3\cdots\geq E_N\geq 0$.

If $Q(\mathbf{E})$ is any function of the eigenvalues, we shall define its average as

$$\langle Q\rangle\equiv\int Qf(\mathbf{E})\,d\mathbf{E}. \tag{3.29}$$

It can be shown that

$$\left\langle E_N^{n_N}\prod_{r=1}^{N-1}\xi_r^{n_r-1}\right\rangle=(N-1)!\,\alpha^{N-M-1}\prod_{r=1}^{N}\frac{n_r!}{r^{n_r}}, \tag{3.30}$$

where

$$M\equiv\sum_{r=1}^{N}n_r. \tag{3.31}$$

In particular, the average spacing between the nearest neighbors E_r and E_{r+1} is given by

$$\langle\xi_r\rangle=2/(\alpha r). \tag{3.32}$$

Note that the average spacing, $\bar{S}_{rm}$, over m consecutive intervals is given by

$$\bar{S}_{rm}=\frac{1}{m\alpha}\sum_{k=r}^{r+m}r^{-1}. \tag{3.33}$$

Since

$$E_r=\sum_{k=r}^{N}\xi_k, \tag{3.34}$$

the moments of the distribution, $\langle E_1^{l_1}E_2^{l_2}\cdots E_N^{l_N}\rangle$, can be evaluated using (3.30). For example, it is easily shown that

$$\langle E_N\rangle=1/(\alpha N) \tag{3.35}$$

and

$$\langle E_r\rangle=\alpha^{-1}\left(N^{-1}+2\sum_{k=r}^{N-1}k^{-1}\right),\quad r=1,2,\ldots,N-1. \tag{3.36}$$

If we let $p_{N,k}(E)$ denote the probability density function of the kth eigenvalue, then by definition

$$p_{N,k}(E)\equiv\int_{E_1\geq E_2\geq\cdots\geq E_N\geq 0}\delta(E_k-E)f(\mathbf{E})\,d\mathbf{E}. \tag{3.37}$$

It is easily shown that

$$p_{N,k}(E)=D_{N,k}\exp[-(k-1)\alpha E]p_{N-k+1,1}(E), \tag{3.38}$$

where

$$p_{n,1}(E)=\eta_n\int_0^E dx_n\int_{x_n}^E dx_{n-1}\cdots\int_{x_3}^E dx_2 f^{(n)}(\mathbf{x}),\quad n>1 =\alpha^{-1}\exp(-\alpha E),\quad n=1. \tag{3.39}$$

Here $f^{(n)}(\mathbf{x})$ is given by (3.28) with $N=n$ and $x_1=E$. The quantities $D_{N,k}$ and η_n are normalization constants.

The global level density $\rho(E)$ is defined as

$$\rho(E)=\sum_{k=1}^{N}p_{N,k}(E). \tag{3.40}$$

Since

$$\overline{Q(E)}\equiv\int_0^{+\infty}Q(E)\rho(E)\,dE=\sum_{k=1}^{N}\langle Q(E_k)\rangle, \tag{3.41}$$

the moments of the level density, $\overline{E^n}$, are given by

$$\overline{E^n}=\sum_{k=1}^{N}\langle E_k^n\rangle. \tag{3.42}$$

The $\langle E_k^n\rangle$ can be evaluated as mentioned above. In particular, it can be shown that

$$\bar{E}=(2N-1)/\alpha. \tag{3.43}$$

When the joint eigenvalue distribution is of the form (3.26) with $F(\mathbf{E})$ defined by (3.27), the level density is given by[18]

$$\sigma(E)\sim\alpha(\pi^2\alpha E)^{-1/2}(2N-\alpha E)^{1/2},\quad 0\leq E\leq 2N, \sim 0,\quad E>2N. \tag{3.44}$$

It is easily shown that

$$\langle E^n\rangle_\sigma=N\pi^{-1}(2N/\alpha)^n\,\Gamma(n+\tfrac{1}{2})\,\Gamma(\tfrac{1}{2})/\Gamma(n+2). \tag{3.45}$$

In particular,

$$\langle E\rangle_\sigma=N^2/2\alpha. \tag{3.46}$$

Thus, comparing (3.42) and (3.46), we see that when there is repulsion between all of the eigenvalues, the "center" of the energy spectrum is pushed up.

The joint distribution for two mth neighbors, E_k and E_{k+m}, is defined by

$$f_{k,m}(E_k, E_{k+m}) = \int_{x_1 \geq x_2 \geq \cdots \geq x_N \geq 0} f(\mathbf{x}) \delta(x_k - E_k) \delta(x_{k+m} - E_{k+m})\, d\mathbf{x}. \tag{3.47}$$

It can be shown that

$$f_{k,m} = \eta_{k,m} \exp(-\alpha k E_k)\, h_{k,m}\, p_{N-k-m+1,1}(E_{k+m}), \tag{3.48}$$

where

$$h_{k,m} = \xi_k, \quad m = 1,$$

$$= \int_{E_{k+m}}^{E_k} dE_{k+m-1} \int_{E_{k+m-1}}^{E_k} dE_{k+m-2} \cdots \int_{E_{k+2}}^{E_k} dE_{k+1} \tag{3.49}$$

$$\times \prod_{r=k}^{k+m-1} \xi_r \exp[-\alpha(E_{k+1} + E_{k+2} + \cdots + E_{k+m-1})], \quad m > 1.$$

If we let $S = E_k - E_{k+m}$, the mth-nearest-neighbor spacing distribution can be shown to be given by

$$P_k^{(m-1)}(S) = \int_0^{+\infty} dT\, f_{k,m}(T + S, T). \tag{3.50}$$

In particular, the nearest-neighbor and next-nearest-neighbor spacing distributions are easily shown to be

$$P_k^{(0)}(S) = (\alpha k)^2 S \exp(-\alpha k S) \tag{3.51}$$

and

$$P_k^{(1)}(S) = \alpha k^2 (k+1)^2 [(\alpha S + 2)\exp(-\alpha S) + (\alpha S - 2)] \times \exp(-\alpha k S), \tag{3.52}$$

respectively.

The "local" spacing distributions are defined as

$$p_k^{(m)}(x) = (r\bar{S})^{-1} \sum_{i=k}^{k+r-1} P_i^{(m)}(\bar{S}x), \tag{3.53}$$

where $\bar{S}$ is the average nearest-neighbor spacing for the region [i.e., $\bar{S}$ is given by (3.33)]. Thus for a region where the average spacing is approximately constant (i.e., $r \gg k$)

$$p^{(0)}(x) \approx 4^{-1} x \exp(-2x). \tag{3.54}$$

To our knowledge the spacing distributions corresponding to (3.26) and (3.27) have not been explicitly studied in the literature.[19] However, for those orthogonal ensembles for which the nearest-neighbor spacing distribution has been studied the distribution is linear in the spacing near the origin as is (3.51).[20,21] On the other hand, for those orthogonal ensembles for which the next-nearest-neighbor spacing distribution has been studied, the distribution is quartic near the origin while $P_k^{(1)}$ as given by (3.48) is cubic.[21] Thus, as expected, the repulsion between next nearest neighbors is now in fact weaker.

It should be noted that for those ensembles which have been studied[20,21]

$$p^{(0)}(x) \approx 2^{-1}\pi x \exp(-4^{-1}\pi x^2). \tag{3.55}$$

Comparing this with (3.54), we see that our ensemble has a larger probability of large spacing. That is, the repulsion effect is now stronger for large spacings.

4. NONORTHOGONAL ENSEMBLES

Here we consider ensembles where not all of the T_{ij} vanish identically. In particular, we consider $P(\mathbf{H})$ of the form (2.4) with

$$\mu(\mathbf{H}) = \sum_\nu \{ \prod_{j>i+1} \delta[R_{ij} - r_{ij}^\nu(\mathbf{H})] \prod_{m>n}{}' \delta[T_{mn} - t_{mn}^\nu(\mathbf{H})] \}, \tag{4.1}$$

where the prime means that only dependent T_{mn} are to be included. The r_{ij}^ν and t_{mn}^ν are defined by the restriction that $\mathbf{H}$ can be diagonalized by a unitary matrix, $\mathbf{A}$, of the form given by (2.7)–(2.12) where $\psi_{k_1}, \psi_{k_2}, \ldots, \psi_{k_p}$, $1 \leq p \leq N-1$, are independent variables, and all other ψ_j are equal to one of the ψ_{k_r} or vanish identically.

Our ensembles will be defined by choosing the $T_{k_r k_r}+1$ as independent variables. Thus, the product in (4.1) includes only $(m,n) \neq (k_r, k_r+1)$, $\forall r$. It can be shown that

$$\left| J\begin{pmatrix} R_{ii}, R_{jj+1}, T_{k_r k_r+1} \\ E_i, \phi_j, \psi_{k_r} \end{pmatrix} \right| = \left| \left(\prod_{k_r} \hat{R}_{k_r k_r+1} \right) J_{\text{ort}} \begin{pmatrix} R_{ii}, R_{jj+1} \\ E_i, \phi_j \end{pmatrix} \right| \tag{4.2}$$

where

$$\hat{R}_{ii+1} = C_i S_i C_{i+1} \Delta_i. \tag{4.3}$$

The range of E_i and ϕ_i will be as given above for the orthogonal case while $0 \leq \psi_{k_r} < 2\pi$, $\forall\ r$.

Clearly, for any case

$$T_N^2 \equiv 2 \sum_{j>i} T_{ij}^2 \tag{4.4}$$

can be expressed in terms of E_i, ϕ_i, and ψ_i by using (2.20). The complexity of the resulting expression increases as p (the number of independent ψ_j) increases. Thus, the analysis becomes more complex as p increases. However, one can obtain up to of order N^2 nonzero T_{ij} with $p=1$. Thus, it is clear that such ensembles offer an opportunity to investigate analytically the effects of the number of nonzero T_{ij} on the statistical properties of the system.

For simplicity we shall consider only cases where $p=1$, (i.e., $\psi_{k_r} = \psi$, $r = 1, 2, \ldots, M$, $\psi_j = 0$, $j \neq k_r$). For definiteness, let $\psi_j = \psi$, $j = 1, 2, \ldots, M$, $\psi_j = 0$, $j > M$. Note that there are $M(N-M)$ nonzero T_{ij} (i.e., $i \leq M < j$). Thus, we can vary the number of nonzero elements from of order N (i.e., $M \ll N$ or $N - M \ll N$) to of order N^2 (i.e., $M \approx N/2$).

It can be shown that

$$f(\mathbf{E}, \phi, \psi) = \eta C_1 S_1 C_2 \Delta_1^2 \prod_{r=2}^{N-1} C_r \Delta_r F(\mathbf{E}) \times \exp(-2\gamma \hat{T}_N^2 \sin^2\psi), \tag{4.5}$$

where

$$\hat{T}_N^2 = \sum_{i=1}^{M} C_i^2 \prod_{r=i}^{M} S_r^2 \Delta_i^2. \tag{4.6}$$

It then follows easily that

$$f(\mathbf{E},\phi)=\eta'\hat{f}(\mathbf{E},\phi)p_{\rm ort}(\mathbf{E},\phi), \tag{4.7}$$

where

$$\hat{f}(\mathbf{E},\phi)=(2\pi\gamma)^{1/2}I_0(\gamma\hat{T}_N^2)\exp(-\gamma\hat{T}_N^2)C_1S_1C_2\Delta_1. \tag{4.8}$$

Here $I_0(z)$ is a modified Bessel function[22] and $p_{\rm ort}$ is given by (3.17). Note that for $\gamma=0$ (i.e., the unitary case),

$$f_{\rm unit}(\mathbf{E},\phi)=2\pi\eta'C_1S_1C_2\Delta_1 f_{\rm ort}(\mathbf{E},\phi). \tag{4.9}$$

Let us consider first the case $M\ll N$. Since we expect only the details and not the conclusions to differ for different M, when M is small, we take $M=1$ for simplicity. For this case, (4.8) simplifies to

$$f(\mathbf{E},\phi)=\eta C_2 h(\beta)p_{\rm ort}(\mathbf{E},\phi), \tag{4.10}$$

where

$$h(\beta)\equiv\sqrt{2\pi}\,\beta I_0(\beta^2)\exp(-\beta^2), \tag{4.11}$$

$$\beta=\sqrt{\gamma}\,\Delta_1C_1S_1, \tag{4.12}$$

and η is a normalization constant. Note that

$$f(\mathbf{E},\phi)\sim\eta C_2 p_{\rm ort}(\mathbf{E},\phi), \tag{4.13}$$

as $\beta\to+\infty$. Since

$$\lim_{\gamma\to\infty}\int G(\mathbf{E},\phi)f(\mathbf{E},\phi)\,d\mathbf{E}\,d\phi$$

$$=\int G(\mathbf{E},\phi)p_{\rm ort}(\mathbf{E},\phi)\,d\mathbf{E}\,d\phi \tag{4.14}$$

for any well-behaved function G, it is clear that there is a measurable region where (4.13) does not hold.[23] From (3.17) and (4.10) it follows that the joint eigenvalue distribution is given by

$$f(\mathbf{E})=\eta\sum_{\mathbf{n}}B_{\mathbf{n}}\hat{f}_{\mathbf{n}}(\mathbf{E})\delta_{m_0N-1}, \tag{4.15}$$

where

$$\hat{f}_n(\mathbf{E})=h_{\mathbf{n}}(E_1,E_2)f_{\mathbf{n}}(\mathbf{E}), \tag{4.16}$$

$$h_{\mathbf{n}}(E_1,E_2)\equiv\Big(\int_0^{a_1}d\phi_1S_1^{2g_1}\int_0^{a_2}d\phi_2S_2^{2g_2}C_2^2h(\beta)\Big)/d'_{\mathbf{n}}, \tag{4.17}$$

and

$$d'_{\mathbf{n}}=\int_0^{a_2}C_2^2S_2^{2g_2+1}\,d\phi_2\int_0^{a_1}S_1^{2g_1}\,d\phi_1. \tag{4.18}$$

Clearly, $\lim_{\gamma\to+\infty}h_{\mathbf{n}}(\mathbf{E})=1$, so that

$$f(\mathbf{E})\sim f_{\rm ort}(\mathbf{E}) \tag{4.19}$$

as $\gamma\to+\infty$.

A detailed analysis of $f(\mathbf{E})$ entails a detailed analysis of $h_{\mathbf{n}}(E_1,E_2)$. For simplicity we shall again limit our discussion to the case when $a_r\to0^+,\forall r$.[24] Clearly, for other ensembles a similar analysis can be done on a term by term basis.

It follows easily that for $\mathbf{a}\to0^+$

$$f(\mathbf{E})=A\,\xi_1f_1(\mathbf{E}), \tag{4.20}$$

where f_1 is defined by (3.25) and where A is the normalization constant. For definiteness, we again assume that $F(E)$ is given by (3.27). Thus,

$$f(\mathbf{E})=(N!(N-1)!\alpha^{2N}/2)\xi_1\prod_{i=1}^{N-1}\xi_i\exp(-\alpha\textstyle\sum E_i). \tag{4.21}$$

One thing which is immediately obvious at this point is the fact that

$$\lim_{\gamma\to+\infty}f(\mathbf{E})\neq f_1(\mathbf{E}). \tag{4.22}$$

In particular, the limit as $\gamma\to+\infty$ and $a_1\to0^+$ depends on the order in which the limits are taken.

An analysis of (4.21) is analogous to that given above for $f_1(\mathbf{E})$. In fact many results can be obtained easily from those given above for f_1. In particular, if we let

$$[Q]\equiv\int Qf(\mathbf{E})\,d\mathbf{E}, \tag{4.23}$$

then when $f(E)$ is given by (4.20),

$$[Q]=\langle\xi_1Q\rangle/\langle\xi_1\rangle. \tag{4.24}$$

Thus, in particular, from (3.30) it follows that

$$[E_N^{n_N}\prod_{r=1}^{N-1}\xi_r^{n_r-1}]$$

$$=\tfrac{1}{2}(N-1)!\,\alpha^{N-M+1}(n_1+1)!\prod_{r=2}^{N}(n_r!/r^{n_r}) \tag{4.25}$$

$$=\tfrac{1}{2}(n_1+1)\;E_N^{n_N}\prod_{r=1}^{N-1}\xi_r^{n_r-1}\;. \tag{4.26}$$

An immediate consequence of (4.26) is that all moments for any local spacing distribution (where E_1 is not involved) corresponding to (4.21) will be identical to those for the orthogonal ensemble. Further, it can be shown that if $\{E^n\}$ are the moments of the level density associated with (4.21), then

$$\{E^n\}=\overline{E^n}+([E_1^n]-\langle E_1^n\rangle), \tag{4.27}$$

$$0\leq[E_1^n]-\langle E_1^n\rangle\leq\frac{n}{2}\langle E_1^n\rangle,\quad\forall\,n\geq0, \tag{4.28}$$

and that

$$\langle E_1^n\rangle/\overline{E^n}\sim(\ln N)/N,\quad n=1,2. \tag{4.29}$$

Thus, for small n, $\{E^n\}\sim\overline{E^n}$ as $N\to+\infty$.

When $M\sim N/2$, the analysis is in general much more difficult than for small M (except, of course, for the limiting case $a_r\to0^+$), and at this point the conclusions are much less definite. It is clear that since $\hat{T}_N$ involves $M+1$ eigenvalues the statistical properties will in general differ significantly from those of the corresponding orthogonal ensemble.

It would appear that, in order to obtain specific conclusions, one would have to resort to numerical calculations. Since the primary purpose here was to introduce the above ensembles, we shall not pursue this case further, other than to note that, as $\gamma\hat{T}_N^2\to+\infty$,

$$f(\mathbf{E},\phi)\sim\hat{f}_M(\mathbf{E},\phi)p_{\rm ort}(\mathbf{E},\phi), \tag{4.30}$$

where

$$\hat{f}_M(\mathbf{E},\phi)\equiv\eta'C_1S_1C_2\Delta_1\hat{T}_N^{-1}. \tag{4.31}$$

Thus, there is a measurable region where (4.30) does not hold.

In conclusion, it should be noted that the ensembles we have considered above can be generalized. In particular, one can generalize the class of unitary matrices $\mathbf{A}$, which diagonalize $\mathbf{H}$. While this would tend to make any resulting conclusions more generally applicable, it

would at the same time make the resulting joint distribution for the eigenvalues and rotation parameters much more complicated than those given above. Since the motivation for introducing the above ensembles was based on the fact that such ensembles are relatively simple and at least offer some hope of obtaining analytic results, such a generalization does not seem desirable at this point.

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[1]See, for example, C.E. Porter, *Statistical Theories of Spectra: Fluctuations* (Academic, New York, 1965), and M.L. Mehta, *Random Matrices and the Statistical Theory of Energy Levels* (Academic, New York, 1967).
[2]N. Rosenzweig, J.E. Monahan, and M.L. Mehta, Nucl. Phys. A **109**, 437 (1968).
[3]M.L. Mehta, Nuovo Cimento B **65**, 107 (1970).
[4]M.L. Mehta, *The International Conference on Statistical Properties of Nuclei*, Albany, New York, August 1971; see *Statistical Properties of Nuclei*, edited by J.B. Garg (Plenum, New York, 1972).
[5]L.D. Favro and J.F. McDonald, Phys. Rev. Lett. **19**, 1254 (1967).
[6]J.F. McDonald, J. Math. Phys. **10**, 1191 (1969).
[7]J.F. McDonald, J. Math. Phys. **15**, 596 (1974).
[8]J.B. French and S.S.M. Wong, Phys. Lett. B **33**, 449 (1970).
[9]O. Bohigas and J. Flores, Phys. Lett. B **34**, 261 (1971).
[10]J.B. French and S.S.M. Wong, Phys. Lett. B **35**, 5 (1971).
[11]O. Bohigas and J. Flores, Phys. Lett. B **35**, 383 (1971).
[12]S.S.M. Wong and J.B. French, Nucl. Phys. A **198**, 188 (1972).
[13]J.F. McDonald and L.D. Favro, J. Math. Phys. **16**, 1057 (1975).
[14]F.J. Dyson, J. Math. Phys. **3**, 140 (1962).
[15]A parametrization for an arbitrary unitary matrix is given in J.F. McDonald, J. Math. Phys. **13**, 1399 (1972). It should be noted that the A being considered here is just $\mathbf{T}^{(N-1)}$ as defined in that article.
[16]Of course, if all (or almost all) of the matrix elements are independent, one would not consider the joint distribution term by term. See, for example, Ref. 1.
[17]See, for example, Ref. 1 above.
[18]H.S. Leff, Phys. Rev. **136**, A355 (1964).
[19]The corresponding unitary case is included in the discussion of D. Fox and P.B. Kahn, Phys. Rev. **134**, B1151 (1964).
[20]M. Gaudin, Nucl. Phys. **25**, 447 (1961).
[21]P.B. Kahn, Nucl. Phys. **41**, 159 (1963).
[22]The definition and properties of $I_0(z)$ required for our discussion can be found in *Applied Mathematics Series, No.* 55: *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964).
[23]In particular, the region $0 \leq y \ll 1/\gamma$, $0 \leq x \leq +\infty$, where $x = \xi_1 \cos(2\phi_1)$, $y = \xi_1 \sin(2\phi_1)$, contributes significantly.
[24]It should be noted that for this limiting case the results are identical $\forall M$.

Neutrinos and Bianchi I universes

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We find that Bianchi I universes allow neutrinos only in the special case $B = C \neq A$, and the neutrinos must be "ghost." The solution is a special case of the Kasner solution. We also discuss massive neutrino solutions in Bianchi I universes. In an appendix we discuss the lack of a Birkhoff-type theorem for plane symmetry.

In this paper we are interested in the much studied Bianchi I type universe described by the metric

$$ds^2 = A^2\,dx^2 + B^2\,dy^2 + C^2\,dz^2 - dt^2, \tag{1}$$

where A, B, and C are functions of t only. For $A \neq B \neq C$ we find this metric does not allow neutrino solutions. For the notation and theory we refer the reader to our previous work.[1-3]

If we specialize the metric to the case $B = C \neq A$ then this metric allows *only* "ghost neutrinos" (vanishing energy and momentum).[1] Since the gravitational field in this case is determined by the vacuum field equations, the solution is a special case of the Kasner metric

$$ds^2 = t^{-2/3}\,dx^2 + t^{4/3}(dy^2 + dz^2) - dt^2. \tag{2}$$

By a coordinate transformation this can be brought to the form

$$ds^2 = (kt+1)^{-1/2}(dx^2 - dt^2) + (kt+1)(dy^2 + dz^2), \tag{3}$$

where k is a constant. This is the time-dependent plane-symmetric ghost neutrino solution that is the counterpart of our static plane-symmetric ghost neutrino solution presented elsewhere, i.e., the type D "ghost neutrino" solution is plane-symmetric but can be either static or the time-dependent solution given in Eq. (3).[1-3]

We note in passing that the vacuum solution (3) requires an extension of Taub's theorem: "A spacetime with plane symmetry which is a solution of the vacuum field equations admits a coordinate system where the line element is independent of t, that is, is static."[4] In the Appendix we discuss this further.

The last case $A = B = C$, the zero curvature Robertson–Walker metric, also does not allow neutrinos.[5]

Recently we have discussed massive neutrinos in general relativity.[5] The zero curvature Robertson–Walker metric allows massive neutrinos, the solution being the Einstein–deSitter dust solution.[5] The general Bianchi I massive neutrino solution is found in the same way and is in fact the Heckmann–Schücking solution[6] with their $9\kappa M/2$ replaced by the constant k^3 found in Ref. 5.

Further results for neutrino solutions in other Bianchi universes may be found in Ref. 7.

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APPENDIX

We will use Taub's notation[4] in the following proof. Consider the case of

$$f'' = g'' = 0, \tag{A1}$$

where

$$A^2 = (f+g)^{-1/2}, \tag{A2}$$

$$B^2 = C^2 = f + g, \tag{A3}$$

$$f = f(x+t) = c_1(x+t), \tag{A4}$$

$$g = g(x-t) = c_2(x-t). \tag{A5}$$

The primes denote derivatives with respect to the arguments and c_1, c_2 are arbitrary constants. The coordinate transformation

$$X + T = (2/k)[c_1(x+t) - 1/2], \tag{A6}$$

$$X - T = (2/k)[c_2(x-t) - 1/2], \tag{A7}$$

$$Y = y, \tag{A8}$$

$$Z = z, \tag{A9}$$

where k is an arbitrary constant transforms the metric to

$$ds^2 = \frac{k^2}{4c_1c_2}(kX+1)^{-1/2}(dX^2 - dT^2) + (kX+1)(dY^2 + dZ^2). \tag{A10}$$

If c_1 and c_2 are both positive or both negative, the metric is the static vacuum solution, i.e., X is a spacelike coordinate. If either c_1 or c_2 is negative, the metric is the homogeneous vacuum (special Kasner) solution, i.e., X is the timelike coordinate. In Ref. 4 only the former case is considered. We can combine both cases into the theorem: "A spacetime with plane symmetry which is a solution of the vacuum field equations admits a coordinate system where the solution is either the static solution of Refs. 1–4 or the special Kasner solution in Eq. (3)."

When one solves the vacuum field equations in the case of spherical symmetry, one finds either the time-dependent homogeneous solution inside the Schwarzschild sphere or the exterior Schwarzschild solution outside. No assumption is made that the variable r occurring in the metric is spacelike or timelike. These two solu-

tions are joined across the Schwarzschild surface $r=2m$ to form a solution to the vacuum field equations everywhere outside the real singularity at $r=0$. Thus, we arrive at the Birkhoff theorem[8]:

"$\cdots$ any C^2 solution of Einstein's empty space equations which is spherically symmetric in an open set V, is locally equivalent to a part of the maximally extended Schwarzschild solution in V."

However, this joining apparently cannot occur in plane symmetry. Here, one has the special Kasner solution for all t between the real singularity $t=-1/k$ and infinity or one can have a static solution between the real singularity $x=-1/k$ and infinity. There is apparently no *natural* way to join these two solutions and obtain a solution in an extended manifold. Therefore, plane symmetry does not have a Birkhoff-type theorem as in spherical symmetry. The vacuum solution in the case of plane symmetry is not *unique*; i.e., it can be either static or homogeneous anywhere. Of course, the vacuum plane-symmetry solutions does allow a fourth killing vector just as in the case of spherical symmetry.[9]

[1]T.M. Davis and J.R. Ray, Phys. Rev. D **9**, 331 (1974).
[2]T.M. Davis and J.R. Ray, J. Math. Phys. **16**, 75 (1975).
[3]T.M. Davis and J.R. Ray, J. Math. Phys. **16**, 80 (1975).
[4]A. Taub, Ann. Math. **53**, 472 (1951).
[5]T.M. Davis and J.R. Ray, Phys. Lett. A **51**, 199 (1975).
[6]O. Heckmann and E. Schücking in *Gravitation*, edited by L. Witten (Wiley, New York, 1962), p. 444.
[7]T.M. Davis, Ph.D. thesis, Clemson University, 1975 (available from University Microfilms, Ann Arbor, Michigan).
[8]S. Hawking and G. Ellis, *The Large Scale Structure of Spacetime* (Cambridge U.P., New York, 1973), p. 369.
[9]H. Goenner, Commun. Math. Phys. **16**, 34 (1970).

Optimal factor group for nonsymmorphic space groups

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The construction of the irreducible representations of single and double nonsymmorphic space groups is discussed. The proof is given that for any symmetry element where the nonsymmorphism plays a role there is a finite group of lowest order such that its irreducible representations engender all the allowable representations of the little group. For most high symmetry elements the order of this optimal factor group is only twice the order of the corresponding point group of the wave vector. The computational advantages of using this group instead of other known factor groups are stressed.

1. INTRODUCTION

All known methods suggested for finding the irreducible representations (hereafter IRREPS) of nonsymmorphic space groups do not start from a detailed analysis of the interaction between the primitive translations and the space operations containing both a point part and a nonprimitive translational part, although this phenomenon is at the heart of the nonsymmorphic degeneracy, the so-called sticking together of dispersion relations on the surface of the Brillouin zone.[1,2]

The projective representation method,[2,3] leaving the ordinary representation theory, enters a domain where some simple and familiar concepts, as, e.g., the class-IRREP relation, are lost; it deals on a different basis with translations and with rotations for the translational part of the little group $G_{\mathbf{k}}$ is described only by multiplicative phase factors while its point part is represented by matrices.

The extension method[4] uses the technique of finding a group G from a group P to which G is homomorphic with a given group H as a kernel; this technique is applied in order to find the allowable representations of $G_{\mathbf{k}}$ but again the roles of translations and of rotations are structurally different so that no insight is possible into the aforementioned interaction.

A third approach is the induction method[5,6] that fully exploits the solvability property of space groups[7]: It is of global nature and it finds the allowable representations of $G_{\mathbf{k}}$ in an over-all way. It may be useful in automatic implementations,[6] but it limits almost completely any insight into the elementary causes of nonsymmorphic degeneracy.

The most popular approach is the factor group method,[8-11] which finds the allowable representations of $G_{\mathbf{k}}$ from some ordinary representations of a factor group simply related to the point group of the wave vector $G^0_{\mathbf{k}}$. The presently known methods in this last class have two distinct disadvantages: The order of the factor group for most symmetry elements is higher than necessary, and, moreover, this order may depend on $\mathbf{k}$ in such a way that points on the same symmetry element have factor groups of different order. Clearly both from a physical and from a computational point of view this is largely unsatisfactory.

In this paper we propose a new factor group method that overcomes both these inconveniences, and we demonstrate that it is possible to define an optimal factor group that reduces to a minimum the amount of computational work required by a method of this class.

With this optimal choice the allowable representations of $G_{\mathbf{k}}$, for all symmetry elements where nonsymmorphism plays a role, are found from the IRREPS of another group $Q_{\mathbf{k}}$ whose order is almost always twice, and never greater than six times, the order of the point group $G^0_{\mathbf{k}}$. The operations of $Q_{\mathbf{k}}$ are the cosets, of a suitable translation subgroup, whose representatives are the operations $(\alpha \mid \tau(\alpha))$, $\alpha \in G^0_{\mathbf{k}}$, together with the products between them and some primitives translations whose images form a cyclic subgroup of order 2, 3, 4, 6. The optimal factor group $Q_{\mathbf{k}}$ is the group of lowest order taking into account the interplay of primitive and nonprimitive translations via point operations.

We divide our exposition as follows: In Sec. 2 the basic concepts about subduced and induced representation theory are summarized; in Sec. 3 the algorithmic tools and the corresponding requirements for factor group methods are described; in the subsequent section the group theoretical proof of our factor group choice is given; then Sec. 5 contains an example and the quantitative comparison of the computational weight for different factor groups; the last section contains the conclusions.

2. INDUCED/SUBDUCED REPRESENTATIONS AND SPACE GROUPS

It is well known that the exigence of describing the physical properties of crystals in terms of the Brillouin zone compels the labelling of the IRREPS of the space group G by the labels of the IRREPS of the translation subgroup.

An exhaustive answer to this problem is given by that part of group representation theory dealing with construction of the IRREPS of a group G starting from the IRREPS of a normal subgroup T of G. The general procedure found in Refs. 11, 12 involves the following manipulations:

—First we construct all the IRREPS $\gamma \equiv \{d(t)\}$ of T and we group them in different *orbits of* T in G, i.e., in sets of IRREPS of T such that any set contains simultaneously $\gamma \equiv \{d(t)\}$ and all nonequivalent $\gamma' \equiv \{d'(t) = d(g^{-1}tg)\}$ for all $g \in G$.

—For every orbit we execute the remaining steps:

—We choose an arbitrary element $\gamma_j \equiv \{d_j(t)\}$ of the orbit and we find its *little group* $L(\gamma_j)$, i. e., the subgroup of G such that for all its elements l the IRREPS $\gamma_j' \equiv \{d_j'(t) = d_j(l^{-1}tl)\}$ of T are equivalent to γ_j;

—then we construct all the *allowable representation* of $L(\gamma_j)$, i. e., the IRREPS of $L(\gamma_j)$ that, when subduced to T, are a multiple of the IRREP γ_j;

—finally for every allowable representation of $L(\gamma_j)$ we induce in G a representation that is irreducible.

The IRREPS of G induced by the allowable representations of the same little group $L(\gamma_j)$ form a so-called *associate set* of representations of G,[11] and we will say also that they are *associated* with the orbit of γ_j in G, a notion we will use extensively in Sec. 4.

Clearly the procedure breaks down for γ_j such that $L(\gamma_j) = G$; anyway it faces us with the problem of finding the allowable representations (not all the IRREPS) of little groups and the various methods for constructing the IRREPS of space groups differ only in the way chosen for this problem.

For space groups the normal subgroup T is the Abélian subgroup of translations whose IRREPS are labelled by a $\mathbf{k}$ not outside the Brillouin zone (BZ), while the different orbits are labelled by a $\mathbf{k}$ not outside the irreducible segment of the Brillouin zone (IBZ). The little group of $\gamma_\mathbf{k}$ is indicated by $G_\mathbf{k}$ and contains all space operations $(\alpha \mid \tau(\alpha) + \mathbf{m})$, whose point part transforms $\mathbf{k}$ into itself or into an equivalent vector. The group $G^0 \approx G/T$ is the point group of G and similarly the group $G_\mathbf{k}^0 \approx G_\mathbf{k}/T$ is the point group of the wave vector $\mathbf{k}$.

As is well known,[13] if $G_\mathbf{k}$ is symmorphic or if $\mathbf{k}$ is within the BZ, then the construction of its allowable representations poses no problems: They are simply found from the IRREPS $\{D_j(\alpha)\}$ of $G_\mathbf{k}^0$ as

$$D_{\mathbf{k}j}((\alpha \mid \tau(\alpha) + \mathbf{m})) = \exp[-i\mathbf{k}\cdot(\tau(\alpha) + \mathbf{m})]D_j(\alpha). \tag{1}$$

Furthermore, this relation holds also for a nonsymmorphic $G_\mathbf{k}$ and $\mathbf{k}$ lying on the surface of the BZ if all the operations $\alpha \in G_\mathbf{k}^0$ transform $\mathbf{k}$ into $\mathbf{k} + \mathbf{K}$ with $\mathbf{K}$ orthogonal to $\tau(\beta)$ for all $\beta \in G_\mathbf{k}^0$. In particular this happens when all such $\mathbf{K}$ are zero, i. e., when there is a $G_{\mathbf{k}'}^0 \supseteq G_\mathbf{k}^0$, $\mathbf{k}'$ lying inside the BZ. This happens, for instance, to the edge K-W and to the vertex K of fcc crystals.

Therefore, a nonsymmorphic space group G requires a special treatment only for the $G_\mathbf{k}$'s satisfying the following conditions: $G_\mathbf{k}$ is nonsymmorphic, $\mathbf{k}$ lies on the surface of the BZ, and at least one element of $G_\mathbf{k}$ transforms $\mathbf{k}$ into an equivalent vector $\mathbf{k} + \mathbf{K}$ with $\mathbf{K}$ not orthogonal to all $\tau(\beta)$, $\beta \in G_\mathbf{k}^0$.

3. FACTOR GROUP METHODS

In the previous section we have shown that the problem of nonsymmorphism amounts to finding the allowable representations of $G_\mathbf{k}$ for most high symmetry elements on the surface of the BZ.

If we now consider that there are 157 nonsymmorphic space groups and at least an average of 10 surface elements for each group we reach ~1500 little groups $G_\mathbf{k}$, every $G_\mathbf{k}$ having an average of, say, four allowable representations. Even assuming only one-dimensional IRREPS and an average of ten distinct point operations in $G_\mathbf{k}$, we obtain 60 000 complex numbers, without speaking of double and magnetic space groups. This implies a large amount of tables so that their realization and the search for data may be inefficient and unreliable. It seems therefore highly preferable to have an algorithm that can generate automatically the allowable representations than to store all this data for a subsequent search.

A basic tool necessary to solve this problem is an algorithm for the, possibly automatic, generation of all the IRREPS of a finite group.

As is shown in Ref. 14, exact (integer arithmetic) algorithms for IRREPS construction are presently available only for symmetric groups while for other groups it is necessary to resort to approximate (floating-point arithmetic) algorithms, where the nonlinearity of the problem increases the difficulties. An exact algorithm exists only for characters of ordinary IRREPS[15] so that a practicable algorithm consists of the exact generation of irreducible characters followed, for instance, by the approximate decomposition of the regular representation using projection operators.[16] The computational weight of this algorithm is proportional to the fourth power of the order of the group for the approximate decomposition and to the fourth power of the number of classes for the exact character generation.

It follows that the highest efficiency, for a constant number of classes, will be reached with the lowest order group such that all the allowable representations of $G_\mathbf{k}$ are found from its IRREPS. It is also clear that this lowest order group will be the most suitable for getting an insight into the geometrical machinery of nonsymmorphism.

We now briefly describe the factor group choice proposed in Ref. 8.

Since the matrices of any allowable representation D^A of $G_\mathbf{k}$ are the images of the elements of $G_\mathbf{k}$ in the homomorphism $G_\mathbf{k} \to D^A$ with kernel containing the normal subgroup $T_\mathbf{k} \equiv \{(\epsilon \mid \mathbf{m}) \mid \exp[-i\mathbf{k}\cdot\mathbf{m}] = 1\}$, it follows that all these representations are engendered by some IRREPS of the factor group $G_\mathbf{k}/T_\mathbf{k}$. Clearly some IRREPS of $G_\mathbf{k}/T_\mathbf{k}$ engender IRREPS of $G_\mathbf{k}$ that are not allowable.[17] The order of the factor group is

$$^0(G_\mathbf{k}/T_\mathbf{k}) = {}^0G_\mathbf{k}^0 \times {}^0(T/T_\mathbf{k}). \tag{2}$$

Expressing $\mathbf{k}$ as $(u_1/v_1)\mathbf{g}_1 + (u_2/v_2)\mathbf{g}_2 + (u_3/v_3)\mathbf{g}_3$, u_i and v_i being relative prime integers, $u_i < v_i$ and the $\mathbf{g}_i$ the reciprocal lattice primitive vectors, we find

$$^0(T/T_\mathbf{k}) = v_1 \wedge v_2 \wedge v_3, \tag{3}$$

where $a \wedge b$ is the least common multiple of a and b. Therefore, the order of the factor group $G_\mathbf{k}/T_\mathbf{k}$ depends on $\mathbf{k}$ in such a way that different points on the same symmetry element have factor groups of different order.

Another factor group has been proposed in Ref. 10 to overcome such a disadvantage, but the order of this group is still not minimal.

In the following section we will show that it is possible to define a lowest order factor group whose order depends only on the symmetry element and such that it reduces the study of nonsymmorphism only to its analysis on the vertices of the IBZ.

4. OPTIMAL FACTOR GROUP

Definition: Given two points $\mathbf{h}$ and $\mathbf{k}$ belonging to the IBZ of a space group G, $\mathbf{h}$ is said to be compatible with $\mathbf{k}$ when $G_{\mathbf{h}}^0 \supseteq G_{\mathbf{k}}^0$ and $\alpha\mathbf{h} = \mathbf{h} + \mathbf{K}$, $\alpha\mathbf{k} = \mathbf{k} + \mathbf{K}$ with the same reciprocal lattice vector $\mathbf{K}$ for any $\alpha \in G_{\mathbf{k}}^0$.

Theorem: If $\mathbf{h}$ is compatible with $\mathbf{k}$, then the set of all the allowable representations of the little group $G_{\mathbf{k}}$ is in a one-to-one onto mapping with the set of all the representations of the group $G_{\mathbf{k}}$ associated with the orbit of $\gamma_{\mathbf{h}}$ in $G_{\mathbf{k}}$. The one-to-one onto mapping is given by

$$D_{\mathbf{k}i}((\alpha \mid \tau(\alpha) + \mathbf{m})) = \exp[i(\mathbf{h} - \mathbf{k}) \cdot (\tau(\alpha) + \mathbf{m})] D_{\mathbf{h}i}((\alpha \mid \tau(\alpha) + \mathbf{m})). \quad (4)$$

Proof: *Step* 1: Under the conditions of the theorem and if $G_{\mathbf{h}}^0 = G_{\mathbf{k}}^0$, the relation (4) defines a one-to-one onto mapping between the set of the allowable representations of $G_{\mathbf{k}}$ and that of $G_{\mathbf{h}}$. In fact let us suppose $\{D_{\mathbf{k}i}\}$ is an allowable representation of $G_{\mathbf{k}}$; then from the irreducibility of the representation $\{D_{\mathbf{k}i}\}$ follows the irreducibility of the set of matrices $\{D_{\mathbf{h}i}\}$; from the allowability of the representation $\{D_{\mathbf{k}i}\}$ and from the mapping it follows that the set of matrices $\{D_{\mathbf{h}i}\}$ subduces on T a multiple of $\gamma_{\mathbf{h}}$. Furthermore, the mapping implies

$$D_{\mathbf{h}i}((\alpha \mid \tau(\alpha) + \mathbf{m})) D_{\mathbf{h}i}((\beta \mid \tau(\beta) + \mathbf{n})) = \exp[-i((\mathbf{h} - \mathbf{k}) - \alpha^{-1}(\mathbf{h} - \mathbf{k})) \cdot \tau(\beta)] \times D_{\mathbf{h}i}((\alpha\beta \mid \tau(\alpha) + \mathbf{m} + \alpha(\tau(\beta) + \mathbf{n})))$$

for all the operations of $G_{\mathbf{k}}$, and owing to the compatibility of $\mathbf{h}$ with $\mathbf{k}$ the phase factor is always 1 so that $\{D_{\mathbf{h}i}\}$ is a representation of $G_{\mathbf{h}}$. Interchanging $\mathbf{h}$ and $\mathbf{k}$ the same reasoning shows that the one-to-one mapping is onto.

Step 2: The application of Step 1 to the space group $G_{\mathbf{k}}$ completes the proof.

Corollary: If $\mathbf{h}$ is compatible with $\mathbf{k}$ and if $\{\Delta_i((\alpha \mid \tau(\alpha) + \mathbf{m})T_{\mathbf{h}})\}$ is an IRREP of $G_{\mathbf{k}}/T_{\mathbf{h}}$ that engenders an IRREP of $G_{\mathbf{k}}$ associated with the orbit of $\gamma_{\mathbf{h}}$ in $G_{\mathbf{k}}$, then the set of matrices $\{\exp[i(\mathbf{h} - \mathbf{k}) \cdot (\tau(\alpha) + \mathbf{m})] \times \Delta_i((\alpha \mid \tau(\alpha) + \mathbf{m})T_{\mathbf{h}})\}$ engenders an allowable representation of $G_{\mathbf{k}}$.

Noting that if $G_{\mathbf{h}}^0 \supseteq G_{\mathbf{k}}^0$ and $(\mathbf{h} - \mathbf{k})$ within the BZ $\mathbf{h}$ is compatible with $\mathbf{k}$, then the previous corollary lets one find all the allowable representations of $G_{\mathbf{k}}$, for any $\mathbf{k}$ not a vertex, from the IRREPS of $G_{\mathbf{k}}/T_{\mathbf{h}}$, where $\mathbf{h}$ is a vertex of the IBZ lying on the same symmetry element of $\mathbf{k}$: Thus ${}^0(T/T_{\mathbf{h}})$ is always lower than ${}^0(T/T_{\mathbf{k}})$. By choosing among the possible vertices one that gives the lowest ${}^0(T/T_{\mathbf{h}})$ we have the optimal factor group $Q_{\mathbf{k}} = G_{\mathbf{k}}/T_{\mathbf{h}}$.

The study of symmetry for points $\mathbf{k}$ on edges or on faces of the IBZ is therefore reduced to the study of factor groups $Q_{\mathbf{k}}$, $\mathbf{h}$ being a suitable vertex compatible with $\mathbf{k}$.

All the preceding results are extended to double nonsymmorphic space groups in a simple way. This leads to the double optimal factor group $\bar{Q}_{\mathbf{k}}$ defined as the factor group of the double little group $\bar{G}_{\mathbf{k}}$ with its normal translation subgroup $T_{\mathbf{h}}$, $\bar{Q}_{\mathbf{k}} = \bar{G}_{\mathbf{k}}/T_{\mathbf{h}}$, $T_{\mathbf{h}}$ being the same normal subgroup used for the single optimal factor group $Q_{\mathbf{k}}$. An analogous extension is possible for magnetic nonsymmorphic space groups.

5. COMPARISON AND EXAMPLE

From the possible values of the coordinates of a vertex of the IBZ[6] and from the relations (2)–(3) it follows that ${}^0Q_{\mathbf{k}} = s^0 G_{\mathbf{k}}^0$, s being equal to 2, 3, 4, 6 and for most symmetry elements equaling 2. Furthermore, the multiplication table of the group $G_{\mathbf{h}}/T_{\mathbf{h}}$ gives the multiplication tables for all the groups $G_{\mathbf{k}}/T_{\mathbf{h}}$, $\mathbf{k}$ being a point, not a vertex, with which the vertex $\mathbf{h}$ is compatible.

By comparing the optimal factor group $Q_{\mathbf{k}}$ with $G_{\mathbf{k}}/T_{\mathbf{k}}$,[8] it follows immediately that if $\mathbf{k}$ is a vertex of the IBZ, then the two groups coincide, but if $\mathbf{k}$ is not a vertex, then the best choice of $\mathbf{k}$ among equivalent points leads to the double optimal factor group $\bar{Q}_{\mathbf{k}}$ defined as the the order of $Q_{\mathbf{k}}$ for symmetry lines, and at least four times the order of $Q_{\mathbf{k}}$ for symmetry planes. A similar comparison of $Q_{\mathbf{k}}$ with the factor group proposed in Ref. 10 shows that the order of the latter is greater than the order of the former by a factor equal to the greatest common divisor of v_1, v_2, v_3, where $\mathbf{h} = (u_1/v_1)\mathbf{g}_1 + (u_2/v_2)\mathbf{g}_2 + (u_3/v_3)\mathbf{g}_3$, $u_i < v_i$. In addition the two groups coincide only for integers v_1, v_2, v_3 relative prime. For instance, the order of the optimal factor groups for the three vertices X, S, and R of the simple orthorhombic system, is always double the order of the corresponding point group while the order of the factor group proposed in Ref. 10 is, respectively, two, four, and eight times the order of the corresponding point group.

It is worthwhile to remember that a simple factor of 2 in the order of the factor group reduces the efficiency of the algorithm for IRREP construction by a factor of 16.

As a simple example of the optimal factor group method, let us obtain the allowable representations of the little group G_D for the space group D_{2h}^{16} (*Pnma*), D being a point on the edge D of the IBZ. According to standard notations $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are the direct lattice primitive vectors and $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ are the reciprocal lattice primitive vectors so that

$$D = \tfrac{1}{2}\mathbf{g}_1 + r\mathbf{g}_2, \quad 0 < r < \tfrac{1}{2},$$
$$G_D^0 = \{\epsilon, C_2^y, \sigma^x, \sigma^z\}, \quad \tau(C_2^y) = \tfrac{1}{2}\mathbf{b},$$
$$\tau(\sigma^x) = \tfrac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c}), \quad \tau(\sigma^z) = \tfrac{1}{2}(\mathbf{a} + \mathbf{c}).$$

TABLE I. Multiplication table of Q_D.

	R_1	R_2	R_3	R_4
R_1	R_1	R_2	R_3	R_4
R_2	R_2	R_1	tR_4	tR_3
R_3	R_3	R_4	t	tR_2
R_4	R_4	R_3	R_2	R_1

The vertices lying on the line D are $X=\frac{1}{2}\mathbf{g}_1$ and $S=\frac{1}{2}(\mathbf{g}_1+\mathbf{g}_2)$ so that ${}^0(T/T_X)=2$ and ${}^0(T/T_S)=2$. We choose $\mathbf{h}=X$ thus $Q_D=G_D/T_X$, where $(\epsilon\,|\,\mathbf{m})=(\epsilon\,|\,m_1\mathbf{a}+m_2\mathbf{b}+m_3\mathbf{c})\in T_X$ when m_1 is even. Let us indicate with R_1, R_2, R_3, R_4, t the cosets of T_X that have coset representatives $(\epsilon\,|\,\mathbf{o})$, $(C_2^y\,|\,\tau(C_2^y))$, $(\sigma^x\,|\,\tau(\sigma^x))$, $(\sigma^z\,|\,\tau(\sigma^z))$, $(\epsilon\,|\,\mathbf{a})$.

As easily verified, $t^2=R_1$ and t commutes with any element of Q_D, so that the multiplication table of Q_D may be directly obtained from its exaustive part shown in Table I.

This table shows the group Q_D is not Abelian and, because ${}^0Q_D=8$, Q_D will have four one-dimensional and one two-dimensional IRREPS. The one-dimensional IRREPS of Q_D are engendered by the IRREPS of G_D and therefore they must be discarded. The only IRREP associated with the orbit of γ_X in G_D is the two-dimensional one.

In order to find this IRREP, let us apply to the group Q_D the concepts of orbit, of little group, and of representations associated with an orbit. From the multiplication table it follows that the direct product group $M=\{R_1,R_2\}\times\{R_1,t\}$ is a subgroup of Q_D of index two and hence a normal subgroup. The two IRREPS of M, γ_1 and γ_2 odd with respect to the element t are shown in Table II and they constitute an orbit, for $R_3^{-1}R_2R_3=R_4$. The representation D_1 of Q_D associated with the orbit of γ_1 is induced by γ_1. Then the matrices of this IRREP are found immediately and are given in Table III.

Finally the set $\{\exp[-ir\mathbf{g}_2\cdot\tau(\alpha)]D_1((\alpha\,|\,\tau(\alpha))T_X)\}$ engenders the unique allowable representation of G_D.

6. CONCLUSIONS

We have shown that for any nonsymmorphic little group it is possible to construct by very simple rules an optimal factor group of lowest order and such that some its IRREPS engender all the allowable representations of the little group.

This optimal factor group allows one to face the problem of nonsymmorphism by making use only of the simple and well-known concepts of ordinary representation theory, e.g., the class concept, the relation between classes and IRREPS, the relation between the IRREP dimensionalities and the group order, the notion of direct and semidirect products.[11]

It is worth-while to note that this results may be also obtained by means of the projective representation theory[18] using the concepts of central extension of a group, of lifting of a projective representation into an ordinary one, and of projecting an ordinary representation into a projective one.[19]

However, we have preferred the simpler approach of ordinary representation theory because this theoretical instrument, which has proved so fruitful in molecular and solid state physics, seems the most suitable to give a physical answer to the not yet solved problem of the sticking together of dispersion relations on the surface of the BZ.

This paper is also intended as a step in this direction and further work is in progress.

TABLE II. Irreducible representations of $M\equiv\{R_1,R_2\}\times\{R_1,t\}$ that are odd with respect to t.

	R_1	R_2	t	tR_2
γ_1	1	1	−1	−1
γ_2	1	−1	−1	1

TABLE III. Irreducible representations of Q_D associated with the orbit of γ_1 in Q_D.

	R_1	R_2	R_3	R_4	t
D_1	1 0 0 1	1 0 0 −1	0 −1 1 0	0 1 1 0	−1 0 0 −1
χ_{D_1}	2	0	0	0	−2

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[1]V. Heine, *Group Theory in Quantum Mechanics* (Pergamon, Oxford, 1960); F. Hund, Z. Phys. 99, 119 (1936).
[2]G. Y. Lyubarskii, *The Application of Group Theory in Physics* (Pergamon, Oxford, 1960).
[3]P. Rudra, J. Math. Phys. 6, 1273 (1965); W. Doring, Z. Naturforsch. 14a, 343 (1959); A. C. Hurley, Phil. Trans. Roy. Soc. London A 260, 1108 (1966).
[4]K. Olbrychski, Phys. Stat. Sol. 3, 1868, 2143 (1963).
[5]I. V. V. Raghavacharyulu, Can. J. Phys. 39, 830 (1961); J. Zak, J. Math. Phys. 1, 165 (1960); M. Glück, Y. Gur, and J. Zak, J. Math. Phys. 8, 787 (1967); A. Casher, M. Glück, and Y. Gur, *The Irreducible Representations of Space Groups*, edited by J. Zak (Benjamin, New York, 1969).
[6]S. C. Miller and W. F. Love, *Tables of Irreducible Representations of Space Groups and Co-Representations of Magnetic Space Groups* (Pruett, Boulder, 1967).
[7]F. Seitz, Ann. Math. 37, 17 (1936).
[8]C. Herring, J. Franklin Inst. 233, 525 (1942).
[9]S. L. Altmann and C. J. Bradley, Rev. Mod. Phys. 37, 33 (1965); D. F. Johnston, Rept. Progr. Phys. 23, 66 (1960); H. Jones, *The Theory of Brillouin Zone and Electronic States in Crystals* (North-Holland, Amsterdam, 1960); L. D. Landau and E. F. Lifshitz, *Statistical Physics* (Pergamon, London, 1958); E. Blokker, J. Comp. Phys. 12, 471 (1973).

[10]M. I. Petrashen and E. D. Trifonov, *Applications of Group Theory in Quantum Mechanics* (M. I. T., Cambridge, 1969).
[11]L. Jansen and M. Boon, *Theory of Finite Groups. Applications in Physics* (North-Holland, Amsterdam, 1967).
[12]J. S. Lomont, *Applications of Finite Groups* (Academic, New York, 1959).
[13]G. F. Koster, Solid State Phys. 5, 173 (1957).
[14]J. J. Cannon, Ph. D. thesis, "Computation in Finite Algebraic Structures," Sydney (1969).
[15]J. D. Dixon, Numer. Math. 10, 446 (1967).
[16]S. Flodmark, Phys. Rev. 132, 1343 (1963); S. Flodmark and E. Blokker, Int. J. Quantum Chem. 1S, 703 (1967).
[17]In particular all the IRREPS of $G_{\mathbf{k}}/T_{\mathbf{k}}$ engendered by the IRREPS of $G^0_{\mathbf{k}}$ must be discarded.
[18]M. Hammermesh, *Group Theory and Its Applications to Physical Problems* (Addison-Wesley, Reading, Mass., 1962).
[19]N. B. Backhouse and C. J. Bradley, Quart. J. Math. 21, 203 (1970); N. B. Backhouse, Quart. J. Math. 21, 277 (1970); L. Dornhoff, *Group Representation Theory* (Dekker, New York, 1971/1972); W. Mackey, Acta Math. 99, 265 (1958).

Wave operators for multichannel scattering by long-range potentials

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The methods of Alsholm in single channel scattering are developed so as to apply to multichannel scattering. For a large class of long-range potentials we prove the existence of partially isometric wave operators, intertwining relations, and the orthogonality of the ranges of these wave operators for distinct channels.

1. INTRODUCTION

In multichannel scattering relatively little work has been done on the proof of existence and/or completeness of wave operators for scattering systems with long-range potentials, i.e., those decreasing at infinity slower than $|\mathbf{x}|^{-1-\epsilon}$, $\epsilon > 0$. The investigation of such scattering systems has thus far been confined to cases in which the potentials are Coulomb or asymptotically Coulomb.[1-6] The convergence of momentum observables in the Heisenberg picture when the Hamiltonian contains long-range repulsive potentials was established for the N-body problem by Lavine,[7] but the existence of the corresponding wave operators was not proved. Postulational schemes for multichannel scattering to accommodate general long-range potentials have been proposed by Prugovečki[8] and by Amrein, Georgescu, and Martin.[9]

In contrast with the situation in multichannel scattering, wave operators for long-range potentials have been thoroughly investigated in the single channel case.[10,11] In particular, quite general results have been obtained by Alsholm,[12] who improved upon earlier results of Buslaev and Matveev.[13] The methods of Alsholm and Kato[14] have recently been extended to treat the problem of scattering by long-range time-dependent potentials.[15]

In the present paper, we apply Alsholm's methods to the case of multichannel scattering and, for a large class of long-range potentials, prove the existence of partially isometric wave operators, the orthogonality of their ranges for distinct channels, and intertwining relations.

In Sec. 2 we formulate the problem giving the motivation and definitions leading up to the statement of our results, which are then proved in the succeeding sections. Because of the length of the proofs, it is desirable to split the estimates into two types. In Sec. 3 we consider those which can be reduced to an application of Alsholm's estimates in single channel scattering. Section 4 then deals with those estimates which cannot be so reduced.

2. FORMULATION

We will consider an N-body ($N \geq 3$) scattering system consisting of spinless distinguishable particles described by the formal Hamiltonian

$$-\sum_{i=1}^{N} \frac{\Delta_{\mathbf{x}_i}}{2m_i} + \sum_{1 \leq i < j \leq N} V_{ij}(\mathbf{x}_i - \mathbf{x}_j) \tag{2.1}$$

in which the two-body local potentials have decompositions of the following form:

$$V_{ij}(\cdot) = V_{ij}{}^{S}(\cdot) + V_{ij}{}^{L}(\cdot); \tag{2.2}$$

where the short-range part $V_{ij}{}^{S}$ satisfies

$$|V_{ij}^{S}(\mathbf{x})| \leq C(1 + |\mathbf{x}|)^{-1-\epsilon(ij)} \tag{2.3}$$

for some constant $\epsilon(ij)$ (depending upon i and j in general) such that $0 < \epsilon(ij) < 1$. For the long-range part $V_{ij}{}^{L}$ we assume that the partial derivatives $\nabla^k V_L(\mathbf{x})$ exist and satisfy

$$|\nabla^k V_{ij}{}^{L}(\mathbf{x})| \leq C(1 + |\mathbf{x}|)^{-k-\alpha_k(ij)}, \tag{2.4}$$

$0 \leq k \leq M < \infty$, for nonnegative integers k and M.

The real-valued constants $\{\alpha_k(ij)\}_{k=0}^{M}$ $(1 \leq i < j \leq N)$ are called decay exponents. We will take over Alsholm's assumptions[12] concerning these exponents except for some trivial changes necessitated by the fact that we allow $k = 0$ in (2.4) whereas he does not. This point will be discussed in more detail below. For the reader's convenience, we summarize these conditions as follows, suppressing the dependence on i and j:

$$1 \geq \alpha_0 > 0, \quad 1 + \alpha_1 > 0, \quad k + \alpha_k > 1 \text{ for } 2 \leq k \leq M. \tag{2.5}$$

Defining $d_k = [k + \alpha_k]$ and $\rho_k = k + \alpha_k - d_k$ for $1 \leq k \leq M$ with the condition $M \geq m + d_m + 1$ for some positive integer $m \geq 1$, we assume

$$\alpha_2 > 0, \tag{2.6}$$

and when $m \geq 2$,

$$\begin{aligned} &k\alpha_1 + \alpha_{k+2} > \max\{0, \rho_{k+2}(\alpha_1 - p_k - \beta(d_{k+2} + p_k + 2)), \\ &\rho_{k+2} + \alpha_1 - 1 - p_k - \beta(d_{k+2} + p_k + 2)\} \end{aligned} \tag{2.7}$$

for $1 \leq k \leq m - 1$ and some $p_k \geq 0$ such that $p_k + d_{k+2} + m \leq M$. When $m \geq 2$,

$$(k-1)\alpha_1 + \beta'(2) + \alpha_{k+1} > \rho_{k+1}(\beta'(2) - p_k - \beta(d_{k+1} + p_k + 3)) \tag{2.8}$$

for $1 \leq k \leq m - 1$ and some $p_k \geq 0$ such that $p_k + d_{k+1} + m + 1 \leq M$.

For $m \geq 1$,

$$\begin{aligned} &m\alpha_1 + \alpha_m > \max\{1, 1 + \rho_m(\alpha_1 - p - \beta(d_m + p + 2)), \\ &\rho_m + \alpha_1 - p - \beta(d_m + p + 2)\} \end{aligned} \tag{2.9}$$

for some $p \geq 0$ such that $p + d_m + 2 \leq M$.

The significance of the positive integer m will be made clear presently, and we have used the notation

$$\beta(k) = \beta(m-2;k) \quad \text{and} \quad \beta'(k) = \beta(m-1;k), \tag{2.10}$$

where

$$\beta(h;k) = \begin{cases} \min\limits_{0 \leq s \leq h} (s\alpha_1 + \alpha_{k+s}), & h \geq 0, k \geq 1, h+k \leq M, \\ \alpha_{k-1}, & h = -1,\ 2 \leq k \leq M+1, \\ \alpha_1, & h = -1, k = 1. \end{cases} \tag{2.11}$$

In later developments we will need to consider potentials of the following form

$$V_{\mathcal{J}_1\mathcal{J}_2}(\mathbf{x}) = \sum_{\substack{i \in \mathcal{J}_1 \\ j \in \mathcal{J}_2}} V_{ij}(\mathbf{x}), \tag{2.12}$$

in which $\mathcal{J}_1$ and $\mathcal{J}_2$ denote certain disjoint sets of positive integers. By using the relations (2.2)–(2.4) for the potentials V_{ij}, it is not difficult to show that similar relations hold for the potential defined by (2.12). We find

$$V_{\mathcal{J}_1\mathcal{J}_2}(\mathbf{x}) = V^S_{\mathcal{J}_1\mathcal{J}_2}(\mathbf{x}) + V^L_{\mathcal{J}_1\mathcal{J}_2}(\mathbf{x}), \tag{2.13}$$

where the short and long range parts satisfy, respectively,[16]

$$\left|V^S_{\mathcal{J}_1\mathcal{J}_2}(\mathbf{x})\right| = \Big|\sum_{\substack{i \in \mathcal{J}_1 \\ j \in \mathcal{J}_2}} V^S_{ij}(\mathbf{x})\Big| \leq C(1+|\mathbf{x}|)^{-1-\epsilon}, \tag{2.14}$$

$$\left|\nabla^k V_{\mathcal{J}_1\mathcal{J}_2}(\mathbf{x})\right| = \Big|\sum_{\substack{i \in \mathcal{J}_1 \\ j \in \mathcal{J}_2}} \nabla^k V^L_{ij}(\mathbf{x})\Big| \leq C(1+|\mathbf{x}|)^{-k-\alpha_k},$$

$$0 \leq k \leq M < \infty, \tag{2.15}$$

with

$$\epsilon = \min_{\substack{i \in \mathcal{J}_1 \\ j \in \mathcal{J}_2}} \epsilon(ij) \tag{2.16}$$

and

$$\alpha_k = \min_{\substack{i \in \mathcal{J}_1 \\ j \in \mathcal{J}_2}} \alpha_k(ij), \quad 0 \leq k \leq M. \tag{2.17}$$

Moreover, it is easily seen that if each decay exponent $\alpha_k(ij)$ $(i \in \mathcal{J}_1,\ j \in \mathcal{J}_2,\ 0 \leq k \leq M)$ satisfies (2.5)–(2.9) then the decay exponents α_k defined by (2.17) will also satisfy conditions of the form (2.5)–(2.9).

The decompositions (2.2) and (2.13) are clearly nonunique. As has been discussed in the case of single channel scattering by long range potentials,[10,12,14] this fact leads to the existence of nonunique wave operators as we shall see later. Moreover, as also happens in single channel scattering, there is a clear connection between this source of nonuniqueness and the nonuniqueness of wave operators previously discussed from the algebraic point of view.[9]

It is easily seen from (2.2)–(2.4) that the two-body potentials V_{ij} satisfy

$$V_{ij}(\circ) \in L^2(R^3) + L^\infty(R^3). \tag{2.18}$$

For this potential class it follows from a well-known result of Kato[17] that the formal differential operator (2.1), as defined on $C_0^\infty(R^{3N})$, has a unique self-adjoint extension H with dense domain $D(H) = D(H_0)$ on the Hilbert space $L^2(R^{3N})$, where H_0 denotes the unique self-adjoint extension of $-\sum_{i=1}^N (\Delta_{\mathbf{x}_i}/2m_i)$.

We now want to make a few remarks concerning the difference between our assumptions on the potentials V_{ij} and Alsholm's assumptions in single channel scattering. For the short range part of the potentials we make essentially the same assumptions as Alsholm and Kato.[14] For the long range part, Alsholm does not make an assumption corresponding to the $k=0$ case in (2.4), but instead shows from his estimates for $k \geq 1$ that his potentials approach a finite (in general nonzero) constant at infinity. We do not follow this procedure. Indeed, it will be seen in Sec. 4 that our proof of the orthogonality of the ranges of the wave operators for distinct channels is not valid if the potentials approach a finite nonzero constant at infinity.[18]

It is clear from a combination of Dollard's formulation of the multichannel scattering problem for Coulomb-like potentials[1-3] and of the work on more general long range potentials in single channel scattering[10,12-14] how the wave operators are to be defined for multichannel scattering with long range potentials. We will follow Hunziker's approach in the case of short range potentials[19-21] and first prove the existence of certain operators associated with cluster decompositions, from which the wave operators are readily obtained. Thus, for a cluster decomposition $D = \{C_1, \ldots, C_n\}$ of the N-body scattering system into $n \geq 2$ clusters, we define the operators $\Omega_D^\pm$ as

$$\Omega_D^\pm = \text{s-}\lim_{t \to \pm\infty} \exp(itH)\exp(-itH_D - iG_t^{(D)}) \tag{2.19}$$

if the strong limits exist.

Here H denotes the self-adjoint extension of (2.1) mentioned after (2.18) and H_D the "free" (self-adjoint) Hamiltonian corresponding to the noninteracting clusters. $G_t^{(D)}$ is a "renormalization" factor designed to cancel the long range effects of the potentials. We define self-adjoint operators $G_t^{(D)(m)}$ by

$$(G_t^{(D)(m)}f)\hat{}\,(\mathbf{k}_1, \ldots, \mathbf{k}_N) = G_t^{(D)(m)}(\mathbf{k}_1, \ldots, \mathbf{k}_N)\hat{f}(\mathbf{k}_1, \ldots, \mathbf{k}_N)$$

for each $f \in L^2(R^{3N})$ in their respective domains. The Lebesgue measurable functions $G_t^{(D)(m)}(\mathbf{k}_1, \ldots, \mathbf{k}_N)$ are defined by the recursive formulas

$$G_t^{(D)(0)} = 0, \quad G_t^{(D)(m)} = \sum_{i<j} G_{t,ij}^{(D)(m)} \quad \text{for } m \geq 1, \tag{2.20a}$$

where

$$G_{t,ij}^{(D)(m)} = \int_0^t V_{ij}^L \{s\mathcal{V}_{C_iC_j} + \nabla G_{s,ij}^{(D)(m-1)}\}\,ds. \tag{2.20b}$$

In (2.20a) the summation runs over all pairs (i,j) linking different clusters and in (2.20b) $\mathcal{V}_{C_iC_j}$ denotes the relative velocity of the two clusters C_i and C_j linked by i and j.

It can be shown that the positive integer $m \geq 1$ which appears in (2.7)–(2.10) and (2.20) labels the minimum number of iterations required in (2.20) in order to have the limits in (2.19) exist, just as in the corresponding situation in single channel scattering.[12,13] In this con-

nection, we note that the iterations in (2.20b) are made for each pair of indices (i,j) independently, i.e., the iterations do not mix in other values of i and j. If we were to use iterations on the total $G_t^{(D)(m)}$ as defined in (2.20a) then when $m \geq 2$ (i.e., when iterations are required) the "renormalization" term for the potential V_{ij} would depend upon potentials for particles other than i and j. Such a situation is not desirable from a physical point of view. This is a new complication which occurs for multichannel scattering with long range potentials when $m \geq 2$. It does not occur in previous work on the subject. We will prove

Theorem 2.1: Consider a scattering system defined by (2.1) with the interparticle potentials V_{ij} satisfying (2.2)–(2.11). Then, for each cluster decomposition $D = \{C_1, \ldots, C_n\}$, $n \geq 2$, the limits in (2.19) exist and define the operators $\Omega_D^{\pm}$ as isometries on the Hilbert space $L^2(R^{3N})$. These operators satisfy the intertwining relations

$$\exp(itH)\Omega_D^{\pm} = \Omega_D^{\pm} \exp(itH_D), \quad -\infty < t < \infty. \tag{2.21}$$

Let α denote a channel consistent[19] with the decomposition D, i.e., such that each bound state fragment of α belongs to some cluster of D. Then the wave operators $\Omega_\alpha^{\pm}$ are defined as the respective restrictions of $\Omega_D^{\pm}$ to the subspace of channel states $\mathcal{H}_\alpha$, i.e., all vectors of $\mathcal{H} = L^2(R^{3N})$ of the form

$$\varphi_\alpha = f(\mathbf{X}_1, \ldots, \mathbf{X}_n) \prod_{j=1}^{n} \psi_j, \tag{2.22}$$

where $f \in L^2(R^{3n})$ and ψ_j denotes a bound state eigenfunction corresponding to the jth fragment. In (2.22) $\mathbf{X}_j$ denotes the center of mass coordinate of the jth fragment and, by convention, we set $\psi_j = 1$ if this fragment is a single particle and call it a simple fragment. A nonsimple fragment is called composite. We have

Proposition 2.1: Impose the assumptions of Theorem 2.1 and let α and β denote distinct channels consistent with cluster decompositions D_1 and D_2, respectively. Then, the ranges of Ω_α^+ and $\Omega_\beta^+ (\Omega_\alpha^-$ and $\Omega_\beta^-)$ are orthogonal.

The proof of these results will be given in the following two sections. Before proceeding with this, however, we note that various special cases of Theorem 2.1 can be considered. As one example, sufficient conditions can be given in order that no iterations are required in (2.20), i.e., we can take $m = 1$. These special cases can be easily derived in analogy with the single channel situation[12] once Theorem 2.1 has been proved. A similar remark also holds for the property of m mentioned at the beginning of the paragraph following (2.20). We will therefore concentrate on the proof of the general results.

3. BEGINNING OF PROOF OF THEOREM 2.1: ESTIMATES REDUCIBLE TO THOSE OF ALSHOLM

The proof of Theorem 2.1 will occupy us in this section and most of the next. In the present section we isolate those estimates which can be put into a form whereby Alsholm's single channel estimates can be directly applied. Then in Sec. 4 we consider those estimates which cannot be treated in this simple way, and for which the necessary bounds are found in a way suggested by Alsholm's approach in single channel scattering.

By the usual argument involving strong differentiability and uniform boundedness, one can verify that it suffices to prove that for some positive constant t_0,

$$Z_D(t) = \left\| \left(H - H_D - \frac{d}{dt} G_t^{(D)(m)}\right) \exp(-itH_D - iG_t^{(D)(m)}) u_D \right\| \tag{3.1}$$

is integrable for $-\infty < t < -t_0$ and $t_0 < t < \infty$ for all u_D belonging to some dense subset of $L^2(R^{3N})$. It will be convenient to choose this subset as that consisting of all vectors of the form

$$u_D = f(\mathbf{X}_1, \ldots, \mathbf{X}_n) \prod_{j=1}^{n} \varphi_j(z_j) \tag{3.2}$$

with Fourier transforms $\hat{\varphi}_j \in C_0^\infty$ and where z_j denotes the collection of internal coordinates of the cluster C_j. In (3.2) we take $f \in \underline{S}_D(R^{3n})$, where we denote by $\underline{S}_D(R^{3n})$ the set of all $f \in L^2(R^{3n})$ with $\hat{f} \in C_0^\infty(R^{3n})$ and $\hat{f}(\mathbf{k}_1, \ldots, \mathbf{k}_n)$ vanishes in an open neighborhood of each of the sets $\{\mathbf{k}_r/M_r = \mathbf{k}_s/M_s\}$ $(1 \leq r < s \leq n)$, where M_r and $\mathbf{k}_r$ $(1 \leq r \leq n)$ denote respectively the mass and the conjugate momenta of the center-of-mass coordinates $\mathbf{X}_r$ of the cluster C_r.

In the derivation of (3.1) one uses the fact that the functions u_D in (3.2) satisfy $u_D \in D(H_0)$ and $\exp(-itH_D - iG_t^{(D)})u_D \in D(H_0) = D(H)$ by Kato's result as summarized in Sec. 2. Here we recall that $G_t^{(D)}$ acts only on the function f in (3.2) and not on the φ_j.

We will only give the proof of Theorem 2.1 for the limit $t \to +\infty$, the argument for the limit $t \to -\infty$ being completely analogous.

We suppose for definiteness that the n clusters of D consist of r simple ones and p composite ones. Following Dollard's treatment of multichannel scattering for Coulomb-like potentials,[1] it is convenient to split (3.1) into three parts corresponding to (1) interaction between simple clusters (particles), (2) interaction between simple and composite clusters, and (3) interaction between composite clusters. We obtain from (3.1)

$$Z_D(t) \leq \sum_{a=1}^{3} Z_D^{(a)}(t), \tag{3.3}$$

where each summand has the following form:

$$Z_D^{(a)}(t) = \sum_{i<j} \left\| \left\{ V_{ij}(\mathbf{x}_i - \mathbf{x}_j) - V_{ij}^L \left(\left(\frac{-\nabla_{\mathbf{X}_{C_i}}}{M_{C_i}} - \frac{(-\nabla_{\mathbf{X}_{C_j}})}{M_{C_j}} \right) t + \nabla G_{t,ij}^{(D)(m-1)} \right) \right\} \times \exp(-itH_D - iG_t^{(D)(m)}) u_D \right\|. \tag{3.4}$$

Here, as in (2.20), the summation extends over all pairs (i,j) linking different clusters, and C_i, C_j denote the clusters linked by i and j. Terms of the form (3.4) for different values of a are distinguished by the choice of simple and/or composite clusters for C_i and C_j according to the discussion preceding (3.3).

We first consider the case $a=1$. It is sufficient to consider (3.4) for a fixed (but arbitrary) pair of the r simple particles, say 1 and 2. Call this term $Z^{(1)}_{D,12}(t)$. There will be at most a finite number of such estimates to obtain the final bound for $Z^{(1)}_D(t)$. By introducing center-of-mass and relative coordinates $\mathbf{R}$ and $\mathbf{y}$, respectively, for particles 1 and 2 along with the appropriate conjugate momenta, we can write $Z^{(1)}_{D,12}(t)$ in the following form:

$$Z^{(1)}_{D,12}(t)=\Big\| \Big[V_{12}(\mathbf{y})-V^L_{12}\Big(\frac{-\nabla_y t}{\mu_{12}}+\nabla G^{(D)(m-1)}_{t,12}\Big)\Big] \times\exp(-itH_{0y}-iG^{(D)(m)}_{t,12})f(\mathbf{y})\Big\| \times\big\|g(\mathbf{R})h(\mathbf{x}_3,\ldots,\mathbf{x}_r,\mathbf{X}_1,\ldots,\mathbf{X}_p)\prod_{j=1}^{p}\varphi_j\big\|, \tag{3.5}$$

where μ_{12} denotes the reduced mass of the two particles and H_{0y} the unique self-adjoint extension of $-\Delta_y/2\mu_{12}$. With the conditions (2.2)–(2.11) on the potential V_{12} and noting that $f\in S(R^3)$, where $S(R^3)$ denotes the set of all $f\in L^2(R^3)$ with $\hat{f}\in C^\infty_0(R^3\backslash\{0\})$, we can use Alsholm's single channel estimates to conclude that (3.5) is integrable for $t_0<t<\infty$ with a suitable $t_0>1$.[22]

For $a=2,3$ we follow Alsholm's technique and find by adding and subtracting a term,

$$Z^{(a)}_D(t)\le Z^{(a)\prime}_D(t)+c^{(a)}_D(t),\quad a=2,3,$$

where $Z^{(a)\prime}_D(t)$ is the same as (3.4) except that the superscript $(m-1)$ is replaced by m and

$$c^{(a)}_D(t)=\sum_{i<j}\Big\|\Big\{V^L_{ij}\Big(\Big(\frac{-\nabla_{\mathbf{x}_{C_i}}}{M_{C_i}}-\frac{(-\nabla_{\mathbf{x}_{C_j}})}{M_{C_j}}\Big)t+\nabla G^{(D)(m)}_{t,ij}\Big) - V^L_{ij}\Big(\Big(\frac{-\nabla_{\mathbf{x}_{C_i}}}{M_{C_i}}-\frac{(-\nabla_{\mathbf{x}_{C_j}})}{M_{C_j}}\Big)t+\nabla G^{(D)(m-1)}_{t,ij}\Big)\Big\}u_D\Big\|. \tag{3.6}$$

Noting that $Z^{(a)\prime}_D(t)$ $(a=2,3)$ depend upon $G^{(D)(m)}_{t,ij}$ but not upon $G^{(D)(m-1)}_{t,ij}$, we will hereafter suppress the dependence on m in our discussion of these quantities.

We next consider estimates for $Z^{(3)\prime}_D(t)$. As was the case for $a=1$, it is sufficient to consider estimates for a fixed pair of clusters C_1 and C_2 which are now, however, taken to be composite. Call this quantity $Z^{(3)\prime}_{D,12}(t)$. Suppose that C_1 consists of particles $r+1, r+2,\ldots,l$ and C_2 consists of particles $l+1,l+2,\ldots,w$. We will introduce center-of-mass and relative coordinates along with the corresponding conjugate momenta for this $(w-r)$-body system, leaving the coordinates of the remaining $N-(w-r)$ particles invariant. We write

$$Z_{D,12}(t)\le\Big\|\Big\{V_{lw}(\mathbf{x})-V^L_{lw}\Big(\frac{-\nabla_x t}{\mu_{lw}}+\nabla G^{(D)}_{t,lw}\Big)\Big\} \times\exp(-itH_{0x}-iG^{(D)}_{t,lw})f(\mathbf{x})\Big\| \times\Big\|g(\mathbf{R})h(\mathbf{x}_1,\ldots,\mathbf{x}_r,\mathbf{X}_3,\ldots,\mathbf{X}_p)\varphi_1(\mathbf{y}_{r+2},\ldots,\mathbf{y}_l) \times\varphi_2(\mathbf{y}_{l+2},\ldots,\mathbf{y}_w)\prod_{j=3}^{p}\varphi_j\Big\| + \Big\|\sum_{\substack{r+1\le i\le l\\ l+1\le j\le w}}\Big\{V_{ij}\Big(\mathbf{x}+\sum_{k=2}^{w}\gamma^{(ij)}_k\mathbf{y}_k\Big)-V^L_{ij}(\mathbf{x})\Big\} \times\exp(-itH_{0x}-iG^{(D)}_{t,lw}) \times f(\mathbf{x})\varphi_1(\mathbf{y}_{r+2},\cdots,\mathbf{y}_l)\varphi_2(\mathbf{y}_{l+2},\ldots,\mathbf{y}_w)\Big\| \times\Big\|g(\mathbf{R})h(\mathbf{x}_1,\ldots,\mathbf{x}_r,\mathbf{X}_3,\ldots,\mathbf{X}_p)\prod_{j=3}^{p}\varphi_j\Big\|, \tag{3.7}$$

where $\mathbf{x},\mathbf{R}$, and $\mathbf{y}_i=\mathbf{x}_{i-1}-\mathbf{x}_i$ $(i\in[r+2,l]\cup[l+2,w])$ denote, respectively, the difference of the center-of-mass vectors of the two clusters, the center-of-mass vector of the two-cluster system, and the relative (internal) coordinates of the clusters. In (3.7) we have introduced the total potential V_{lw} acting between the chosen clusters C_1 and C_2 in accordance with the definition (2.12). The quantity $G^{(D)}_{t,lw}$ is given by (2.20) in terms of this potential.

We have denoted the reduced mass of the two clusters by μ_{lw} and the unique self-adjoint extension of $-\Delta_x/2\mu_{lw}$ by H_{0x}. The scalars $\{\gamma^{(ij)}_k\}$ have the property $|\gamma^{(ij)}_k|\le 1$ and depend only upon the particle masses. In general, they have different values for different pairs (i,j). Also, we have set

$$\mathbf{y}_{l+1}=0 \tag{3.8}$$

in the second term of (3.7). This device permits us to write the summation over the variables $\{\mathbf{y}_k\}$ in a more compact manner.

Using conditions (2.2)–(2.11) on the potentials V_{ij} and noting that $f\in S(R^3)$, we again use Alsholm's single channel estimates to conclude that the first term of (3.7) is integrable for $t_0<t<\infty$ with a suitable $t_0>1$, Here one notes that the above conditions on the V_{ij} imply the conditions (2.13)–(2.17) on the potential V_{lw} as well as conditions analogous to (2.5)–(2.9) according to the discussion following (2.17), and one makes use of the results noted in Ref. 22.

Estimates for the case $a=2$ follow as a special case of the above discussion for $a=3$. One considers the situation in which one of the clusters C_1 or C_2 is simple instead of composite. An expression of the general form of (3.7) is obtained but somewhat simpler in structure.

We will complete the present section by showing that (3.6) is integrable for $t_0<t<\infty$ with an appropriate $t_0>1$. It is clearly sufficient to consider the case for a given pair of clusters C_1 and C_2. Call this term $c^{(a)}_{D,12}(t)$. As in the case of $Z^{(a)\prime}_D(t)$ we will only consider $a=3$. The necessary bounds for $a=2$ will then follow as a special case. By introducing the same coordinates as before we can write

$$c^{(3)}_{D,12}(t)=\Big\|\Big\{V^L_{lw}\Big(\frac{-\nabla_x t}{\mu_{lw}}+\nabla G^{(D)(m)}_{t,lw}\Big)-V^L_{lw}\Big(\frac{-\nabla_x t}{\mu_{lw}}+\nabla G^{(D)(m-1)}_{t,lw}\Big)\Big\} \times f(\mathbf{x})\Big\|\Big\|g(\mathbf{R})h(\mathbf{x}_1,\ldots,\mathbf{x}_r,\mathbf{X}_3,\ldots,\mathbf{X}_p) \times\varphi_1(\mathbf{y}_{r+2},\ldots,\mathbf{y}_l)\varphi_2(\mathbf{y}_{l+2},\ldots,\mathbf{y}_w)\prod_{j=3}^{p}\varphi_j\Big\|. \tag{3.9}$$

For the moment we will assume that each $V_{ij}^L \in C^\infty(R^3)$. It will be shown presently that this involves no loss in generality. It follows from (2.15) that this property then also holds for V_{lw}^L. One easily shows from the mean value theorem,[23] (2.15), (2.17), the analog of (2.9) for the decay exponents defined by (2.17), and the following estimate (valid for $1 \leq m \leq M$):

$$\left|\nabla G_{t,lw}^{(D)(m)}(\mathbf{p}) - \nabla G_{t,lw}^{(D)(m-1)}(\mathbf{p})\right| \leq C_K(1+t^{1-(m-1)\alpha_1-\alpha_m}), \quad (3.10)$$

that (3.9) is integrable for $t_K < t < \infty$. Here $\mathbf{p}=(p_1,p_2,p_3)$ denote the respective conjugate momenta of the variables $\mathbf{x}=(x_1,x_2,x_3)$ used in (3.7).

One can establish (3.10) as Alsholm did for a similar estimate in Lemma 6 of Ref. 12, showing in the process that these estimates are valid for $\mathbf{p} \in K$ with K any compact subset of $R^3 - \{0\}$ and the positive constants C_K and t_K depend on K. These restrictions suffice for our purposes (as they also did for Alsholm) because f in (3.9) denotes any element of $\underline{S}(R^3)$. Following Alsholm, we use the estimates (3.10) under the stipulation that no positive integral linear combination of the $\alpha_k(ij)$ is equal to unity. It can be shown that this involves no loss in generality. In particular, we can assume that $0 < \alpha_1(ij) < 1$. Naturally, similar remarks hold for the α_k defined by (2.17). In the derivation of (3.10) one also uses the condition $\beta(2) \geq 0$ which Alsholm has shown follows from (2.6) and (2.7).

We must now show that it is permissible to take each $V_{ij}^L \in C^\infty(R^3)$.[24] The proof involves the same basic ideas as in single channel scattering,[12,14] but the argument becomes more involved due to the more complicated kinematical structure of the multichannel situation. Consider a fixed pair (i,j). For a potential V_{ij} satisfying (2.2)–(2.4) with decay exponents satisfying (2.5)–(2.11) one defines the convolution $\bar{V}_{ij}^L = \omega^* V_{ij}^L$, where $\omega \in C_0^\infty(R^3)$, $\omega \geq 0$, $\|\omega\|_{L^1(R^3)}=1$, and sets $\bar{V}_{ij}^S = V_{ij}^S + V_{ij}^L - \bar{V}_{ij}^L$.

Then, $V_{ij} = \bar{V}_{ij}^S + \bar{V}_{ij}^L$ is also a decomposition of the potential V_{ij} into short and long range parts, respectively, satisfying (2.3) and (2.4) with decay exponents satisfying (2.5)–(2.11). One has $\bar{V}_{ij}^L \in C^\infty(R^3)$. Defining operators $\overline{G_t^{(D)(m)}}$ by (2.20) in terms of the $\bar{V}_{ij}^L$, one easily shows that if the strong limits

$$\text{s-lim}_{t\to\pm\infty} \exp(itH)\exp(-itH_D - i\overline{G^{(D)(m)}})$$

exist, then the limits (2.19) exist provided that the following strong limits also exist:

$$G_\pm = \text{s-lim}_{t\to\pm\infty} \exp[i(\overline{G_t^{(D)(m)}} - G_t^{(D)(m)})].$$

In order to prove the existence of the latter limits it suffices to show that

$$\left\| \sum_{i<j} \{\overline{V_{ij}}(t\vert_{C_iC_j} + \nabla\overline{G_{t,ij}^{(D)(m-1)}}) - V_{ij}^L(t\vert_{C_iC_j} + \nabla G_{t,ij}^{(D)(m-1)})\}u_D \right\| \quad (3.11)$$

is integrable for $-\infty < t < -t_0$ and $t_0 < t < \infty$ with some $t_0 > 1$ for all u_D of the form (3.2) with $f \in \underline{S}_D(R^{3n})$. Since the summation in (3.11) runs over all pairs (i,j) connecting different clusters, we can restrict ourselves to a fixed pair and consider the three cases of the discussion preceding (3.3), as we have done for the previous estimates in this section. For $a=1$ the estimates are reduced to those involving potentials for a single pair of particles, say (1,2). The required integrability then follows from a result of Alsholm.[25] For $a=3$ we have a similar type of estimate except that the potentials are V_{lw}^L and $\bar{V}_{lw}^L$, such as occur in (3.7). Here we have defined $\bar{V}_{lw}^L$ in terms of the $\bar{V}_{ij}^L$ as in (2.15). The required integrability for this case again follows from Alsholm's estimates[25] if we note, as we previously did in the case of (3.7), that the conditions (2.4)–(2.11) on the V_{ij}^L imply (2.15) and (2.17) and also conditions on V_{lw}^L analogous to (2.5)–(2.9). A similar argument applies to the $\bar{V}_{ij}^L$ and $\bar{V}_{lw}^L$. The integrability for $a=2$ follows as a special case of the argument for $a=3$.

This completes the proof of existence of the operators $G_\pm$.

4. CONCLUSION OF PROOF OF THEOREM 2.1: PROOF OF PROPOSITION 2.1

We now have to consider estimates for the following norm which occurs in the second term of (3.7):

$$W_D(t) = \left\| \sum_{\substack{r+1\leq i\leq l \\ l+1\leq j\leq w}} \{V_{ij}(\mathbf{x} + \sum_{b=2}^{w} \gamma_b^{(ij)}\mathbf{y}_b) - V_{ij}^L(\mathbf{x})\}\exp(-iY)f(\mathbf{x})\chi_D \right\|, \quad (4.1)$$

where we have set $Y = Y_t^{(D)} = tH_{0_x} + G_{t,lw}^{(D)}$ and

$$\chi_D = \varphi_1(\mathbf{y}_{r+2}, \ldots, \mathbf{y}_l)\varphi_2(\mathbf{y}_{l+2}, \ldots, \mathbf{y}_w). \quad (4.2)$$

The norm (4.1) is appropriate for the case $a=3$ but, as we have noted in Sec. 3, the corresponding object for $a=2$ can be obtained as a special case. Using the decompositions (2.2), we write

$$W_D(t) \leq W_D^S(t) + W_D^L(t),$$

where

$$W_D^S(t) = \sum_{\substack{r+1\leq i\leq l \\ l+1\leq j\leq w}} \left\| V_{ij}^S(\mathbf{x} + \sum_{b=2}^{w} \gamma_b^{(ij)}\mathbf{y}_b)\exp(-iY)f(\mathbf{x})\chi_D \right\| \quad (4.3)$$

and

$$W_D^L(t) = \sum_{\substack{r+1\leq i\leq l \\ l+1\leq j\leq w}} \left\| \{V_{ij}^L(\mathbf{x} + \sum_{b=2}^{w} \gamma_b^{(ij)}\mathbf{y}_b) - V_{ij}^L(\mathbf{x})\}\exp(-iY)f(\mathbf{x})\chi_D \right\|. \quad (4.4)$$

Estimates for (4.4) will be considered first. Using the result proved at the end of Sec. 3 that we can take each $V_{ij}^L \in C^\infty(R^3)$ and the mean value theorem, we write,

$$W_D^L(t) \leq C \sum_{\substack{r+1\leq i\leq l \\ l+1\leq j\leq w}} W_{D,ij}^L(t)$$

where

$$W_{D,ij}^L(t) = \left\| (1 + \left|\mathbf{x} + \theta \sum_{b=2}^{w} \gamma_b^{(ij)}\mathbf{y}_b\right|)^{-1-\alpha_1(ij)} \exp(-iY)f(\mathbf{x})\psi_D \right\| \quad (4.5)$$

with

$$\psi_D = \sum_{b=2}^{w} |\mathbf{y}_b|\chi_D. \quad (4.6)$$

Here we have used the estimate (2.4) for the potential gradients, and the parameter $\theta \in (0,1)$ comes from our application of the mean value theorem.[23]

We write the following operator identity which is obtained by Alsholm's technique,[12,14]

$$(\mathbf{x}+\theta\sum_{b=2}^{w}\gamma_b^{(ij)}y_b)\cdot\mathbf{p}\exp(-iY) = \exp(-iY)\left[tQ(|\mathbf{p}|)+\left(\mathbf{x}+\theta\sum_{b=2}^{w}\gamma_b^{(ij)}\mathbf{y}_b\right)\cdot\rho\right] \tag{4.7}$$

This identity is derived in the momentum representation using $x_j = i\partial/\partial p_j$ $(j=1,2,3)$. We have also used the fact that each component of each $\mathbf{y}_b$ commutes with each component of $\mathbf{p}$ and have defined

$$Q = Q(|\mathbf{p}|) = |\mathbf{p}|^2/\mu_{1w} + (|\mathbf{p}|/t)DG_{t,1w}^{(D)}. \tag{4.8}$$

This latter quantity is the same as a similar one used by Alsholm[12,14] in the single channel case except for a trivial change involving the reduced mass of the clusters, so that we will be able to take over his estimates involving Q to the multichannel case. The operator D in (4.8) is defined by[12,14]

$$\begin{aligned} Du &= \mathcal{F}^{-1}\frac{\partial}{\partial|\mathbf{p}|}\hat{u}, \quad \text{when } u=u(x), \\ Dv &= \frac{\partial}{\partial|\mathbf{p}|}v, \qquad \text{when } v=v(p), \end{aligned} \tag{4.9}$$

where $\mathcal{F}$ means Fourier transform.

Since by our assumptions V_{1w}^L satisfies Alsholm's conditions with regard to the decay exponents, we can take over the following estimates:

$$\begin{aligned} &|\nabla^k DG_{t,1w}^{(D)(m)}(\mathbf{p})| \le C_K(1+t^{1-\beta(k+1)}) \\ &\text{for } k\ge 0,\ k+m-1\le M, \end{aligned} \tag{4.10}$$

which are subject to the same restrictions concerning the momenta $\mathbf{p}$ and the decay exponents as was discussed in connection with (3.10).

From (4.8) and (4.10) we conclude with Alsholm that $Q^{-1}(|\mathbf{p}|)$ exists for $|\mathbf{p}|\neq 0$ for sufficiently large $|t|$ since $\beta(1)=\alpha_1>0$.

In order to obtain bounds for each norm (4.5), we will use (4.7) and an interpolation theorem of Alsholm[26] which states that if B is a positive self-adjoint operator (not necessarily bounded) on a Hilbert space, then for any $u\in D(B)$ and $0\le\rho\le 1$,

$$\|B^\rho u\| \le \|u\|^{1-\rho}\|Bu\|^\rho. \tag{4.11}$$

We will follow a straightforward variant of Alsholm's procedure and consider estimates for $\|A_{ij}^k\exp(-iY)f\psi_D\|$, $k\ge 0$, with A_{ij} the operator of multiplication by

$$(1+|\mathbf{x}+\theta\sum_{b=2}^{w}\gamma_b^{(ij)}\mathbf{y}_b|)^{-1}.$$

By applying (4.7) we obtain

$$\begin{aligned} \|A_{ij}^{k+1}\exp(-iY)f\psi_D\| &\le t^{-1}\|A_{ij}^k\exp(-iY)|\mathbf{p}|Q^{-1}f\psi_D\| \\ &\quad + t^{-1}\|A_{ij}^{k+1}\exp(-iY)(\mathbf{x}+\theta\sum_{b=2}^{w}\gamma_b^{(ij)}\mathbf{y}_b)\cdot\mathbf{p}Q^{-1}f\psi_D\| \\ &\le t^{-1}\|A_{ij}^k\exp(-iY)|\mathbf{p}|Q^{-1}f\psi_D\| \end{aligned} \tag{4.12}$$

$$+ t^{-1}\|A_{ij}^k\exp(-iY)(\mathbf{x}+\theta\sum_{b=2}^{w}\gamma_b^{(ij)}\mathbf{y}_b)\cdot\mathbf{p}Q^{-1}f\psi_D\|. \tag{4.13}$$

In particular, we find from (4.13), with $k=0$,

$$\|A_{ij}\exp(-iY)f\psi_D\| \le t^{-1}\||\mathbf{p}|Q^{-1}f\psi_D\| + t^{-1}\|\mathbf{x}\cdot\mathbf{p}Q^{-1}f\psi_D\| + t^{-1}\|\sum_{b=2}^{w}\gamma_b^{(ij)}\mathbf{y}_b\cdot\mathbf{p}Q^{-1}f\psi_D\|. \tag{4.14}$$

Using the bounds[12]

$$|\nabla^k Q^{-1}(|\mathbf{p}|)| \le C_K(1+t^{-\beta(k+1)}) \tag{4.15}$$

for $k\ge 0$, $m+k-1\le M$, and $\mathbf{p}\in K$, $t\ge t_K$ for any compact subset K of $R^3-\{0\}$, we find in a similar manner as Alsholm,

$$\|\mathbf{x}\cdot\mathbf{p}Q^{-1}f\psi_D\| \le C_K(\|f\|+\|Df\|)\|\psi_D\|, \tag{4.16}$$

for $K=\operatorname{supp}\hat{f}$.

To obtain an estimate for the last norm in (4.14), we follow a similar procedure as was used to derive (4.16). That is, we use the representation $y_{bh}=i(\partial/\partial q_{bh})(b\in[2,l]\cup[l+2,w]$, $h=1,2,3)$ where q_{bh} denotes the conjugate momentum to y_{bh} and obtain, taking into account (3.8),

$$\|\sum_{b=2}^{w}\gamma_b^{(ij)}\mathbf{y}_b\cdot\mathbf{p}Q^{-1}f\psi_D\| \le C_K\|f\|\sum_{b=2}^{w}\|D_b\psi_D\|,$$

$K=\operatorname{supp}\hat{f}$. Here we have used the commutativity property mentioned following (4.7) and have defined the operators D_b in terms of the derivatives[27] $\partial/\partial|\mathbf{q}_b|$ completely analogously to the definition of the operator D in (4.9). The final estimate for (4.14) now becomes

$$\|A_{ij}\exp(-iY)f\psi_D\| \le C_K t^{-1}[(\|f\|+\|Df\|)\|\psi_D\| + \|f\|\sum_{b=2}^{w}\|D_b\psi_D\|], \tag{4.17}$$

for $t\ge t_K$, where $K=\operatorname{supp}\hat{f}$. We will prove the following inequality:

$$\|A_{ij}^k\exp(-iY)f\psi_D\| \le C_K t^{-k}[(1+t^{-q-\beta(k+q+1)})\|f\|\sum_{a=0}^{k+q}\sum_{b=2}^{w}\|D_b^a\psi_D\| + t^{-q}\|D^{k+q}f\|\sum_{a=0}^{k+q-1}\sum_{b=2}^{w}\|D_b^a\psi_D\|] \tag{4.18}$$

for $t\ge t_K$, $K=\operatorname{supp}\hat{f}$, $k\ge 0$, $q\ge 0$, $k+q+m-1\le M$, and $f\in\underline{S}(R^3)$. ψ_D is of course defined by (4.6). The constant C depends on w as well as on the support of $\hat{f}$. The numbers $\beta(k)$ are defined by (2.10) and (2.11) in terms of the decay exponents of V_{1w}^L, which have a definition of the form (2.17).

Following the ideas of Alsholm's proof of an analogous result in the single channel case, we will prove (4.18) by induction in k and q. For $k=0$, (4.18) obviously holds for all $q\ge 0$ with $q+m-1\le M$, and for $k=1$, (4.17) shows that (4.18) holds for $q=0$.[28] Assume that, for some $k\ge 0$, (4.18) holds for all $q\ge 0$ such that $k+q+m-1\le M$. We shall prove (4.18) with k replaced by $k+1$ and for all $q\ge 0$ such that $k+q+m\le M$.

By using (4.18) with $q=0$ for the terms on the right side of (4.13) one shows that (4.18) holds with $q=0$ and k replaced by $k+1$. In deriving this result we make use of the following inequalities

$$\left.\begin{aligned}\|D^k|\mathbf{p}|Q^{-1}f\| &\le C_K[(1+t^{-\beta(k+1)})\|f\| + \|D^k f\|] \\ \|D^k \mathbf{x}\cdot\mathbf{p}Q^{-1}f\| &\le C_K[(1+t^{-\beta(k+2)})\|f\| + \|D^{k+1}f\|]\end{aligned}\right\}, \quad (4.19)$$

$$K=\operatorname{supp}\hat{f}, \quad (4.20)$$

$$\|D_b^a y_{h\lambda}\psi_D\| \le C\sum_{r=1}^{a+1}\|D^r{}_b\psi_D\|, \quad (4.21)$$

which are easily obtained where, in the cases of (4.19) and (4.20), we use (4.15) and the following interpolation inequality of Alsholm:

$$(1+t^{-\beta(i+1)})\|D^{j-i}w\| \le C_K[(1+t^{-\beta(j+1)})\|w\| + \|D^j w\| \quad (4.22)$$

valid for $t \ge t_K$, with $K=\operatorname{supp}w$, $w\in \underline{S}(R^3)$. We emphasize that (4.22) has only been applied to norms involving f and its derivatives and not to the function ψ_D or its derivatives.[27]

Now we use induction in q and assert that (4.18) holds with k replaced by $k+1$ and q replaced by $q+1$. The truth of this assertion follows from using (4.12) with the first term on the right side estimated by (4.18) with q replaced by $q+1$, and the remaining term estimated by (4.18) with k replaced by $k+1$. In deriving this result we have again used (4.19)—(4.21) as well as the interpolation inequalities (4.22) and the following inequality of Alsholm:

$$t^{-1}\|Dw\| \le C_K[\|w\| + t^{-k-q-2}\|D^{k+q+2}w\|]$$

for $t\ge t_K$, $K=\operatorname{supp}\hat{w}$, $w\in\underline{S}(R^3)$. This completes the proof of (4.18).

We can now obtain the required estimate for (4.5) by using (4.18) along with (4.11) wherein the operator B is taken as A_{ij}^k in (4.18) and we set $k\rho = 1+\alpha_1(ij)$. It is then seen that, since we have taken $0<\alpha_1(ij)<1$, it suffices to have $k\ge 2$ in order that $\rho<1$. In particular, for $k=2$ we obtain

$$\begin{aligned}W_{D,ij}^L(t) \le C_K t^{-1-\alpha_1(ij)}&\|f\|^{[1-\alpha_1(ij)]/2}\ \|\psi_D\|^{[1-\alpha_1(ij)]/2} \\ &\times[\|f\| + \|D^{q+2}f\|]^{[1+\alpha_1(ij)]/2} \\ &\times\Big(\sum_{a=0}^{q+2}\sum_{b=2}^{w}\|D_b^a\psi_D\|\Big)^{[1+\alpha_1(ij)]/2},\end{aligned} \quad (4.23)$$

where we have used the fact that there exists a $q\ge 0$ such that[12]

$$q+\beta(q+3)>0. \quad (4.24)$$

Since $\alpha_1(ij)>0$, it follows that $W_{D,ij}^L(t)$ is integrable for all $f\in\underline{S}(R^3)$ and $t\ge t_K$, $K=\operatorname{supp}\hat{f}$, subject to the conditions that $D_b^a\psi_D$ $(0\le a\le q+2,\ b\in[2,l]\cup[l+2,w])$ exist and are square integrable over the appropriate space. Subject to these conditions, the required integrability of $W_D^L(t)$ immediately follows.

To obtain an estimate for (4.3), we use the bounds (2.3) to write

$$W_D^S(t) \le C\sum_{\substack{r+1\le i\le l\\ l+1\le j\le w}} W_{D,ij}^S(t),$$

where

$$W_{D,ij}^S(t) = \|(1+|\mathbf{x}+\sum_{b=2}^{w}\gamma_b^{(ij)}\mathbf{y}_b|)^{-1-\epsilon(ij)}\exp(-iY)f\chi_D\|. \quad (4.25)$$

It is seen that (4.25) is of the same form as (4.5) with $\alpha_1(ij)$ replaced by $\epsilon(ij)$ and ψ_D replaced by χ_D. In view of the conditions on $\epsilon(ij)$ noted after (2.3), it is clear that the same method applies as in our analysis of (4.5). We obtain a bound of the form (4.23) with $\alpha_1(ij)$ replaced by $\epsilon(ij)$ and ψ_D replaced by χ_D so that (4.25) is indeed integrable for all $f\in\underline{S}(R^3)$ for $t\ge t_K$, $K=\operatorname{supp}\hat{f}$, subject, of course, to the conditions stated after (4.24) wherein ψ_D is replaced by χ_D. With this stipulation, the required integrability condition for $W_D^S(t)$ immediately follows.

In order to show that the stated conditions on the functions χ_D and ψ_D are indeed satisfied, we note that, by the definition of the functions u_D stated after (3.2), we have $\varphi_1\in C_0^\infty(R^{3[l-(r+1)]})$ and $\hat{\varphi}_2\in C_0^\infty(R^{3[w-(l+1)]})$. Thus, in particular, $\varphi_1\in\mathcal{S}(R^{3[l-(r+1)]})$ and $\varphi_2\in\mathcal{S}(R^{3[w-(l+1)]})$, where $\mathcal{S}$ denotes the space of C^∞ functions of rapid decrease at infinity of Schwartz. It immediately follows that $D_b^a\chi_D$ and $D_b^a\psi_D$ $(0\le a\le q+2,\ b\in[2,l]\cup[l+2,w])$ exist and are square integrable over the appropriate space.

With the existence of the limits (2.19) now established, the fact that $\Omega_D^\pm$ are isometries follows from their being strong limits of unitary operators.

In order to establish the intertwining relations (2.21), we first note that the long range part of the effective potential which appears in $G_t^{(D)}$, as defined in (2.20a), consists of a sum of potentials of the form (2.15) each with a set of decay exponents $\{\alpha_k, 0\le k\le M\}$ with α_k defined by (2.17). We write

$$G_{t+s}^{(D)(m)} - G_t^{(D)(m)} = \sum_{C_iC_j}(G_{t+s,C_iC_j}^{(D)(m)} - G_{t,C_iC_j}^{(D)(m)}), \quad (4.26)$$

where the summation runs over all distinct clusters as indicated in (2.20a). For each pair of clusters (C_i, C_j) we can now introduce a momentum variable $\mathbf{p}=(p_1,p_2,p_3)$, each component of which is conjugate to the corresponding component of a coordinate variable of the type of $\mathbf{x}=(x_1,x_2,x_3)$ used in (3.7). Then we find that

$$G_{t+s,C_iC_j}^{(D)(m)}(\mathbf{p}) - G_{t,C_iC_j}^{(D)(m)}(\mathbf{p}) \to 0, \quad 1\le m\le M,$$

as $t\to\pm\infty$ for $-\infty<s<\infty$ and $\mathbf{p}$ belonging to any compact subset of $R^3-\{0\}$. Since there are only a finite number of terms in the summation in (4.26), it follows that

$$\operatorname*{s-lim}_{t\to\pm\infty}\exp[i(G_{t+s}^{(D)(m)} - G_t^{(D)(m)})] = I$$

for $1\le m\le M$ and $-\infty<s<\infty$. The intertwining relations are now easily established from this result and a standard construction. This concludes the proof of Theorem 2.1.

In order to prove Proposition 2.1, we first define the wave operators $\Omega_\alpha^\pm$, for a channel α consistent with a given cluster decomposition D, as the respective restrictions of $\Omega_D^\pm$ to the subspace of channel states (2.22), as previously noted in Sec. 2. We will conclude the paper by proving that the ranges of Ω_α^+ and Ω_β^+ are orthogonal for distinct channels α and β. The proof for Ω_α^- and Ω_β^- is similar.

The simplest method of proof seems to be to show that

$$\text{s-}\lim_{t\to+\infty}\frac{d}{dt}\exp(-iG_t^{(D)})h=0 \tag{4.27}$$

for all h belonging to a dense subset of $\mathcal{H}_\alpha$, in which α is a channel consistent with D. A condition similar to (4.27) has been discussed by Amrein, Georgescu, and Martin,[9] in their postulational approach to multichannel scattering, who show that their condition coupled with certain well-known properties of the channel Hamiltonians is sufficient to establish the desired orthogonality. By following their argument, one easily shows that orthogonality also follows if their condition is replaced by (4.27).

Returning to the description of an arbitrary cluster decomposition given following (3.2), we will prove (4.27) for all h of the form (2.22) with $f\in\underline{S}_D(R^{3n})$, where α denotes a channel consistent with the decomposition D. Noting that

$$\left|\nabla G_{t,ij}^{(D)(m-1)}(\mathbf{p})\right|\leq C_K(1+t^{1-\beta(1)}),\quad 1\leq m\leq M, \tag{4.28}$$

(for $t\geq t_K$, where K denotes any compact subset of $R^3-\{0\}$) which follows from an inequality of Alsholm, we use the momentum representation to see that the argument of each V_{ij}^L in (2.20b) is an increasing function of t since we may assume that each $\alpha_1(ij)$ is less than unity.

By splitting the quantity $\|(d/dt)\exp(-iG_t^{(D)(m)})h\|$ into three cases, as was done earlier in the proof of existence of the operators $\Omega_D^\pm$, and using (2.20) and (4.28) coupled with the estimate (2.4) for $k=0$ and (2.5), one easily verifies that (4.27) holds for all h of the stated type. This completes the proof of Proposition 2.1.

We note from the proof of Theorem 2.1, in particular the discussion centering around the operators $G_\pm$, that $\Omega_D^\pm$ are generally not unique. This leads to nonunique wave operators $\Omega_\alpha^\pm$, as we have indicated in the paragraph following (2.17).

After the present paper was written, the author received a preprint[29] in which a theory of multichannel scattering by time-dependent potentials is developed by a generalization of the approach of Ref. 15.

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[1]J.D. Dollard, thesis, Princeton University, 1963.
[2]J.D. Dollard, J. Math. Phys. **5**, 729 (1964).
[3]J.D. Dollard, Rocky Mt. J. Math. **1**, 5 (1971); **2**, 217(E) (1972).
[4]C. Chandler and A.G. Gibson, J. Math. Phys. **15**, 291 (1974).
[5]E. Prugovečki and J. Zorbas, Nucl. Phys. A **213**, 541 (1973).
[6]J. Zorbas, J. Phys. A **7**, 1557 (1974).
[7]R.B. Lavine, Commun. Math. Phys. **20**, 301 (1971).
[8]E. Prugovečki, J. Math. Phys. **14**, 957 (1973); **16**, 442(E) (1975). See in particular Sec. 3.
[9]W.O. Amrein, V.Georgescu, and Ph.A. Martin, in *Physical Reality and Mathematical Description*, edited by Ch.P. Enz and J. Mehra (Reidel, Dordrecht, The Netherlands, 1974).
[10]A nice review of this work has been given by W.O. Amrein, in *Scattering Theory in Mathematical Physics*, edited by J. La Vita and J.-P. Marchand (Reidel, Dordrecht, The Netherlands, 1974).
[11]For a treatment of classical scattering see I.W. Herbst, Commun. Math. Phys. **35**, 193 (1974).
[12]P.K. Alsholm, thesis, University of California, Berkeley, 1972. See also Ref. 14.
[13]V.S. Buslaev and V.B. Matveev, Teor. Mat. Fiz. **2**, 367 (1970) [Theoret. Math. Phys. **2**, 266 (1970)].
[14]P. Alsholm and T. Kato, in *Proceedings of the Symposium on Pure Mathematics* (Am. Math. Soc., Providence, R.I., 1971), Vol. XXIII, pp. 393–99.
[15]J.H. Hendrickson, J. Math. Phys. **16**, 768 (1975).
[16]The constant C in (2.3), (2.4), (2.14), and 2.15) generally has different values in each of these inequalities, although we have used the same symbol in each case. We will follow this practice throughout the paper, using the symbol C for a generic constant.
[17]T, Kato, Trans. Amer. Math. Soc. **70**, 195 (1951). See also Section V.5 of T. Kato, *Perturbation Theory for Linear Operators* (Springer, New York, 1966).
[18]For potentials of the type just described, (4.27) is not satisfied.
[19]W. Hunziker, J. Math. Phys. **6**, 6 (1965).
[20]W. Hunziker, Helv, Phys. Acta **39**, 451 (1966).
[21]W. Hunziker, in *Lectures in Theoretical Physics*, edited by A.O. Barut and W.E. Brittin (Gordon and Breach, New York, 1968), Vol. XA.
[22]This conclusion follows from Alsholm's estimates if $\alpha_1(12)\leq 1$, an inequality which is easily derived from (2.5) by use of the method of proof of Proposition 3 in Appendix 1 of Ref. 12.
[23]We use the formulation given by T.M. Apostol, *Mathematical Analysis* (Addison-Wesley, Reading, Mass., 1958), p. 117, Theorem 6-17.
[24]The proof of these statements follows from Lemma 1 of Ref. 12 with exception of those involving the decay exponent α_0, with which Alsholm was not concerned. However, the proof of these follows immediately from the properties of the quantities involved.
[25]See the proof of Lemma 2 in Ref. 12.
[26]This result is actually a special case of Theorem 4.1, p. 49, of-M.A. Krasnosel'skii, *Topological Methods in the Theory of Nonlinear Integral Equations* (Pergamon, London, 1964).
[27]We have not yet shown that the indicated differentiations are permitted. This will be discussed later in this section.
[28]Here one uses the condition $\beta(2)\geq 0$ previously noted in our discussion of (3.10).
[29]J.H. Hendrickson, "n-Body Scattering into Cones with Long-Range Time-Dependent Potentials," J. Math. Phys. (to be published).

A spectral representation on ordinary linear difference equation with operator-valued coefficients of the second order*

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The spectral theory associated with two-dimensional linear partial difference operators of the second order on the pseudo-Hilbert space originated by Berezanskii is studied. The present discussion, partly in Govindaraju's style, is essentially based on the Kodaira's method.

1. INTRODUCTION

In the investigation of spectral properties of two- or three-dimensional harmonic lattices in the nearest neighbor interaction approximation, Asahi[1] has proposed a method in which partial difference systems of the second order are reduced to ordinary ones by using a matrix whose elements are operators. But the system considered by Asahi is restricted finitely in the y direction and extended infinitely in the x direction; the present author intends to make the theory complete by extending it to the system infinitely spreaded in both directions in the case of bounded operators.

On the other hand, Berezanskii[2] has constructed a pseudo-Hilbert space in order to treat the operator-coefficient difference equations with application to the system of partial difference operators of the second order. Since Berezanskii has performed the proof of spectral expansion theory by using orthonormal operator-valued polynomials, the present author intends, therefore, to develop the spectral theory of partial difference operators of the second order in the x direction and of any even order in the y direction, in a manner different from Berezanskii. Namely, the methods the present article depends on are those of Kodaira's[3-6] and Govindaraju's[7] types, but using the pseudo-Hilbert space of Berezanskii.

This article, partly reported,[8] is composed of two parts: Part I is devoted to the investigation of algebraic structure of partial difference operator of second order in the x direction, the results of which are summarized in classification of operators. In Part II we study the spectral expansion theory. The application of the spectral theory to physical systems, two-dimensional lattice crystals, will be discussed later.

PART I

2. DIFFERENCE EXPRESSION

We consider an ordinary linear formally self-adjoint difference expression of order two with operator coefficients given by

$$(Lu)(x)=Q^{-1}(x)\{P_1(x)\,u(x+1)+P_0(x)\,u(x)+P_1(x-1)\,u(x-1)\}, \tag{2.1}$$

where x denotes an integer, which runs through a subset $\mathbf{D}$ of $\mathbf{Z}$, the set of all integers, and $Q(x)$, $P_1(x)$, and $P_0(x)$ are all bounded Hermitian operators on a Hilbert space H. We also assume that $Q(x)$ and $P_1(x)$ are positive-definite for all $x\in\mathbf{D}$; i.e., the inner product $(Q(x)v,v)_H$ and $(P_1(x)v,v)_H$ are positive for every non-zero element v belonging to H. Since the inverse of $Q(x)$ exists for all $x\in\mathbf{D}$, $(Q(x)v,v)_H=0$ implies that $v=0$ for all $x\in\mathbf{D}$, which condition holds also for $P_1(x)$.

Although $u(x)$ appeared in Eq. (2.1) is supposed as an element of H, we treat in what follows the corresponding difference equation for the operator $U(x)$ from H into H, given by

$$(LU)(x)=Q^{-1}(x)\{P_1(x)\,U(x+1)+P_0(x)\,U(x)+P_1(x-1)\,U(x-1)\}, \tag{2.2}$$

where x belongs to $\mathbf{D}$.

By $L(H_1,H_2)$ we denote a set of all bounded linear operators from a Hilbert space H_1 into a Hilbert space H_2. Let us define an operator $L_x\in L(H,H)$ by $(LU)(x)=L_xU(x)$. Then, the operator L corresponds one-to-one to a sequence $(\cdots,L_x,L_{x+1},\cdots)$ which belongs to a space $\sum_{x=a}^{b}\oplus L(H,H)$, where a and b $(a<b)$ stand for the boundary points, being allowed to be $a=-\infty$ and $b=+\infty$. By putting $H'=\sum_{x=a}^{b}\oplus H$ as in Berezanskii, we can suppose L belongs to a Hilbert space $H_0=L(H,H')$. The construction of a Hilbert space H_0 is discussed on the Appendix.

3. THE DIFFERENCIAN AND THE LAGRANGE'S FORMULA

We introduce a product for the operators in H defined by

$$\langle A,B\rangle_H(x)=A^*(x)\,Q(x)\,B(x). \tag{3.1}$$

Since $P_1(x)$, $P_0(x)$, and $Q(x)$ are assumed to be Hermitian, it then holds that

$$\langle LU,V\rangle_H(x)-\langle U,LV\rangle_H(x)=[U,V](x)-[U,V](x-1), \tag{3.2}$$

where we have put

$$[U,V](x)=U^*(x+1)\,P_1(x)V(x)-U^*(x)\,P_1(x)\,V(x+1), \tag{3.3}$$

which we call the *differencian* associated with the operator L. Furthermore, we introduce a symbol for summation given by

$$\mathbf{S}_y^z \cdots \Delta x \equiv \begin{cases} \sum_{x=y+1}^{z} \cdots, & \text{for } z \geq y+1, \\ 0, & \text{for } z = y, \\ -\sum_{x=z+1}^{y} \cdots, & \text{for } y \geq z+1. \end{cases}$$

Then it follows from Eq. (3.2) that

$$\mathbf{S}_y^z \{\langle LU, V\rangle_H(x) - \langle U, LV\rangle_H(x)\}\Delta x = [U, V](z) - [U, V](y), \tag{3.4}$$

which is called the *Lagrange's formula*.

For later convenience, we give another expression for the differencian:

$$[U, V](x) = (W^*[U]BW[V])(x), \tag{3.5}$$

where we have put

$$B(x) = \begin{pmatrix} 0 & -P_1(x) \\ P_1(x) & 0 \end{pmatrix} \quad \text{and} \quad W[V] = \begin{pmatrix} V(x) \\ V(x+1) \end{pmatrix}. \tag{3.6}$$

It is easily seen that the differencian has the following properties:

$$\begin{aligned} &[U+V, X](X) = [U, X](x) + [V, X](x), \\ &[U, V]^*(x) = -[V, U](x). \end{aligned} \tag{3.7}$$

4. SOME RESULTS FROM THE LAGRANGE'S FORMULA

Let E_H be the unity operator in H, and denote by $\hat{l}$ for each complex number l the operator lE_H, of which the main property we use is the commutativity to any operators in H.

If $U(x)$ and $V(x)$ satisfy the equations $(LU)(x, l) = U(x, l)\hat{l}$ and $(LV)(x, m) = V(x, m)\hat{m}$ respectively, then we obtain from the Lagrange's formula (3.4) an expression $(\bar{l} - m)\mathbf{S}_y^z\langle U, V\rangle_H(x)\,\Delta x = [U, V](z) - [U, V](y)$, where we have used the property $\hat{l}^* = \bar{l}E_H$. If the operator $U(x)$ can be considered as a function of complex number l, $U(x) = U(x, l)$, then we can define a complex conjugate operator $\bar{U}(x, l)$ of $U(x, l)$ by $\bar{U}(x, l) = U(x, \bar{l})$. Furthermore, we define for the operator L in $L(H, H')$ the complex conjugate by

$$\begin{aligned} (\bar{L}U)(x) = {} & [Q^{-1}(x)]^* \{P_1^*(x)\,U(x+1) + P_0^*(x)\,U(x) \\ & + P_1^*(x-1)\,U(x-1)\}. \end{aligned} \tag{4.1}$$

Then, from the assumption of Hermicity of $Q(x)$, $P_1(x)$, and $P_0(x)$ for all $x \in \mathbf{D}$, we have $\bar{L} = L$, which gives the relation $(L\bar{U})(x, l) = \bar{U}(x, l)\hat{l}^*$.

It holds from the Lagrange's formula that $0 = (\bar{l} - l) \times \mathbf{S}_y^z\langle U, \bar{U}\rangle_H(x)\Delta x = [U, \bar{U}](z) - [U, \bar{U}](y)$, which implies that, for $U(x, l)$ satisfying the equation $(LU)(x, l) = U(x, l)\hat{l}$, the differencian $[U, \bar{U}](x)$ does not depend on x. In such cases we write $[U, \bar{U}]$ instead of $[U, \bar{U}](x)$.

By putting $V = U$ and consequently $m = l$, in other words, when $V(x, m)$ satisfies the same equation for $U(x, l)$, the Lagrange's formula is reduced to

$$-2i\,\mathrm{Im}(l)\,\mathbf{S}_y^z\langle U, U\rangle_H(x)\Delta x = [U, U](z) - [U, U](y), \tag{4.2}$$

which we call the *Green's formula*.

By the way we define the *transpose* of U by

$$\begin{aligned} &U^t(x, l) = \overline{U^*(x, l)}, \\ &(U^t(x, l)v, v)_H = (v, \overline{U(x, l)}v)_H. \end{aligned} \tag{4.3}$$

5. A CANONICAL SYSTEM OF FUNDAMENTAL SOLUTIONS

By the canonical system of fundamental solutions of the equation

$$(LU)(x, l) = U(x, l)\hat{l}, \quad x \in \mathbf{D}, \tag{5.1}$$

we mean the set of solutions $S_1(x, l)$ and $S_2(x, l)$ satisfying the following three conditions simultaneously:

$$[S_j(l), S_k(l)] = \epsilon_{jk}E_H \quad j, k = 1, 2, \tag{5.2}_1$$

$$\overline{S_j(x, \bar{l})} = S_j(x, l), \quad j = 1, 2, \tag{5.2}_2$$

and

$$S_j(x, l), \quad j = 1, 2, \text{ are integral functions of } l, \tag{5.2}_3$$

where the matrix $[\epsilon_{jk}]$ is given by

$$[\epsilon_{jk}] = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{5.3}$$

We can prove the existence of such a system of solutions by using the transfer-matrix method: We write Eq. (5.1) in a matrix form

$$W[U](x) = T(x) \cdot W[U](x-1), \tag{5.4}$$

where we have put

$$T(x) = \begin{pmatrix} 0 & E_H \\ -P_1^{-1}(x)P_1(x-1) & P_1^{-1}(x)\{Q(x)\hat{l} - P_0(x)\} \end{pmatrix}. \tag{5.5}$$

Successive applications of Eq. (5.4) give us the relation $W[U](x) = (T(x) \cdots T(c+1)) \cdot W[U](c)$, from which we have

$$U(x) = (T(x) \cdots T(c+1))_{11}\,U(c) + (T(x) \cdots T(c+1))_{12}\,U(c+1), \tag{5.6}$$

where c is a fixed integer contained in $\mathbf{D}$.

Since $(U(c), U(c+1))$ is a two-dimensional vector, we have two independent solutions of Eq. (5.1) by constructing two suitable independent vectors as $(U(c), U(c+1))$. Now we proceed to construct such two vectors: First, solving the eigenvalue problem $B(x)Y = \lambda Y$, we have two eigenvalues $\lambda_1 = iP_1(x)$ $(= -\lambda_2)$ with the corresponding normalized eigenvectors Y_1 and Y_2 given by

$$Y_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} iE_H \\ E_H \end{pmatrix} \quad \text{and} \quad Y_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} -iE_H \\ E_H \end{pmatrix}.$$

We introduce real (Hermitian-operator-component) vectors W_1 and V_1 by putting $Y_1 = (1/\sqrt{2})(W_1 + iV_1) \times \exp(-i\beta)$, β being any given real number. Then W_1 and V_1 are expressed in the form

$$W_1 = \begin{pmatrix} -\sin\beta \\ \cos\beta \end{pmatrix}E_H \quad \text{and} \quad V_1 = \begin{pmatrix} \cos\beta \\ \sin\beta \end{pmatrix}E_H.$$

Let us put

$$D(x)=(W_1, V_1)\begin{pmatrix}-1/\sqrt{P_1(x)} & 0\\ 0 & \sqrt{P_1(x)}\end{pmatrix}$$
$$=\begin{pmatrix}\sin\beta & \cos\beta\\ -\cos\beta & \sin\beta\end{pmatrix}P_1^{-1/2}(x).$$

Then it is easily seen that

$$D^t(x)B(x)D(x)=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}E_H.$$

If we choose $S_j(c)=e_j^{(0)}$ and $S_j(c+1)=e_j^{(1)}$, $j=1,2$, as

$$\begin{pmatrix}e_1^{(0)} & e_2^{(0)}\\ e_1^{(1)} & e_2^{(1)}\end{pmatrix}=D(c),$$

and put

$$S_j(x,l)=(T(x)\cdots T(c+1))_{11}e_j^{(0)}+(T(x)\cdots T(c+1))_{12}e_j^{(1)}, \tag{5.7}$$

then the condition $(5.2)_1$ is satisfied, and furthermore $S_j(c)$ and $S_j(c+1)$, $j=1,2$, are Hermitian. Since the domain and range of $P_1(c)$ is the whole space H, we see from the construction of the operators $S_j(x,l)$, $j=1,2$, that $S_j(x,l)$ has domain and the range H for $j=1,2$, for all $x\in\mathbf{D}$.

Conditions $(5.2)_2$ and $(5.2)_3$ are easily verified to be satisfied by the operators given by Eq. (5.7).

It is easily shown from the Lagrange's formula that the following formula holds:

$$-2i\,\mathrm{Im}(l)\,\mathbf{S}_c^z\langle S_j(l),S_k(l)\rangle_H(x)\Delta x$$
$$=[S_j(l),S_k(l)](z)-\epsilon_{jk}E_H, \tag{5.8}$$

where we have used the relations $(5.2)_1$.

6. SOME RELATIONS FROM THE GREEN'S FORMULA

For later use we develop some formulae related to the Green's formula. First of all, it is easily seen that, for any $A\in H$,

$$(\mathbf{S}_c^z\langle S_j(l),S_j(l)\rangle_H(x)\Delta x\cdot A,A)_H$$
$$=\mathbf{S}_c^z(Q(x)S_j(x,l)A,S_j(x,l)A,S_j(x,l)A)_H\,\Delta x. \tag{6.1}$$

Since the operator $Q(x)$ is positive-definite, we see the operator $\mathbf{S}_c^z\langle S_j(l),S_j(l)\rangle_H(x)\,\Delta x$ is also positive-definite for $z\geq c+1$. Hence it turns out that, for $\mathrm{Im}(l)\neq 0$, the operator $[-2i\,\mathrm{Im}(l)]^{-1}[S_j(l),S_j(l)](z)$, $j=1,2$, is also positive-definite:

$$-[1/2i\,\mathrm{Im}(l)][S_j(l),S_j(l)](z)>0,\quad j=1,2,$$

and it is easily shown that this operator is Hermitian.

Next we derive some useful relations in later sections. For brevity we introduce some notations:

$$F(x,l)=W[S_1(l)](x)=\begin{pmatrix}S_1(x,l)\\ S_1(x+1,l)\end{pmatrix},$$
$$H(x,l)=W[S_2(l)](x)=\begin{pmatrix}S_2(x,l)\\ S_2(x+1,l)\end{pmatrix}, \tag{6.2}$$

$$K(x,l)=(FH)(x,l)=\begin{pmatrix}S_1(x,l) & S_2(x,l)\\ S_1(x+1,l) & S_2(x+1,l)\end{pmatrix}.$$

Then the relation $(5.2)_1$ is expressed in the form

$$(K^*B\bar{K})(x,l)=J\quad\text{or}\quad(K^tBK)(x,l)=J, \tag{6.3}$$

where $J=[\epsilon_{jk}E_H]$. It holds that $(K^*BK)(x,l)$ $=(K^*B\bar{K}\bar{K}^{-1}K)(x,l)=J(\bar{K}^{-1})(x,l)$, so that $[(K^*BK)J^{-1}](x,l)$ $=J(\bar{K}^{-1}K)(x,l)J^{-1}$, which provides the relation $[(K^*BK)J^{-1}(K^tB\bar{K})](x,l)=J$. Since $J^{-1}=J$, we obtain

$$[(K^*BK)J(K^tB\bar{K})](x,l)=-J. \tag{6.4}$$

From the identity

$$(K^*BK)(x,l)=\begin{pmatrix}(F^*BF) & (F^*BH)\\ (H^*BF) & (H^*BH)\end{pmatrix}(x,l),$$

Eq. (6.4) is reduced to

$$[(F^*BH)(F^tB\bar{F})](x,l)-[(F^*BF)(H^tB\bar{F})](x,l)=0, \tag{6.5}_1$$
$$[(F^*BH)(F^tB\bar{H})](x,l)-[(F^*BF)(H^tB\bar{H})](x,l)=E_H, \tag{6.5}_2$$
$$[(H^*BH)(F^tB\bar{F})](x,l)-[(H^*BF)(H^tB\bar{F})](x,l)=-E_H \tag{6.5}_3$$
$$[(H^*BH)(F^tB\bar{H})](x,l)-[(H^*BF)(H^tB\bar{H})](x,l)=0. \tag{6.5}_4$$

Now we can prove the following relation:

$$(F^*BF)(x,l)+(H^tB\bar{H})^{-1}(x,l)$$
$$=[(F^*BH)(H^*BH)^{-1}(H^*BF)](x,l). \tag{6.6}$$

Since $(H^*BH)(x,l)$ has its inverse by the property that $(H^*BH)(x,l)=-[2i\,\mathrm{Im}(l)]^{-1}[S_2(l),S_2(l)](x)>0$ for all $\mathrm{Im}(l)\neq 0$, we have, from Eq. $(6.5)_4$, $(F^tB\bar{H})(x,l)$ $=[(H^*BH)^{-1}(H^*BF)(H^tB\bar{H})](x,l)$, so that it holds that $[(F^*BH)(F^tB\bar{H})](x,l)=[(F^*BH)(H^*BH)^{-1}(H^*BF)(H^tB\bar{H})]$ $\times(x,l)$. Using Eq. $(6.5)_2$, we obtain $[(F^*BH)(H^tB\bar{H})](x,l)$ $+E_H=[(F^*BH)(H^*BH)^{-1}(H^*BF)(H^tB\bar{H})](x,l)$, from which we have Eq. (6.6).

7. RADIUS OPERATOR

Since the operator $-[2i\,\mathrm{Im}(l)]^{-1}[S_2(l),S_2(l)](x)$ is positive-definite, we define the operator $R(x,l)$ by

$$R(x,l)=-i\{[S_2(l),S_2(l)](x)\}^{-1}, \tag{7.1}$$

which we call the *radius operator*. This operator is easily found to be Hermitain and has the property

$$R(x,l)\begin{cases}>0, & \text{for } \mathrm{Im}(l)>0,\\ <0, & \text{for } \mathrm{Im}(l)<0.\end{cases} \tag{7.2}$$

By making use of the Green's formula, we can express this radius operator in the form

$$R(x,l)=[1/2\,\mathrm{Im}(l)]\{\mathbf{S}_c^z\langle S_2(l),S_2(l)\rangle_H(x)\,\Delta x\}^{-1}. \tag{7.3}$$

We see that the operator $P(z,l)=\mathbf{S}_c^z\langle S_2(l),S_2(l)\rangle_H(x)\,\Delta x$ is nonnegative and nondecreasing:

$$0\leq P(c,l)\leq P(c+1,l)\leq\cdots\leq P(z,l)\leq\cdots, \tag{7.4}$$

because of the following relation, for $z > y+1$,

$$((P(z,l)-P(y,l))A, A)_H = \mathbf{S}_{y+1}^{z}(Q(x)S_2(x,l)A, S_2(x,l)A)_H \Delta x > 0.$$

Furthermore, we can state the following:

Lemma 7.1: The operator $P(x,l)$ defined above is strictly increasing at step 2 in the sense of positive-definiteness. Here by strictly increasing at step n we mean the property of a sequence $\{A(x)\}$ to satisfy an inequality $A(x+n) \geq A(x)$ for all x. //

Proof: If there exists x such that $P(x,l)=P(x+1,l)=P(x+2,l)$, then we have, for any given $A \in H$, $((P(x+1,l)-P(x,l))A, A)_H = 0$ and $((P(x+2,l)-P(x+1,l))A, A)_H = 0$, from which it follows, by using the transfer matrix method, that $S_2(y,l)$ is identically zero for $y \geq x$ and also identically zero for $y < x$. Since the identically zero solution for $S_j(x,l)$ is excluded in our consideration by the condition $(5.2)_1$, the operator $P(x,l)$ must increase strictly at step 2, which proves the lemma. //

Next we consider the convergence of the operator $R(x,l)$ as $x \to b$. To this end we prove the following:

Lemma 7.2: Let A and B be Hermitian and positive-definite operators in the Hilbert space H. If A and B satisfy the relation $0 < A \leq B$, then it follows that $A^{-1} \geq B^{-1} > 0$. //

Proof: Since A is an Hermitian and positive-definite operator in H, there exists its inverse, which is also Hermitian and positive-definite. Hence there exists a unique Hermitian and positive-definite operator $A^{-1/2}$, by making use of which we define an Hermitian and positive-definite operator $\Gamma = A^{-1/2}BA^{-1/2}$. Hence the relations $B - A \geq 0$ and $E_H = A^{-1/2}AA^{-1/2}$ imply that $\Gamma - E_H \geq 0$, since $A^{-1/2}$ maps H onto H.

Now we derive the positive-definiteness of $E_H - \Gamma^{-1}$. Since $\Gamma - E_H$ is positive-definite, it follows that, for any $v \in H$,

$$0 \leq ((\Gamma - E_H)v, v)_H = (\Gamma^{1/2}v, \Gamma^{1/2}v)_H - (v,v)_H = \|\Gamma^{1/2}v\|_H^2 - \|v\|_H^2.$$

If we put $u = \Gamma^{1/2}v$, then we have $\|u\|_H^2 - \|\Gamma^{-1/2}u\|_H^2 \geq 0$, which implies the relation $((E_H - \Gamma^{-1})u, u)_H \geq 0$. Since u ranges over the whole H as v runs over H, we obtain $E_H - \Gamma^{-1} \geq 0$.

Since it holds that $E_H = (A^{-1/2}AA^{-1/2})^{-1} = A^{1/2}A^{-1}A^{1/2}$ and $\Gamma^{-1} = (A^{-1/2}BA^{-1/2})^{-1} = A^{1/2}B^{-1}A^{1/2}$, we arrive at the relation $0 \leq E_H - \Gamma^{-1} = A^{1/2}(A^{-1} - B^{-1})A^{1/2}$, which implies that, for any $v \in H$, $((A^{-1} - B^{-1})A^{1/2}v, A^{1/2}v) \geq 0$. Since the range of $A^{1/2}$ is the whole H, we finally have $A^{-1} - B^{-1} \geq 0$. Thus the lemma is proved. QED

Since there exists, from the Lemma 7.1, a sequence of numbers, $c = c_0 < c_1 < \cdots$, such that $0 < P(c_0,l) < P(c_1,l) < \cdots$, it holds from the Lemma 7.2 that

$$\begin{aligned} &R(c_0,l) > R(c_1,l) > \cdots > 0, \quad \text{for } \mathrm{Im}(l) > 0, \\ &R(c_0,l) < R(c_1,l) < \cdots < 0, \quad \text{for } \mathrm{Im}(l) < 0. \end{aligned} \tag{7.5}$$

Therefore, we can see that $R(x,l)$ converges to an Hermitian operator $R_b(l)$ as $x \to b$ in the strong operator topology, by using the following:

Theorem 7.1: If a sequence of Hermitian operators, $A_1, A_2, \ldots$ in H, is monotone-increasing (or decreasing) and has upper (or lower) bound, then the sequence converges to an Hermitain operator in the strong operator topology. //

We omit the proof of this theorem, since it is seen in elementary textbooks of operator analysis.

Remark: The property of monotone increase (or decrease), not strictly monotone property, provides the proof of convergence of $R(x,l)$ to $R_b(l)$. The convergence of $R(x,l)$ to $R_a(l)$ as x tends to a is also proved similarly.

8. DEFINITION OF BOUNDARY CONDITIONS

A general solution of Eq. (5.1) is expressed in the form

$$\Psi(x,l) = S_1(x,l)\cdot\hat{f}_1 + S_2(x,l)\cdot\hat{f}_2. \tag{8.1}$$

Let $\chi(x)$ be an Hermitain operator in $L(H,H)$ satisfying the so-called *self-adjoint conditions* at a and b:

$$\text{s-}\lim_{x\to t}[\chi,\chi](x) = 0, \quad t = a \text{ and } b, \tag{8.2}$$

where a and b $(a < b)$ designate the boundary points. In what follows $f(a)$ and $f(b)$ represent the operators $\text{s-}\lim_{x\to a} f(x)$ and $\text{s-}\lim_{x\to b} f(x)$ respectively. We put

$$X(t) = \text{s-}\lim_{r\to t}\begin{pmatrix} \chi(r) \\ \chi(r+1) \end{pmatrix}, \quad t = a \text{ or } b. \tag{8.3}$$

Now we define the *boundary condition* at a or b for Ψ by

$$\text{s-}\lim_{x\to t}(X^*BW[\Psi])(x) = 0, \quad t = a \text{ or } b, \tag{8.4}$$

which is simply rewritten in the form $[\chi,\Psi](t) = 0$, $t = a$ or b.

Since it holds that $W[\Psi](x) = W[S_1(l)](x)\hat{f}_1 + W[S_2(l)](x)\hat{f}_2$, Eq. (8.4) is reduced to $(X^*BF)(t,l)\hat{f}_1 + (X^*BH)(t,l)\hat{f}_2 = 0$. If the operator $(X^*BH)(t,l)$ has its inverse, then we get

$$\hat{f}_2 = -Z_t(l)\hat{f}_1, \quad t = a \text{ or } b, \tag{8.5}$$

where we have put

$$Z_t(l) = -[(X^*BH)^{-1}(X^*BF)](t,l), \quad t = a \text{ or } b. \tag{8.6}$$

From the linearity of the operator L, scalar multiplication to Ψ is immaterial. Thus we can put $\hat{f}_1 = E_H$, giving the solution satisfying the boundary condition at t $(= a$ or $b)$ in the form

$$\Psi_t(x,l) = S_1(x,l) + S_2(x,l)Z_t(l). \tag{8.7}$$

To prove the existence of inverse of $(X^*BH)(b,l)$, we deal with the following boundary-value problem (Govindaraju):

$$\begin{aligned} &(LY)(x,l) = Y(x,l)\hat{l}, \quad Y(x,l) \in L(H,H), \\ &(W^*[Y]BH)(c) = 0 \text{ and } (W^*[Y]BX)(b) = 0, \end{aligned} \tag{8.8}$$

where $X(t)$ satisfies the self-adjoint condition at $t = b$: $(X^*BX)(t) = 0$. The general solution of $(LY)(x,l) = Y(x,l)\hat{l}$ is described as $\Psi(x,l) = S_1(x,l)\hat{f}_1 + S_2(x,l)\hat{f}_2$. Since $H(c)$ satisfies the condition $(H^*BH)(c) = 0$, we can put $X(c) = H(c)$. Substituting Ψ into the boundary condition at c,

we have $(H^*BH)(c)\hat{f}_2+(F^*BH)(c)\hat{f}_1=0$, which gives the solution satisfying the boundary condition at c in the form $\Psi_c(x,l)=S_2(x,l)\hat{f}_2$. From the fact that $\Psi_c(x,l)$ satisfies the boundary condition at b, we get $(H^*BX)(b,l)\hat{f}_2=0$. In order that $\hat{f}_2\neq 0$, $(H^*BX)(b,l)$ must be the zero operator and l is an eigenvalue.

On the other hand, it is well known that this boundary-value problem has real eigenvalues, so that it holds that $(H^*BX)(b,l)\neq 0$ for $\mathrm{Im}(l)\neq 0$, which means that $(X^*BH)(b,l)$ has its inverse for $\mathrm{Im}(l)\neq 0$. The existence of inverse of $(H^*BX)(z,l)$ is shown in a similar way for $\mathrm{Im}(l)\neq 0$.

9. SOME PROPERTIES OF $Z_b(l)$

We can easily show the following:

Lemma 9.1: Let $\chi(x)$ and $f(x)$ be two operators in $L(H,H)$. Then the relations $[\chi,\chi](x)=0$ and $[\chi,f](x)=0$ imply that $[f,f](x)=0$. //

Proof: From the relation $[\chi,\chi](x)=0$, we see that the vector $W[\chi](x)$ is orthogonal to the vector $(BW[\chi])(x)$. Similarly, from $[\chi,f](x)=0$, it follows that the vector $W[f](x)$ is orthogonal to the vector $(BW[\chi])(x)$. Hence the vector $W[f](x)$ is linearly dependent to $W[\chi](x)$, namely $W[f](x)=\alpha W[\chi](x)$, which provides the relation $[f,f](x)=\alpha[\chi,\chi](x)=0$. This proves the lemma. //

Now we put

$$G_b(x,l)=W[\Psi_b(l)](x)=F(x,l)+H(x,l)Z_b(l). \tag{9.1}$$

From the fact that $\Psi_b(x,l)$ satisfies the boundary condition at b, one obtains

$$(X^*BG_b)(b,l)=0. \tag{9.2}$$

Since X in Eq. (9.2) does not depend on l, it holds from Lemma 9.1 that

$$[G_b^*(l')BG_b(l)](b)=0. \tag{9.3}$$

If we put $l'=l$ and $l=\bar{l}$ in Eq. (9.3), we get

$$Z_b^*(l)=Z_b(\bar{l}). \tag{9.4}$$

This is an important property of $Z_b(l)$.

Secondly, we see from the Green's formula that

$$-2i\,\mathrm{Im}(l)\mathbf{S}_c^b\langle\Psi_b(l),\Psi_b(l)\rangle_H(x)\,\Delta x = [G_b^*BG_b](b,l)-[G_b^*BG_b](c,l).$$

Since the boundary condition at b gives us the relation $(G_b^*BG_b)(b,l)=0$ and easy calculation gives us $(G_b^*BG_b)(c,l)=\bar{Z}_b(l)-Z_b(l)$, it follows that

$$\mathbf{S}_c^b\langle\Psi_b(l),\Psi_b(l)\rangle_H(x)\,\Delta x=-\frac{1}{\mathrm{Im}(l)}\,\mathrm{Im}[Z_b(l)]. \tag{9.5}$$

This implies that

$$\mathrm{Im}[Z_b(l)]\begin{cases}>0, & \text{for } \mathrm{Im}(l)<0,\\ <0, & \text{for } \mathrm{Im}(l)>0.\end{cases} \tag{9.6}$$

10. CENTER OPERATOR AND EQUATION OF CIRCLE

We define a *center operator* at b, $C_b(l)$, by

$$C_b(l)=-[(H^*BH)^{-1}(H^*BF)](b,l). \tag{10.1}$$

Then the relation

$$C_b^*(l)=C_b(\bar{l}) \tag{10.2}$$

is obtained, since we have, from Eq. $(6.5)_4$,

$$[(H^*BH)^{-1}(H^*BF)](x,l)=[(F^tB\bar{H})(H^tB\bar{H})^{-1}](x,l). \tag{10.3}$$

Secondly we construct the equation of the circle: From the boundary condition at b, the following relation holds: $g_b(l)\equiv[G_b^*BG_b](b,l)=[(F^*+Z_b^*H^*)B(F+HZ_b)](b,l)=0$. By the definition of the radius operator and Eq. (6.6), this expression turns out to be $g_b(l)=[Z_b(l)-C_b(l)]^*\times[iR_b(l)]^{-1}[Z_b(l)-C_b(l)]-iR_b(\bar{l})$. If we define a function of operators by

$$f_b(A)=[A-C_b(l)]^*R_b^{-1}(l)[A-C_b(l)]-R_b(\bar{l}), \tag{10.4}$$

then Eq. (10.4) gives us that

$$f_b(Z_b(l))=0. \tag{10.5}$$

It is seen natural from the form of Eq. (10.4) to give the name "equation of the circle" to the equation $f_b(A)=0$ for $A\in L(H,H)$, with its center $C_b(l)$ and its radius $R_b(l)$.

One of properties for the center operator is obtained as follows: We get from the Green's formula that

$$-2i\,\mathrm{Im}(l)\,\mathbf{S}_c^b([S_1(l)+S_2(l)C_b(l)]^*Q[S_1(l)+S_2(l)C_b(l)])(x)\,\Delta x=-iR_b(l)+2i\,\mathrm{Im}[C_b(l)], \tag{10.6}$$

where we have used the definitions of radius operator and center operator and Eq. (6.6). Since it holds that $R_b(l)<0$ for $\mathrm{Im}(l)>0$ and $>$ for $\mathrm{Im}(l)<0$, we have from Eq. (10.1) that

$$\mathrm{Im}[C_b(l)]\begin{cases}>0, & \text{for } \mathrm{Im}(l)<0,\\ <0, & \text{for } \mathrm{Im}(l)>0.\end{cases} \tag{10.7}$$

11. CONVERGENCE OF $Z_r(l)$ as $r\to b$

Now we examine the limit of $Z_r(l)$ as r goes to b. For $r'>r+1$, we have

$$-2i\,\mathrm{Im}(l)\,\mathbf{S}_c^{r'}\langle\Psi_r(l),\Psi_r(l)\rangle_H(x)\,\Delta x = if_{r'}(Z_r(l))+2i\,\mathrm{Im}[Z_r(l)],$$

which gives us the relation

$$0<\mathbf{S}_r^{r'}\langle\Psi_r(l),\Psi_r(l)\rangle_H(x)\,\Delta x=-\frac{1}{2\,\mathrm{Im}(l)}f_{r'}(Z_r(l)).$$

It then follows that

$$f_{r'}(Z_r(l))\begin{cases}>0, & \text{for } \mathrm{Im}(l)<0,\\ <0, & \text{for } \mathrm{Im}(l)>0.\end{cases} \tag{11.1}$$

Similarly, for $r>r'+1$, we have

$$0<\mathbf{S}_{r'}^{r}\langle\Psi_r(l),\Psi_r(l)\rangle_H(x)\,\Delta x=\frac{1}{2\,\mathrm{Im}(l)}f_{r'}(Z_r(l)),$$

from which one obtains

$$f_{r'}(Z_r(l))\begin{cases}>0, & \text{for } \mathrm{Im}(l)>0,\\ <0, & \text{for } \mathrm{Im}(l)<0.\end{cases} \tag{11.2}$$

By the relation $if_r(C_r(l))=-iR_r(\bar{l})$ obtained in Sec. 10,

it holds that $f_r(C_r(l)) > 0$ for $\mathrm{Im}(l) > 0$ and < 0 for $\mathrm{Im}(l) < 0$.

Now we define the circle at r, $N_r(l)$, associated with the operator L by

$$N_r(l) = \{A \mid f_r(A) = 0,\ A \in L(H,H)\}, \tag{11.3}$$

and its interior at r, $M_r(l)$, by

$$M_r(l) = \{A \mid f_r(A) > 0,\ \mathrm{Im}(l) > 0,\ A \in L(H,H)\}. \tag{11.4}$$

Then we see from the discussions in Sec. 7 that

$$M_x(l) \subset M_y(l), \quad \text{for } y > x+1. \tag{11.5}$$

Since the radius operator $R(r,l)$ tends strongly to an operator $R_b(l)$ as $r \to b$, if $R_b(l)$ is a nonzero operator in H, then the circle tends to a limiting circle $N_b(l)$. In this case $Z_b(l)$ depends on the boundary condition at b, which will be called the *limit circle case*. If the limit radius operator becomes a zero operator, then the circle at r tends to a point, namely the center operator $C_b(l)$. In this case the operator $Z_r(l)$ tends to the operator $C_b(l)$ and does not depend on the boundary condition at r previously imposed, which is called the *limit point case*.

Since the arguments about the other boundary points a are discussed similarly, we can classify the operator L as follows:

(i) limit point type at both end points,

(ii) limit point type at a and limit circle type at b,

(iii) limit circle type at a and limit point type at b,

(iv) limit circle type at both end points.

The corresponding classifications of one-dimensional operators of the second order are seen in Ref. 5.

PART II

12. NULL-PRODUCT OPERATOR

For the purpose of constructing a Green's function we introduce the so-called null-product in the following way: As to two general solutions $\Psi(x,l;f) = S_1(x,l)\hat{f}_1 + S_2(x,l)\hat{f}_2$ and $\Psi(x,l;g) = S_1(x,l)\hat{g}_1 + S_2(x,l)\hat{g}_2$, we define the *null product* by

$$[[f,g]](l) = [\Psi(\cdot,l;f), \bar{\Psi}(\cdot,l;g)](x), \tag{12.1}$$

which is reduced to

$$[[f,g]](l) = (\bar{f}_2\bar{g}_1 - \bar{f}_1\bar{g}_2)E_H \tag{12.2}$$

by using the property of canonical system of fundamental solutions. We continue to construct the null-product operator. If we impose the boundary conditions at a and b,

$$(X^*BW[\Psi])(t) = 0, \quad t = a,\ b, \tag{12.3}$$

then one obtains a set of two solutions

$$\Psi_t(x,l) = S_1(x,l) + S_2(x,l)\,Z_t(l), \quad t = a,\ b, \tag{12.4}$$

where $Z_a(l)$ and $Z_b(l)$ are determined by, for $t = a,\ b$,

$$Z_t(l) = -[(X^*BH)^{-1}(X^*BF)](t,l),$$

in the limit circle case at t, (12.5)

$$Z_t(l) = -[(H^*BH)^{-1}(H^*BF)](t,l),$$

in the limit point case at t.

If we put, for brevity,

$$h_1 = \begin{pmatrix} E_H \\ Z_a(l) \end{pmatrix} \text{and} \quad h_2 = \begin{pmatrix} E_H \\ Z_b(l) \end{pmatrix}, \tag{12.6}$$

then we get $[[h_1,h_2]](l) = \bar{Z}_a(l) - \bar{Z}_b(l)$. Now we define the matrix operator by

$$\mathcal{J}(l) = \begin{pmatrix} [[h_1,h_1]](l) & [[h_1,h_2]](l) \\ [[h_2,h_1]](l) & [[h_2,h_2]](l) \end{pmatrix}, \tag{12.7}$$

which we call the *null-product operator*. If, for simplicity, we put

$$Z(l) = Z_b(l) - Z_a(l), \tag{12.8}$$

then it follows that

$$\mathcal{J}(l) = \begin{pmatrix} 0 & -\bar{Z}(l) \\ \bar{Z}(l) & 0 \end{pmatrix}. \tag{12.9}$$

Since it holds from the definitions of $W[f]$ and $B(x)$ that $(W^*[\Psi_a]BW[\bar{\Psi}_a])(x,l) = (W^*[\Psi_b]BW[\bar{\Psi}_b])(x,l) = 0$ and $(W^*[\Psi_a]BW[\bar{\Psi}_b])(x,l) = -(W^*[\Psi_b]BW[\bar{\Psi}_a])(x,l) = [[h_1,h_2]](l)$, we get

$$(Y^*BY)(x,l) = \mathcal{J}(l) \quad \text{and} \quad (\bar{Y}\mathcal{J}^{-1}Y^*)(x,l) = B^{-1}(x), \tag{12.10}$$

where we have put

$$Y(x,l) = \begin{pmatrix} \Psi_a(x,l) & \Psi_b(x,l) \\ \Psi_a(x+1,l) & \Psi_b(x+1,l) \end{pmatrix}.$$

Then the relations between elements in Eq. (12.10) are written down in the forms

$$(\bar{\Psi}_a^{(j)}\bar{Z}^{-1}\Psi_b^{*(k)})(x,l) - (\bar{\Psi}_b^{(j)}\bar{Z}^{-1}\Psi_a^{*(k)})(x,l) = \mathrm{sgn}(j-k)(1-\delta_{jk})\,P_1^{-1}(x), \quad j,k = 0,1, \tag{12.11}$$

which will be used to derive some properties of a Green's function constructed in the following section. Here we have used a notation $\Psi^{(n)}(x,l) = \Psi(x+n,l)$.

13. GREEN'S FUNCTION

The construction of a Green's function is the key point for the spectral expansion theorem. We put

$$G(x,y;l) = \begin{cases} \Psi_a(y,l)Z^{-1}(l)\,\Psi_b^t(x,l), & \text{for } y \le x, \\ \Psi_b(y,l)Z^{-1}(l)\,\Psi_a^t(x,l), & \text{for } y > x, \end{cases} \tag{13.1}$$

and, for any $A(x) \in L(H,H)$,

$$U(x,l) = \mathbf{S}_a^b\langle G(x,\cdot\,;l), A\rangle_H(y)\,\Delta y. \tag{13.2}$$

After elementary calculations, taking into account the concrete forms for $G(x,y;l)$, Eq. (13.1), we arrive at the relation

$$(LU)(x,l) = \bar{l}U(x,l) + A(x). \tag{13.3}$$

Secondly we define the *Green's operator* $G(l)$ by

$$(GA)(x,l) = \mathbf{S}_a^b\langle G(x,\cdot\,;l), A(\cdot)\rangle_H(y)\,\Delta y, \tag{13.4}$$

by which Eq. (13.3) is expressed in the form $[(L-\bar{l})G(l)A](x) = A(x)$. We omit the proof of the relation $[G(l)(L-\bar{l})A](x) = A(x)$. Now, from these last two for-

mulas, we can describe the Green's operator define by Eq. (13.4) in the form $G(l)=(L-\bar{l})^{-1}$.

14. OPERATOR MATRIX $M(l)$

The matrix obtained in this section is directly related to the spectral expression of operator associated with L. The Green's function defined by Eq. (13.1) is expressed by means of canonical system of fundamental solutions in the forms

$$G(x,y;l)=(S_1(y,l),S_2(y,l))M(l)\begin{pmatrix}S_1^t(x,l)\\ S_2^t(x,l)\end{pmatrix}$$

$$\text{for } y\leqslant x, \tag{14.1}$$

where the matrix defined by

$$M(l)=\begin{pmatrix} Z^{-1}(l) & Z^{-1}(l)Z_b^t(l)\\ Z_a(l)Z^{-1}(l) & Z_a(l)Z^{-1}(l)Z_b^t(l)\end{pmatrix} \tag{14.2}$$

satisfies the relation $M(l)-M^t(l)=-J$, because $Z^t(l)=Z(l)$. The expression of $G(x,y;l)$ for $y>x$ is obtained by putting $M^t(l)$ in Eq. (14.1) instead of $M(l)$.

15. CONSTRUCTION OF A SELF-ADJOINT OPERATOR FROM L

Consider a subdomain $\mathcal{D}$ of the defining domain of the operator L given by $\mathcal{D}=\{U\mid U\in H_0,\ LU\in H_0\}$, and let T be the operator obtained from L by restricting its domain within $\mathcal{D}$: $T=L\mid\mathcal{D}$ (or $TU=LU$ if $U\in\mathcal{D}$). Furthermore, let us put $\mathcal{D}_a=\{U\mid U\in\mathcal{D},\ [\chi,U](a)=0\}$, $\mathcal{D}_b=\{U\mid U\in\mathcal{D},\ [\chi,U](b)=0\}$ and $\mathcal{D}_0=\mathcal{D}_a\cap\mathcal{D}_b$. Let T_0 be an operator obtained from T by restricting its domain within $\mathcal{D}_0$. Then it is easily proved that T_0 is symmetric and self-adjoint. The detail discussions are seen in Ref. 6, though some modifications should be required. We put $H=T_0$ in what follows.

16. CONSTRUCTION OF A SPECTRAL OPERATOR FUNCTION. I

We treat in this section the operator H instead of L. As in the case of the Green's operator of L, the operator $G(l)$ given by Eq. (13.4) is a resolvent operator of $H-l$. Since H is self-adjoint, we have the spectral decomposition of H in the form

$$H=\int_{-\infty}^{\infty}\lambda dE(\lambda),\quad E(\lambda)\in L(H_0,H_0), \tag{16.1}$$

where $\{E(\lambda)\}$ is the resolution of the identity. Let us put $U(x,\lambda)=[E(\lambda)-E(0)]U(x)$, $U(x,\Delta)=E(\Delta)U(x)=U(x,\lambda)-U(x,\mu)$ for $\Delta=]\mu,\lambda]$, $U\in H_0$, and $U(x,\Delta)=\mathbf{S}_a^b\langle G(x,\cdot\,;l),V(\Delta)\rangle_H(y)\,\Delta y=(G(l)V(\Delta))(x)$. Then it follows that, for $m=-1,0,1$,

$$U^{(m)}(x,l)=U(x+m,l)=\mathbf{S}_a^b\langle G^{(m)}(x,\cdot\,;l),V(\Delta)\rangle_H(y)\,\Delta y$$
$$=\langle G^{(m)}(x,\cdot\,;l),V(\Delta)\rangle_{H_0}.$$

Since it holds that $V(x,\Delta)=[(H-l)U(\Delta)](x)=[\int_\Delta(\lambda-l)dE(\lambda)U](x)$, we obtain

$$U^{(m)}(x,\Delta)=\langle\int_\Delta(\lambda-l)dE(\lambda)G^{(m)}(x,\cdot\,;l),U\rangle_{H_0}. \tag{16.2}$$

From Eq. (14.1) we get

$$G^{(m)}(c,y;l)$$
$$=\begin{cases}\sum_{k=1}^{2}\sum_{j=1}^{2}S_k(y,l)M_{kj}(l)e_j^{(m)}, & \text{for } y\leqslant c,\\ \sum_{k=1}^{2}\sum_{j=1}^{2}S_k(y,l)(M^t(l))_{kj}e_j^{(m)}, & \text{for } y>c,\end{cases} \tag{16.3}$$

because $S_k^t(c+m)=e_k^{(m)}$ for $m=-1,0,1$.

If we put

$$\Gamma_j(y,l)=\begin{cases}\sum_{k=1}^{2}S_k(y,l)(M(l))_{kj}, & \text{for } y\leqslant c,\\ \sum_{k=1}^{2}S_k(y,l)(M^t(l))_{kj}, & \text{for } y>c,\end{cases} \tag{16.4}$$

then we get

$$G^{(m)}(c,y;l)=\sum_{j=1}^{2}\Gamma_j(y,l)e_j^{(m)}, \tag{16.5}$$

from which $U^{(m)}(c,\Delta)$ in Eq. (16.2) turns out to be

$$U^{(m)}(c,\Delta)=\sum_{j=1}^{2}e_j^{(m)}\langle\int_\Delta(\lambda-l)dE(\lambda)\Gamma_j(\cdot,l),U\rangle_{H_0},$$

where we have used the relation $(e_j^{(m)})^*=e_j^{(m)}$ and $e_j^{(m)}\in L(H,H)$.

Secondly putting

$$\xi_j(y,\Delta)=\int_\Delta(\lambda-l)dE(\lambda)\Gamma_j(y,l), \tag{16.6}$$

we obtain

$$U^{(m)}(c,\Delta)=\sum_{j=1}^{2}e_j^{(m)}\langle\xi_j(\cdot,\Delta),U\rangle_{H_0}, \tag{16.7}$$

or setting

$$U^j(\Delta)=\langle\xi_j(\cdot,\Delta),U\rangle_{H_0}, \tag{16.8}$$

we get finally

$$U^{(m)}(c,\Delta)=\sum_{j=1}^{2}e_j^{(m)}U^j(\Delta). \tag{16.9}$$

17. INTEGRO-DIFFERENCE EQUATION FOR OBTAINING SPECTRA

We treat in this section the equation

$$(LU)(x,\Delta)=\int_\Delta\mu\,dU(x,\mu), \tag{17.1}$$

which is used to get the spectral expansion formula. It is easily shown that the expression

$$U_0(x,\Delta)=\int_\Delta\sum_{j=1}^{2}S_j(x,\mu)\,dU^j(\mu), \tag{17.2}$$

satisfies Eq. (17.1). We now seek for the solution of Eq. (17.1) under the initial condition

$$\sum_{j=1}^{2}e_j^{(m)}U^j(\Delta)=U^{(m)}(c,\Delta),\quad m=1,0,-1. \tag{17.3}$$

Putting $U(x,\Delta)=U_0(x,\Delta)+T(x,\Delta)$, and substituting it into Eq. (17.1), we have

$$(LU)(x,\Delta)=\int_\Delta\mu\,dU_0(x,\mu)+(LT)(x,\Delta). \tag{17.4}$$

On the other hand, it holds that $(LU)(x,\Delta)=\int_\Delta\mu dU_0(x,\mu)+\int_\Delta\mu dT(x,\mu)$, from which we get

$$(LT)(x,\Delta)=\int_\Delta\mu dT(x,\mu). \tag{17.5}$$

From the relation $U^{(m)}(c,\Delta)=U_0^{(m)}(c,\Delta)+T(c,\Delta)$ and Eq. (17.2), we have

$$U_0^{(m)}(c,\Delta)=\int_\Delta\sum_{j=1}^{2}S_j^{(m)}(c,\lambda)\,dU^j(\lambda)=\sum_{j=1}^{2}e_j^{(m)}U^j(\Delta).$$

Therefore, $T^{(m)}(x,\Delta)$ must satisfy the initial condition

$$T^{(m)}(c,\Delta)=0,\quad m=-1,0,1. \tag{17.6}$$

We can easily show that the solution $T(x,\lambda)$ of Eq. (17.5) under the initial condition (17.6) is zero operator, which implies that the solution $U(x,\lambda)=U_0(x,\lambda)$ is a unique solution of Eq. (17.1) under the condition (17.3).

18. CONSTRUCTION OF A SPECTRAL OPERATOR FUNCTION. II

As shown in Sec. 17, the solution of Eq. (17.1) under the initial condition (16.8) is expressed, by using Eq. (16.7), in the form

$$U(x,\Delta)=\int_\Delta \sum_{j=1}^{2} S_j(x,\mu)\,d\langle \xi_j(\cdot,\mu), U\rangle_{H_0}. \tag{18.1}$$

Since we can put $U(x,\lambda)=\xi_k(x,\lambda)$, we have

$$\xi_k(x,\Delta)=\int_\Delta \sum_{j=1}^{2} S_j(x,\mu)\,d\langle \xi_j(\cdot,\mu), \xi_k(\cdot,\mu)\rangle_{H_0}. \tag{18.2}$$

Putting

$$\rho^{jk}(\Delta)=\langle \xi_j(\cdot,\Delta), \xi_k(\cdot,\Delta)\rangle_{H_0}, \tag{18.3}$$

and therefore, by using Eq. (16.6),

$$\rho^{jk}(\Delta)=\int_\Delta |\mu-l|^2 d\langle E(\mu)\Gamma_j(\cdot,l), \Gamma_k(\cdot,l)\rangle_{H_0},$$

we obtain

$$\int_{-\infty}^{\infty} |\lambda-l|^{-2} d\rho^{jk}(\lambda)=\langle \Gamma_j(\cdot,l), \Gamma_k(\cdot,l)\rangle_{H_0}. \tag{18.4}$$

It follows from Eqs. (16.5) and (5.8) that

$$\begin{aligned}[\langle \Gamma_j, \Gamma_k\rangle(l)] &= -[2i\,\mathrm{Im}(l)]^{-1}[M^*JM-(M^t)^*JM^t](l)\\ &\quad -[2i\,\mathrm{Im}(l)]^{-1}[(KM^t)^*B(KM^t)](b)\\ &\quad -[2i\,\mathrm{Im}(l)]^{-1}[(KM)^*B(KM)](a).\end{aligned}$$

The boundary conditions in the forms $(G_t^*BG_t)(t,l)=0$ yields $[(KM)^*B(KM)](t)=0$, for $t=a$ and b, from which we get

$$[\langle \Gamma_j(l), \Gamma_k(l)\rangle_{H_0}]=-[2i\,\mathrm{Im}(l)]^{-1}[M^*JM-(M^t)^*JM^t](l). \tag{18.5}$$

The elementary matrix calculations of right-hand side of Eq. (18.5) gives us the relation $[M^*JM-(M^t)^*JM^t](l)=M(\bar{l})-M(l)=-2i\,\mathrm{Im}[M(l)]$, where we have used the property $M^*(l)=M(\bar{l})$. Consequently, Eq. (18.4) is reduced to

$$\int_{-\infty}^{\infty} |\lambda-l|^{-2}\,\mathrm{Im}(l)\,d\mathbf{P}(\lambda)=\mathrm{Im}[M(l)], \tag{18.6}$$

where we have put

$$\mathbf{P}(\lambda)=[\rho^{jk}(\lambda)]. \tag{18.7}$$

The inverse formula of Eq. (18.6) is expressed in the form

$$\mathbf{P}(\lambda)=-\lim_{\epsilon\to+0}\pi^{-1}\int_0^\lambda \mathrm{Im}[M(\mu+i\epsilon)]\,d\mu, \tag{18.8}$$

and has the properties $\mathbf{P}(\lambda)\geq 0$ and $\mathbf{P}^*(\lambda)=\mathbf{P}(\lambda)$.

19. EXPANSION FORMULA

Since we have from Eqs. (18.2) and (18.3)

$$\xi_k(x,\Delta)=\int_\Delta \sum_{j=1}^{2} S_j(x,\mu)\,d\rho^{jk}(\mu), \tag{19.1}$$

substitution of this formula into Eq. (18.1) provides

$$U(x,\Delta)=\int_\Delta \sum_{j=1}^{2} S_j(x,\mu)\,dV_j(\mu),$$

$$V_j(\Delta)=\mathbf{S}_a^b\Big(\int_\Delta \sum_{k=1}^{2} S_k(x,\mu)\,d\rho^{kj}(\mu)\Big)^*\,Q(x)\,U(x)\,\Delta x,$$

or formally, making $\lambda\to\infty$ and $\mu\to-\infty$ in $\Delta=]\mu,\lambda]$,

$$U(x)=\mathbf{S}_a^b \sum_{j,k=1}^{2} \int_{-\infty}^{\infty} S_j(x,\mu)\,d\rho^{kj}(\mu)S_k^*(y,\mu)\,Q(y)\,U(y)\,\Delta y. \tag{19.2}$$

APPENDIX: CONSTRUCTION OF A HILBERT SPACE H_0

As to the results in this appendix, reference should be made to Berezanskii.[2] Let H be a Hilbert space with inner product $(\cdot,\cdot)_H$, and the norm $\|u\|_H=(u,u)_H$. Next we introduce a direct sum of H: $H'=\sum_{x=a}^{b}\oplus H$, where a and b may be improper. In this space the inner product is defined by $(\mathbf{u},\mathbf{v})_{H'}=\sum_{x=a}^{b}(u_x,v_x)_{H'}$ and also any $u\in H'$ designates $(\cdots u_x,u_{x+1},\cdots)$.

Let $L(H,H)$ be a set of all bounded linear operators from H into H, which is a vector space under ordinary addition of operators. If we assume that $u_x\in L(H,H)$ for all $x\in\mathbf{D}$, and put $\mathbf{u}=(\cdots,u_x,u_{x+1},\cdots)$, then $\mathbf{u}$ is an element of a direct sum of $L(H,H)$: $\mathbf{u}\in\sum\oplus L(H,H)$. We define a product of this $\mathbf{u}$ and any $A\in H$ such that $\mathbf{u}A=(\cdots,u_xA,u_{x+1}A,\cdots)$. Then $\mathbf{u}$ becomes a linear operator from H into H'. Hence we denote by H_0 the set of all bounded linear operator from H' into H'. The operator L considered in the main text can be regarded as an operator belonging to H_0.

Now we construct a Hilbert space H_0. First of all we define an inner product in H_0 by

$$\langle \mathbf{u},\mathbf{v}\rangle_{H_0}=\mathbf{u}^*Q\mathbf{v}\quad[\in L(H,H)], \tag{A1}$$

where $\mathbf{u}$, $\mathbf{v}\in H_0$ and Q is a fixed positive-definite operator $H'\to H'$, and furthermore we have defined $\mathbf{u}^*$ as an operator H' into H by $(\mathbf{u}^*A,B)_H=(A,\mathbf{u}B)_{H'}$, $B\in H$, $A\in H'$. The inner product defined by Eq. (A1) has the properties: $\langle \mathbf{u},\mathbf{v}+\mathbf{w}\rangle_{H_0}=\langle \mathbf{u},\mathbf{v}\rangle_{H_0}+\langle \mathbf{u},\mathbf{w}\rangle_{H_0}$, $\langle \mathbf{u}+\mathbf{v},\mathbf{w}\rangle_{H_0}=\langle \mathbf{u},\mathbf{w}\rangle_{H_0}+\langle \mathbf{v},\mathbf{w}\rangle_{H_0}$, $\langle \mathbf{u},\mathbf{v}\Lambda\rangle_{H_0}=\langle \mathbf{u},\mathbf{v}\rangle_{H_0}\cdot\Lambda$, for $\Lambda\in L(H,H)$, $\langle \mathbf{u}\Lambda,\mathbf{v}\rangle_{H_0}=\Lambda^*\langle \mathbf{u},\mathbf{v}\rangle_{H_0}$, and $\langle \mathbf{u},\mathbf{v}\rangle^*_{H_0}=\langle \mathbf{v},\mathbf{u}\rangle_{H_0}$. The positive-definiteness of $\langle \mathbf{u},\mathbf{u}\rangle_{H_0}$ is shown by the relation $(\langle \mathbf{u},\mathbf{u}\rangle_{H_0}\cdot v,v)_H=(\mathbf{u}^*Q\mathbf{u}v,v)_H=(Q\mathbf{u}v,\mathbf{u}v)_{H'}\geq 0$. Furthermore, the operator $\langle \mathbf{u},\mathbf{u}\rangle_{H_0}$ is easily shown to be Hermitian in H.

Now we introduce a topology in H_0, which is a strong operator topology in H':

Definition A.1: A sequence $\{\mathbf{u}^{(n)}\}$ in H_0 converges to a $\mathbf{u}\in H_0$ if and only if, for any given $\epsilon>0$ and for each $v\in H$, there exists a positive integer N such that $\|\mathbf{u}^{(n)}v-\mathbf{u}v\|_{H'}<\epsilon$ for all $n>N$. //

With respect to this topology, H_0 becomes complete. To show this, we define Cauchy sequence in H_0:

Definition A.2: A sequence $\{\mathbf{u}^{(n)}\}$ in H_0 is a Cauchy sequence if and only if, for any given $\epsilon>0$ and for each $v\in H$, there exists a positive integer N such that $\|\mathbf{u}^{(n)}v-\mathbf{u}^{(m)}v\|_{H'}<\epsilon$ for all $n,m>N$. //

Then, we easily prove in the usual manner the following:

Theorem A.1: The space H_0 is complete in the sense that any Cauchy sequence converges. //

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[1]T. Asahi, Suppl. Prog. Theor. Phys., No. 23, 59 (1963).

[2]Ju. M. Berezanskii, *Expansions in Eigenfunctions of Selfadjoint Operators*, Amer. Math. Soc. Math. Mono., Vol. 17 (Amer. Math. Soc., Providence, R.I., 1968).

[3]K. Kodaira, Amer. J. Math. **71**, 921 (1949).

[4]K. Kodaira, Amer. J. Math. **72**, 502 (1950).

[5]M. Fukushima, "Spectral theory of ordinary difference operators of the second order, I. General theory," Soka Univ. Sci. Lab. Mimeo-Series, No. 1 (1971).

[6]M. Fukushima, "On the eigenvalue problem of the difference operators of any even order and the corresponding eigenfunction expansions, I. General theory," Soka Univ. Sci. Lab. Mimeo-Series, No. 2 (1972).

[7]R. V. Govindaraju, Trans. Amer. Math. Soc. **154**, 113 (1971).

[8]M. Fukushima, "Operator-valued-measure approach to spectra of two-dimensional classical harmonic lattices," in *Lecture Notes in Physics, Vol.* **39** (Springer, New York, 1975), pp. 528–31.

Uniform bounds of the pressures of the $\lambda\phi_3^4$ field model

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We show that the pressures of the $\lambda\phi_3^4$ field model with free and with periodic boundary conditions are bounded uniformly in space cutoff.

I. INTRODUCTION

In this paper we study the partition function $Z(a,b,c)$ $[Z^P(a,b,c)]$ and the pressure $\alpha(a,b,c)$ $[\alpha^P(a,b,c)]$ for the $\lambda\phi_3^4$ quantum field theory in a finite box $\Omega = a\times b\times c$ centered at the origin with free (periodic) boundary conditions. The partition function $Z(a,b,c)$ is defined as the limit of momentum cutoff quantities:

$$Z_\kappa(a,b,c) = \langle \exp[-V_\kappa(a,b,c)]\rangle ,$$

where $V_\kappa(a,b,c)$ is the doubly cutoff (momentum cutoff κ and space cutoff $\Omega = a\times b\times c$) interaction action of the $\lambda\phi_3^4$ field model and $\langle\circ\rangle$ stands for the expectation of the Gaussian measure with mean zero and covariance $(-\Delta + m_0^2)^{-1}$. For detailed definitions we refer the reader to Glimm and Jaffe[1] and Feldman.[2] Glimm and Jaffe have obtained bounds uniform in κ, of the form:

$$Z_\kappa(a,b,c) \leq (\text{const})^{abc}. \tag{1.1}$$

Feldman[2] has shown that $Z_\kappa(a,b,c)$ converges as $\kappa \to 1$ and thus the bounds apply also to the limit function

$$Z(a,b,c) = \lim_{\kappa\to 1} Z_\kappa(a,b,c). \tag{1.2}$$

Thus the pressure defined by

$$\alpha(a,b,c) = (abc)^{-1}\log Z(a,b,c)$$

is bounded above uniformly in the volume Ω. The corresponding quantities $Z^P(a,b,c)$ and $\alpha^P(a,b,c)$ for periodic boundary conditions are defined similarly in terms of the periodic action $V_\kappa^P(a,b,c)$ with periodic boundary conditions on $\partial\Omega$, see Ref. 3. The periodic partition function $Z^P(a,b,c)$ also satisfies a bound of the form (1,1). Finally we will consider the partition functions $Z_\delta^P(a,b,c)$ of the lattice approximation with periodic boundary conditions defined by Park,[3] and the corresponding pressures $\alpha_\delta^P(a,b,c)$. Here δ denotes the lattice spacing parameter and as has been shown by Park,[3] $Z_\delta^P(a,b,c)$ also satisfies a bound of the form (1.1) uniformly in δ and converges to $Z^P(a,b,c)$ as δ tends to zero.

Our principal results for the partition functions are given in the following theorem.

Theorem 1.1: There are constants d_1 and d_2 independent of a,b,c,δ, such that:

(a) $\exp(-d_1abc) \leq Z(a,b,c) \leq \exp(d_2abc)$,

(b) $\exp(-d_1abc) \leq Z^P(a,b,c) \leq \exp(d_2abc)$,

(c) $\exp(-d_1abc) \leq Z_\delta^P(a,b,c) \leq \exp(d_2abc)$.

As an immediate corollary we obtain

Corollary 1.2: The finite volume pressures $\alpha(a,b,c)$, $\alpha^P(a,b,c)$, and $\alpha_\delta^P(a,b,c)$ are bounded uniformly in a, b, c, and δ.

A comment on our result and method of its proof might be useful. Recently the existence of the weakly coupled $\lambda\phi_3^4$ field model has been established by Feldman and Osterwalder[4] and Magnen and Seneor[5] independently. The next step might involve the method of $P(\phi)_2$[6] to establish the existence of the strongly coupled $\lambda\phi_3^4$ field model. It has been suggested that controlling the pressures controls the Schwinger functions.[7,8] Our result is the first step in controlling the pressure of the $\lambda\phi_3^4$ field model. The method we will use is very simple and looks useful. The main techniques are the method of transfer matrix, Nelson's symmetry and Hölder's inequality. We believe that by using our method one may obtain the exponential bounds of the $\lambda\phi_3^4$ field model. Also it will be interesting to show the convergence of the pressures as the volume of the box Ω tends to infinity.

II. PROOF OF THE MAIN RESULTS

In this section we give the proof of Theorem 1.1. The method we will use is the method of transfer matrix, Nelson's symmetry and Hölder's inequality.[6] The main procedure is as follows: To show Theorem 1.1 for $Z(a,b,c)$ we first transfer the partition function into transfer matrix form and then use Hölder's inequality to contract length c of one side into length $2\epsilon, \epsilon > 0$. This allows one to compare the lower bound of $Z(a,b,c)$ with that of $Z(a,b,2\epsilon)$. Nelson's symmetry gives us the relation $Z(a,b,2\epsilon) = Z(2\epsilon,a,b)$. We use the above procedure two more times. The exponential (lower) bound of $Z(a,b,c)$ can be obtained from the fact that $Z(\epsilon,\epsilon,\epsilon) > \frac{1}{2}$ for small ϵ. The above method will be also applied for $Z^P(a,b,c)$ and $Z_\delta^P(a,b,c)$. The above method has been used by Guerra for the $p(\phi)_2$ model.[6] We will modify Guerra's method slightly to control the divergent wavefunction renormalization. Let $H_\kappa(a,b)$ be the doubly cutoff (momentum cutoff κ and space cutoff $a\times b$) interaction Hamiltonian. See Ref. 1, Sec. 1.1 for the detailed definition. In this section we will always assume that there is no momentum cutoff in the interaction action $V_\kappa(a,b,c)$ in the time direction (see Ref. 1, Sec. 1.1). The partition function and the Hamiltonian are related through[1]

$$Z_\kappa(a,b,c) = \langle \exp[-cH_\kappa(a,b)]\rangle \exp[\Lambda_\kappa(a,b) + T_\kappa(a,b,c)], \tag{2.1}$$

where $\Lambda_\kappa + T_\kappa$ is the wavefunction renormalization[1]. In the notation of Glimm and Jaffe, $\Lambda_\kappa = \Lambda_2(\kappa) + \Lambda_3(\chi)$

and $T_\kappa = T_2(\kappa) + T_3(\kappa)$. Here we have written the wave-function renormalization into two parts to separate the time independent divergent term $\Lambda_\kappa(a,b)$ from the time dependent regular term $T_\kappa(a,b,c)$. Eventually we will be able to control the divergent term Λ_κ. First note that from Ref. 1, Sec. 1.1 for $a,b,c \geq \epsilon > 0$ there is a constant, independent of the box $\Omega = a\times b\times c$ and momentum cutoff κ such that

$$|T_\kappa(a,b,c)| \leq \text{const}(\epsilon)abc. \tag{2.2}$$

For notational convenience we write

$$\begin{aligned}\hat{Z}_\kappa(a,b,c) &= \langle \exp[-cH_\kappa(a,b)]\rangle \exp[\Lambda_\kappa(a,b)],\\ \hat{Z}(a,b,c) &= \lim_{\kappa\to\infty} \hat{Z}_\kappa(a,b,c).\end{aligned} \tag{2.3}$$

The above limits exists by (1.2), (2.1), and (2.2). From (1.1), (2.1), and (2.2) it also follows that

$$\exp[-O(abc)]Z_\kappa(a,b,c) \leq \hat{Z}_\kappa(a,b,c) \leq \exp[O(a,b,c)]. \tag{2.4}$$

The above relation also holds between $Z(a,b,c)$ and $\hat{Z}(a,b,c)$. The Hölder's inequality yields

$$\frac{\langle \exp[-cH_\kappa(a,b)]\rangle}{\langle \exp[-\epsilon H_\kappa(a,b)]\rangle} \geq \left[\frac{\langle \exp[-2\epsilon H_\kappa(a,b)]\rangle}{\langle \exp[-\epsilon H_\kappa(a,b)]\rangle}\right]^{(c-\epsilon)/\epsilon} \tag{2.5}$$

for $(c-\epsilon)/\epsilon \geq 1$. The above is a modification of Guerra's method.[6] From Nelson's symmetry in the lattice approximation and convergence of the lattice approximation as lattice spacing tends to zero,[9] we also obtain

$$Z(a,b,c) = Z(c,a,b) = Z(b,c,a). \tag{2.6}$$

Proof of Theorem 1.1(a): We only need to prove the first inequality. From (2.4)–(2.6) it follows that for $(c-\epsilon)/\epsilon \geq 1$

$$\begin{aligned}
Z(a,b,c) &\geq \exp[-O(abc)]\lim_{\kappa\to\infty}\hat{Z}_\kappa(a,b,c) \text{ by (2.4)} && (2.4)\\
&\geq \exp[-O(abc)]\lim_{\kappa\to\infty}\left[\frac{\langle \exp[-cH_\kappa(a,b)]\rangle}{\langle \exp[-\epsilon H_\kappa(a,b)]\rangle}\right]\\
&\quad\times \hat{Z}_\kappa(a,b,\epsilon) \text{ by (2.3)} && (2.3)\\
&\geq \exp[-O(abc)]\lim_{\kappa\to\infty}[\hat{Z}_\kappa(a,b,2\epsilon)]^{(c-\epsilon)/\epsilon}\\
&\quad\times[\hat{Z}_\kappa(a,b,\epsilon)]^{-(c-2\epsilon)/\epsilon} \text{ by (2.5)} && (2.5)\\
&\geq \exp[-\text{const}(\epsilon)abc]\lim_{\kappa\to\infty}[\hat{Z}_\kappa(a,b,2\epsilon)]^{(c-\epsilon)/\epsilon}\\
&\qquad\text{by (2.4) and (1.1)}\\
&\geq \exp[-\text{const}(\epsilon)abc][Z(a,b,2\epsilon)]^{(c-\epsilon)/\epsilon}\\
&\qquad\text{by (2.4) and (1.1)}\\
&\geq \exp[-\text{const}(\epsilon)abc][Z(2\epsilon,a,b)]^{(c-\epsilon)/\epsilon} \text{ by (2.6).}
\end{aligned}$$

Applying the above procedure two more times, we arrive at

$$Z(a,b,c) \geq \exp[-\text{const}(\epsilon)abc][Z(2\epsilon,2\epsilon,2\epsilon)]^{(a-\epsilon)(b-\epsilon)(c-\epsilon)/\epsilon^3}. \tag{2.7}$$

Using Feldman's method,[2] it is not hard to show that $Z(\epsilon,\epsilon,\epsilon) \to 1$ as $\epsilon \to 0$. Choose ϵ sufficiently small such that $Z(2\epsilon,2\epsilon,2\epsilon) \geq \frac{1}{2}$. Theorem 1.1(a) then follows from (2.7). ∎

We next prove Theorem 1.1(b) and (c). We denote by $V_\kappa^P(a,b,c)$ the momentum cutoff interaction action of the $(\lambda\phi^4 - \sigma\phi^2 - \mu\phi)_3$ field model with periodic boundary conditions. See Ref. 3 for detailed discussions and definitions. In general we allow that α and μ can be different from zero. We also define $V_\kappa^{HP}(a,b,c)$ by $V_\kappa^{HP}(a,b,c) = V_\kappa(a,b,c)$ where $V_\kappa(a,b,c)$ is the action corresponding to free boundary conditions. The half periodic partition function is defined by

$$Z_\kappa^{HP}(a,b,c) = \langle \exp[-V_\kappa^{HP}(a,b,c)]\rangle,$$

where we understand that $\langle\cdot\rangle$ stands for the expectation with respect to the Gaussian measure for periodic boundary conditions on $\partial\Omega$. Using a formula relating two Wick orderings and using the explicit definitions of the actions,[1,3] it is easy to check that

$$\begin{aligned}
&V_\kappa^{HP}(a,b,c) = V_\kappa^P(a,b,c) + b(\kappa)\int_\Omega :\phi_\kappa^2(x):_P dx + c(\kappa,\Omega),\\
&|b(\kappa)| \leq \text{const} \qquad \text{uniformly in } \kappa,\\
&|c(\kappa,\Omega)| \leq \text{const } abc \qquad \text{uniformly in } \kappa.
\end{aligned} \tag{2.8}$$

Here we note that two divergence terms arose from the change in the mass and vacuum counter terms in (2.8), but these cancelled each other out. The relation (2.8) implies that, to prove Theorem 1.1(b), it is sufficient to show that $Z^{HP}(a,b,c) \geq \exp[-O(abc)]$ for the $(\lambda\phi^4 - \sigma\phi^2 - \mu\phi)_3$ model in general. From (2.8) and the result of Ref. 3 it follows that

$$Z^{HP}(a,b,c) = \lim_{\kappa\to\infty} Z_\kappa^{HP}(a,b,c)$$

exists. Let $H_0^P(a,b)$ be the free Hamiltonian in a periodic square $a\times b$ and let $H_\kappa^P(a,b)$ be the momentum cutoff (half periodic) interaction Hamiltonian of the $(\lambda\phi^4 - \sigma\phi^2 - \mu\phi)_3$ field model. Following Ref. 10 we have

$$\begin{aligned}
&Z_\kappa^{HP}(a,b,c)\\
&\quad= \frac{T_\gamma\{\exp[-cH_\kappa^P(a,b)]\}}{T_\gamma\{\exp[-cH_0^P(a,b)]\}}\exp[\Lambda_\kappa(a,b) + T_\kappa(a,b,c)].
\end{aligned} \tag{2.9}$$

We again use Hölder's inequality to obtain

$$\frac{T_\gamma\{\exp[-cH_\kappa^P(a,b)]\}}{T_\gamma\{\exp[-\epsilon H_\kappa^P(a,b)]\}} \geq \left[\frac{T_\gamma\{\exp[-2\epsilon H_\kappa^P(a,b)]\}}{T_\gamma\{\exp[-\epsilon H_\kappa^P(a,b)]\}}\right]^{(c-\epsilon)/\epsilon} \tag{2.10}$$

for $(c-\epsilon)/\epsilon \geq 1$. An explicit computation yields $(c \geq \epsilon > 0)$

$$\exp[-O(abc)] \leq T_\gamma\{\exp[-cH_0^P(a,b)]\} \leq \exp[O(abc)]. \tag{2.11}$$

From (2.4) and the upper bound of the partition function[3] we also have

$$Z_\kappa^{HP}(a,b,c) \leq \exp[O(abc)]. \tag{2.12}$$

From Nelson's symmetry for the half periodic partition function we have

$$Z^{HP}(a,b,c) = Z^{HP}(c,a,b). \tag{2.13}$$

We are now ready to prove Theorem 1.1(b) and (c).

Proof of Theorem 1.1 (b) and (c): We follow the method used in the proof of part (a). From (2.9)–(2.13) it follows that for

$$\begin{aligned}
Z^{HP}(a,b,c) &\geq \exp[-O(abc)]\lim_{\kappa\to\infty}\frac{T_\gamma\{\exp[-cH_\kappa^P(a,b,c)]\}}{T_\gamma\{\exp[-\epsilon H_\kappa^P(a,b)]\}}\\
&\quad\times Z_\kappa^{HP}(a,b,\epsilon) \text{ by (2.9) and (2.11)}
\end{aligned}$$

$$\geq \exp[-\text{const}(\epsilon)abc] \lim_{\kappa \to 1} [Z_\kappa^{HP}(a,b,2\epsilon)]^{(c-\epsilon)/\epsilon}$$
$$\times [Z_\kappa^{HP}(a,b,\epsilon)]^{-(c-2\epsilon)/\epsilon} \quad \text{by (2.10) and (2.11)}$$
$$\geq \exp[-\text{const}(\epsilon)abc] \lim_{\kappa \to 1} [Z_\kappa^{HP}(a,b,2\epsilon)]^{(c-\epsilon)/\epsilon} \quad \text{by (2.12)}$$
$$= \exp[-\text{const}(\epsilon)abc][Z^{HP}(a,b,2\epsilon)]^{(c-\epsilon)/\epsilon}$$
$$= \exp[-\text{const}(\epsilon)abc][Z^{HP}(2\epsilon,a,b)]^{(c-\epsilon)/\epsilon} \quad \text{by (2.13)}$$
$$\geq \exp[-\text{const}(\epsilon)abc][Z^{HP}(2\epsilon,2\epsilon,2\epsilon)]^{(a-\epsilon)(b-\epsilon)(c-\epsilon)/\epsilon^3}.$$

In Ref. 3 it has been shown that, for any ϵ, $Z^P(2\epsilon,2\epsilon,2\epsilon) > 0$ for the $(\lambda\phi^4 - \sigma\phi^2 - \mu\phi)_3$ model. From (2.8) we also have that $Z^{HP}(2\epsilon,2\epsilon,2\epsilon) > 0$. This gives us

$$Z^{HP}(a,b,c) \geq \exp[-O(abc)]. \tag{2.14}$$

To show the above bound for $Z^P(a,b,c)$ we choose $\sigma = \lim_{\kappa \to 1} b(\kappa)$ and $\mu = 0$. Theorem 1.1(b) now follows from (2.8) and (2.14).

We now give a brief discussion of the proof of Theorem 1.1(c). Notice that the relations corresponding to (2.9), (2.10), and (2.13) hold for the lattice approximation. Also the relations corresponding to (2.8) and (2.12) hold for the lattice approximation (uniformly in δ). Hence, if one follows the procedure used in the proof of Theorem 1.1(b), one may obtain that

$$Z_\delta^{HP}(a,b,c) \geq \exp[-\text{const}(\epsilon)abc] \times [Z_\delta^{HP}(2\epsilon,2\epsilon,2\epsilon)]^{(a-\epsilon)(b-\epsilon)(c-\epsilon)/\epsilon^3}.$$

From the convergence of the lattice approximation and from the argument used in the later part of the proof of Theorem 1.1(b) we have proven Theorem 1.1(c). This complete the proof. ∎

Note added in manuscript: E. Seiler and B. Simon have independently developed techniques similar to ours in "Nelson's Symmetry and All That in Yukawa$_2$ and $(\phi^4)_3$ Field Theories" (Princeton University Preprint, 1975).

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[1]J. Glimm and A. Jaffe, Fortschr. Physik. **21**, 327 (1973).
[2]J. Feldman, Commun. Math. Phys. **37**, 93 (1974).
[3]Y. Park, J. Math. Phys. **16**, 2183 (1975).
[4]J. Feldman and K. Osterwalder, "The Wightman Axioms and the Mass Gap for Weakly Coupled $\lambda\phi_3^4$ Quantum Field Theories," Harvard Preprints.
[5]J. Magnen and R. Sénéor, "Infinite Volume Limit of the $\lambda\phi_3^4$ Model," Preprint.
[6]B. Simon, "The $p(\phi)_2$ Euclidean (Quantum) Field Theory" (Princeton U.P., Princeton, N.J., 1974).
[7]F. Guerra, "Exponential Bounds in Lattice Field Theory," Preprint in preparation.
[8]J. Fröhlich, "The Irreducible Quantum Fields and Dynamical Symmetric Breaking in Symanski—Nelson Positive Quantum Field Theory," Princeton Preprint.
[9]Y. Park, J. Math. Phys. **16**, 1065 (1975).
[10]F. Guerra, L. Rosen, and B. Simon, Commun. Math. Phys. **41**, 19 (1975).