Tensor operators and twisted group algebras

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Two generalizations of Frame's theory of the conjugating representation of a finite group G are explored and applied to the problem of forming tensor operators out of a group algebra. In each case the group G acts on the group algebra $A(\bar{G})$, where $\bar{G}$ either contains G or covers G as a central extension. By construction, an affirmative answer is given to the question, raised by de Vries and van Zanten, as to whether or not $\bar{G}$ may be found such that $A(\bar{G})$ carries all the irreducible representations of G. Several examples are given, with the groups chosen from among the crystallographic point groups.

1. INTRODUCTION

From the earliest days of quantum mechanics the notion of a set of tensor operators for a group has been of utmost importance, particularly in angular momentum studies (Refs. 1—3). Although it is often the case that tensor operators in quantum mechanics are constructed from physical observables using the various operations of the tensor calculus, there is some virtue in working within a more abstract setting. In particular there has been interest recently in the construction of tensor operators for a finite group G out of its own group algebra $A(G)$ (Refs. 4—8). We recall that $A(G)$ has elements which are complex linear combinations of a set of basis members in one-to-one correspondence with, and for convenience actually denoted by, the set of elements of G. The multiplication in $A(G)$ is given as the linear extension of the product in G itself. Of course, $A(G)$ provides a module for the regular representation of G, but it also has a G-module structure relative to the action $a \to gag^{-1}$, for $a \in A(G)$, $g \in G$. In the pure group theory literature this action has been termed the *conjugating representation*, originally discussed by Frame in Ref. 9 and more recently by Solomon, Roth, and Formanek (Refs. 10—12). It is precisely this action which has been considered by Gamba, Killingbeck, and Van Zanten and de Vries (Refs. 4—8), independently of the above-mentioned authors.

It is at once clear that the center Z of G acts trivially on $A(G)$, the implication being that irreducible tensor operators may only be associated with those irreducible representations (reps) of G which give rise to ordinary reps of G/Z. Contrary perhaps to instinct, by following trials with simple examples and some theoretical results of Roth (Ref. 11), it was shown in Ref. 12 by Formanek and in Ref. 8 by van Zanten and de Vries that $A(G)$ does not necessarily carry all the reps of G/Z. However, the latter were able to show that each rep of G/Z occurs as a constituent of at least one of the modules in the sequence $\otimes^n A(G)$, $n = 1, 2, \cdots$. Indeed, it follows that there is an integer N, such that $\otimes^n A(G)$ contains every rep of G/Z whenever $n \geq N$. The same authors left open the question of associating tensor operators, in an analogous fashion, with all the reps of G.

The aim of the present paper is to offer some generalizations of the above-mentioned work, incidentally dealing in principle with the lacuna noted in Ref. 8 by van Zanten and de Vries. For the sake of simplicity we have separated the generalizations into two types. In the first case in Sec. 2 we allow G to act in a conjugating manner on $A(\bar{G})$, where $\bar{G}$ is a finite group containing G. In particular we analyze $A(\bar{G})$ as a G-module into its irreducible G-submodules, and we also look at some other natural G-submodules. Section 3 contains the results of applying Sec. 2 to two main choices for $\bar{G}$: first as the full permutation group on the elements of G and secondly as the holomorph of G. The second generalization is considered in Sec. 4, where G acts on $A(\bar{G})$, $\bar{G}$ containing a central subgroup K such that $\bar{G}/K \approx G$. We quickly specialize to the choice $\bar{G} = G^{\omega}$, the linearizing group of the projective representations of G with factor system ω. Here we find that $A(\bar{G})$ has a natural image $A(G; \omega)$, called a twisted group algebra, on which G may act in tensor fashion. We note that it is necessary to widen the notion of a tensor operator, as given for example in Sec. 2 of Ref. 8, to include the possibility that G acts via a projective representation, a not uncommon situation. The analysis is similar to that given in Sec. 2. We conclude by noting that any point group may act in accordance with Sec. 4 on a subalgebra of the group algebra of its associated double group.

2. G AS A SUBGROUP OF $\bar{G}$

If the group G is contained as a subgroup in the group $\bar{G}$, then $A(\bar{G})$, the group algebra of $\bar{G}$, can be considered as a G-module relative to the action $a \to gag^{-1}$, for $a \in A(\bar{G})$ and $g \in G$. Clearly, if $g \in \bar{Z} \cap G$, where $\bar{Z}$ is the center of $\bar{G}$, then g acts trivially on $A(\bar{G})$; hence the latter can be alternatively considered as a $[G/(\bar{Z} \cap G)]$-module. But if $g \in G - \bar{Z} \cap G$, then g acts nontrivially on $A(\bar{G})$, so that, *a fortiori*, $A(\bar{G})$ is a faithful $[G/(\bar{Z} \cap G)]$-module. It now follows from a theorem of Burnside (for a particularly simple proof see Ref. 13) that every irreducible $[G/(\bar{Z} \cap G)]$-module occurs as a constituent of at least one of the tensor power modules $\otimes^n A(\bar{G})$, $n = 1, 2, \cdots$. This conclusion is noted for the special case $\bar{G} = G$ in Ref. 8. The hope is that with the greater freedom now allowed to us, by a suitable choice of $\bar{G}$, we will be able to accommodate all the reps of G. We return to this point in Sec. 3.

$A(\bar{G})$ has as basis the set $\{\bar{g} : \bar{g} \in \bar{G}\}$, which may be used to determine the character function, $\chi^{\bar{G}}$, of the generalized conjugating representation carried by $A(\bar{G})$. In fact, for $g \in G$, $\chi^{\bar{G}}(g) = |\bar{N}(g)| = |\bar{G}|/|\bar{C}(g)|$, where $\bar{N}(g)$ is the normalizer (centralizer) of g in $\bar{G}$ and where $\bar{C}(g)$ denotes the conjugacy class of $\bar{G}$ containing g. Now let $\{\chi^{\mu}\}$ denote the set of irreducible characters of G, and χ_i^{μ} denote the value of χ^{μ} on the ith conjugacy class, C_i, of G. Then, if $\chi^{\bar{G}} = \sum_{\mu} a_{\mu} \chi^{\mu}$, we have

$$a_{\mu} = \frac{1}{|G|} \sum_i |C_i| \chi_i^{\bar{G}} \chi_i^{\mu}, \tag{2.1}$$

since $\chi_i^{\bar{\mathbf{G}}}$ is real,

$$= \frac{|\bar{\mathbf{G}}|}{|\mathbf{G}|} \sum_i \frac{|\mathbf{C}_i|}{|\bar{\mathbf{C}}_i|} \chi_i^\mu \tag{2.2}$$

$$= \sum_i \frac{|\bar{\mathbf{N}}(c_i)|}{|\mathbf{N}(c_i)|} \chi_i^\mu, \tag{2.3}$$

where $c_i \in \mathbf{C}_i$ and $\bar{\mathbf{C}}_i$ and where the barred and unbarred symbols refer, respectively, to $\bar{\mathbf{G}}$ and $\mathbf{G}$. Notice that the coefficient of χ_i^μ is a positive integer since $\mathbf{N}(c_i)$ is a subgroup of $\bar{\mathbf{N}}(c_i)$. Equations (2.2) and (2.3) generalize the result of Frame, also noted in Refs. 4, 8, that, for $\bar{\mathbf{G}} = \mathbf{G}$, $\chi^{\mathbf{G}} = \sum_\mu b_\mu \chi^\mu$, where $b_\mu = \sum_i \chi_i^\mu$, the sum of the entries in the μth row of the character table of $\mathbf{G}$. This latter sum is therefore a nonnegative integer, as is a_μ.

Consider now the character afforded by the power module $\otimes^n A(\bar{\mathbf{G}})$, for $n \geq 1$. Clearly it is $(\chi^{\bar{\mathbf{G}}})^n$, and it contains χ^μ with frequency

$$a_\mu^{(n)} = \sum_i \frac{|\bar{\mathbf{N}}(c_i)|^n}{|\mathbf{N}(c_i)|} \chi_i^\mu, \tag{2.4}$$

which reduces in the case $\bar{\mathbf{G}} = \mathbf{G}$ to

$$b_\mu^{(n)} = \sum_i |\mathbf{N}(c_i)|^{n-1} \chi_i^\mu, \tag{2.5}$$

being equivalent to Eq. (23) of Ref. 8.

We turn now to a consideration of certain natural $\mathbf{G}$-submodules of $A(\bar{\mathbf{G}})$, namely those generated by elements of single classes in $\bar{\mathbf{G}}$. Clearly the character of the representation afforded by $A(\mathbf{D}_i)$, where $\mathbf{D}_i$ denotes both the ith conjugacy class of $\bar{\mathbf{G}}$ and the submodule of $A(\bar{\mathbf{G}})$ which it generates, is given by $\chi^{\mathbf{D}_i}(g) = |\bar{\mathbf{N}}(g) \cap \mathbf{D}_i|$. Then we have

Theorem 1: Let d_i be a fixed member of the class $\mathbf{D}_i$ of $\bar{\mathbf{G}}$, and let 1_i denote the trivial character of the normalizer subgroup $\bar{\mathbf{N}}(d_i)$. Then

$$\chi^{\mathbf{D}_i} = (1_i \uparrow \bar{\mathbf{G}}) \downarrow \mathbf{G}. \tag{2.6}$$

In particular $\mathbf{D}_i$ carries a monomial representation.

Proof: Write the coset decomposition $\bar{\mathbf{G}} = \sum_j h_j \bar{\mathbf{N}}(d_i)$. Then it is easy to see that $\mathbf{D}_i$ can be written as the set $\{h_j^{-1} d_i h_j : \text{all } j\}$. Consider $(1_i \uparrow \bar{\mathbf{G}})(g)$, for $g \in \mathbf{G}$, which is equal to the number of j's for which $h_j g h_j^{-1} \in \bar{\mathbf{N}}(d_i)$. This, however, equals the number of j's for which $h_j^{-1} d_i^{-1} h_j g h_j^{-1} d_i h_j = g$, a characterization which immediately implies (2.6). This concludes the proof.

In the special case that $\bar{\mathbf{G}} = \mathbf{G}$, this result appears in the proof of Lemma 1.5 of Ref. 11, and it is also equivalent, through the Frobenius reciprocity theorem, to Theorem 1 and its corollary of Ref. 8. The following is a simple consequence of the Mackey subgroup theorem (see, for example, Ref. 14).

Corollary 1: Let $\bar{\mathbf{G}} = \sum_\alpha \mathbf{G} h_\alpha \bar{\mathbf{N}}(d_i)$ be a double coset decomposition of $\bar{\mathbf{G}}$. Write $\mathbf{L}_\alpha = \mathbf{G} \cap \bar{\mathbf{N}}(h_\alpha d_i h_\alpha^{-1})$ and let 1_α denote the trivial character of $\mathbf{L}_\alpha$. Then

$$\chi^{\mathbf{D}_i} = \sum_\alpha 1_\alpha \uparrow \mathbf{G}. \tag{2.7}$$

To conclude, we return to the choice $\bar{\mathbf{G}} = \mathbf{G}$ and note the result of Frame that $\chi^{\mathbf{G}} = \sum_\mu \chi^\mu \chi^{*\mu}$, where $\chi^{*\mu}$ is the complex conjugate of the character χ^μ and where the summation is over all inequivalent characters of $\mathbf{G}$. This formula, which is implicit in Eq. (18) of Ref. 8, is easily proved using the orthogonality properties of irreducible characters, for example, see Theorem (1.2) of Ref. 11. However, it is perhaps interesting to obtain it in the following direct manner. For suppose we reduce the left regular representation of $\mathbf{G}$ into its primary parts, and concentrate attention on the two-sided ideal J^μ of $A(\mathbf{G})$ which carries the rep D^μ with multiplicity d_μ $(= \dim D^\mu)$. If we assume that g is represented by $D^\mu(g) \otimes I_\mu$, where I_μ is the $d_\mu \times d_\mu$ identity matrix, then a matrix basis for J^μ is the set $\{E^{rs} \otimes I_\mu : (E^{rs})_{pq} = \delta_{rp}\delta_{sq}$, for $1 \leq r, s \leq d_\mu\}$. A simple calculation shows that, under the conjugating action of $g \in \mathbf{G}$, $E^{rs} \otimes I_\mu$ is sent to the matrix

$$\sum_{p,q} [D^\mu(g) \otimes D^{*\mu}(g)]_{pq,rs} (E^{pq} \otimes I_\mu). \tag{2.8}$$

Thus J^μ carriers $D^\mu \otimes D^{*\mu}$, and Frame's theorem follows on summing over the μ's to fill out the whole of $A(\mathbf{G})$.

If we write the Kronecker product formula $\chi^\mu \chi^\nu = \sum_\lambda g_{\mu\nu}^\lambda \chi^\lambda$, then $b_\lambda = \sum_i \chi_i^\lambda = \sum_\mu g_{\mu\bar{\mu}}^\lambda$, so that b_λ is zero if and only if every $g_{\mu\bar{\mu}}^\lambda$ is zero. The dual situation, in the sense given in Refs. 15, 16, is also of interest. For the dual of $\sum_\mu \chi^\mu \chi^{*\mu}$ is the class sum $\sum_i \mathbf{C}_i \mathbf{C}_{i'} / |\mathbf{C}_i|$, which can be variously calculated as $\sum_{i,k} (h_{ii',k} / |\mathbf{C}_i|) \mathbf{C}_k$ and $\sum_{k,\mu} (\chi_k^\mu / d_\mu) \mathbf{C}_k$, where the numbers $h_{ii',k}$ are class multiplication coefficients. Since the latter are nonnegative integers, it follows that $\sum_\mu \chi_k^\mu / d_\mu$ is zero if and only if $h_{ii',k} = 0$ for all i, and this if and only if $\mathbf{C}_k$ has no elements of the form $aba^{-1}b^{-1}$. We reach the well-known result that $\mathbf{C}_k$ consists only of commutators if and only if $\sum_\mu \chi_k^\mu / d_\mu \neq 0$. Of course, it is crucial in the proof to note that a class either has no commutators or consists entirely of commutators. Further to this, it is shown in Ref. 8 that

$$\sum_\mu \frac{\chi_k^\mu}{d_\mu} \left(= \sum_i \frac{h_{ii',k}}{|\mathbf{C}_i|} \right)$$

measures the number of ways an element of $\mathbf{C}_k$ can be written as a commutator.

3. EXAMPLES

It is perhaps trivial, but nevertheless often useful, to regard the relationship $\mathbf{G} \leq \bar{\mathbf{G}}$ as having arisen in the following situation. Suppose $\mathbf{G}$ acts as a transformation group on a set S, that is, with each $g \in \mathbf{G}$ there is associated a one-to-one transformation, T_g, of the set S onto itself, such that T_e is the trivial transformation and $T_{g_1 g_2} = T_{g_1} T_{g_2}$, for all $g_1, g_2 \in \mathbf{G}$. But S may very well possess one-to-one transformations other than the T_g's, $g \in \mathbf{G}$. So there may exist many transformation groups $\bar{\mathbf{G}}$ lying between $\mathbf{G}$ and $\mathbf{P}(S)$, the full permutation group of the set S. For example, suppose it is possible to write $S = \cup_i S_i$, where the sets S_i have the same cardinality and are $\mathbf{G}$-invariant. Clearly we may embed $\mathbf{G}$ in several subgroups of $\mathbf{P}(S)$ simply by the adjunction of transformations which bodily interchange some or all of the sets S_i in a consistent fashion. This is a situation which occurs when a complex molecule is symmetrically built from equivalent subunits which themselves possess symmetry. In Ref. 17, Boyle has successfully exploited this feature of complex molecules, and, by

using the theory of induced representations, has developed the method of ascent of symmetry as a useful tool in molecular studies.

For the present purpose, however, we content ourselves with the choice $S=\mathbf{G}$ and let $\mathbf{G}$ act on itself by left translations. Thus, if $g\in\mathbf{G}$, the left translation λ_g acts on $g'\in\mathbf{G}$ to give gg'. In the first example we take $\bar{\mathbf{G}}=\mathbf{S}_{|\mathbf{G}|}$, the full permutation group on $|\mathbf{G}|$ symbols, of order $|\mathbf{G}|!$. We first remark that, except in the trivial case $|\mathbf{G}|=2$, $\mathbf{S}_{|\mathbf{G}|}$ has trivial center so that $\mathbf{G}/\bar{\mathbf{Z}}\cap\mathbf{G}=\mathbf{G}$. It follows that irreducible tensor operators may be associated with every rep of $\mathbf{G}$ by employing the $\mathbf{G}$-module $A(\mathbf{S}_{|\mathbf{G}|})$ and its powers. This settles in principle the question asked by van Zanten and de Vries towards the end of Sec. 3 in Ref. 8. We now decompose $A(\mathbf{S}_{|\mathbf{G}|})$ by computing the integers a_μ, as given in Eq. (2.3). For each $g\in\mathbf{G}$ we need to consider the normalizer of λ_g in $\mathbf{S}_{|\mathbf{G}|}$. Suppose $\pi\in\bar{\mathbf{N}}(\lambda_g)$, then $(\pi\lambda_g)g'=(\lambda_g\pi)g'$ for all $g'\in\mathbf{G}$. It follows that $\pi(gg')=g\pi(g')$ for all $g'\in\mathbf{G}$, which means that π is essentially only a function of the cosets of $\langle g\rangle$ in $\mathbf{G}$, where $\langle g\rangle$ denotes the cyclic group of order $m(g)$ generated by g. Hence $|\bar{\mathbf{N}}(\lambda_g)|=|\mathbf{G}|!/[|\mathbf{G}|-r(g)]!$, where $r(g)=|\mathbf{G}|/m(g)$. Finally

$$a_\mu=\sum_i\frac{|\mathbf{G}|!}{(|\mathbf{G}|-r_i)!}\frac{|\mathbf{C}_i|}{|\mathbf{G}|}\chi_i^\mu, \tag{3.1}$$

where $r_i=r(c_i)$ for $c_i\in\mathbf{C}_i$. We are guaranteed that $a_\mu\geq 0$, but this may be strengthened.

Theorem 2: $a_\mu>0$ for all μ unless $|\mathbf{G}|=2$.

Proof: Write

$$a_\mu=\frac{|\mathbf{G}|!}{|\mathbf{G}|}d_\mu+\sum_{i\neq 0}\frac{|\mathbf{G}|!}{(|\mathbf{G}|-r_i)!}\frac{|\mathbf{C}_i|}{|\mathbf{G}|}\chi_i^\mu,$$

where the second term is an integer, positive, negative, or zero, whose magnitude does not exceed

$$\frac{|\mathbf{G}|!}{|\mathbf{G}|}d_\mu\sum_{i\neq 0}\frac{|\mathbf{C}_i|}{(|\mathbf{G}|-r_i)!}.$$

Suppose m is the least order of the nontrivial elements of $\mathbf{G}$, and r is $|\mathbf{G}|/m$. It follows that

$$\sum_{i\neq 0}\frac{|\mathbf{C}_i|}{(|\mathbf{G}|-r_i)!}$$

does not exceed

$$\frac{1}{(|\mathbf{G}|-r)!}\sum_{i\neq 0}|\mathbf{C}_i|=\frac{|\mathbf{G}|-1}{(|\mathbf{G}|-r)!}.$$

Thus $a_\mu=(|\mathbf{G}|!/|\mathbf{G}|)d_\mu(1+a)$, where $|a|\leq(|\mathbf{G}|-1)/(|\mathbf{G}|-r)!$. We will have established our result if we can show that $|a|<1$. Actually this condition is violated for $|\mathbf{G}|=2$, 3, 4, but the validity of the theorem for the cases $|\mathbf{G}|=3$, 4 can be verified directly (see the final sentence of Sec. 3). To deal with larger values of $|\mathbf{G}|$, we note that $r\leq|\mathbf{G}|/2$ if $|\mathbf{G}|$ is even and $r\leq(|\mathbf{G}|-1)/2$ if $|\mathbf{G}|$ is odd. Hence $|a|\leq(|\mathbf{G}|-1)/(|\mathbf{G}|/2)!$ if $|\mathbf{G}|$ is even and $|a|\leq(|\mathbf{G}|-1)/[(|\mathbf{G}|+1)/2]!$ if $|\mathbf{G}|$ is odd. These numbers are less than $(|\mathbf{G}|-1)/|\mathbf{G}|$ and $(|\mathbf{G}|-1)/(|\mathbf{G}|+1)$, respectively, if $|\mathbf{G}|>4$. Hence $|a|<1$ for all μ if $|\mathbf{G}|>4$. With the cases $|\mathbf{G}|=3$, 4, we have that $a_\mu>0$ for all μ for $|\mathbf{G}|\geq 3$. There remains the exception, when $|\mathbf{G}|=2$. This completes the proof.

We have shown therefore that $A(\mathbf{S}_{|\mathbf{G}|})$ carries every rep of $\mathbf{G}$ when $\mathbf{G}$ acts in the conjugating fashion. Perhaps this is hardly surprising when one considers the enormity of $\mathbf{S}_{|\mathbf{G}|}$ when $|\mathbf{G}|$ is not small. It would be interesting to have more information about pairs of groups $(\mathbf{G},\bar{\mathbf{G}})$ with $\mathbf{G}\leq\bar{\mathbf{G}}$ and where the generalized conjugating representation of $\mathbf{G}$ on $A(\bar{\mathbf{G}})$ contains every rep of $\mathbf{G}$. There is strong empirical evidence to suggest that $\bar{\mathbf{G}}=\mathbf{G}=\mathbf{S}_n$ is such a case, except for $n=2$.

For our second example we take $\bar{\mathbf{G}}$ as the *holomorph* of $\mathbf{G}$, denoted hol$\mathbf{G}$. hol$\mathbf{G}$ is a subgroup of $\mathbf{S}_{|\mathbf{G}|}$ and consists of the pairs $\lambda_g\sigma$, $g\in\mathbf{G}$ and $\sigma\in\text{aut}\mathbf{G}$. Clearly $\lambda_g\sigma$ sends g' into $g\,\sigma(g')$, from which it follows quickly that the elements of hol$\mathbf{G}$ may be represented in the form (g,σ), with the product law

$$(g_1,\sigma_1)(g_2,\sigma_2)=(g_1\sigma_1(g_2),\sigma_1\sigma_2). \tag{3.2}$$

for g_1, $g_2\in\mathbf{G}$ and σ_1, $\sigma_2\in\text{aut}\mathbf{G}$. It is now easy to check that hol$\mathbf{G}$ is indeed a group, having identity $(e,1)$, and where the inverse of (g,σ) is $(\sigma^{-1}(g^{-1}),\sigma^{-1})$. Furthermore, the elements (e,σ), $\sigma\in\text{aut}\mathbf{G}$, form a subgroup isomorphic to aut$\mathbf{G}$, and the elements $(g,1)$, $g\in\mathbf{G}$, make up a normal subgroup isomorphic to $\mathbf{G}$. Finally, hol$\mathbf{G}$ is the semidirect product of $\mathbf{G}$ by aut$\mathbf{G}$, written hol$\mathbf{G}=\mathbf{G}\circledS\text{aut}\mathbf{G}$. We now calculate the center of hol$\mathbf{G}$.

Lemma 1: $\mathbf{Z}(\text{hol}\mathbf{G})=\{(z,1):z\in\mathbf{Z}(\mathbf{G})\text{ and }\sigma(z)=z\text{ for all }\sigma\in\text{aut}\mathbf{G}\}$.

Proof: If (g,σ) is central, then $(g,\sigma)(g',\sigma')$ $(g'\sigma')(g,\sigma)$, for all $(g',\sigma')\in\text{hol}\mathbf{G}$. Hence

$$\left.\begin{aligned} g\sigma(g')&=g'\sigma'(g)\\ \sigma\sigma'&=\sigma'\sigma\end{aligned}\right\}, \tag{3.3}$$

for all $(g',\sigma')\in\text{hol}\mathbf{G}$. In particular Eqs. (3.3) hold when σ' is the identity. Then $g\sigma(g')=g'g$, for all $g'\in\mathbf{G}$, with the result that σ is the inner automorphism corresponding to the element g^{-1}. Putting this information back into (3.3) we see that $g=\sigma'(g)$ for all $\sigma'\in\text{aut}\mathbf{G}$. In particular g is a member of $\mathbf{Z}(\mathbf{G})$ and hence σ is trivial. This concludes the proof.

Although $\mathbf{Z}(\text{hol}\mathbf{G})$ is not trivial, in general, the following result provides a certain amount of encouragement.

Theorem 3: Let $\mathbf{G}$ be a finite Abelian group whose Sylow 2-subgroup is $\mathbf{C}(2^{\alpha_1})\times\mathbf{C}(2^{\alpha_2})\times\cdots\times\mathbf{C}(2^{\alpha_r})$, where $\mathbf{C}(2^\alpha)$ is cyclic of order 2^α, and $\alpha_1\geq\alpha_2\geq\cdots\geq\alpha_r$. Then $\mathbf{Z}(\text{hol}\mathbf{G})$ is trivial unless $\alpha_1>\alpha_2$. In the exceptional cases $\mathbf{Z}(\text{hol}\mathbf{G})$ is generated by the unique element of order 2 in $\mathbf{C}(2^{\alpha_1})$, as a subgroup of hol$\mathbf{G}$.

Proof: The proof is a rather elementary, but long-winded exercise. We merely state that the essential point is the discovery of a sufficient number of automorphisms of $\mathbf{G}$.

Theorem 3 tells us that the very worst groups from the point of view of the ordinary conjugating representation, namely the Abelian groups, are very good candidates for the employment of the generalized conjugating representation acting on the holomorph.

We now consider some simple examples. For each group $\mathbf{G}$, we choose a suitable group $\bar{\mathbf{G}}$ containing $\mathbf{G}$, but with trivial center, and then decompose $\chi^{\bar{\mathbf{G}}}$ using (2.2). We take the examples from among the crystallographic point group, taking notation from Ref. 14.

$\mathbf{C}_2$: The smallest group containing $\mathbf{C}_2$ and having trivial center is $\mathbf{C}_{3v}$ (or $\mathbf{D}_3$)—both $\mathbf{S}_{|\mathbf{G}|}$ and holG are of order two and hence unsuitable. Then $\chi^{\bar{\mathbf{G}}} = 4A + 2B$.

$\mathbf{C}_3$: In this case we choose $\bar{\mathbf{G}}$ as $\mathbf{C}_{3v}$ (or $\mathbf{D}_3$). In fact this choice of $\bar{\mathbf{G}}$ is also a realization of $\mathbf{S}_{|\mathbf{G}|}$ and holG. Then $\chi^{\bar{\mathbf{G}}} = 4A + {}^1E + {}^2E$.

$\mathbf{C}_4$: By Theorem 3, holG has nontrivial center, and indeed holG can be identified with $\mathbf{D}_4$. However, $\mathbf{S}_{|\mathbf{G}|} = \mathbf{S}_4$, which can be identified with $\mathbf{O}$, the proper cubic group. Then

$$\chi^{\bar{\mathbf{G}}} = 10A + 6B + 4\,{}^1E + 4\,{}^2E.$$

$\mathbf{D}_2$: In this case $\mathbf{S}_{|\mathbf{G}|} = \mathbf{S}_4$, which this time can be identified with the full tetrahedral group $\mathbf{T}_d$. Also, it is clear, by considering the possible bases for $\mathbf{D}_2$, that autG $= \mathbf{S}_3$. Indeed, holG $= \mathbf{T}_d$ again. However, $\mathbf{T}_d$ is larger than is absolutely necessary for our purposes. We need look no further than $\bar{\mathbf{G}} = \mathbf{T}$. We find $\chi^{\bar{\mathbf{G}}} = 6A + 2B_1 + 2B_2 + 2B_3$.

$\mathbf{D}_4$: This is a group which Killingbeck (Ref. 7) was unable to treat fully. We choose $\bar{\mathbf{G}} = \mathbf{O}$. Then we find $\chi^{\bar{\mathbf{G}}} = 8A_1 + 2A_2 + 4B_1 + 2B_2 + 4E$.

This concludes our set of examples. We observe finally that we have established directly the validity of Theorem 2 for $|\mathbf{G}| = 3, 4$.

4. TWISTED GROUP ALGEBRAS

Suppose $\bar{\mathbf{G}}$ is a finite group containing a central subgroup $\mathbf{K}$, where $\bar{\mathbf{G}}/\mathbf{K} \approx \mathbf{G}$. Then we claim that $\mathbf{G}$ acts tensorially on $A(\bar{\mathbf{G}})$. To see this let π be the canonical epimorphism of $\bar{\mathbf{G}}$ onto $\mathbf{G}$, and let σ be a section of the extension $\mathbf{1} \to \mathbf{K} \xrightarrow{i} \bar{\mathbf{G}} \xrightarrow{\pi} \mathbf{G} \to \mathbf{1}$; that is, σ is a map: $\mathbf{G} \to \bar{\mathbf{G}}$, where $\pi \circ \sigma$ is the identity on $\mathbf{G}$, thus providing us with a set of coset representatives of $\mathbf{K}$ in $\bar{\mathbf{G}}$. Then, if $g \in \mathbf{G}$ and $a \in A(\bar{\mathbf{G}})$, g sends a to $\sigma(g)\, a\, \sigma(g)^{-1}$. Since $\mathbf{K}$ is central, it is clear that the action is independent of the choice of the section σ. Evidently $A(\bar{\mathbf{G}})$ is a faithful $(\mathbf{G}/\mathbf{Z})$-module, hence $A(\bar{\mathbf{G}})$ and its powers exhaust all irreducible $(\mathbf{G}/\mathbf{Z})$-modules. Again, since $\mathbf{K}$ is central, the character of the action of $\mathbf{G}$ on $A(\bar{\mathbf{G}})$ is the projection onto $\mathbf{G}$ of the character $\sum_\mu \chi^\mu \chi^{*\mu}$, where μ runs over all the rep labels of $\bar{\mathbf{G}}$.

Although it is possible to develop further the above analysis, it is perhaps more profitable to look at a special case which is closer to the experience of mathematical physicists. We suppose that ω is a factor system for the group $\mathbf{G}$, where the values assumed by ω are nth roots of unity for some n. Then we consider the extension $\mathbf{1} \to \mathbf{C}_n \to \mathbf{G}^\omega \to \mathbf{G} \to 1$, where $\mathbf{C}_n$ is the cyclic group of nth roots of unity. It will be recalled from Mackey (Ref. 18) that $\mathbf{G}^\omega$ is the group which linearises the ω-representations of $\mathbf{G}$. More concretely, $\mathbf{G}^\omega$ has underlying set $\mathbf{G} \times \mathbf{C}_n$, and possesses the multiplication law

$$(g_1,\ z_1)(g_2, z_2) = (g_1 g_2,\ \omega(g_1,\ g_2) z_1 z_2), \tag{4.1}$$

for $g_1,\ g_2 \in \mathbf{G}$, and $z_1,\ z_2 \in \mathbf{C}_n$. The set $\mathbf{C}_n^\circ = \{(e,\ z) : z \in \mathbf{C}_n\}$ is a central subgroup of $\mathbf{G}^\omega$, and $\mathbf{G}^\omega/\mathbf{C}_n^\circ \approx \mathbf{G}$. Hence $\mathbf{G}$ acts tensorially on $A(\mathbf{G}^\omega)$. However, it is also true that $\mathbf{G}$ acts tensorially on a natural image of $A(\mathbf{G}^\omega)$, namely the twisted group algebra $A(\mathbf{G};\ \omega)$. This algebra, which has been discussed by several authors (Refs. 19–22), is a module over the complex field, with basis the set of objects $\{\nu(g) : g \in \mathbf{G}\}$, and further has a multiplication which is the linear extension of the law

$$\nu(g_1)\nu(g_2) = \omega(g_1,\ g_2)\, \nu(g_1 g_2), \tag{4.2}$$

for all $g_1,\ g_2 \in \mathbf{G}$. The link with $A(\mathbf{G}^\omega)$ is seen in the following manner. Choose a faithful matrix ω-representation of $\mathbf{G}$, and lift it to a matrix representation of $A(\mathbf{G}^\omega)$ in which the element $(e,\ z) \in \mathbf{C}_n^\circ$ and the scalar $\gamma \in \mathbf{C}$ are represented by diag(z) and diag(γ), respectively. Then $A(\mathbf{G};\ \omega)$ is isomorphic with the algebra generated by the representation matrices of the elements $(g,\ 1)$, which are precisely the ω-representation matrices of the elements $g \in \mathbf{G}$. We now show directly that the transformation rule $a \to \nu(g)\, a\, \nu(g)^{-1}$, $a \in A(\mathbf{G};\ \omega)$ and $g \in \mathbf{G}$, turns $A(\mathbf{G};\ \omega)$ into a $\mathbf{G}$-module. Here, $\nu(g)^{-1} = \nu(g^{-1})/\omega(g,\ g^{-1})$. We calculate $\nu(g_1)\nu(g_2)\, a\, \nu(g_2)^{-1}\nu(g_1)^{-1}$ as

$$\frac{\omega(g_1,\ g_2)\omega(g_2^{-1},\ g_1^{-1})\omega(g_1 g_2,\ (g_1 g_2)^{-1})}{\omega(g_2,\ g_2^{-1})\,\omega(g_1,\ g_1^{-1})} \times \nu(g_1 g_2)\, a\, \nu(g_1 g_2)^{-1}, \tag{4.3}$$

the numerator of which becomes

$$\omega(g_2,\ g_2^{-1} g_1^{-1})\,\omega(g_1,\ g_1^{-1})\,\omega(g_2^{-1},\ g_1^{-1}) \tag{4.4}$$

$$= \omega(g_2,\ g_2^{-1})\,\omega(g_1,\ g_1^{-1}), \tag{4.5}$$

using the simple properties of factor systems. It follows that (4.3) becomes $\nu(g_1 g_2)\, a\, \nu(g_1 g_2)^{-1}$, confirming that we have a true action.

Before analysing this $\mathbf{G}$-module we recall some notions and results (see Refs. 21, 22). An element $g \in \mathbf{G}$ is termed ω-regular if $\omega(g,\ g') = \omega(g',\ g)$ for all $g' \in \mathbf{N}(g)$, the centralizer of g. ω-regularity is a class property and respects inversion. A fact which simplifies calculations is that ω can be so adjusted that $\omega(g,\ g') = \omega(gg'g^{-1},\ g)$ for all $g' \in \mathbf{G}$ if g is ω-regular. Another useful result is that, for any given $g \in \mathbf{G}$, $g' \to \omega(g,\ g')/\omega(g',\ g)$ is a linear character on $\mathbf{N}(g)$. Finally, this same result establishes that the subset of $\mathbf{Z}$ which consists of ω-regular elements, forms a subgroup $\mathbf{Z}_\omega$, say.

Consider now the result of the action of $g \in \mathbf{G}$ on a basis element

$$\nu(g') \to \nu(g)\nu(g')\nu(g)^{-1} \tag{4.6}$$

$$= \frac{\omega(g,\ g')\omega(gg',\ g^{-1})}{\omega(g,\ g^{-1})}\, \nu(gg'g^{-1}) \tag{4.7}$$

$$= \frac{\omega(g,\ g')}{\omega(gg'g^{-1},\ g)}\, \nu(gg'g^{-1}). \tag{4.8}$$

It follows that g acts trivially on $A(\mathbf{G};\ \omega)$ if and only if $g \in \mathbf{Z}$ and g is ω-regular. Hence $A(\mathbf{G};\ \omega)$ is a faithful $(\mathbf{G}/\mathbf{Z}_\omega)$-module. If χ_ω is the character function for the representation of $\mathbf{G}$ on $A(\mathbf{G};\ \omega)$, then

$$\chi_\omega(g) = \sum{}' \omega(g,\ g')/\omega(g',\ g), \tag{4.9}$$

where the prime restricts the summation to elements $g' \in \mathbf{N}(g)$. Clearly if g is ω-regular, $\chi_\omega(g) = |\mathbf{N}(g)| = |\mathbf{G}|/|\mathbf{C}(g)|$, but if g is not ω-regular, the orthogonality relations for the characters of $\mathbf{N}(g)$ imply $\chi_\omega(g) = 0$. It quickly follows, if $\chi_\omega = \sum_\mu c_\mu \chi^\mu$, that

$$c_\mu = \sum_i{}' \chi_i^\mu, \tag{4.10}$$

where the prime restricts the summation to the ω-regular classes.

Several of the results of Sec. 2 carry over. In particular, $\chi_\omega = \sum_\lambda \theta^\lambda \theta^{*\lambda}$, where the summation is over the inequivalent ω-characters θ^λ of G. Also, Theorem 1 and Corollary 1 have analogs.

5. EXAMPLES

We begin with a theoretical example for which $\mathbf{Z}_\omega$ may well be smaller than $\mathbf{Z}$. In fact let $\mathbf{G}$ be a finite Abelian group, and let $\mathbf{G}(\omega)$ be the subset of ω-regular elements of $\mathbf{G}$. Since $\mathbf{Z}_\omega = \mathbf{G}(\omega)$, the latter is a subgroup of $\mathbf{G}$. We have $\chi_\omega(g) = |\mathbf{G}|$ if $g \in \mathbf{G}(\omega)$, but is zero otherwise. Also $c_\mu = \sum_{g \in \mathbf{G}(\omega)} \chi^\mu(g)$ is $|\mathbf{G}(\omega)|$ if $\chi^\mu \downarrow \mathbf{G}(\omega)$ is trivial, but zero otherwise. It follows from this that

$$\chi_\omega = |\mathbf{G}(\omega)|(1_\omega \uparrow \mathbf{G}), \tag{5.1}$$

by the Frobenius reciprocity theorem, where 1_ω is the trivial character on $\mathbf{G}(\omega)$. It is clear that $A(\mathbf{G}; \omega)$ contains all irreducible modules of $\mathbf{G}/\mathbf{G}(\omega)$. Further results relating to the ω-rep theory of Abelian groups may be found in Refs. 23, 24.

For a specific example take $\mathbf{G} = \mathbf{D}_2$, with elements e, a, b, ab, where $a^2 = b^2 = e$ and $ab = ba$. Define ω by $\omega(a, a) = \omega(b, b) = 1$, $\omega(a, b) = -\omega(b, a) = i$, and extended bilinearly to the whole of $\mathbf{D}_2$. We find that $\mathbf{G}(\omega) = \{e\}$; hence $\chi_\omega = 1 \uparrow \mathbf{D}_2$, the regular representation of $\mathbf{D}_2$. This agrees with Frame's theorem, for there is just one equivalence class of ω-reps of $\mathbf{D}_2$, given for example by

$$e \to \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad a \to \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad b \to \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad ab \to \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix},$$

and for this we find that $\sum_\lambda \theta^\lambda \theta^{*\lambda}$ has value 4 at $g = e$ and zero elsewhere.

This example leads on to a class of groups familiar to mathematical physicists, namely the class of point groups. Here ω is chosen as the factor system naturally associated with the 2 : 1 homomorphism of $\mathbf{SU}(2)$ onto $\mathbf{SO}(3)$. The reader may consult Refs. 22, 25, where it is shown that if $\mathbf{P}$ is a point group, then $\mathbf{P}^\omega$ can be identified with the double group $\tilde{\mathbf{P}}$, and further that the conclusions of Opechowski's theorem can be related to the ω-regular class structure of $\mathbf{P}$. To continue, when $\mathbf{P}$ acts on $A(\mathbf{P}; \omega)$, the latter carries a representation whose character is $\sum_\lambda \theta^\lambda \theta^{*\lambda}$, where θ^λ ranges over the irreducible double-valued representation of $\mathbf{P}$. Also, the frequency of χ^μ in χ_ω is $\sum' \chi_i^\mu$, where the prime indicates summation only over the ω-regular classes of $\mathbf{P}$. We recall from Ref. 22 that a class of $\mathbf{P}$ is ω-regular if either it contains no twofold rotation, or, if it does contain a twofold rotation R, there is no twofold rotation in $\mathbf{P}$ whose axis is normal to that of R.

We conclude with a concrete example, choosing $\mathbf{P} = \mathbf{T}$, the proper tetrahedral group. From our interpretation of Opechowski's theorem, it is clear that $\mathbf{T}$ has three ω-regular classes, namely the identity class and the two classes of threefold rotations. The remaining class, containing the twofold rotations is not ω-regular. We deduce from the ordinary character table of $\mathbf{T}$ that $\chi_\omega = 3A + 3T$. Although $A(\mathbf{T}; \omega)$ does not carry the nontrivial linear characters of $\mathbf{T}$, these do appear on $\otimes^2 A(\mathbf{T}; \omega)$.

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Vector potentials and physical optics

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The general problem considered is to obtain solutions w to the vector equation $v = \mathrm{curl}(w)$, where v is a given divergence-free vector field with singularities. Two methods are discussed: A special method, which applies when v is of the type which occurs in the Kirchhoff theory of diffraction, and a general method, which applies to any divergence-free vector field whatever. As an example the general method is used to obtain the Maggi–Rubinowicz representations of the Kirchhoff–Helmholtz (double) integral as a line integral. The singularities of the solutions w are known to produce important optical effects, and the nature of these singularities is largely determined by topological properties of the domain on which v is regular.

I. INTRODUCTION

A. Statement of problem

In this paper we shall discuss methods for the calculation of vector potentials; i.e., we are interested in obtaining solutions $\mathbf{w}$ to the equation

$$\mathbf{v} = \nabla \times \mathbf{w} \tag{1.1}$$

where $\mathbf{v}$ is a given divergence free (solenoidal) vector field. If $\mathbf{v}$ has no singularities, then a solution to (1.1) is given by

$$\mathbf{w}(\mathbf{r}) = -\int_0^1 t\mathbf{r} \times \mathbf{v}(t\mathbf{r})\, dt = -\mathbf{r} \times \int_0^1 t\mathbf{v}(t\mathbf{r})\, dt. \tag{1.2}$$

If $\mathbf{v}$ has singularities, as is always the case in optical applications, then complications ensue.

The result (1.2) is a particular example of a much more general theorem, the *Poincaré lemma*, which is well known to differential geometers. See, e.g., Refs. 1 and 2. A simple direct proof will be given in Sec. 2B. [There is also a well-known solution given in terms of volume integrals (see, e.g., Ref. 3, p. 2, or Ref. 4), which will not be used in this paper.]

We shall present two methods for solving (1.1) when $\mathbf{v}$ has singularities: a *special method*, which is only applicable to vector fields of the type which occur as integrands in the Kirchhoff theory of diffraction, and a *general method*, which is applicable to any divergence free vector field whatever.

One matter to receive some attention in this paper is that of showing how singularities in $\mathbf{v}$ produce singularities in the solution $\mathbf{w}$ to (1.1). It may happen that *every* solution $\mathbf{w}$ will have more singularities than $\mathbf{v}$. It is well known that certain topological properties of the domain on which $\mathbf{v}$ is regular determine whether or not this is possible. Certain other conditions determine whether or not two different solutions $\mathbf{w}$ to (1.1) must necessarily differ by the gradient of a scalar function. These questions will be discussed in Sec. 1C. The analysis of the singularities of the vector potentials $\mathbf{w}$ is of considerable importance, since in the Miyamoto–Wolf theory of diffraction these singularities play an essential role in producing geometrical optics effects. (See Sec. 1B below for references.)

B. Motivation

Let S be an aperture in an opaque screen, and let $u = u(\mathbf{r})$ be the space-dependent part of a monochromatic wave incident on the screen, so that u satisfies the scalar wave equation

$$\nabla^2 u + k^2 u = 0, \quad (k = 2\pi/\lambda). \tag{1.3}$$

In the Kirchhoff theory of physical optics the field u_K diffracted through S is given by

$$4\pi u_K(P) = \int\int_S \mathbf{v} \cdot \eta\, dA, \tag{1.4}$$

where $\mathbf{v}$ is the "Helmholtz" vector field

$$\mathbf{v}(\mathbf{r}) = u(\mathbf{r})\nabla \frac{\exp(ikr)}{r} - \frac{\exp(ikr)}{r}\nabla u(\mathbf{r}). \tag{1.5}$$

In these relations P is the field point (= point at which the diffracted field is measured), $\mathbf{r}$ is the position vector $\mathbf{PQ}$ of a general point Q, and η is the unit normal to S, which generally, by convention, points away from the sources on the illuminated side of the screen. The vector field $\mathbf{v}$ is divergence free by virtue of (1.3). Hence if $\mathbf{w}$ is a solution to (1.1), and S contains no singularities of $\mathbf{w}$, then Stokes' theorem can be applied to obtain

$$4\pi u_K(P) = \int_{\partial S} \mathbf{w} \cdot d\mathbf{r}, \tag{1.6}$$

where ∂S denotes the boundary of S. If $\mathbf{w}$ has singularities, then certain terms must be adjoined to the right-hand side. See Refs. 5, 6.

The transformation of the double integral (1.4) into the line integral (1.6) has much practical value because it greatly reduces the costs of machine calculation. (See, e.g., Ref. 7.) From the standpoint of theory these line integral representations are very interesting because they show very clearly how the Kirchhoff theory predicts certain geometrical optics effects, and, qualitatively at least, certain edge effects which are implied by the Fermat principle and Keller's "Geometrical Theory of Diffraction."[8–10]

Methods for solving (1.1) when $\mathbf{v}$ is a vector field of the Helmholtz type (1.5) have been discussed by Miyamoto–Wolf[5] and by Rubinowicz.[4,6,11] In particular, for an historical survey see Ref. 4.

C. Generalities: Existence and uniqueness of solutions

(i) *Existence.* To facilitate discussion, whenever a vector field $\mathbf{v}$ has singularities it is to be understood that these singularities are to be excluded from its

"domain" (of definition or regularity). We shall say that a domain D has *Property* 1 if for every divergence free vector field $\mathbf{v}$ with domain D there exists a solution to (1.1) which is regular everywhere in D. It is well known that Property 1 is a topological property of a domain, and hence remains invariant when the domain is continuously deformed. We shall illustrate this notion with a few examples. (The topologically sophisticated reader will recognize that Property 1 is equivalent to the vanishing of the second Betti number of the deRham cohomology of the domain. See, e.g., Refs. 1, 2.)

Example 1.1: In the solution (1.2) $\mathbf{r}$ is the position vector of a general point drawn from a fixed but *arbitrary* origin. The proof consists merely of calculating the curl of the right-hand side, using some vector identities and integration by parts. Therefore, the solution is valid in any region in which the integration paths $t \to t\mathbf{r}$ do not hit singularities of $\mathbf{v}$. Hence a region bounded by a spherical surface has Property 1.

Example 1.2: Since Property 1 is a topological property, any region obtained by continuously deforming a spherical region also has Property 1. For example, a tubular region having the shape of the letter **S** has Property 1, a fact which is not at all apparent from the solution (1.2).

Example 1.3: A domain D *fails* to have Property 1 if and only if there exists a divergence free vector field $\mathbf{v}$ with domain D which is *not* the curl of a field $\mathbf{w}$ with domain D. As a corollary to Stokes' theorem it is known that a divergence free vector field $\mathbf{v}$ is the curl of some other vector field without singularities only if $\iint_S \mathbf{v}\cdot\eta\, dA = 0$ for every *closed* surface S. Therefore, a domain D fails to have Property 1 if (and only if, see below) there exists a divergence free vector field $\mathbf{v}$ with domain D and a closed surface S in D such that $\iint_S \mathbf{v}\cdot\eta\, dA \neq 0$. For example, the region obtained by removing a point from Euclidean 3-space $\mathbf{E}^3$ fails to have Property 1. To prove this we only need to note that $\iint_S \nabla(1/r)\cdot\eta\, dA = -4\pi$ when S is a sphere enclosing the origin.

Example 1.4: A domain obtained by removing one point, or a discrete set of points, from any of the domains described in the first two examples fails to have Property 1.

Remark 1.1: According to the first example, every regular point of a divergence free vector field $\mathbf{v}$ has, say, a spherical neighborhood in which (1.1) has a solution. Also, the entire domain of $\mathbf{v}$ can be filled up with such neighborhoods. However, according to the last two examples, these "local" solutions cannot always be joined together to form a smooth solution to (1.1) which is valid everywhere in the domain.

Let $\mathbf{v}$ be a divergence free vector field with domain D. Then the failure of D to have Property 1 does not at all imply that $\mathbf{v}$ is not a curl. (This remark is trivial: Let $\mathbf{w}$ be an arbitrary field with a prescribed set of singularities and set $\mathbf{v} = \nabla\times\mathbf{w}$.) There is in fact a well-known criterion for $\mathbf{v}$ to be a curl, half of which has already been discussed in Example 1.3, viz., a divergence free vector field $\mathbf{v}$ is the curl of some other vector field with domain (of regularity) D if and only if $\iint_S \mathbf{v}\cdot\eta\, dA = 0$ for *every* closed surface S in D.

(ii) *Uniqueness*: From the identity $\nabla\times\nabla f = 0$ it follows that if $\mathbf{w}$ is a solution to (1.1), then so is $\mathbf{w} + \nabla f$ where f is any scalar valued function. Hence solutions are not unique, and we now pose the question as to when any two solutions must necessarily differ by the gradient of a scalar function. Since the difference between any two solutions to (1.1) is curl free, this question reduces to determining when a curl free vector field is necessarily the gradient of some function. Again, as in the case of existence, there is a topological condition on domains D which guarantee that every curl free vector field $\mathbf{w}$ with domain (of regularity) D is a gradient, and there is an analytical condition which insures that a vector field $\mathbf{w}$ is a gradient, and which applies whether or not its domain has this topological property.

We shall say that a domain D has *Property* 2 if every curl free vector field with domain D is the gradient of some scalar function with domain D. The following results are well known.

Proposition 1: A domain D has Property 2 if and only if it is *simply connected*; i.e., if and only if every closed circuit in D can be continuously deformed into a point without leaving D.

Proposition 2: A curl free vector field $\mathbf{w}$ with domain D is the gradient of some function if and only if $\int_\gamma \mathbf{w}\cdot d\mathbf{r} = 0$ for every closed curve γ.

We recall that if $\mathbf{w}$ is a curl free vector field defined on a simply connected domain D, then $\mathbf{w} = \nabla f$, where $f(P) = \int_{\Gamma(P)} \mathbf{w}\cdot d\mathbf{r}$, and where $\Gamma(P)$ is *any* curve joining a fixed but arbitrary origin to P. [The simple connectivity of D is needed to establish, by means of Stokes' theorem, that the value of $f(P)$ does not depend of the particular choice of the curve Γ.] Hence, if D is $\mathbf{E}^3$ we can write

$$f(\mathbf{r}) = \int_0^1 \mathbf{r}\cdot\mathbf{w}(t\mathbf{r})\, dt = \mathbf{r}\cdot\int_0^1 \mathbf{w}(t\mathbf{r})\, dt. \tag{1.7}$$

Remark 1.2: Both (1.2) and (1.7) are particular examples of the Poincaré lemma, which contains these results and a countably infinite number of others of a like nature.

Example 1.5: The domains obtained by removing a point from $\mathbf{E}^3$ or a spherical region have Property 2 but not Property 1. The domains obtained by removing an entire line from $\mathbf{E}^3$ have neither Property 1 nor Property 2.

Example 1.6: There are certain properties of the vector field $\mathbf{v} = \nabla(1/r)$ which will be used in the sequel. Although $\nabla\cdot\nabla(1/r) = \nabla^2(1/r) = 0$, this field (whose domain is $\mathbf{E}^3$ with a point removed) cannot be represented as a curl on this domain because for every closed surface S

$$\iint_S \nabla(1/r)\cdot\eta\, dA = \begin{cases} -4\pi & \text{if } S \text{ encloses the origin,} \\ 0 & \text{otherwise.} \end{cases} \tag{1.8}$$

To represent $\nabla(1/r)$ as a curl in a more restricted domain, we remove a line l from $\mathbf{E}^3$, let x, y, z be rectangular coordinates with $x^2 + y^2 + z^2 = r^2$ and l corresponding to the z axis, and set

$$\psi = [\psi_x, \psi_y, \psi_z] = (z/r)(x^2+y^2)^{-1}[-y, x, 0].$$

Then a straightforward calculation shows that

$$\nabla(1/r) = \nabla \times \psi \quad \text{on } \mathbf{E}^3 - 1.$$

Since the domain $\mathbf{E}^3 - 1$ is *not* simply connected, it is not necessarily true that any two such representations of $\nabla(1/r)$ as a curl will differ by the gradient of some function.

Finally, another property of $\nabla(1/r)$ which will be useful in the sequel is the following: On a surface S the infinitesimal element $d\Omega$ of solid angle subtended by the origin is given by

$$d\Omega = \pm \frac{\mathbf{r}}{r^3} \cdot \eta \, dA = \mp \nabla(1/r) \cdot \eta \, dA,$$

the sign depending on various conventions. The sign convention will be used consistently so that the solid angle subtended by a *closed* surface S is zero when S does not enclose the origin. With this understanding, for any open or closed surface S we shall write [cf. (1.8)]

$$\int\int_S \nabla(1/r) \cdot \eta \, dA = \pm \text{ solid angle subtended by } S \text{ at the origin.} \tag{1.9}$$

II. THE SPECIAL METHOD

A. Statement of results

The main result of this section is contained in the following proposition.

Proposition: Let $\mathbf{v} = \mathbf{v}(\mathbf{r})$ be a vector field of the Helmholtz type (1.5). Then

$$\mathbf{v}(\mathbf{r}) = u(0)\nabla(1/r) + \nabla \times \mathbf{w}(\mathbf{r}), \tag{2.1a}$$

where

$$\mathbf{w}(\mathbf{r}) = \frac{\mathbf{r}}{r} \times \int_0^1 \exp(ikt r) \nabla u(t\mathbf{r}) \, dt. \tag{2.1b}$$

In these relations $u(0)$ is the value of the unperturbed incident radiation at the field point P (where $r = 0$), and the origin must be taken at P. The singularities of $\mathbf{w}$ are contained in the set of line segments PQ where Q varies over the set of singularities of u.

As we mentioned at the end of the last section, the vector field $\nabla(1/r)$ can be expressed in various nonequivalent ways as a curl on domains consisting of $\mathbf{E}^3$ with a line removed.

According to (1.9) the contribution of the first term of the right-hand side of (2.1a) to the Helmholtz integral (1.4) is the solid angle subtended by S at P. Therefore, one might conclude that this term would become negligible as P recedes to the far field. However, this solid angle is comparable in magnitude to the contribution from the other term. In fact, in the plane and spherical wave case, this solid angle combines with a certain part of the other term to produce the geometrical optics field (cf. Sec. 3C).

The line integral in (2.1b) is very similar to the Miyamoto–Wolf representations,[5] except that it is an integral over a finite rather than an infinite interval.

The Miyamoto–Wolf representations do not contain any explicit appearance of a term analogous to the first term on the right-hand side of (2.1a), and we suspect that this may be related to the fact that the derivation of our result (2.1) does not require that the incident field u or its derivatives satisfy any conditions at infinity (the Sommerfeld conditions) as is the case in the Miyamoto–Wolf theory.

In the next paragraph we shall give a direct proof of (1.2), and in Sec. 2C we shall show how this derivation can be easily modified to give (2.1).

B. Derivation of (1.2)

Let $\mathbf{w}$ be the vector field defined by (1.2). We have to show that $\nabla \times \mathbf{w} = \mathbf{v}$. From the identity

$$\nabla \times (A \times B) = (B \cdot \nabla)A - B(\nabla \cdot A) - (A \cdot \nabla)B + A(\nabla \cdot B),$$

we get

$$\begin{aligned}\nabla \times [\mathbf{r} \times \mathbf{v}(t\mathbf{r})] &= [\mathbf{v}(t\mathbf{r}) \cdot \nabla]\mathbf{r} - \mathbf{v}(t\mathbf{r})(\nabla \cdot \mathbf{r}) - (\mathbf{r} \cdot \nabla)\mathbf{v}(t\mathbf{r}) \\ &\quad + \mathbf{r}[\nabla \cdot \mathbf{v}(t\mathbf{r})] \\ &= \mathbf{v}(t\mathbf{r}) - 3\mathbf{v}(t\mathbf{r}) - t\frac{d}{dt}\mathbf{v}(t\mathbf{r}) + 0 \\ &= -2\mathbf{v}(t\mathbf{r}) - t\frac{d}{dt}\mathbf{v}(t\mathbf{r}).\end{aligned}$$

Hence

$$\nabla \times \mathbf{w}(\mathbf{r}) = \int_0^1 \left(2t\mathbf{v}(t\mathbf{r}) + t^2 \frac{d}{dt}\mathbf{v}(t\mathbf{r})\right) dt.$$

Integrating by parts, we obtain

$$\nabla \times \mathbf{w}(r) = t^2 \mathbf{v}(t\mathbf{r})\big|_{t=0}^1. \tag{2.2}$$

This completes the proof since (in this case) it is assumed that $\mathbf{v}$ is a smooth field with no singularities.

C. Derivation of (2.1)

We now have to consider the case when $\mathbf{v}$ is given by (1.5), and thus has a singularity at $r = 0$. We *define*

$$\mathbf{w}(\mathbf{r}) = -\int_{0+}^1 t\mathbf{r} \times \mathbf{v}(t\mathbf{r}) \, dt. \tag{2.3}$$

As in the previous case [cf. (2.2)] we get

$$\nabla \times \mathbf{w}(\mathbf{r}) = t^2 v(t\mathbf{r})\big|_{t=0+}^1. \tag{2.4}$$

Expanding $\nabla[\exp(ikr)/r]$ in (1.5), we get

$$\mathbf{v}(\mathbf{r}) = \exp(ikr)\left[u(\mathbf{r})\left(\frac{ik}{r} - \frac{1}{r^2}\right)\frac{\mathbf{r}}{r} - \frac{1}{r}\nabla u(\mathbf{r})\right], \tag{2.5}$$

so that

$$\lim_{t \to 0+} [t^2 v(t\mathbf{r})] = -u(0)\mathbf{r}/r^3 = u(0)\nabla(1/r).$$

Substituting into (2.4), we get

$$\nabla \times \mathbf{w}(\mathbf{r}) = \mathbf{v}(\mathbf{r}) - u(0)\nabla(1/r).$$

Finally, to complete the proof we have to show that the field $\mathbf{w}$ as defined by (2.3) is the same as that given in (2.1b). But this is an easy consequence of (2.3), (2.5), and the relation $\mathbf{r} \times \mathbf{r} = 0$.

Remark 2.1: The quadrature involved in the right-hand side of (2.1b) must be expressed in closed form if this result is to be usefully applied in the reduction of the double integral (1.4) to the line integral (1.6) (for the purpose of reducing the costs of machine calculations). The corresponding result for the general method (discussed in the next section) requires the solution the exact differential equation $dF = A\,dr + B\,d\theta + C\,d\varphi$ for the function F, and our experience has been that the quadratures involved in the general method are likely to be easier than those involved in (2.1b). There is however, one case in which the quadrature in (2.1b) is very easy; viz., in the plane wave case, $u(\mathbf{r}) = \exp[ik\mathbf{r}\cdot\xi]$ and one easily obtains

$$\mathbf{w}(\mathbf{r}) = \frac{\xi\times\mathbf{r}}{|\xi\times\mathbf{r}|^2}(1-\cos\theta)(1-\exp[ikr(1+\cos\theta)])$$

where $\cos\theta = (\mathbf{r}\cdot\xi)/r$.

Remark 2.1: As mentioned in Sec. 1A, the solution (1.2) can be obtained directly from the proof of the Poincaré lemma, as given, say, in Ref. 2, pp. 155, 156 . To the vector field $\mathbf{v} = [v_x, v_y, v_z]$ one associates the differential 2-form $^*v = v_x\,dy\wedge dz + v_y\,dz\wedge dx + v_z\,dx\wedge dy$. Then $^*v$ is closed when v is divergence free, in which case one can write $^*v = d\,w$ where $w = h\,^*v$, h being the chain homotopy operator used in the proof of the Poincaré lemma, which sends k-forms into $(k-1)$-forms, and satisfies $dh + hd = \text{identity}$.

III. THE GENERAL METHOD

A. Introductory remarks

The general method is based on the following "well-known" proposition, which is a generalization of the Poincaré lemma, and involves the idea of de Rham cohomology.[1,2]

Proposition: Let v be a divergence free vector field, with singularities. Then there exists an integer N depending only on the topological structure of the domain of regularity of v, such that if $\mathbf{v}_1, \cdots, \mathbf{v}_N$ is a set of *any* N divergence free vector fields whose domains of regularity contain that of v, there exist constants a_0, $a_1, \cdots, a_N$ not all zero such that $a_0\mathbf{v} + a_1\mathbf{v}_1 + \cdots a_N\mathbf{v}_N$ is the curl of some vector field w whose singularities (if they exist) are contained in the set of singularities of v.

In fact, if the set of singularities of v consists of a discrete set of points and/or lines, then w will have no singularities. The integer N is the second Betti number of the de Rham cohomology of the domain of v.

The general method consists of the following steps.

(i) By an appropriate choice of the $\mathbf{v}_1, \cdots, \mathbf{v}_N$ we can write

$$\mathbf{v} = a_1\mathbf{v}_1 + \cdots + a_N\mathbf{v}_N + \nabla\times\mathbf{w} \tag{3.1}$$

where the constants $a_1, \ldots, a_N$ and the vector field w can be determined as follows.

(ii) To solve (3.1) for $a_1, \cdots, a_N$ we construct a set of closed surfaces $S_1, \cdots, S_N$ with the property that

$$\int\int_{S_i}\mathbf{v}_i\cdot\eta\,dA \neq 0 \quad\text{and}\quad \int\int_{S_i}\mathbf{v}_j\cdot\eta\,dA = 0 \quad\text{when } i\neq j,$$

so that

$$a_i = \left(\int\int_{S_i}\mathbf{v}_i\cdot\eta\,dA\right)^{-1}\int\int_{S_i}\mathbf{v}\cdot\eta\,dA.$$

(iii) The constants $a_1, \cdots, a_N$ having been determined, we then solve (3.1) for w. In fact, we reduce (3.1) to an exact differential equation (cf. Remark 2.1) by translating the equation into an equation involving differential forms.

Example 3.1: Let v be the Helmholtz vector field (1.5) corresponding to a plane wave $u(\mathbf{r}) = \exp[ik\mathbf{r}\cdot\xi]$. Then v has only a single singular point at the field point $P(r=0)$, and $N=1$. We take $\mathbf{v}_1 = \nabla(1/r)$, and $S_1 = a$ small sphere centered at P. It turns out that $a_1 = 1$, so that

$$\mathbf{v}(\mathbf{r}) = \nabla(1/r) + \nabla\times\mathbf{w} \tag{3.2}$$

which, formally at least, is the same as (2.1a). However, in the present case [(3.2)], w is guaranteed *not* to have any singularities at all. *In effect, we have used the vector field* $\nabla(1/r)$ *to wipe out the singularity of* v.

Example 3.2: Let v be the Helmholtz vector field corresponding to a spherical wave. Then v has two singularities, at $r=0$ and $r_0=0$, where r, $\mathbf{r}_0$ are the position vectors of a general point drawn from the field point and source point, respectively. In this case $N=2$, $\mathbf{v}_1 = \nabla(1/r)$, $\mathbf{v}_2 = \nabla(1/r_0)$, S_1 and S_2 are small spheres centered at $r=0$ and $r_0=0$, respectively, and we get

$$\mathbf{v} = \nabla(1/r) + \nabla(1/r_0) + \nabla\times\mathbf{w}$$

where w *has no singularities*. In effect, we have used the vector fields $\nabla(1/r)$ and $\nabla(1/r_0)$ to wipe out the two singularities of v.

In Sec. 3C we shall show how the general method can be used to reproduce the Maggi–Rubinowicz line integral representations for the Helmholtz integrals (1.4) corresponding to plane and spherical wave radiation. In the next paragraph we shall reduce the Maggi–Rubinowicz results to a form which is convenient for this purpose.

B. The Maggi–Rubinowicz representations

Notation: S = an open surface in Euclidean 3-space which, physically, will correspond to an aperture in an opaque screen. It will always be assumed that S is finite in extent, ∂S = boundary of S, η = unit normal to S, and ∂S is always oriented so that a point moving in a positive direction around ∂S appears to move in a counterclockwise direction when η is pointing towards the observer. The Helmholtz integral (1.4) is given by the right-hand side of the relation

$$4\pi u_K(P) = \int\int_S\{u\,\mathrm{grad}\,H - H\,\mathrm{grad}\,u\}\cdot\eta\,dA \tag{3.3}$$

where for convenience we set $H = \exp(ikr)/r$, r being the vector drawn from the field point P to a variable point in space.

Let ξ be a unit vector, which in our applications will correspond to the normal to the unperturbed incident wave front at the field point P, and let l be the axis which passes through P and is parallel to ξ. Let φ be the angular coordinate which corresponds to a rotation

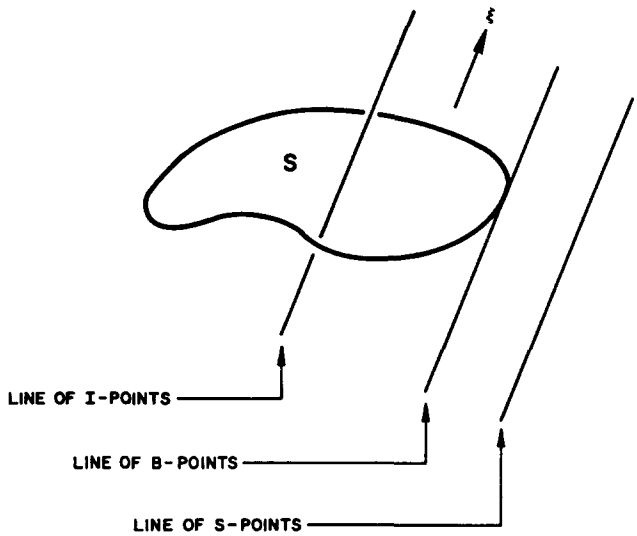

FIG. 1. I, B, and S-points.

around l, so that if a special xyz coordinate system is chosen with $\mathbf{e}_z = \xi$, we have

$$d\varphi = (x\,dy - y\,dx)/(x^2 + y^2). \tag{3.4}$$

Equivalently, if F is a function, the line integral $\int_{\partial S} F d\varphi$ can be written

$$\int_{\partial S} F d\varphi = \int_{\partial S} F \frac{(\xi \times \mathbf{r}) \cdot d\mathbf{r}/dt}{|\xi \times \mathbf{r}|^2}\, dt \tag{3.5}$$

where $\mathbf{r} = \mathbf{r}(t)$ is any parametric representation of ∂S with respect to a fixed origin lying on l. Then we shall say that P is an I-point, a B-point, or an S-point according as to whether ∂S winds around l, l intersects ∂S, or l falls outside of ∂S. (See Fig. 1.) Analytically, the condition that P be an I-point is that $\int_{\partial S} d\varphi = \pm 2\pi$ (the sign depending on the orientation of ∂S), and the condition that P be an S-point is $\int_{\partial S} d\varphi = 0$. If P is a B-point, the form $\int_{\partial S} d\varphi$ is indeterminate. Physically, the set of I-points, B-points, and S-points correspond (respectively) to the geometrical optics illuminated zone, shadow boundary zone, and shadow zone.

The Maggi–Rubinowicz results can now be expressed as follows (cf. Ref. 12 p. 79).

Plane Wave Case; Let all vectors and angles be as shown in Fig. 2, and let $u(\mathbf{r}) = \exp(ik\mathbf{r} \cdot \xi)$. Then

$$\int\int_S \{u\,\mathrm{grad}\, H - H\,\mathrm{grad}\, u\} \cdot \eta\, dA$$

$$= c - \int_{\partial S} (1 - \cos\theta) \exp[ikr(1 + \cos\theta)]\, d\varphi \tag{3.6}$$

$$\text{where } c = \begin{cases} 0 & \text{if } P \text{ is an } S\text{-point} \\ 4\pi & \text{if } P \text{ is an } I\text{-point.} \end{cases}$$

Spherical Wave Case: Let all vectors and angles be as is shown in Fig. 3, and let P_0 be the source of a spherical wave $u(\mathbf{r}) = (1/r_0)\exp(ikr_0)$ where $\mathbf{r}_0$ is the vector drawn from P_0 to a variable point in space. Then

$$\int\int_S \{u\,\mathrm{grad}\, H - H\,\mathrm{grad}\, u\} \cdot \eta\, dA$$

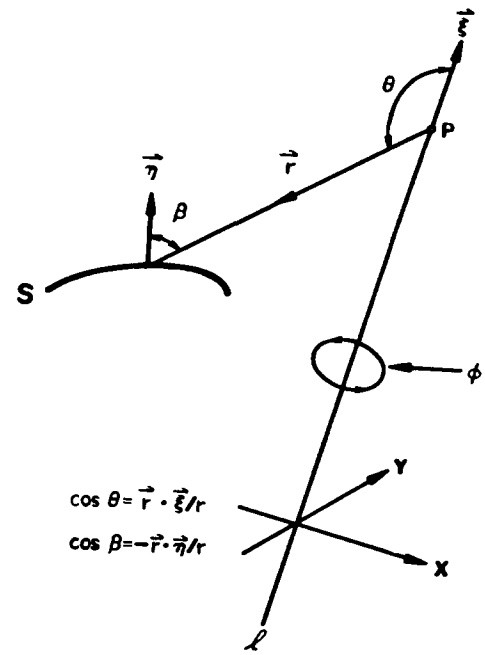

FIG. 2. Plane wave case.

$$= \frac{\exp(ikR)}{R}\left\{c - \int_{\partial S} [1 - \cos(\theta - \theta_0)] \exp[ik(r_0 + r - R)]\, d\varphi\right\}$$

where $c = 0$ or 4π as before. (3.7)

C. A derivation of the Maggi–Rubinowicz representations

As mentioned in Sec. 3A, the reduction of (3.1) to an

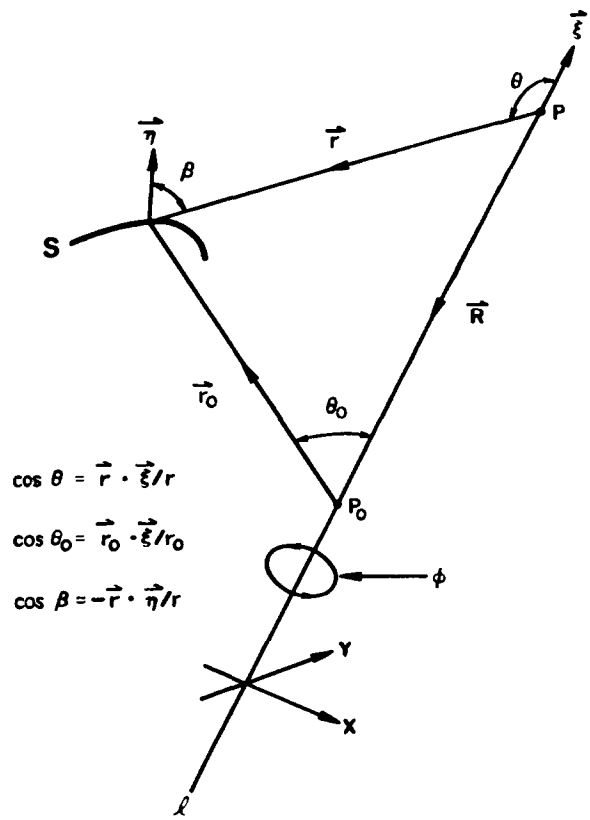

FIG. 3. Spherical wave case.

exact differential equation will involve translating the problem from vector language to the language of differential forms. In the translation the Helmholtz vector field $\mathbf{v}=[v_x, v_y, v_z]$ will correspond to a differential 2-form $\omega = v_x\, dy\wedge dz + v_y\, dz\wedge dx + v_z\, dx\wedge dy$, and the property of v being divergence free translates into ω being closed.

Let *, d, and $\wedge$ be the usual operators employed in the calculus of differential forms. (See, e.g., Refs. 1, 2, 13.) For smooth functions f, g recall that

$$d*df=\nabla^2 f, \quad df\wedge *dg=\nabla f\cdot\nabla g, \qquad \int_S *df=\int_S \nabla f\cdot\eta\, dA \text{ for any surface } S. \tag{3.8}$$

Let

$$\omega = *(u\,dH - H\,du). \tag{3.9}$$

Then the Helmholtz integral, i.e., the right-hand side of (1.4), is merely $\int_S\omega$; and ω is a closed form: $d\omega=0$. For from (3.9) we have

$$d\omega = u(d*d)H - H(d*d)u + du\wedge *dH - dH\wedge *du.$$

The last two terms cancel, and the first two terms cancel because $\nabla^2 u + k^2 u = 0$ and $\nabla^2 H + k^2 H = 0$.

Our detailed proof will be confined to the plane wave case—not because this case is any much simpler than the spherical wave case (it isn't), but because it provides a better illustration of a certain matter involving constants of integration.

Let

$$\omega_0 = -\frac{1}{r^2}*dr = *d(1/r). \tag{3.10}$$

Then $d\omega_0=0$, and

$$\int_S \omega_0 = \int_S \frac{\cos\beta}{r^2}dA \tag{3.11}$$

where $\cos\beta = -\eta\cdot\nabla r$, and η = normal to S. Hence

$$\int_S \omega_0 = \text{solid angle subtended by } S \text{ at } P. \tag{3.12}$$

From general principles (de Rham cohomology) we can assert the existence of a constant a and a 1-form ψ such that

$$\omega = a\omega_0 + d\psi. \tag{3.13}$$

We shall now show that $a=1$, so that

$$\omega = \omega_0 + d\psi. \tag{3.13'}$$

Proof: Let S_ρ be a sphere of radius ρ centered at P. Then from (3.12) and (3.13) we get $\int_{S_\rho}\omega = a\int_{S_\rho}\omega_0 = 4\pi a$. Expanding (3.9) we get

$$\omega = \left\{\left(\frac{ik}{r}-\frac{1}{r^2}\right)*dr - \frac{ik}{r}*\xi\right\}\exp[ik(r+\mathbf{r}\cdot\xi)] \tag{3.14}$$

(where the vector $\xi=[\xi_1,\xi_2,\xi_3]$ is identified with the 1-form $\xi=\xi_1\,dx+\xi_2\,dy+\xi_3\,dz$, the xyz coordinate system being chosen as in (3.4)—see Eq. (3.16) below.) But $d\omega=0$ implies S_ρ is independent of $\rho>0$. Hence allowing $\rho\to 0$, we get

$$\int_{S_\rho}\omega = -\int_{S_\rho}\frac{*dr}{r^2} + o(\rho) = 4\pi.$$

Hence $a=1$. So we can write (3.13') as

$$\omega = -\frac{1}{r^2}*dr + d\psi. \tag{3.15}$$

We now have to solve this last equation for ψ. Again, the angle θ is defined as shown in Fig. 2, and an xyz rectangular coordinate system is chosen so that (3.4) holds, and so that $\xi=\mathbf{e}_z$. We shall also identify the vector ξ with the differential form $\xi=dz$. Hence we have

$$r^2=x^2+y^2+z^2, \quad x=r\sin\theta\cos\varphi, \quad y=r\sin\theta\sin\varphi, \quad z=r\cos\theta, \quad \xi=\mathbf{e}_z, \quad \xi=dz. \tag{3.16}$$

We also have

$$*dx=dy\wedge dz, \quad *dy=dz\wedge dx, \quad *dz=dx\wedge dy, \quad *(dy\wedge dz)=dx, \quad *(dz\wedge dx)=dy, \quad *(dx\wedge dy)=dz. \tag{3.17}$$

From (3.4), (3.16), and (3.17) we get

$$*\xi = dx\wedge dy = r\sin^2\theta\, dr\wedge d\varphi + r^2\sin\theta\cos\theta\, d\theta\wedge d\varphi, \quad *dr = r^2\sin\theta\, d\theta\wedge d\varphi. \tag{3.18}$$

[This last equation can be obtained by taking the wedge product of (3.4) with the relation $-\sin\theta\, d\theta = d(\cos\theta) = d(z/r) = (r\,dz - z\,dr)/r^2$.]

From (3.14), (3.15), and (3.18) we finally get

$$d\psi = (A\,dr + B\,d\theta)\wedge d\varphi, \text{ where}$$
$$A = -ik\sin^2\theta\exp[ikr(1+\cos\theta)], \tag{3.19}$$
$$B = \sin\theta + [-\sin\theta + ikr\sin\theta(1-\cos\theta)]\exp[ikr(1+\cos\theta)].$$

Now since $d\psi$ is exact, we should have $A\,dr + B\,d\theta = dF$ where $F=F(r,\theta)$. Integrating $\partial F/\partial r = A$, we get

$$F = -(1-\cos\theta)\exp[ikr(1+\cos\theta)] + G(\theta), \tag{3.20}$$

where G is a function of θ only. The function G is obtained by solving the equation $\partial F/\partial\theta = B$. Hence

$$B = \frac{\partial F}{\partial\theta} = [-\sin\theta + ikr\sin\theta(1-\cos\theta)]\exp[ikr(1+\cos\theta)] + G'(\theta).$$

Comparing this last equation with (3.19), we get

$$G(\theta) = b - \cos\theta \tag{3.21}$$

where b is a constant.

Caution: The value of the constant b is not arbitrary. For we have $d\psi = dF\wedge d\varphi = d(F\,d\varphi)$, so that $\psi = F\,d\varphi$ is a solution. But this last relation must hold everywhere in space, and φ is singular on the axis l. Hence we must choose b so that $F=0$ on l. The axis l is given by $\theta=0$ and $\theta=\pi$. Hence $b=1$, and from (3.20) and (3.21) we get

$$F(r,\theta) = F_1 + F_2, \text{ where}$$
$$F_1 = 1-\cos\theta, \tag{3.22}$$
$$F_2 = -(1-\cos\theta)\exp[ikr(1+\cos\theta)].$$

Combining these results, we get

$$\omega = -\frac{*dr}{r^2} + d(F\,d\varphi).$$

Applying Stokes' theorem we have

$$\int_S \omega = -\int_S \frac{*dr}{r^2} + \int_{\partial S} F\,d\varphi$$

$$= -\int_S \frac{*dr}{r^2} + \int_{\partial S} F_1\,d\varphi + \int_{\partial S} F_2\,d\varphi.$$

The use of Stokes' theorem is justified because the form $F\,d\varphi$ has no singularities.

To complete the proof we have to show that

$$c = -\int_S \frac{*dr}{r^2} + \int_{\partial S} F_1\,d\varphi \quad (=0 \text{ or } 4\pi).$$

Case 1. *P is an S-point*: Then $dF_1 \wedge d\varphi$ has no singularities on S, so that we can apply Stokes' theorem to obtain

$$\int_{\partial S} F_1\,d\varphi = \int_S dF_1 \wedge d\varphi = \int_S d(1-\cos\theta) \wedge d\varphi$$

$$= \int_S \sin\theta\,d\theta \wedge d\varphi.$$

But $\sin\theta\,d\theta \wedge d\varphi = (*dr)/r^2$. Hence in this case $c = 0$.

Case 2. *P is an I-point*: Let α be small, and let D be the small disc-like subset of S whose boundary is given by $\theta = \pi - \alpha$, and let A be the annular subset of S which is complementary to D. Then

$$\int_{\partial S} F_1\,d\varphi = \int_{\partial S} F_1\,d\varphi - \int_{\partial D} F_1\,d\varphi + \int_{\partial D} F_1\,d\varphi$$

$$= \int_A dF_1 \wedge d\varphi + 2\pi(1+\cos\alpha)$$

$$= \int_A \frac{*dr}{r^2} + 2\pi(1+\cos\alpha).$$

Hence as $\alpha \to 0$ we have

$$c = -\int_S \frac{*dr}{r^2} + \int_A \frac{*dr}{r^2} + 2\pi(1+\cos\alpha) \to 0 + 4\pi = 4\pi,$$

and this completes the derivation.

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Useful extremum principle for the variational calculation of matrix elements. II

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Recent work [Phys. Rev. A 9, 108 (1974)] on variational principles for diagonal bound state matrix elements of arbitrary Hermitian operators is extended. In particular, it is shown that the previously derived minimum principle for the trial auxiliary function appearing in such variational principles can be constructed using a modified Hamiltonian possessing not heretofore recognized positive definite properties. Thus there is at least one alternative to the particular modified Hamiltonian on which the results of Phys. Rev. A 9, 108 (1974) originally were based.

I. INTRODUCTION

A constantly recurring problem in quantum theory is the estimation of the diagonal matrix element

$$W_{nn}=\phi_n^\dagger W\phi_n\equiv(\phi_n, W\phi_n) \tag{1}$$

of an arbitrary known linear Hermitian operator W, where the nth bound state normalized eigenfunction ϕ_n—corresponding to eigenenergy E_n of the given Hamiltonian H—is well specified but inexactly known. A natural procedure for the estimation of W_{nn} is a variational approach. In addition to having a trial estimate ϕ_{nt} of the exact ϕ_n, making use of such variational principles for W_{nn} characteristically requires having a trial estimate L_{nt} of an "auxiliary" function L_n satisfying the inhomogeneous equation

$$(H-E_n)L_n=q(\phi_n), \tag{2}$$

where

$$q(\phi_n)=-W\phi_n+\phi_n^\dagger W\phi_n.$$

The variational principle is given by

$$(\phi_n^\dagger W\phi_n)_{\rm var}=\phi_{nt}^\dagger W\phi_{nt}+2Re\ L_{nt}^\dagger(H-E_{nt})\phi_{nt}.$$

The determination of a reasonable L_{nt} is very much more difficult than might seem at first to be the case. The source of the difficulty has only recently been completely understood, and a method for by-passing the difficulty introduced.[1] Briefly, L_n can be defined to be orthogonal to ϕ_n, the solution of the associated homogeneous equation, and no singularity problem arises on inverting $H-E_n$. In practice, of course, neither ϕ_n nor E_n is known precisely. If we replace E_n by E_{nt}, there is no solution Ω to the homogeneous equation $(H-E_{nt})\Omega=0$. We *cannot* require L_{nt}, the solution of

$$(H-E_{nt})L_{nt}=q(\phi_{nt}), \tag{3a}$$

to be orthogonal to anything, and the inversion of $H-E_{nt}$ in the determination of L_{nt} leads to a near singularity. As a consequence the variational principle breaks down if the trial auxiliary function is chosen as the solution of (3a), as shown in Ref. 1. We must then modify (3a), preferably in a way which enables us to determine trial auxiliary functions by means of a well-defined, reliable approximation procedure.

The above authors[1] discuss sequences of equations

$$(H_t-E_{nt})L_{nt}=q_t(\phi_{nt}) \tag{3b}$$

whose solutions $L_{nt}\to L_n$ as $\phi_{nt}\to\phi_n$, where q_t may differ from q, where

$$E_{nt}=\phi_{nt}^\dagger H\phi_{nt}, \tag{4}$$

and where the "trial" Hamiltonian H_t need not $\to H$ as $\phi_{nt}\to\phi_n$. They further show that for any proposed ϕ_{nt} the desired L_{nt} satisfying (3b) can itself be estimated from a variational principle. Moreover, given a set of sufficiently accurate trial bound state eigenfunctions ϕ_{it}, $i=1,\ldots,n$ satisfying

$$\phi_{it}^\dagger\phi_{jt}=\delta_{ij}, \tag{5}$$

the variational principle for L_{nt} becomes a minimum principle provided H_t in (3b) is chosen to be

$$H_{{\rm mod},t}^{(n)}=H-\sum_{i=1}^{n}\frac{HP_{it}H}{E_{it}}, \tag{6}$$

where

$$\phi_{it}^\dagger H\phi_{jt}=E_{it}\delta_{ij} \tag{7}$$

and the projection operators are defined as

$$P_{it}=\phi_{it}\phi_{it}^\dagger. \tag{8}$$

The aforementioned minimum principle is expected to greatly facilitate the task of finding accurate estimates L_{ntt} of the L_{nt} exactly solving Eq. (3b), just as the Rayleigh–Ritz minimum principle greatly facilitates the task of accurately estimating the exact ϕ_n satisfying

$$(H-E_n)\phi_n=0. \tag{9}$$

The possibility of constructing a minimum principle for L_{nt}, i.e., of finding a functional $M(L_{ntt})$ which achieves its minimum value when $L_{ntt}=L_{nt}$ solving (3b), rests primarily on the fact that the operator $H_{{\rm mod},t}^{(n)}-E_{nt}$ is positive definite, i.e., that

$$(\psi,[H_{{\rm mod},t}^{(n)}-E_{nt}]\psi)>0 \tag{10}$$

in the space of quadratically integrable functions.

A very much more detailed account of the origins of the difficulty of estimating L_{nt} and of the methods of

bypassing that difficulty, and references to earlier work, can be found in Ref. 1.

We note that the alternative Hamiltonian defined by (11) below has been discussed in the past.[2,3] Indeed, the possibility of using $\hat{H}^{(1)}_{\mathrm{mod},t}$ for precisely the purposes of the present paper was suggested by Aranoff and Percus,[3] who also made some use of the operator. They did not, however, obtain conditions on ϕ_{1t} which guarantee the positivity of $\hat{H}^{(1)}_{\mathrm{mod},t}$.

II. AN ALTERNATIVE MODIFIED HAMILTONIAN

The main objective of this paper is demonstrating that—for sufficiently accurate (a phrase made precise below) ϕ_{it} obeying (5) and (7)—an alternative (to $H^{(n)}_{\mathrm{mod},t}$) choice for H_t in (3b) is the operator $\hat{H}^{(n)}_{\mathrm{mod},t}$ defined by the sequence

$$\hat{H}^{(i)}_{\mathrm{mod},t}=P_{it}\hat{H}^{(i-1)}_{\mathrm{mod},t}P_{it}+(1-P_{it})\hat{H}^{(i-1)}_{\mathrm{mod},t}(1-P_{it}),\quad i=1,\ldots,n \tag{11}$$

where 1 is the unit operator and

$$\hat{H}^{(0)}_{\mathrm{mod},t}\equiv H. \tag{12}$$

The operator $\hat{H}^{(n)}_{\mathrm{mod},t}$ is positive definite in the space of quadratically integrable functions ψ orthogonal to ϕ_{it}, $i=1,\ldots,n$; i.e., provided the ϕ_{it} are sufficiently accurate,

$$(\psi,[\hat{H}^{(n)}_{\mathrm{mod},t}-E_{nt}]\psi)>0 \tag{13}$$

if

$$\phi^{\dagger}_{it}\psi=0,\quad i=1,\ldots,n. \tag{14}$$

Consequently (as will be amplified below) an alternative minimum principle for L_{nt} can be obtained by using $\hat{H}^{(n)}_{\mathrm{mod},t}$ instead of the original $H^{(n)}_{\mathrm{mod},t}$ specified by (6).

We now prove Eq. (13). For simplicity, we assume none of the states ϕ_i are degenerate, so that the ordering of the exact ϕ_i can be supposed consistent with $E_i<E_j$ whenever $i<j$. The needed modifications in the proof to make it applicable in the case of degeneracy are straightforward and essentially the same as are needed[1] to extend the validity domain of Eq. (10) from nondegenerate to degenerate ϕ_i. Suppose first that $n=1$, i.e., that in the desired matrix element (1) the quantity $\phi_n\equiv\phi_1$ is the ground state eigenfunction. Denote by χ_i any complete orthonormal set whose first element is $\chi_1=\phi_{1t}$, the estimate of ϕ_1. Then one easily sees that in the χ representation

$$\hat{H}^{(1)}_{\mathrm{mod},t}=\begin{pmatrix} E_{1t} & 0 & 0 & \cdots \\ 0 & H_{22} & H_{23} & \cdots \\ 0 & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \tag{15}$$

where

$$H_{ij}=\chi^{\dagger}_i H\chi_j \tag{16}$$

and E_{1t} is defined by Eq. (7).

The basis for the submatrix

$$\bar{H}^{(1)}=\begin{pmatrix} H_{22} & H_{23} & \cdots \\ H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \end{pmatrix} \tag{17}$$

in (15) is a complete set of functions orthogonal to ϕ_{1t}. This basis approaches the function space spanned by the exact ϕ_2, ϕ_3, $\cdots$, in the limit that $\phi_{1t}\to$ the exact ϕ_1. In this limit, therefore, the exact E_2 is approached by $\bar{E}^{(1)}_2$, the lowest eigenvalue of $\bar{H}^{(1)}$. It follows that for sufficiently accurate ϕ_{it} we surely will have

$$E_{1t}<\bar{E}^{(1)}_2. \tag{18}$$

But Eq. (18) is sufficient to guarantee that Eq. (13) subject to (14) will hold in the case $n=1$ QED. We show in Appendix A that a sufficient condition for (18) to hold is

$$E_{1t}<\tfrac{1}{2}(E_1+E_2). \tag{19}$$

If there is only one bound state, E_2 must be replaced by E_{thr}, the threshold energy for the beginning of the continuum spectrum associated with H.

Suppose next that $n=2$, i.e., that ϕ_n in the desired matrix element (1) is the first excited state eigenfunction. We now denote by χ_i any complete orthonormal set whose first two elements obeying (7) are $\chi_1\equiv\phi_{1t}$, $\chi_2=\phi_{2t}$. Then because Eq. (11) constructs $\hat{H}^{(2)}_{\mathrm{mod},t}$ from $\hat{H}^{(1)}_{\mathrm{mod},t}$ by the same projection technique as was used to construct $\hat{H}^{(1)}_{\mathrm{mod},t}$ from H, it is clear that in the present χ representation we have

$$\hat{H}^{(2)}_{\mathrm{mod},t}=\begin{pmatrix} E_{1t} & 0 & 0 & 0 & \cdots \\ 0 & E_{2t} & 0 & 0 & \cdots \\ 0 & 0 & H_{33} & H_{34} & \cdots \\ 0 & 0 & H_{43} & H_{44} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \tag{20}$$

where E_{1t}, E_{2t} are defined by (7). As previously, for sufficiently accurate ϕ_{1t}, ϕ_{2t} the lowest eigenvalue $\bar{E}^{(2)}_3$ of

$$\bar{H}^{(2)}=\begin{pmatrix} H_{33} & H_{34} & \cdots \\ H_{43} & H_{44} & \\ \vdots & \vdots & \end{pmatrix} \tag{21}$$

surely will obey

$$E_{2t}<\bar{E}^{(2)}_3, \tag{22}$$

which is sufficient to guarantee (13) for functions ψ orthogonal to ϕ_{1t} and ϕ_{2t}. It is shown in Appendix A that a sufficient condition for (22) to hold is

$$E_{2t}<\tfrac{1}{2}(E_2+E_3)-[(E_{1t}-E_1)(E_3-E_1)/(E_2-E_1)]. \tag{23}$$

If there are only two bound states, E_3 must be replaced by E_{thr}.

Appendix A makes it obvious that when ϕ_n is the nth bound state, Eq. (13) subject to (14) is guaranteed by relations similar to (23) and (19), though of course for

large n they will be rather more complicated than (23) and more tedious to derive. Once (13) subject to (14) has been assured, it is obvious from Eqs. (2.1)—(2.4), (3.15)—(3.18), and (3.24)—(3.32) of I that for quadratically integrable $L_{ntt} \equiv \psi$ satisfying (14) the functional

$$M(L_{ntt}) = L_{ntt}^{\dagger}(\hat{H}_{\mathrm{mod},t}^{(n)} - E_{nt})L_{ntt} - L_{ntt}^{\dagger}q_t - q_t^{\dagger}L_{ntt} \tag{24}$$

attains its minimum value $M(L_{nt})$ when (for given ϕ_{it}) the quantity L_{ntt} equals the unique function L_{nt} satisfying

$$(\hat{H}_{\mathrm{mod},t}^{(n)} - E_{nt})L_{nt} = -W\phi_{nt} + \sum_{i=1}^{n} P_{it}W\phi_{nt} \equiv q_t \tag{25}$$

subject to the orthogonality conditions (14); moreover, this function L_{nt} is a suitable trial auxiliary function in the variational principle

$$\langle W_{nn}\rangle_{\mathrm{var}} = \phi_{nt}^{\dagger}W\phi_{nt} + L_{nt}^{\dagger}[(H - E_{nt})\phi_{nt}] + [(H - E_{nt})\phi_{nt}]^{\dagger}L_{nt} \tag{26}$$

providing a variational estimate of the desired exact W_{nn} of Eq. (1).

With the above, we have achieved our main objective.

Whether the present $\hat{H}_{\mathrm{mod},t}^{(n)}$ of Eq. (11) generally will be more or less convenient to employ than the former $H_{\mathrm{mod},t}^{(n)}$ of Eq. (6) will have to be determined by experience. It is true that the orthogonality conditions (14) on L_{ntt}—which can make the minimization of (24) awkward to carry out—do not[1] have to be imposed when $H_{\mathrm{mod},t}^{(n)}$ is employed. Also, it is shown in Appendix B that the trial ϕ_{1t} needed to ensure the desired positive definite property (13) of $\hat{H}_{\mathrm{mod},t}^{(1)}$ always will have to be more accurate than the trial ϕ_{1t} needed to ensure the corresponding positive definite property (10) of $H_{\mathrm{mod},t}^{(1)}$. Nevertheless, when $\hat{H}_{\mathrm{mod},t}^{(n)}$ is used, satisfying the inequality

$$E_{nt} < \bar{E}_{n+1}^{(n)} \tag{27}$$

[which, with $\bar{E}_{n+1}^{(n)}$ obviously defined, is the analog of (18) and (22) needed to guarantee (13) subject to (14)] should not be a serious problem with any reasonably accurate estimate of $E_{1t}, E_{2t}, \ldots, E_{nt}$, e.g., with the E_{it} estimated via the Rayleigh—Ritz applied to linear combinations of n orthogonal functions $u_1, \ldots, u_n$. For example, with hydrogenic energy levels $E_n = -R/n^2$, Eq. (19) merely requires

$$E_{1t} - E_1 < 3R/8, \tag{28a}$$

while Eq. (23) demands

$$E_{2t} - E_2 < \frac{5R}{72} - \frac{32}{27}(E_{1t} - E_1); \tag{28b}$$

the inequalities (28) are satisfied if E_{1t} and E_{2t} are accurate to four percent, i.e., if

$$E_{1t} - E_1 < R/25,$$

$$E_{2t} - E_2 < R/100.$$

Furthermore, as discussed in Appendix B, the inequalities (19) and (23) are merely sufficient—not necessary—conditions for (18) and (22), respectively; it is possible to have trial ϕ_{it} which satisfy (13) subject to (14) even though (19), (23) and their analogs for higher n are not obeyed. In any event, failure of (13) subject to (14) should be easily recognizable in practice; when (13) fails the functional $M(L_{ntt})$ will not steadily converge to a minimum value as the number of arbitrary parameters in the trial functions L_{ntt} is steadily increased. In this circumstance, presumably possible only if (18), (22) or their analogs (27) for $n > 2$ fail, it will be necessary to introduce a more accurate set of trial eigenfunctions ϕ_{it} and associated trial energies E_{it}.

APPENDIX A: CONDITIONS ON TRIAL ENERGIES

Let ϕ_{1t} be a normalized trial ground state wavefunction which provides the energy estimate E_{1t} via Eq. (4). We will prove that if χ is a normalized function orthogonal to ϕ_{1t} but otherwise arbitrary, then the inequality

$$\chi^{\dagger}H\chi > E_{1t} \tag{A1}$$

is satisfied provided that E_{1t} obeys the inequality (19). Since the eigenvalue $\bar{E}_2^{(1)}$ is the minimum value of $\chi^{\dagger}H\chi$ for normalized χ orthogonal to ϕ_{1t} [recall the form of the matrix $\bar{H}^{(1)}$, Eq. (17)], this proof implies that (19) indeed suffices to guarantee (18).

Before proceeding with the aforementioned proof, we shall give a simplified argument which makes the result plausible. Suppose neither ϕ_{1t} nor χ have projections on states with energies above E_2; in effect we are supposing that H describes a two-level system. Then ϕ_{1t} has the expansion

$$\phi_{1t} = (\cos\theta)\phi_1 + (\sin\theta)\phi_2, \tag{A2}$$

where for simplicity we further assume the expansion coefficients $\cos\theta$ and $\sin\theta$ are real, so that θ is a real angle. The quantity χ orthogonal to ϕ_{1t} now is represented by

$$\chi = -(\sin\theta)\phi_1 + (\cos\theta)\phi_2. \tag{A3}$$

Accordingly,

$$E_{1t} = E_1\cos^2\theta + E_2\sin^2\theta, \tag{A4}$$

and

$$\chi^{\dagger}H\chi = E_1\sin^2\theta + E_2\cos^2\theta. \tag{A5}$$

The inequality (A1) now becomes

$$(E_2 - E_1)(\cos^2\theta - \sin^2\theta) > 0, \tag{A6}$$

which is satisfied whenever $\sin^2\theta < \frac{1}{2}$. But if $\sin^2\theta < \frac{1}{2}$, Eq. (A4) yields

$$E_{1t} = E_1 + (E_2 - E_1)\sin^2\theta < E_1 + (E_2 - E_1)/2 \tag{A7}$$

which is precisely the inequality (19). Conversely, if (19) holds in the present effectively two-level case, then (A7) implies $\sin^2\theta < \frac{1}{2}$ and (A6) is obeyed, which in turn implies (A1) surely holds.

The above discussion can be roughly restated as follows. The condition $\phi_{1t}^{\dagger}\chi = 0$ represents a linear constraint on χ. It follows from Sylvester's theorem,[4] or alternatively from the mini-max property[5] of the eigenvalues, that the spectrum S of eigenvalues in the space orthogonal to ϕ_{1t} interlaces the spectrum $E_1, E_2, E_3, \ldots$ of H. Thus the lowest eigenvalue of the spectrum S, which we have denoted by $\bar{E}_2^{(1)}$, satisfies $E_1 \leq \bar{E}_2^{(1)} \leq E_2$. The statement that $E_t < \frac{1}{2}(E_1 + E_2)$ implies that the

probability of finding the particle in state 1 is more than $\frac{1}{2}$. The orthogonality of χ and ϕ_{1t} then implies that the probability of a particle with a wavefunction χ being found in state 1 is less than $\frac{1}{2}$. The lowest energy associated with χ is then above the value associated with probabilities of $\frac{1}{2}$ each for finding the particle in states 1 and 2, that is, above $\frac{1}{2}(E_1+E_2)$, or above the value associated with ϕ_{1t}.

We now proceed to the promised proof that (19) implies (A1) even when the expansions of ϕ_{1t} and χ are not restricted to the forms (A2) and (A3). In particular, suppose these expansions are

$$\phi_{1t}=\sum_i a_{1i}\phi_i, \tag{A8}$$

$$\chi=\sum_i b_i\phi_i \tag{A9}$$

in terms of the exact assumedly nondegenerate eigenfunctions of H, ordered so that $E_1<E_2<E_3<\cdots$; as $\phi_{1t}\to\phi_1$, $|a_{11}|^2\to 1$. Here and subsequently the index i in $\sum_i$ runs over all ϕ_i starting from $i=1$, with the understanding that the discrete sum is replaced by an integral when ϕ_i lies in the continuum. The normalization and orthogonality conditions on ϕ_{it} and χ take the form

$$\sum_i |a_{1i}|^2=1, \tag{A10a}$$

$$\sum_i |b_i|^2=1, \tag{A10b}$$

$$\sum_i b_i^* a_{1i}=0. \tag{A10c}$$

From the expansion

$$\chi^\dagger H\chi=\sum_i |b_i|^2 E_i \tag{A11}$$

we obtain a lower bound on $\chi^\dagger H\chi$, namely

$$\begin{aligned}\chi^\dagger H\chi &\geq |b_1|^2E_1+E_2[|b_2|^2+|b_3|^2+\cdots]\\ &=|b_1|^2E_1+E_2[1-|b_1|^2].\end{aligned}$$

In other words, we have

$$\chi^\dagger H\chi\geq |b_1|^2(E_1-E_2)+E_2. \tag{A12}$$

Because $E_1-E_2<0$, its factor $|b_1|^2$ in (A12) can be replaced by any quantity $\geq|b_1|^2$, e.g., by 1, we then obtain the trivial result $\chi^\dagger H\chi\geq E_1$. To obtain an improved upper bound on $|b_1|^2$, and thence an improved lower bound on $\chi^\dagger H\chi$, we make use of the following general result. Let **A** and **B** be normalized orthogonal vectors. The orthogonality condition is

$$\begin{aligned}0&=\sum_i B_i^*A_i\\ &=B_n^*A_n+\sum_{j\neq n}B_j^*A_j\end{aligned} \tag{A13}$$

where n is arbitrary and will be chosen for convenience. From (A13) and the Schwarz inequality we have

$$\begin{aligned}|B_n|^2|A_n|^2&=\Big|\sum_{j\neq n}B_j^*A_j\Big|^2\\ &\leq\Big\{\sum_{j\neq n}|B_j|^2\Big\}\Big\{\sum_{j\neq n}|A_j|^2\Big\}.\end{aligned} \tag{A14}$$

Use of the normalization conditions

$$\sum_i |A_i|^2=\sum_i |B_i|^2=1$$

in (A14) then gives

$$|B_n|^2|A_n|^2\leq(1-|B_n|^2)(1-|A_n|^2) \tag{A15}$$

which may be written

$$|A_n|^2+|B_n|^2\leq 1. \tag{A16}$$

Applying this general result to the case at hand, wherein ϕ_{1t} and χ having the expansions (A8) and (A9) are the pair of normalized orthogonal vectors, we obtain

$$|b_1|^2\leq 1-|a_{11}|^2. \tag{A17}$$

Inserting (A17) in (A12) then yields

$$\chi^\dagger H\chi\geq[1-|a_{11}|^2](E_1-E_2)+E_2. \tag{A18}$$

Moreover, we have the expansion

$$E_{1t}=\sum_i |a_{1i}|^2E_i, \tag{A19}$$

which—as in the derivation of (A12)—implies

$$E_{1t}\geq|a_{11}|^2(E_1-E_2)+E_2. \tag{A20}$$

The inequality (A20) can be rewritten in the form

$$\begin{aligned}&E_2-E_{1t}\leq|a_{11}|^2[E_2-E_1],\\ &|a_{11}|^2\geq(E_2-E_{1t})/(E_2-E_1),\end{aligned} \tag{A21a}$$

which is the so-called Eckart lower bound[6] for the overlap of ϕ_1 and ϕ_{1t}. From (A21a), we have

$$1-|a_{11}|^2\leq 1-\frac{E_2-E_{1t}}{E_2-E_1}=\frac{E_{1t}-E_1}{E_2-E_1}. \tag{A21b}$$

Inserting into (A18) the upper bound (A21b) on $[1-|a_{11}|^2]$, we find that

$$\chi^\dagger H\chi\geq E_1+E_2-E_{1t}. \tag{A22}$$

The condition that this lower bound on $\chi^\dagger H\chi$ shall exceed E_{1t} is seen to be precisely the inequality (19) QED. It is clear from the above derivation that if there is only one bound state, E_2 must be replaced by $E_{\rm thr}$, the threshold energy of the continuum; in so doing we are presuming that $E_{\rm thr}\leq 0$, which of course must be the case for any system of particles with interaction potentials vanishing at infinity.

The proof that (23) guarantees (22) is a generalization of the proof given immediately above. Equations (A8)–(A10) are retained, but we now introduce as well the expansion

$$\phi_{2t}=\sum_i a_{2i}\phi_i. \tag{A23}$$

The relations

$$\sum_i |a_{2i}|^2=1, \tag{A24a}$$

$$\sum_i b_i^* a_{2i}=0, \tag{A24b}$$

$$\sum_i a_{2i}{}^* a_{1i}=0 \tag{A24c}$$

express the fact that ϕ_{2t} is normalized and orthogonal to ϕ_{1t} and to χ, which now represents any function in the space orthogonal to both ϕ_{1t} and ϕ_{2t}. In place of the manipulations leading to (A12) we now write

$$\chi^\dagger H\chi\geq|b_1|^2E_1+|b_2|^2E_2+E_3(|b_3|^2+|b_4|^2+\cdots)$$

$$= |b_1|^2 E_1 + |b_2|^2 E_2 + E_3(1 - |b_1|^2 - |b_2|^2).$$

Thus

$$\chi^\dagger H \chi \geq |b_1|^2(E_1 - E_3) + |b_2|^2(E_2 - E_3) + E_3 \tag{A25}$$

replaces (A12). From (A24) and the general result (A16) we have

$$|b_2|^2 \leq 1 - |a_{22}|^2 \tag{A26}$$

in addition to our still valid (A17). Using (A17) and (A26) in (A25) yields

$$\chi^\dagger H \chi \geq [1 - |a_{11}|^2](E_1 - E_3) + [1 - |a_{22}|^2](E_2 - E_3) + E_3. \tag{A27}$$

When ϕ_{1t} and ϕ_{2t} are good trial functions, $|a_{11}|^2$ and $|a_{22}|^2$ in (A10a) and (A24a) are close to unity. An upper bound on $[1 - |a_{22}|^2]$ is obtained by generalizing the derivation of (A21b), which remains valid. We have

$$E_{2t} = \sum_i |a_{2i}|^2 E_i, \tag{A28}$$

which as in the derivation of (A25) implies

$$E_{2t} \geq |a_{21}|^2(E_1 - E_3) + |a_{22}|^2(E_2 - E_3) + E_3. \tag{A29}$$

Since $\phi_{1t}^\dagger \phi_{2t} = 0$ we have, from (A16) and (A24c),

$$|a_{21}|^2 \leq 1 - |a_{11}|^2, \tag{A30}$$

so that (A29) becomes

$$E_{2t} \geq (1 - |a_{11}|^2)(E_1 - E_3) + |a_{22}|^2(E_2 - E_3) + E_3. \tag{A31}$$

This is equivalent to

$$|a_{22}|^2 \geq \frac{E_3 - E_{2t}}{E_3 - E_2} - [1 - |a_{11}|^2]\left(\frac{E_3 - E_1}{E_3 - E_2}\right), \tag{A32a}$$

or

$$1 - |a_{22}|^2 \leq [1 - |a_{11}|^2]\left(\frac{E_3 - E_1}{E_3 - E_2}\right) + \frac{E_{2t} - E_2}{E_3 - E_2}. \tag{A32b}$$

Equation (A32b) is the desired upper bound on $[1 - |a_{22}|^2]$. Using it in (A27), we find

$$\chi^\dagger H \chi \geq E_3 + E_2 - E_{2t} + 2(E_1 - E_3)[1 - |a_{11}|^2], \tag{A33}$$

which, making use of (A21b), becomes

$$\chi^\dagger H \chi \geq E_3 + E_2 - E_{2t} + 2(E_1 - E_3)\,\frac{E_{1t} - E_1}{E_2 - E_1}. \tag{A34}$$

The condition that this lower bound on $\chi^\dagger H \chi$ shall exceed E_{2t} is precisely the inequality (23) QED. For $E_{1t} = E_1$ this combination reduces to $E_{2t} < (E_2 + E_3)/2$ as might have been expected from our earlier discussion in this appendix. Since $E_{2t} \geq E_2$ always, the condition (23) guaranteeing (22) can be satisfied only if the right-hand side of (23) exceeds E_2. This leads to the requirement that ϕ_{1t} must be sufficiently accurate that

$$E_{1t} < E_1 + \left(\frac{E_3 - E_2}{2}\right)\left(\frac{E_2 - E_1}{E_3 - E_1}\right). \tag{A35}$$

It can be seen (probably as might have been expected) that the condition (A35) on E_{1t}—needed to ensure that (23) and thus (22) really can be satisfied—always is more stringent than the condition (19) merely needed to ensure (18). Evidently in (A34), (A35), and (23) E_3 must be replaced by E_{thr} if there are but two bound states.

The derivation of the inequality guaranteeing (27) would proceed along precisely the above lines. For instance, in the case $n = 3$ we would have (in an obvious notation)

$$\chi^\dagger H \chi \geq [1 - |a_{11}|^2](E_1 - E_4) + [1 - |a_{22}|^2](E_2 - E_4) + [1 - |a_{33}|^2](E_3 - E_4) + E_4,$$

$$1 - |a_{33}|^2 \leq [1 - |a_{11}|^2]\left(\frac{E_4 - E_1}{E_4 - E_3}\right) + [1 - |a_{22}|^2] \times \left(\frac{E_4 - E_2}{E_4 - E_3}\right) + \frac{E_{3t} - E_3}{E_4 - E_3}$$

in place of (A27) and (A32b), respectively; the sought for sufficient condition follows on using (A21b), (A32b), and (A37) in (A36). The results for arbitrary n follow from (A36) and (A37) by inspection.

APPENDIX B: COMPARATIVE STRINGENCY OF POSITIVE DEFINITE REQUIREMENTS

The required positive definite property (10) of $H^{(n)}_{\text{mod},t}$ can be guaranteed by sufficiency conditions[1] on the accuracies of the trial E_{nt}, akin to the sufficiency conditions (19) and (23) guaranteeing, respectively, the required positive definite property (13) of $\hat{H}^{(1)}_{\text{mod},t}$ and $\hat{H}^{(2)}_{\text{mod},t}$. Evidently the comparative stringency of these sufficiency conditions on E_{nt} will have some bearing on the comparative ease with which $\hat{H}^{(n)}_{\text{mod},t}$ or $H^{(n)}_{\text{mod},t}$ can be employed, although (as we have stated above) the overall comparative convenience of $\hat{H}^{(n)}_{\text{mod},t}$ and $H^{(n)}_{\text{mod},t}$ surely will have to be determined by experience. Therefore, it is interesting that in the case $n = 1$—i. e., in the case that $\phi_n \equiv$ the ground state ϕ_1 in the desired matrix element (1)—we can show these sufficiency conditions on E_{1t} always are more stringent for our present $\hat{H}^{(1)}_{\text{mod},t}$ than for our earlier[1] $H^{(1)}_{\text{mod},t}$. The argument is trivial. According to Eq. (3.12b) of I, a sufficient condition for (10) to hold in the case $n = 1$ is

$$E_{1t} < -(E_1 E_2)^{1/2}. \tag{B1}$$

But

$$\tfrac{1}{2}(E_1 + E_2) \leq -(E_1 E_2)^{1/2}, \tag{B2}$$

because we have

$$|E_1| + |E_2| - 2|E_1 E_2|^{1/2} = [\,|E_1|^{1/2} - |E_2|^{1/2}]^2 \geq 0. \tag{B3}$$

Hence, as asserted, the sufficiency condition (19) always is more stringent than the sufficiency condition (B1).

The above argument is not immediately germane to the comparative difficulties of guaranteeing the positive definite properties (10) and (13), because neither (19) nor (B1) are necessary conditions; they are merely sufficient. This claim is readily illustrated for the condition (19), using the expansions and notation in Appendix A. Suppose for simplicity that the three lowest states have the equally spaced energies $E_1 = -2\alpha$, $E_2 = -\alpha$, $E_3 = 0$, with $\alpha > 0$; suppose further that the particular ϕ_{1t} being employed has projections only on ϕ_1 and ϕ_3. Then from (A19) we have

$$E_{1t} = -2\alpha a_{11}^2, \tag{B4}$$

where for simplicity we are assuming a_{11} is real. We will have

$$E_{1t} > (E_1 + E_2)/2 = -3\alpha/2 \tag{B5}$$

if

$$a_{11}^2 < 3/4. \tag{B6}$$

With the present ϕ_{1t} it is obvious that the χ minimizing (A11) subject to (A10c) can have no projections on those eigenfunctions ϕ_i for which $i > 3$, i. e., can have no projections on the positive energy continuum eigenfunctions. Thus (A10) and (A11) become

$$b_1^2 + b_2^2 + b_3^2 = 1, \tag{B7a}$$

$$b_1 a_{11} + b_3 a_{13} = 0, \tag{B7b}$$

$$\chi^\dagger H \chi = -2\alpha b_1^2 - \alpha b_2^2, \tag{B7c}$$

where, since a_{11} has been supposed real, we now lose no significant generality in supposing a_{13}, b_1, b_2, and b_3 are real as well. Equations (B7a) and (B7b) can be solved for b_3 and b_2 in terms of b_1, thereby converting (B7c) to

$$\begin{aligned}\chi^\dagger H \chi &= -2\alpha b_1^2 - \alpha\{1 - (1 + a_{11}^2/a_{13}^2) b_1^2\} \\ &= -\alpha + b_1^2 \alpha\{a_{11}^2/a_{13}^2 - 1\}.\end{aligned} \tag{B8}$$

According to Eq. (B8), if $a_{11}^2/a_{13}^2 > 1$, then the minimum value of $\chi^\dagger H \chi$ is $-\alpha = E_2$, obtained with $b_1^2 = 0$. In the range consistent with (B6),

$$a_{13}^2 > \tfrac{1}{4}, \quad a_{11}^2/a_{13}^2 < 3. \tag{B9}$$

Also, recalling (B4), we will have $E_{1t} < E_2 = -\alpha$ if

$$a_{11}^2 > \tfrac{1}{2}, \quad a_{11}^2/a_{13}^2 > 1.$$

Therefore, if a_{11} and a_{13} are chosen so that

$$1 < a_{11}^2/a_{13}^2 < 3,$$

in particular, if

$$a_{11}^2 = \tfrac{2}{3}, \quad a_{13}^2 = \tfrac{1}{3}, \quad a_{11}^2/a_{13}^2 = 2,$$

we will have (in the simple case under present discussion)

$$(E_1 + E_2)/2 < E_{1t} < (\chi^\dagger H \chi)_{\min} = \bar{E}_2^{(1)}. \tag{B10}$$

Equation (B10) demonstrates that (18)—and consequently (13)—can hold even though the particular ϕ_{1t} used to construct $\hat{H}^{(1)}_{\mathrm{mod},t}$ via (11) fails to obey (19). Since we explained in Appendix A that (23) reduces to $E_{2t} < \frac{1}{2}(E_2 + E_3)$ when E_{1t} is exact, it is obvious that we can construct a similar illustration—involving a ϕ_{2t} with projections only on the equally spaced bound states ϕ_2 and ϕ_4—demonstrating that (23) is not a necessary condition for (22) to hold.

On the other hand, we can prove rigorously that whenever $\hat{H}^{(1)}_{\mathrm{mod},t}$ —constructed via (11) with a given choice of ϕ_{1t}—obeys

$$(\psi, [\hat{H}^{(1)}_{\mathrm{mod},t} - E_{1t}]\psi) > 0 \tag{B11a}$$

for quadratically integrable functions ψ obeying

$$\phi_{1t}^\dagger \psi = 0, \tag{B11b}$$

then surely $H^{(1)}_{\mathrm{mod},t}$ —constructed via (6) with the same ϕ_{1t}—obeys

$$(\psi, [H^{(1)}_{\mathrm{mod},t} - E_{1t}]\psi) > 0 \tag{B12}$$

for quadratically integrable ψ unrestricted by (B11b). The converse does not hold however; if $H^{(1)}_{\mathrm{mod},t}$ constructed with a given ϕ_{1t} obeys (B12), we cannot be sure that $\hat{H}^{(1)}_{\mathrm{mod},t}$ constructed from the same ϕ_{1t} will obey (B11a) for functions ψ subject to (B11b). Moreover, when ϕ_{1t} equals the exact ϕ_1 it follows from the discussion following Eq. (17), and from Eq. (3.11) of I, that E_2 is the lowest eigenvalue of $H^{(1)}_{\mathrm{mod},t}$ and of $\hat{H}^{(1)}_{\mathrm{mod},t}$. Therefore, as ϕ_{1t} is made increasingly accurate starting from a very poor ϕ_{1t}, the positive definite requirement (B11) on $\hat{H}^{(1)}_{\mathrm{mod},t}$ cannot be satisfied before the positive definite requirement (B12) on $H^{(1)}_{\mathrm{mod},t}$ is satisfied, although with sufficiently accurate ϕ_{1t} both (B11) and (B12) surely will be satisfied.

The above claims concerning the relationship between (B11) and (B12) for the same ϕ_{1t}—which account for the assertion in the text immediately preceding Eq. (27)—are proved as follows. Introduce the projection operator

$$Q_{1t} = 1 - P_{1t} \tag{B13a}$$

obeying, by virtue of the definition (8),

$$P_{1t} Q_{1t} = Q_{1t} P_{1t} = P_{1t} - P_{1t}^2 = 0. \tag{B13b}$$

From (6), recalling the definition (4) of E_{1t}, one readily verifies that

$$P_{1t} H^{(1)}_{\mathrm{mod},t} = H^{(1)}_{\mathrm{mod},t} P_{1t} = 0.$$

Therefore, we have

$$Q_{1t} H^{(1)}_{\mathrm{mod},t} Q_{1t} = (1 - P_{1t}) H^{(1)}_{\mathrm{mod},t} (1 - P_{1t}) = H^{(1)}_{\mathrm{mod},t}. \tag{B14}$$

Thus, returning to (6), we have

$$\begin{aligned} Q_{1t} H Q_{1t} &= Q_{1t} H^{(1)}_{\mathrm{mod},t} Q_{1t} + Q_{1t} H P_{1t} H Q_{1t}/E_{1t} \\ &= H^{(1)}_{\mathrm{mod},t} + Q_{1t} H P_{1t} H Q_{1t}/E_{1t}. \end{aligned} \tag{B15}$$

In (B15) the coefficient of $1/E_{1t}$ is

$$(Q_{1t} H \phi_{1t})(\phi_{1t}^\dagger H Q_{1t}) = (Q_{1t} H \phi_{1t})(Q_{1t} H \phi_{1t})^\dagger$$

since the definition (B13a) makes $Q_{1t}^\dagger = Q_{1t}$. Consequently, once ϕ_{1t} has been chosen accurate enough that $E_{1t} < 0$ [as it must be if there is to be any chance of satisfying either (10) or (13)], we will have the operator inequality

$$Q_{1t} H Q_{1t} \leq H^{(1)}_{\mathrm{mod},t}. \tag{B16}$$

Equation (B16) means that the lowest eigenvalue of $H^{(1)}_{\mathrm{mod},t}$ in the space of quadratically integrable functions ψ never lies below the lowest eigenvalue of $Q_{1t} H Q_{1t}$ in the same space. But this lowest eigenvalue of $Q_{1t} H Q_{1t}$ is precisely the lowest eigenvalue $\bar{E}_2^{(1)}$ of $\bar{H}^{(1)}$, Eq. (17), because one easily sees that in the representation (spanning the entire space of ψ) which yields (15) for $\hat{H}^{(1)}_{\mathrm{mod},t}$ the operator $Q_{1t} H Q_{1t}$ is given by

$$Q_{1t} H Q_{1t} = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & H_{22} & H_{23} & \cdots \\ 0 & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \\ \vdots & \vdots & \vdots & \end{pmatrix}. \tag{B17}$$

Since it is presumed that the lowest bound state energy E_1 of H is <0, it follows from Sylvester's theorem[4] (as in Appendix A) that $\bar{E}_2^{(1)}$ is <0, i.e., it is certain that $E_2^{(1)}$ lies below the lowest eigenvalue, zero, associated with the matrix (B17); correspondingly, (B17) shows that the eigenfunction of $Q_{1t}HQ_{1t}$ belonging to its lowest eigenvalue $\bar{E}_2^{(1)}$ lies in the subspace orthogonal to ϕ_{1t}. Indeed, according to (11), we have

$$\hat{H}^{(1)}_{\mathrm{mod},t} = P_{1t}HP_{1t} + Q_{1t}HQ_{1t}. \tag{B18}$$

Consequently, since

$$\begin{aligned} &P_{1t}\chi = \chi^\dagger P_{1t} = 0, \\ &Q_{1t}\chi = \chi \end{aligned} \tag{B19}$$

for any normalized χ perpendicular to ϕ_{1t}, Eqs. (B18) and (B19) imply that for such χ

$$\chi^\dagger \hat{H}^{(1)}_{\mathrm{mod},t}\chi = \chi^\dagger Q_{1t}HQ_{1t}\chi = \chi^\dagger H\chi. \tag{B20a}$$

Equation (B20a) in turn implies that for normalized χ orthogonal to ϕ_{1t}

$$\min\{\chi^\dagger \hat{H}^{(1)}_{\mathrm{mod},t}\chi\} = \min\{\chi^\dagger Q_{1t}HQ_{1t}\chi\} = \min\{\chi^\dagger H\chi\} = \bar{E}_2^{(1)}. \tag{B20b}$$

As the accuracy of ϕ_{1t} is improved starting from comparatively inaccurate ϕ_{1t}, Eq. (B12) will begin to hold when the lowest eigenvalue of $H^{(1)}_{\mathrm{mod},t}$ becomes greater than E_{1t}. The preceding results—especially (B16) and (B20b)—have demonstrated that for such ϕ_{1t}, barely satisfying (B12), we generally will have $\bar{E}_2^{(1)} < E_{1t}$, in which event the inequality (B11a) will fail for some functions ψ consistent with (B11b). This demonstrates the claims made above concerning the relationship between (B11) and (B12) for the same ϕ_{1t}.

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Perturbative-variational approximations to the spectral properties of semibounded Hilbert space operators, based on the moment problem with finite or diverging moments. Application to quantum mechanical systems

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We introduce in a systematic way the properly defined arctangent of the mean value of the resolvent of a Hilbert space operator. We consider more precisely the case of semibounded self-adjoint operators H, in the region of the discrete spectrum. The arctangent of the Padé approximations to the mean value of the resolvent are constructed out of the moments. They are shown to provide converging monotonic increasing sequences of lower bounds to the arctangent of the resolvent. Consequently bounds with the same properties are derived for the discrete eigenvalues of H and, most remarkable, *the ordering* of the corresponding poles of the approximations reproduces the ordering of the exact poles. The Padé method is shown to provide a way to fully exploit the content of the Rayleigh-Ritz variational method, by providing a simple mechanical procedure to build up the variational subspaces: It defines a powerful both perturbative and variational approximation to semibounded operators. The difficulties of the Ritz method in the degenerate case are overcome by the fact that all bounds in the Padé method are *strict* bounds. In a second part, we consider the important case in which the moments are given by diverging algorithms. By properly regularizing them, we show that the Padé–Ritz variational principle generalizes to produce absolute maxima of the arctangent of the Padé approximations in the regulator and that these maxima form monotonic converging sequences of lower bounds. In the last part, we discuss an application to quantum mechanical systems for which the perturbative variational method is applied to the *energy*, allowing us to treat the case of strong coupling. As a consequence it appears possible to solve (approximately) the R-dimensional anharmonic oscillator in a purely *algebraic* way.

INTRODUCTION

In quantum mechanics, one is often faced with the problem of calculating the matrix element of the resolvent of an Hamiltonian H. This operator H is, for physical reasons, a semibounded self-adjoint Hilbert space operator. The use of the polarisation theorem allows one to consider only mean values of the resolvent of H:

$$R_\varphi(\lambda) = \langle \varphi | [1 - \lambda H]^{-1} | \varphi \rangle. \tag{1}$$

$R_\varphi(\lambda)$ enjoys a remarkable property: It can be written as a dispersion relation with a nonnegative weight function.

Introducing the "moments of H"

$$\mu_n = \langle \varphi | H^n | \varphi \rangle \tag{2}$$

which are the Taylor expansion coefficients of $R_\varphi(\lambda)$, the method of moments[1,2] gives us a powerful tool to build up approximations to $R_\varphi(\lambda)$. However, it is necessary that the numbers μ_n exist, that is, that $|\varphi\rangle$ be chosen in such a way to belong to the domain of any power of H. This is always so when H is a bounded self-adjoint operator. In such a case, the method of moments gives converging approximations to $R_\varphi(\lambda)$ whose formal and practical aspects are discussed in Ref. 2.

However, the operators H, with which we are faced in quantum mechanics are generally only semibounded. For this class of operators, the moment method suffers from two types of difficulties:

(i) Even if all the μ_n exist, a certain indeterminacy on $R_\varphi(\lambda)$ still survives, when the moment problem is indeterminate. While when the problem is determinate, the knowledge of the μ_n is sufficient to rebuild $R_\varphi(\lambda)$. Only a *sufficient* condition (Carleman[3]) on the μ_n is known for the problem to be determinate. [Practically μ_n must not increase faster than $(2n)!$].

(ii) If for some $n \geq N$, the μ_n do not exist any more. This case appears very frequently, in particular in the so-called problem of singular interactions.

If the moment problem is determinate, then one can extend the results valid for the case of bounded operators to this last case.[3]

The purpose of this paper is to explore and to state some further properties of the moment method, more particularly keeping in mind the case of semibounded operators.

In this work, we consider a generic semibounded self-adjoint operator H and we want to explore the properties of $R_\varphi(\lambda)$ in the region of the discrete spectrum. The resolvant having a very violent behaviour in this region, we completely smooth it out, by considering systematically the properly well-defined arctangent of it. We build up for $\arctan \lambda R_\varphi(\lambda)$ a monotonic sequence of bounds, which, as a consequence, allows to construct a monotonically decreasing sequence of upper bounds for the distinct eigenvalues of H.

The tool of our investigation is the Padé approximation technique, which has been extensively analyzed in the recent literature.[4–7]

We give now a brief description of the content of our work:

In Sec. I.A, we fix our notations and definitions.

In Sec. I.B, we show a simple property of monotonicity in the parameter λ for the $\arctan \lambda R_\varphi(\lambda)$ as well as

for arctan $\lambda[N-1/N]$, where we have considered the Padé approximant $[N-1/N]$ to $R_\varphi(\lambda)$ built up from the first $2N$ moments $\langle\varphi|H^n|\varphi\rangle$ $(n=0,\ldots,2N-1)$. Furthermore, one proves that the sequence $\{\arctan\lambda[N-1/N]\}$ is monotonic in the index N.

In Sec. I.C, we show that $\arctan\lambda[N-1/N]$ is bounded from above (or from below, according to the properties of H) by $\arctan\lambda R_\varphi(\lambda)$. Here we also discuss the possibility of more general monotonic approximations to $\arctan\lambda R_\varphi(\lambda)$, using the variational method of Rayleigh–Ritz. It is well known that the Padé approximants are particular versions of the Ritz method.[2,4,6]

In Sec. I.D, we state the convergence of $\arctan\lambda[N-1/N]$ as $N\to\infty$. When the moment problem is determinate, the limit is the correct function $\arctan\lambda R_\varphi(\lambda)$. In this case we have, as a by-product, that the poles of the Padé approximants converge to the corresponding exact poles of the resolvent of H (the distinct inverse eigenvalues of H).

In Sec. I.E, we consider and discuss what analogous results can be expected from the variational Ritz method.

With respect to the general variational procedure (the Ritz method), the Padé approximants enjoy some useful advantages, such as the control of the convergence and the possibility of obtaining further important information on the spectral function of $R_\varphi(\lambda)$. Therefore, in Appendix H, we recall the connection of the Padé approximants with the tridiagonalization method of Jacobi[1,8] and the Lanczoz method.[2,9] Then, in Appendix I, we discuss how one can obtain bounds on the residues of the poles of $R_\varphi(\lambda)$ and, furthermore, how one can localize the discrete spectrum embedded in the continuous spectrum.

In the second part of this work, we are faced with the difficulties of the type (ii) for the method of moments. In this case, one cannot expand $R_\varphi(\lambda)$ in a power series of λ with coefficients given by $\langle\varphi|H^n|\varphi\rangle$. We give a procedure to overcome this difficulty. One introduces a suitable regularization of the operator H, as a family of operators $H(\epsilon)$ for which the moments $\langle\varphi|H^n(\epsilon)|\varphi\rangle$ exist and the moment problem is determinate. If the regularization parameter ϵ is chosen in an appropriate way, one can show that absolute maxima, as a function of ϵ, of the $\arctan\lambda[N-1/N]$ exist which give monotonic converging approximations to $\arctan\lambda R_\varphi(\lambda)$.

The usefulness of such a procedure, which extends the Padé–Ritz variational principle to include cutoff parameters, has been proven to be very efficient in computing physical quantities (phase shifts which appear as the arctan of the resolvant of a symmetric operator) in the theory of singular interactions.[10] A possible application of the method could be to consider, variational properties of the phase shifts in field theory as function of the regulators.

We conclude this work with a brief discussion of the applications to quantum mechanical problems. In particular, we consider the R-dimensional anharmonic oscillator.

The method developed here, enables one to consider new perturbative variational expansions in quantum mechanisms, where the expansion parameter is not a coupling constant, but the inverse of the energy, which allows consideration of the case of strong coupling. Starting with a trial vector $|\varphi\rangle$ which may depend on a certain number of variational parameters $\{\rho_i\}$, one computes a given Padé approximation. Then the poles of this approximation which form *ordered* sequences, approximating the exact ones, can always be optimized by exploiting their variational properties with respect to the $\{\rho_i\}$, obtaining upper bounds for the discrete distinct eigenvalues of H (excited states). Such procedure can give very rapidly converging approximations as has been shown in the particular context of potential scattering theory for operators of the Hilbert–Schmidt type.[11]

For the R-dimensional anharmonic oscillator, whose Hamiltonian is an arbitrary polynomial in R variables, we show that, by conveniently choosing the trial vector $|\varphi\rangle$, it is possible to render the calculation, at any order purely algebraic, avoiding any of the difficulties connected with the calculation of multiple integrals.

I.

A. The class of operators—notations and definitions

In this paper, we consider self-adjoint Hilbert space operators H, having the positive part of their essential spectrum reduced to a point: the origin. This means that their continuous spectrum must be nonpositive, while the positive part of the spectrum must be discrete with only one point of accumulation, the origin (some other type of operators are briefly discussed). Such operators can be compact, bounded or semibounded.

Our aim is to compute approximations to the mean value of the resolvent of H in the positive region, and in particular of the positive discrete spectrum (isolated poles of the resolvent).

Let $|\varphi\rangle$ be a vector in Hilbert space, such that it belongs to the domain of any power of H, and consider the mean value of the resolvent of H

$$R_\varphi(\lambda)=\langle\varphi|[1-\lambda H]^{-1}|\varphi\rangle \tag{I.A.1}$$

and μ_K be the K^{th} moment

$$\mu_K=\langle\varphi|H^K|\varphi\rangle. \tag{I.A.2}$$

Due to the hypothesis on the vector $|\varphi\rangle$ all the μ_K are finite. The case where some or all μ_K do not exist, but admit finite regularizations will be the object of the second part of this paper.

Using the spectral representation for H, we can rewrite (I.A.1)

$$R_\varphi(\lambda)=\langle\varphi|\int_{-\infty}^{+\infty}\frac{dP_t}{1-\lambda t}|\varphi\rangle=\int_{-\infty}^{+\infty}\frac{d\mu}{1-\lambda t} \tag{I.A.3}$$

with

$$d\mu=\langle\varphi|dP_t|\varphi\rangle>0, \tag{I.A.4}$$

where $d\mu$ is a positive measure. By expanding (I.A.3) in power of λ, we obtain formally

$$R_\varphi(\lambda)=\sum_{n=0}^{\infty}\lambda^n\int_{-\infty}^{+\infty}t^n\,d\mu=\sum_{n=0}^{\infty}\lambda^n\langle\varphi|H^n|\varphi\rangle=\sum_{n=0}^{\infty}\lambda^n\mu_n. \tag{I.A.5}$$

We see that $R_\varphi(\lambda)$ is an extended Stieltjes function.

The problem of computing $R_\varphi(\lambda)$, knowing the μ_n, is equivalent to the "moment problem," of constructing a positive measure $d\mu$ from the knowledge of the moments:

$$\mu_K = \int_{-\infty}^{+\infty} t^k \, d\mu. \tag{I.A.6}$$

It is known that if the series

$$\sum_{k=1}^{\infty} [\mu_{2K}]^{-1/2k} \tag{I.A.7}$$

diverges, the moment problem is determinate (I.A.6 has a unique solution) and one can reconstruct unambiguously $R_\varphi(\lambda)$ for complex value of λ, from the μ_K, using the $[N-1/N]$ Padé approximations to $R_\varphi(\lambda)$. These Padé approximations converge uniformly in λ, in any compact region of the upper or lower λ half complex plane, to the resolvent $R_\varphi(\lambda)$.

Condition (I.A.7) is roughly equivalent to $|\mu_K| \lesssim K!$. In fact, in our case, condition (I.A.7) can be replaced by the much less stringent condition that the series

$$\sum_{k=1}^{\infty} |\mu_K|^{-1/2K} \tag{I.A.8}$$

diverges. The reason is that we deal here, with operators H which can, by a finite translation, be changed into negative operators $\bar{H}$. This translation induces an homographical transformation on the variable λ of $\lambda R(\lambda)$, transformation for which the Padé approximations are covariant.

Furthermore, it is not difficult to show that when (I.A.8) is verified the translated moments fulfill the Carlemen condition for the Stieltjes case, and therefore the moment problem is determinate for $\bar{H}$.

Combining those two results, we see that (I.A.8) is sufficient to have, in our case, the moment problem determinate.

We want now to explore the properties of the resolvent and its Padé approximations on the real axis among the singularities.

B. Some preliminary theorems

To analyse the properties of the resolvent on the semipositive axis where we have as a function of λ only isolated poles accumulating at infinity, we shall introduce systematically the arctan of λ times the resolvent. This function has very remarkable properties of monotonicity in λ, and, furthermore, is holomorphic in λ for real λ positive; the poles have been changed into points of holomorphy and therefore it is now easier to obtain bounds for the resolvent and for the position of the poles.

1. A property of the arctangent of λ times the resolvent of an operator H

Let us consider the function

$$\lambda R_\varphi(\lambda) = \lambda \int_{-\infty}^{+\infty} \frac{d\mu}{1-\lambda t} = \lambda \int_{-\infty}^{0} \frac{d\mu}{1-\lambda t} + \lambda \int_{0}^{+\infty} \frac{d\mu}{1-\lambda t}. \tag{I.B.1}$$

For t positive, we have by hypothesis only isolated poles

$$d\mu = \sum_i \rho_i \delta(t - 1/\lambda_i)\, dt \tag{I.B.2}$$

with $\rho_i > 0$ and $\lambda_i > 0$. We can, therefore, rewrite (I.B.1):

$$\lambda R_\varphi(\lambda) = \lambda \int_{-\infty}^{0} \frac{d\mu}{1-\lambda t} + \sum_i \rho_i \frac{\lambda \lambda_i}{\lambda_i - \lambda}. \tag{I.B.3}$$

We see that for Re $\lambda > 0$, $\lambda R_\varphi(\lambda)$ is meromorphic in λ. It is trivial to check that

$$\frac{d}{d\lambda}\left[\frac{1}{\lambda} R_\varphi\left(\frac{1}{\lambda}\right)\right] < 0 \tag{I.B.4}$$

for $\lambda > 0$ and $\lambda \neq \lambda_i$.

Therefore, $(d/d\lambda)[\lambda R_\varphi(\lambda)]$ is for $\lambda > 0$, and $\neq \lambda_i$, always positive.

Defining the positive inverse spectrum of H by the equation

$$\lambda_i H |\Psi_i\rangle = |\Psi_i\rangle \tag{I.B.5}$$

we shall therefore consider two cases:

(A) If the positive inverse spectrum accumulates at $+\infty$, we write

$$0 < \lambda_1 < \lambda_2 < \cdots < \lambda_N < \lambda_{N+1} < \cdots, \tag{I.B.6}$$

where we have classified only the distinct inverse-eigenvalues such that $|\varphi\rangle$ has nonzero projection on the respective eigenspaces, and we define the quantity

$$\delta^A(\lambda) = \arctan \lambda R(\lambda) \quad \text{for } \lambda \geq 0. \tag{I.B.7}$$

$R(0^+)$ being equal to μ_0 is finite, and we define the arctan by continuity, starting from the value

$$\delta^A(0^+) = 0. \tag{I.B.8}$$

We see that

$$\frac{d}{d\lambda}\delta^A(\lambda) = \frac{1}{1+\lambda^2 R_\varphi^2(\lambda)} \frac{d}{d\lambda}[\lambda R_\varphi(\lambda)] > 0 \tag{I.B.9}$$

for $\lambda > 0$. Furthermore, $\lambda R(\lambda)$ being meromorphic for Re $\lambda > 0$, we see that $(d/d\lambda)[\delta^A(\lambda)]$ is holomorphic for $\lambda > 0$ and therefore $\delta^A(\lambda)$ is also holomorphic in the vicinity of the semipositive axis.

Finally, $\delta^A(\lambda)$, which is a monotonic increasing function of λ, passes through the value $(2k-1)\frac{1}{2}\pi$ for $\lambda = \lambda_k$ and tends to $+\infty$, for $\lambda \to +\infty$, if there are infinitely many discrete states, or tends to a finite limit $\delta^A(+\infty)$, with

$$(2N-1)\tfrac{1}{2}\pi < \delta^A(+\infty) < (2N+1)\tfrac{1}{2}\pi \tag{I.B.10}$$

if there are N finite states.

(B) If the discrete positive inverse spectrum accumulates at point $a > 0$, then we set

$$\lambda_1 > \lambda_2 > \cdots > \lambda_N > \lambda_{N+1} > \cdots > a > 0. \tag{I.B.11}$$

In such a case, we define the arctangent by normalizing it at $\lambda = +\infty$, and following it by continuity down to $\lambda = a^+$.

We set

$$\delta^B(+\infty) = \arctan \lim_{\lambda \to +\infty} \lambda R(\lambda) \tag{I.B.12}$$

with $-\pi/2 < \delta^B(+\infty) \leq +\pi/2$. (I.B.13)

We see that $\delta^B(\lambda)$ is a monotonously increasing function

of λ, holomorphic in λ in the vicinity of the semipositive axis, and tending to $-\infty$ when $\lambda \to a^+$. Finally, $\delta^B(\lambda)$ passes through the values $-(2k-1)\frac{1}{2}\pi$, when $\lambda = \lambda_k$.

If the number of poles is finite and equal p on the positive axis, then it is immediate to relate $\delta^A(\lambda)$ and $\delta^B(\lambda)$:

$$\delta^B(\lambda) = \delta^A(\lambda) - p\pi. \tag{I.B.14}$$

2. Properties of monotonicity in the variable λ, and in the index N, of the arctangent of the [N-1/N] Padé approximant to the resolvent of an operator

We shall first recall the following fundamental theorem, whose demonstration, for completeness will be found in Appendix A.

Theorem I: Let H be a symmetric operator, and $|\varphi\rangle$ a vector in the field of any power of H. We set

$$R_\varphi(\lambda) = \langle\varphi|[1-\lambda H]^{-1}|\varphi\rangle, \tag{I.B.15}$$

$$\mu_k = \langle\varphi|H^k|\varphi\rangle < \infty. \tag{I.B.16}$$

The Padé approximation $[N-1/N]_{R_\varphi}(\lambda)$ constructed out of the first $2N$ moments μ_k $(k=0,1,2,\ldots,2N-1)$ is equal to the mean value of the resolvent of the finite rank symmetric operator $P_N H P_N$:

$$[N-1/N]_{R_\varphi}(\lambda) = \langle\varphi|[1-\lambda P_N H P_N]^{-1}|\varphi\rangle, \tag{I.B.17}$$

where P_N is the projector onto the N-dimensional space $\mathcal{E}^{(N)}$ spanned by the vectors $\{|\varphi\rangle; H|\varphi\rangle; H^2|\varphi\rangle; \cdots H^{N-1}|\varphi\rangle\}$, supposed to be linearly independent. In the accidental case where this set is linearly dependent, $[N-1/N]_{R_\varphi}(\lambda)$ is equal to $R_\varphi(\lambda)$ itself.

We see as a consequence of this theorem and of the previous properties that the function

$$\delta_N(\lambda) = \arctan\lambda\,[N-1/N]_{R_\varphi}(\lambda) = \arctan[N/N]_{\lambda R_\varphi}(\lambda) \tag{I.B.18}$$

is an holomorphic function of λ, for λ in a neighbourhood of the real axis, monotonically increasing in λ.

In Case A, we define the arctan, as before, by the condition

$$\delta_N^A(0) = 0, \tag{I.B.19}$$

while in Case B we use the normalization

$$\delta_N^B(+\infty) = \arctan \lim_{\lambda\to+\infty} [N/N]_{\lambda R_\varphi}(\lambda). \tag{I.B.20}$$

However, since the number of poles is finite and equal to N, these two functions are connected by (I.B.14).

We shall now state the following theorem, whose demonstration will be found in Appendix B.

Theorem II: The function $\delta_{N+1}^A(\lambda)$ is, for $\lambda > 0$, always greater than $\delta_N^A(\lambda)$. If in one point $\bar\lambda > 0$, $\delta_{N+1}^A(\bar\lambda) = \delta_N^A(\bar\lambda)$, then all $\delta_{N+k}^A(\lambda)$, $k \geq 0$ are identical to $\delta_N^A(\lambda)$, itself equal to $\delta^A(\lambda)$. The same extends to $\lambda < 0$, by changing "greater than" by "less than." Furthermore, at point $\lambda = 0$, $\delta_{N+1}^A(\lambda)$ and $\delta_N^A(\lambda)$ have a contact of order $(2N+1)$ in λ.

As a consequence of this theorem, we see that for $\lambda > 0$ the family of functions $\delta_N^A(\lambda)$ from a monotonically increasing set of increasing functions

$$\delta_1^A(\lambda) < \delta_2^A(\lambda) < \cdots < \delta_N^A(\lambda) < \delta_{N+1}^A(\lambda) < \cdots. \tag{I.B.21}$$

If p is the number of poles located on the positive real axis (that is, the number of positive eigenvalues of the operator $P_N H P_N$), $\delta_N^A(\lambda)$ reaches at $\lambda = +\infty$ a value between $(2p-1)\pi/2$ and $(2p+1)\pi/2$ as consequence of (I.B.10). Furthermore, due to the orthogonality properties of the denominators of the $[N-1/N]_{R_\varphi}(\lambda)$ Padé approximations,[1,2,7] we see that, between two poles of the $[N/N]_{\lambda R_\varphi}$, we have *exactly* one pole of the $[N+1/N+1]_{\lambda R_\varphi}$, except between the two of opposite sign nearest to the origin of the $[N/N]_{\lambda R_\varphi}$, for which we have two poles of the $[N+1/N+1]_{\lambda R_\varphi}$, one positive and one negative. Therefore, the number of positive poles of $[N+1/N+1]_{\lambda R_\varphi}$ is either p or $p+1$ depending if the last pole of $[N+1/N+1]_{\lambda R_\varphi}$ occurs at the right of the rightmost pole of $[N/N]_{\lambda R_\varphi}$ or at the left of the leftmost pole of $[N/N]_{\lambda R_\varphi}$. Finally, we want to point out that if we order the positive poles of $[N/N]_{\lambda R_\varphi}$ and $[N+1/N+1]_{\lambda R_\varphi}$ following the scheme

$$0 < \lambda_1^N < \lambda_2^N < \cdots < \lambda_p^N, \tag{I.B.22}$$

$$0 < \lambda_1^{N+1} < \lambda_2^{N+1} < \cdots < \lambda_p^{N+1} < \lambda_{p+1}^{N+1} \tag{I.B.23}$$

(the last one λ_{p+1}^{N+1} may not exist), we have, as a consequence of (I.B.21), that

$$\lambda_k^{N+1} < \lambda_k^N, \quad k = 1,2,\ldots,p. \tag{I.B.24}$$

The poles of the $[N-1/N]_{R_\varphi}(\lambda)$ Padé approximant form *ordered* monotonically decreasing sequences.

We come now to theorems concerned with the functions $\delta_N^B(\lambda)$.

Theorem III: If H is a positive operator, then the function $\delta_{N+1}^B(\lambda)$ is for real λ always smaller than $\delta_N^B(\lambda)$. If in one point $\bar\lambda > 0$, $\delta_{N+1}^B(\bar\lambda) = \delta_N^B(\bar\lambda)$, then all $\delta_{N+k}^B(\lambda)$, $k \geq 0$, are identical to $\delta_N^B(\lambda)$, itself equal to $\delta^B(\lambda)$.

At point $\lambda = 0$ we have

$$\delta_{N+1}^B(\lambda) - \delta_N^B(\lambda) = -\pi + O(\lambda^{2N+1}). \tag{I.B.25}$$

When H is positive, all the poles of $[N/N]_{\lambda R_\varphi}$ are also positive (because they are the eigenvalues of $P_N H P_N$ which is positive). Therefore, applying formula (I.2.14) we see that

$$\delta_N^B(0) - \delta_{N+1}^B(0) = [\delta_N^A(0) - \delta_{N+1}^A(0)] - [N-(N+1)]\pi$$

$$= \pi. \tag{I.B.26}$$

This proves formula (I.B.25), taking into account the last part of Theorem II. Furthermore, $\delta_{N+1}^B(0)$ being smaller than $\delta_N^B(0)$, we see by an argument identical to the one of Appendix B that $\delta_{N+1}^B(\lambda)$ will remain everywhere smaller than $\delta_N^B(\lambda)$. Now by ordering the poles of the Padé approximations from right to left, we find similarly that they form *ordered* monotonically *increasing* sequences:

$$\lambda_i^N < \lambda_i^{N+1}. \tag{I.B.27}$$

C. Bounds provided by the arctangent of the [N/N] P.A. to the resolvent of an operator H

We shall consider a more general type of approximation (the so-called variational approximation) to the re-

solvent of an operator H, than the Padé approximation, and prove for it a property of bound to the exact resolvent. We assume that $|\varphi\rangle$ belongs to D, where D is the domain of H.

Let us consider a sequence of finite-dimensional spaces $\{\mathcal{E}_1;\mathcal{E}_2;\mathcal{E}_3;\cdots;\mathcal{E}_N;\mathcal{E}_{N+1};\cdots\}$ which are subspaces of D, such that the $(N+1)$-dimensional space $\mathcal{E}_{N+1}$ always contains the N-dimensional space $\mathcal{E}_N$:

$$\mathcal{E}_1\subset\mathcal{E}_2\subset\cdots\subset\mathcal{E}_N\subset\mathcal{E}_{N+1}\subset\cdots\subset\mathcal{H}. \tag{I.C.1}$$

If we introduce the projectors $P_1, P_2, \cdots, P_N, P_{N+1}, \cdots$ which project into the corresponding spaces, we see that the operators P_i form a monotonic increasing sequence of positive operators:

$$0<P_1<P_2<\cdots<P_N<P_{N+1}<\cdots<I. \tag{I.C.2}$$

We introduce the restriction H_N of H to the space $\mathcal{E}_N$:

$$H_N=P_NHP_N. \tag{I.C.3}$$

The resolvent $R_\varphi(\lambda)$ to H is

$$R_\varphi(\lambda)=\langle\varphi|[1-\lambda H]|\varphi\rangle. \tag{I.C.4}$$

It is interesting to consider the approximate resolvent $R_\varphi^N(\lambda)$:

$$R_\varphi^N(\lambda)=\langle\varphi|[1-\lambda P_NHP_N]^{-1}|\varphi\rangle, \tag{I.C.5}$$

where the vector $|\varphi\rangle$ is restricted to belong to *all* spaces $\mathcal{E}_N$ $(N=1,2,\cdots)$, $P_N|\varphi\rangle=|\varphi\rangle$.

We have the following theorem whose demonstration will be found in Appendix C.

Theorem IV: If the operator H has a purely discrete positive inverse spectrum with only one point of accumulation at $+\infty$, then for $\lambda\geq 0$

$$\arctan\lambda R_\varphi^N(\lambda)\leq\arctan\lambda R_\varphi(\lambda), \tag{I.C.6}$$

where the arctan are followed by continuity from $\lambda=0^+$ where they are put equal to zero

A corollary of this theorem is

Theorem V: The sequence of $\arctan\lambda k_\varphi^N(\lambda)$ is for $\lambda\geq 0$ a monotonic nondecreasing sequence of increasing functions:

$$0\leq\arctan\lambda R_\varphi^1(\lambda)\leq\arctan\lambda R_\varphi^2(\lambda)\leq\cdots\leq\arctan\lambda R_\varphi^N(\lambda)\leq \arctan\lambda R_\varphi^{N+1}(\lambda)\leq\cdots\leq\arctan\lambda R_\varphi(\lambda). \tag{I.C.7}$$

We have seen in I.B.1 that the arctan of $\lambda R_\varphi^N(\lambda)$ is an increasing function of λ, equal to zero at $\lambda=0$. Furthermore, noticing that

$$P_NH_{N+1}P_N=H_N \tag{I.C.8}$$

and that H_{N+1} is an H-operator, we see that

$$\arctan\lambda R_\varphi^N(\lambda)\leq\arctan\lambda R_\varphi^{N+1}(\lambda) \tag{I.C.9}$$

by using Theorem IV applied to the restriction H_N of H_{N+1}.

This proves simply Theorem V.

Remark: We notice that while the bounds (I.C.7) are loose, the bounds on the Padé approximations are *strict*: If in *one point* $\bar\lambda$ there is equality, then the equality extends to all values of λ and all P.A. of larger order which become identical among themselves and to the exact resolvent. It can be shown with explicit examples that this is *not* the case for the variational approximation in general.

D. Convergence of the [N-1/N] Padé approximation to the resolvent of an H operator on the positive semiaxis in the determinate case

For a given value $\lambda=\bar\lambda>0$, formula (I.C.6) shows clearly that the $\arctan[\lambda[N-1/N]_{R_\varphi}(\lambda)]$ has a limit when $N\to+\infty$, because they form monotonically increasing sequences of real positive bounded numbers. The limit being smaller or equal to $\arctan\lambda R_\varphi(\lambda)$.

We shall now show, that when the moment problem is determinate, the limit is effectively $\arctan\lambda R_\varphi(\lambda)$. For λ complex this result is well known,[3] and we shall therefore extend it to the real positive values of λ among and including the discrete poles of the resolvent.

We shall first recall that if we order the p positive poles of the $[N/N]$ Padé approximation to $\lambda R_\varphi(\lambda)$

$$0<\lambda_1^{(N)}<\lambda_2^{(N)}<\cdots\lambda_i^{(N)}<\lambda_{i+1}^{(N)}<\cdots<\lambda_p^{(N)}, \tag{I.D.1}$$

as well as those of the exact function $\lambda R_\varphi(\lambda)$,

$$0<\lambda_1<\lambda_2<\cdots<\lambda_i<\lambda_{i+1}<\cdots, \tag{I.D.2}$$

then for a fixed i we have (see formula I.B.24)

$$\lambda_i<\cdots<\lambda_i^{N+1}<\lambda_i^N<\cdots<\lambda_i^{N_0}, \tag{I.D.3}$$

where $N_0\geq i$ is sufficiently large for the $[N_0/N_0]$ Padé approximation to have i positive poles. The fact that such N_0 exists is trivially connected to the fact that when $N\to+\infty$, the number p of positive poles of $[N/N]_{\lambda R_\varphi}(\lambda)$ also tends to infinity. This last argument is evident if the moment problem is determinate because then the approximated measure of the Padé approximation can be shown to tend to the exact measure, which can happen only if the number of positive poles of the approximations tends to the number of the positive poles of the resolvent. If the moment problem is indeterminate, then all self-adjoint extensions of the symmetrical operator associated with this indeterminate problem[1] have the same essential spectrum, because the defect index is finite.[1] Therefore, an analogous conclusion applies.

The sequence λ_i^N $(N=N_0;N_0+1;N_0+2,\cdots)$, being a positive decreasing bounded-from-below sequence, has a limit L_i for $N\to+\infty$ with

$$\lambda_i\leq L_i \tag{I.D.4}$$

and clearly

$$L_i\leq L_{i+1}, \tag{I.D.5}$$

also,

Theorem VI: The Padé approximation $[N/N]$ to $\lambda R_\varphi(\lambda)$ converges uniformly to an analytic function of λ, holomorphic in any compact of the λ complex plane, in which for $N>N_0$ the sequences of $[N/N]_{\lambda R_\varphi}(\lambda)$ have no poles. If the moment problem is determinate this analytic function is $\lambda R_\varphi(\lambda)$ itself. (See Appendix D for the proof.)

It is not difficult to show (See Appendix E) the following:

Theorem VII: If the moment problem is determinate, then $\lambda_i = L_i$, $i = 1, 2, \cdots$.

We have shown that the positive poles of the Padê approximation converge to the poles of the resolvent in the determinate case in a monotonic way: the ith pole of the approximation being monotonically decreasing in the index N, bound of the ith pole of the resolvent. We now extend this result to any point of the real positive axis.

Theorem VIII: In the determinate case the arctan $[N/N]_{\lambda R_\varphi}(\lambda)$ form, for $\lambda > 0$, a monotonically increasing sequence tending, when $N \to +\infty$, to arctan $\lambda R_\varphi(\lambda)$. (See proof in Appendix F.)

Finally, we want to point out that if, for convenience, one uses the normalization of the arctan at $+\infty$ (Case B of Sec. I. B) nothing is changed in the conclusions of all this chapter except that we have decreasing sequences instead of increasing ones, and therefore a certain number of inequalities have to be reversed.

E. Extension of the previous results to the variational Rayleigh-Ritz method and comparison of our inequalities with the standard variational inequalities

As consequence of Theorem IV, we can construct a monotonically decreasing sequence of upper bounds to each of the discrete inverse eigenvalues of H (to be specific, we will consider only Case A).

We have shown that these upper bounds converge to exact values when we use the Padê approximation method and the moment problem is determinate. We shall extend now these results to the Ritz variational method. We first recall the meaning of the standard variational upper bounds (mini-max principle, Poincarê inequalities).[12]

Let us call $\tilde{\lambda}_i$ $(i = 1, 2, \cdots)$ the inverse positive discrete eigenvalues of H (in general nondistinct) ordered in a nondecreasing way,

$$0 < \tilde{\lambda}_1 \leq \tilde{\lambda}_2 \leq \cdots, \tag{I.E.1}$$

corresponding to the orthogonal set of eigenvectors $\{\tilde{\Psi}_1, \tilde{\Psi}_2, \cdots\}$, $\mathcal{E}_N$ being an N-dimensional subspace of the domain D of H and P_N the corresponding projector; we consider the operator $H_N = P_N H P_N$, and its inverse positive eigenvalues $\tilde{\lambda}_i^N$ $(i = 1, 2, \ldots, M \leq N)$.

We have, as a consequence of the mini-max principle,

$$\tilde{\lambda}_1 \leq \tilde{\lambda}_1^N, \quad \tilde{\lambda}_2 \leq \tilde{\lambda}_2^N, \cdots, \tilde{\lambda}_M \leq \tilde{\lambda}_M^N. \tag{I.E.2}$$

It is unfortunately not true that, if we consider the *distinct* inverse positive eigenvalues $\bar{\lambda}_i$ of H and $\bar{\lambda}_i^N$ of H_N,

$$\bar{\lambda}_1 \leq \bar{\lambda}_1^N, \quad \bar{\lambda}_2 \leq \bar{\lambda}_2^N, \ldots, \bar{\lambda}_{M'} \leq \bar{\lambda}_{M'}^N, \quad M' \leq M, \tag{I.E.3}$$

except for the first inequality which is always true.

Let us now introduce a subsequence extracted from the sequence $\{\bar{\lambda}_i\}$ in the following way: Given $|\varphi\rangle$ in the Hilbert space we associate with $|\varphi\rangle$ the sequence

$$S|\varphi\rangle = \{\lambda_1(\varphi) < \lambda_2(\varphi) < \cdots\}, \tag{I.E.4}$$

where $\lambda_1(\varphi)$ is the first term of the sequence $\{\bar{\lambda}_i\}$ for which $|\varphi\rangle$ has a nonzero projection in the corresponding eigenspace, $\lambda_2(\varphi)$ is the second term of the sequence having the same property and so on [obviously the $\lambda_i(\varphi)$ are the poles of the resolvent $R_\varphi(\lambda)$]

For an arbitrary projector P_N, it is still untrue that

$$\lambda_1(\varphi) \leq \lambda_1^N(\varphi), \quad \lambda_2(\varphi) \leq \lambda_2^N(\varphi) \cdots. \tag{I.E.5}$$

However, as shown previously, these inequalities become true if we choose the special choice of P_N associated with the Padê approximation method or even more generally if $|\varphi\rangle$ belongs to all spaces $\mathcal{E}_N$:

$$P_N|\varphi\rangle = |\varphi\rangle. \tag{I.E.6}$$

We come back now to the problem of convergence of arctan $\lambda R_\varphi^N(\lambda)$ to arctan $\lambda R_\varphi(\lambda)$ when (I.E.6) is fulfilled. Introducing a succession of linear manifolds $\mathcal{E}_N$ such that $\mathcal{D} \supset \mathcal{E}_{N+1} \supset \mathcal{E}_N$ with $\mathcal{E}_1 = \{|\varphi\rangle\}$. It is clear that the sequence generates an infinite-dimensional manifold $\mathcal{E}_\infty \subseteq \mathcal{D}$.

Let us suppose that (1) $\mathcal{E}_\infty$ is dense in the $\mathcal{H}$ (Hilbert space) in which we work; (2) the transforms of $\mathcal{E}_\infty$ by $H \pm iI$ are dense in $\mathcal{H}$.

(1) Implies that $P_N \to I$ for $N \to +\infty$ (P_N projects on $\mathcal{E}_N$), that is, $P_N H P_N \to H$ in $\mathcal{E}_\infty$ but not necessary in $\mathcal{D}$ (convergence in the strong sense).

If (1) and (2) are fulfilled, then

$$\langle\varphi|[1 - \lambda H_N]^{-1}|\varphi\rangle \underset{N\to\infty}{\to} \langle\varphi|[1 - \lambda H]^{-1}|\varphi\rangle, \quad \mathrm{Im}\,\lambda \neq 0, \tag{I.E.7}$$

and the convergence is uniform for λ belonging to any compact not intersecting the real axis. (See Ref. 8 for the proofs.)

Condition (2) is specific of unbounded operators; in fact, for bounded operators only condition (1) is necessary to prove the convergence of the resolvent (see Appendix G). By analogy with the fact that, for a bounded operator, the moment problem is always determinate, we can say that condition (2) represents, for the Ritz variational principle, the analogous condition of the determination for the Padê approximation method. Therefore, when (2) is verified, we shall say that the variational Rayleigh–Ritz method is *determinate*.

Introducing the spectral families $E(\lambda)$ and $E_N(\lambda)$ associated to H and H_N, we now have for the determinate problem

$$\lim_{N\to\infty} \langle\varphi|E^N(\lambda)|\varphi\rangle = \langle\varphi|E(\lambda)|\varphi\rangle \tag{I.E.8}$$

in any point for which $\langle\varphi|E(\lambda)|\varphi\rangle$ is continuous.[8]

From this last inequality, together with the fact that the arctan $\lambda R_\varphi^N(\lambda)$ form a monotonically converging increasing sequence, we can deduce that

$$\lim_{N\to\infty} \lambda_i^N(\varphi) = \lambda_i(\varphi). \tag{I.E.9}$$

As consequence of this result, and of the Vitali's theorem,[13] we get the following:

Theorem IX: If the Ritz variational problem is determinate, then

$$\lim_{N\to\infty} \arctan \lambda\langle\varphi|[1 - \lambda P_N H P_N]^{-1}|\varphi\rangle = \arctan \lambda\langle\varphi|[1 - \lambda H]^{-1}|\varphi\rangle. \tag{I.E.10}$$

II. THE MOMENT PROBLEM WITH DIVERGING MOMENTS

Introduction

When the moments do exist, the method of Padé approximations appears to the very useful, giving an explicit and simple way to construct and choose the space $\mathcal{E}_N$ of the variational method. In fact, the Padé approximation method allows one to obtain rapidly converging answers. (For compact operators the spectrum is approached exponentially rapidly[2]; this feature seems to be general.) This convergence can even be improved, exploiting the variational aspects of the method.[11] Because of the systematic feature of the moment method, its rapidity of convergence, its possibility to sum up strongly diverging series, it is extremely useful to consider the extension of the method to the case in which the moments themselves are given by diverging algorithms.[14]

To set up the problem, let us suppose the vector $|\varphi\rangle$ does not belong to domains of H^n.

This condition is too restrictive, and can be enlarged to the case in which the first p moments exist, and only the $p+1$, $p+2, \cdots$ are infinite, and to the indeterminate moment problem. However, for definiteness, we shall stick to the first case. To make use of the moment meth od, we introduce a sequence of auto-adjoint operators $H(\epsilon)$ regularizing H and fulfilling

$$|\mu_n(\epsilon)| = |\langle\varphi|H^n(\epsilon)|\varphi\rangle| < +\infty, \quad n=1,2,\cdots. \tag{II.1}$$

Let us suppose that it is possible to regularize in such a way that

(i) $H(\epsilon)$ gives rise to a determinate moment problem for $\epsilon<\epsilon_0$ [for instance, we can choose $H(\epsilon)$ to be bounded];

(ii) $\lim_{\epsilon\to\epsilon_0} \arctan \lambda\langle\varphi|[1-\lambda H(\epsilon)]^{-1}|\varphi\rangle = \arctan \lambda\langle\varphi|[1-\lambda H]^{-1}|\varphi\rangle$ (with the ordinary convention on the definition of the arctan); and

(iii) $\arctan \lambda\langle\varphi|[1-\lambda H(\epsilon')]^{-1}|\varphi\rangle > \arctan \lambda\langle\varphi|[1-\lambda H(\epsilon)]^{-1}|\varphi\rangle$, $\epsilon<\epsilon'<\epsilon_0$. (II.2)

That such regularization can be effectively worked out is explicitly shown in a rather general example in Ref. 10.

When condition (i), (ii), (iii) are fulfilled, we can state the following theorem.

Notation

$$\delta(\lambda,\epsilon) = \arctan \langle\varphi|\lambda[1-\lambda H(\epsilon)]^{-1}|\varphi\rangle, \tag{II.3}$$

$$\delta^N(\lambda,\epsilon) = \arctan \lambda[N-1/N]_{R(\epsilon,\lambda)}(\lambda,\epsilon). \tag{II.4}$$

We have

(i) $\delta(\lambda,\epsilon)$ is, for fixed $\lambda>0$, a monotonically nondecreasing function of ϵ (for $\epsilon<\epsilon_0$) having its maximum value at $\epsilon=\epsilon_0$ equal to $\delta(\lambda)$;

(ii) $\delta^N(\lambda,\epsilon)$ is, for fixed $\lambda>0$, bounded by $\delta(\lambda,\epsilon)$ from above and by 0 from below and has, therefore, an absolute maximum $\bar{\delta}^N(\lambda,\epsilon_N)$ (if the absolute maximum is achieved in more than one point, we take for ϵ_N the nearest to ϵ_0);

(iii) for fixed λ and ϵ, the $\delta^N(\lambda,\epsilon)$ form a monotonically increasing sequence tending to $\delta(\lambda,\epsilon)$ for $\epsilon<\epsilon_0$.

As a consequence of (i), (ii), (iii) we have the following theorem:

Theorem X: The maxima $\bar{\delta}^N(\lambda,\epsilon_N)$ form a monotonically increasing sequence tending to $\delta(\lambda)$ when $N\to+\infty$, $\epsilon_N\to\epsilon_0$ $(N\to\infty)$.

The proof of this theorem can be found in Ref. 10.

Furthermore, the function $\bar{\delta}^N(\lambda,\epsilon_N(\lambda))$ is a monotonically continuous nondecreasing function of λ, which provides a lower bound to $\delta(\lambda)$; therefore, we again can obtain an upper bound for each inverse eigenvalue of the positive discrete spectrum.

As can be seen from the previous considerations, the extension of the method to the case of the problem of moments which diverge consists in a *supervariational principle*. In fact, two variations are used: the first, at fixed cutoff ϵ, produces the Padé approximation in the framework of the Ritz–Rayleigh method in which the projectors $P_N(\epsilon)$ are built up from the iterated vectors $H^n(\epsilon)|\varphi\rangle$ $(n=0,1,\ldots N-1)$; the second variation exploits the dependence of $P_N(\epsilon)$ on ϵ and its effect on $\delta^N(\lambda,\epsilon)$.

The explicit construction of proper regularizations for the operator H will be the content of future work for specific problems where a precise knowledge of H is given.

III. AN APPLICATION TO QUANTUM MECHANICAL SYSTEMS

We shall give here very briefly a direct application of the previous theorems to a quantum mechanical system whose Hamiltonian is H. We suppose we have an N-body Hamiltonian of the form

$$H = H(p_1, p_2, \ldots, p_N, q_1, \ldots q_N) \tag{III.1}$$

where $[p_k, q_j] = -i\delta_{kj}$. We suppose H to be self-adjoint and bounded from below, with a discrete spectrum to the left of the continuous spectrum extending to $+\infty$. Then by constructing the moment

$$\mu_k = \langle\varphi|H^k|\varphi\rangle \tag{III.2}$$

for a suitable $|\varphi\rangle$, such that the μ_k exist for all k and do not increase faster than $(2k)!$ (and also that the μ_k are easily numerically computable), we can apply the previous technique.

We first compute $\mu_1, \mu_2, \ldots, \mu_{2N-1}$. Then we construct the denominators of the Padé approximations to the resolvent by a recursive algebraic method.[15] Look for the classified zeros and obtain in the discrete region of the spectrum *strict* upper bounds for the ith excited state provided by the ith zero of the Nth approximation $(i<N)$. These upper bounds form a monotonic sequence in N decreasing rapidly to the exact ith excited state when N tends to infinity. Furthermore, at *a given* fixed N, it is in principle possible to adjust $|\varphi\rangle$ variationally in such way to obtain the exact value by looking for the minimum as a function of $|\varphi\rangle$ of the approximate ith zero of the denominator of the approximation. All bounds are always *strict* bounds, if, for *any* of the bounds, equality is achieved at a given step; then the exact solution is reached simultaneously for all the eigenvalues.

Such properties make a large improvement in the vari-

ational method, because all bounds are *strict*, as well as in the perturbative method, because we can start with a series diverging as fast as $(2n)!$ and still achieve a rapid convergence (which has been proved to be exponential for the completely continuous case, and very likely is the same in the general case). The method can be extended to *singular* interactions by introducing regularized Hamiltonians $H(\epsilon)$ for which the moments

$$\mu_K(\epsilon) = \langle \varphi | H^k(\epsilon) | \varphi \rangle \tag{III.3}$$

exist and the moment problem is determinate.

Then, as shown previously in the section devoted to the infinite moment problem, the arctan of the Padé approximation constructed on the resolvent of $H(\epsilon)$ have absolute maximums in ϵ which provide a lower bound to the arctan of the exact resolvent. As a consequence we again find upper bounds for the ith excited state which converge very rapidly to the expected exact value. See Ref. 10 for an example of the application of this method to the theory of singular potentials.

To end we shall propose an explicit and *algebraic* way of treating Hamiltonians which are polynomials in the p_i and q_i.

The case of polynomial interaction of N particles: Let us suppose

$$H(p_1, p_2, \ldots p_N, q_1, \ldots, q_N) \tag{III.4}$$

is a polynomial in the variables p_i and q_i.

In such a case the moment

$$\mu_k = \langle \varphi | H^k | \varphi \rangle \tag{III.5}$$

can be computed algebraically if one chooses a vector $|\varphi\rangle$ of the form

$$\langle q_1, q_2, \ldots, q_N | \varphi \rangle = P(q_1, q_2, \ldots, q_N) \exp\left(-\sum_{i=1}^{N} \gamma_i q_i^{2s}\right) \tag{III.6}$$

where P is a polynomial and $\gamma_i > 0$ and $s > 0$. We obtain

$$\mu_K = \int dq_1\, dq_2 \cdots dq_N\, P^*(q_1, q_2 \cdots q_N) \exp\left(-\sum_{i=1}^{N} \gamma_i q_i^{2s}\right) \times H^k(p_1 p_2 \cdots p_N, q_1, q_2, \cdots q_N) P(q_1 \cdots q_N) \exp\, -\sum \gamma_i q_i^{2s} \tag{III.7}$$

with

$$p_i = -i \frac{\partial}{\partial q_i}. \tag{III.8}$$

The result for μ_K is of the form

$$\mu_K = \sum_{(\delta)} C_\delta \prod_{i=1}^{N} \int_{-\infty}^{+\infty} q_i^{\delta_i} \exp(-\gamma_i q_i^{2s})\, dq_i, \tag{III.9}$$

but

$$\int_{-\infty}^{+\infty} q_i^{\delta_i} \exp(-\gamma_i q_i^{2s})\, dq_i = \begin{cases} 0 & \text{if } \delta_i \text{ is odd} \\ \dfrac{\Gamma[(\delta+1)/2s]}{s\gamma_i[(\delta+1)/2s]} & \text{if } \delta \text{ is even.} \end{cases} \tag{III.10}$$

We remark that the calculation necessitates only the knowledge of, at most, a finite number of values of $\Gamma(z)$ for z rational (if we choose s integer):

$$z_1 = 1/2s, \quad z_2 = 2/2s, \cdots z_i = \frac{\delta_i + 1}{2s}, \cdots z_N = \frac{\delta_N + 1}{2s}. \tag{III.11}$$

The $C_{(\delta)}$ can be computed by purely formal algebraical manipulations; therefore, the μ_K can be calculated by formal languages on computers.

Still, by algebraical manipulations, we compute the denominators of the Padé approximations (using for instance recursive algebraic method[15]); then, the zero being ordered, and separated by the zeros of the previous approximation, it is not difficult by standard method to compute them.

We obtain in such a way upper bounds for the ith excited state. Convergence is achieved if the moment problem is determinate, for instance, if the μ_K does not increase faster than $(2k)!$. This can be obtained by suitably choosing s as a function of the degree of the polynomial. (For a complete analysis of this case see Ref. 16.) Finally, we point out that this method can be greatly improved by varying the γ_i and the coefficient of the polynomial P in front of the exponential in the definition of $|\varphi\rangle$. This is so because

$$E_i < E_i^N(\varphi), \tag{III.12}$$

where E_i is the energy of the ith excited state and E_i^N is the ith eigenvalue of the Nth Padé approximation. Therefore,

$$E_i \leq \inf_{|\varphi\rangle} E_i^N(\varphi). \tag{III.13}$$

The method is independent of the coupling constant, which can be as large as one wants, because the expansion is done on the resolvent, that is, in the inverse of the energy. At a given fixed $|\varphi\rangle$ the convergence towards the exact eigenvalue is very likely exponential.

If the interaction is singular but can be approached by a family of polynomials, then by combining the previous arguments with the method explained for the infinite moment problem one obtains upper bounds for the ith excited state. All the technique extends to the eigenstates embedded in the continuum by use of the results of Appendix I.

To summarize, we can say that the method allows us to construct what would be called the successive approximations of the standard variational method in a regular and systematic way avoiding the loose bounds of the general variational method.

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APPENDIX A: PROOF OF THE FUNDAMENTAL THEOREM I

We shall first suppose the vectors $H^i|\varphi\rangle$, $i = 0, 1, \cdots, N-1$, spanning $\mathcal{E}^{(N)}$, linearly independent. In such a case it is clear that

$$(P_N H P_N)^l |\varphi\rangle = H^l |\varphi\rangle, \quad l \leq N-1. \tag{A1}$$

Instead, if the vectors $H^i|\varphi\rangle$, $i=0,1,\ldots,N-1$, are linearly dependent, then, for any l, $H^l|\varphi\rangle$ belongs to the space $\mathcal{E}^{(P)}$ $(P<N)$ generated by the vectors $H^i|\varphi\rangle$, $i=0,1,\ldots,N-1$. It is clear that in such case

$$(P_N H P_N)^l |\varphi\rangle = H^l |\varphi\rangle \text{ for any } l, \tag{A2}$$

and in this case the moments μ_l of $R_\varphi(\lambda)$ are identical for any l to those μ_l^N of $[N-1/N]_{R_\varphi}(\lambda)$ which appears to be identical to $R_\varphi(\lambda)$.

Let us come back to the case where $\mathcal{E}^{(N)}$ effectively has N dimension; taking the conjugate of (A1), we get

$$\langle\varphi|(P_N H P_N)^{l'} = \langle\varphi|H^{l'}, \quad l' \leq N-1, \tag{A3}$$

and multiplying (A1) by $P_N H P_N$ once more, we get

$$(P_N H P_N)^{l+1} |\varphi\rangle = P_N H^{l+1} |\varphi\rangle, \quad l \leq N-1, \tag{A4}$$

and combining (A3) and (A4),

$$\langle\varphi|(P_N H P_N)^{l'+l+1} |\varphi\rangle = \langle\varphi|H^{l'+l+1}|\varphi\rangle, \quad l+l'+1 \leq 2N-1. \tag{A5}$$

Therefore,

$$\mu_k^N = \mu_k \text{ for } k=0,1,2,\ldots,2N-1. \tag{A6}$$

Expanding $R_\varphi(\lambda)$ and $\langle\varphi|1/(1-\lambda P_N H P_N)|\varphi\rangle$ as power of λ

$$R_\varphi(\lambda) = \sum_0^\infty \lambda^K \langle\varphi|H^k|\varphi\rangle = \sum_0^\infty \lambda^k \mu_k, \tag{A7}$$

$$\langle\varphi|\frac{1}{1-\lambda P_N H P_N}|\varphi\rangle = \sum_0^\infty \lambda^k \langle\varphi|(P_N H P_N)^k|\varphi\rangle = \sum_0^\infty \lambda^k \mu_k^N. \tag{A8}$$

We see that

$$R_\varphi(\lambda) - \langle\varphi|\frac{1}{1-\lambda P_N H P_N}|\varphi\rangle = O(\lambda^{2N}). \tag{A9}$$

On the other hand, $P_N H P_N$ is a finite-rank Hermitian operator for which a spectral decomposition can be written:

$$P_N H P_N = \sum_{i=1}^N h_i^{(N)} p_i^{(N)} \tag{A10}$$

and

$$\langle\varphi|\frac{1}{1-\lambda P_N H P_N}|\varphi\rangle = \langle\varphi|P_N \frac{1}{1-\lambda P_N H P_N} P_N|\varphi\rangle = \langle\varphi|\frac{I_N}{I_N - \lambda P_N H P_N}|\varphi\rangle, \tag{A11}$$

where I_N is the unit operator acting in $\mathcal{E}^{(N)}$.

Using (A10) we get

$$\langle\varphi|\frac{1}{1-\lambda P_N H P_N}|\varphi\rangle = \sum_{i=1}^N \frac{\langle\varphi|p_i^{(N)}|\varphi\rangle}{1-\lambda h_i^{(N)}}. \tag{A12}$$

(A12) shows that $\langle\varphi|1/(1-\lambda P_N H P_N)|\varphi\rangle$ is a rational fraction of degree N at denominator and degree $N-1$ at numerator, and (A9) shows that it differs from $R_\varphi(\lambda)$ by order λ^{2N}; it is, therefore, the $[N-1/N]$ Padé approximation to $R_\varphi(\lambda)$.

APPENDIX B: PROOF OF THEOREM II

We want to prove here Theorem II.

We first recall a well-known identity[17]:

$$[N/N+1]_{R_\varphi}(\lambda) - [N-1/N]_{R_\varphi}(\lambda) = \lambda^{2N} \frac{\Delta(0,N)}{\Delta(0,N-1)} \frac{1}{Q_N(\lambda) Q_{N+1}(\lambda)}, \tag{B1}$$

where we have set

$$[N-1/N]_{R_\varphi}(\lambda) = \frac{P_{N-1}(\lambda)}{Q_N(\lambda)} \text{ with } Q_N(0) = +1. \tag{B2}$$

$P_{N-1}(\lambda)$ is a polynomial of degree $N-1$ in λ and $Q_N(\lambda)$ is a polynomial of degree N in λ [the normalization $Q_N(0) = +1$ can always be chosen when the first moment is finite, which is the case here] and

$$\Delta(0,N) = \begin{vmatrix} \mu_0 & \mu_1 \cdots & \mu_N \\ \mu_1 & \mu_2 \cdots & \mu_{N+1} \\ & \cdots & \\ \mu_N & \mu_{N+1} \cdots & \mu_{2N} \end{vmatrix}. \tag{B3}$$

It is well known that for a self-adjoint operator all $\Delta(0,N)$ are positive.

If, for some N_0, $\Delta(0,N_0)=0$, then all $\Delta(0,N_0+k)$ are zero, $k \geq 0$, and the mean value of the resolvent reduces to a rational fraction, identical to its $[N_0-1/N_0]_{R_\varphi}(\lambda)$ Padé approximant.[18]

Formula (B1) shows clearly that, if there exists a $\bar{\lambda} \neq 0$ such that $\delta_{N+1}^A(\bar{\lambda}) = \delta_N^A(\bar{\lambda})$, then the determinant $\Delta(0,N)$ would be zero and therefore

$$[N-1/N]_{R_\varphi}(\lambda) = [N/N+1]_{R_\varphi}(\lambda) \tag{B4}$$

and the Padé approximant $[N-1/N]_{R_\varphi}(\lambda)$ would reduce to the exact solution.

Leaving aside this exceptional case, we see that $\delta_{N+1}^A(\lambda)$ and $\delta_N^A(\lambda)$ cannot intersect for $\lambda \neq 0$, and, therefore, their relative value in the vicinity of the origin will fix their relative position everywhere for real λ.

In fact, we deduce from (B1) that

$$\delta_{N+1}^A(\lambda) - \delta_N^A(\lambda) = \frac{\Delta(0,N)}{\Delta(0,N-1)} \lambda^{2N+1} + O(\lambda^{2N+2}). \tag{B6}$$

Therefore, we obtain that for $\lambda > 0$

$$\delta_N^A(\lambda) < \delta_{N+1}^A(\lambda). \tag{B7}$$

APPENDIX C: PROOF OF THEOREM IV

To prove Theorem IV, we introduce the linear operator

$$H(x) = [x + (1-x)P_N] H [x + (1-x)P_N] \tag{C1}$$

which interpolates linearly between

$$H_N = P_N H P_N = H(0) \tag{C2}$$

and

$$H = H(1). \tag{C3}$$

By considering the mean value of the resolvent of $H(x)$,

$$R_\varphi(\lambda, x) = \langle\varphi|[1-\lambda H(x)]^{-1}|\varphi\rangle, \tag{C4}$$

and also the restriction $\mathcal{R}^N(z)$ of the resolvent of H,

$$\mathcal{R}^N(z) = P_N [1 - zH]^{-1} P_N, \tag{C5}$$

we have the first lemma:

Lemma I:

$$R_\varphi(\lambda,x)=\langle\varphi|[I^{(N)}-(1-x^2)\mathcal{R}^N(\lambda x^2)]^{-1}x^2\mathcal{R}^N(\lambda x^2)|\varphi\rangle. \tag{C6}$$

This lemma allows us to express the interpolating resolvent as a rational fraction of the matrix elements of an operator of rank N: $\mathcal{R}^N(\lambda x^2)$

This lemma is a consequence of the identity

$$[I-BP_N]^{-1}=I+BP_N[I-P_NBP_N]^{-1}P_N. \tag{C7}$$

In fact, we can write

$$R_\varphi(\lambda;x)=\langle\varphi|[x+(1-x)P_N][1-\lambda[x+(1-x)P_N]\times H[x+(1-x)P_N]]^{-1}[x+(1-x)P_N]|\varphi\rangle, \tag{C8}$$

because

$$P_N|\varphi\rangle\equiv|\varphi\rangle; \tag{C9}$$

then using the identities

$$A[1-\lambda AHA]^{-1}A=A^2[1-\lambda HA^2]^{-1}=[1-\lambda A^2H]^{-1}A^2, \tag{C10}$$

we obtain

$$R_\varphi(\lambda;x)=\langle\varphi|[1-\lambda H[x^2+(1-x^2)P_N]]^{-1}|\varphi\rangle$$
$$=\langle\varphi|[1-\lambda[x^2+(1-x^2)P_N]H]^{-1}|\varphi\rangle \tag{C11}$$

$$R_\varphi(\lambda;x)=\langle\varphi|[1-\lambda(1-x^2)(1-\lambda x^2H)^{-1}HP_N]^{-1}\times(1-\lambda x^2H)^{-1}|\varphi\rangle \tag{C12}$$

and using identity (C7), we can rewrite

$$R_\varphi(\lambda;x)=\langle\varphi|[1-X_N]^{-1}\mathcal{R}^N(\lambda x^2)|\varphi\rangle \tag{C13}$$

with

$$X_N=\frac{(1-x^2)}{x^2}[\mathcal{R}^N(\lambda x^2)-P_N]. \tag{C14}$$

We consider now the expression

$$\eta_N(\lambda)=\arctan\lambda R_\varphi(\lambda)-\arctan\lambda R_\varphi^N(\lambda)$$
$$=\arctan[\lambda R_\varphi(\lambda;1)]-\arctan[\lambda R_\varphi(\lambda;0)]. \tag{C15}$$

We see that we can write

$$\eta_N(\lambda)=\int_{0+}^{1}\frac{(\partial/\partial x)[\lambda R_\varphi(\lambda;x)]}{1+\lambda^2R_\varphi^2(\lambda;x)}\,dx, \tag{C16}$$

or, introducing the variable $z=\lambda x^2$,

$$\eta_N(\lambda)=\int_{0+}^{\lambda}\frac{(\partial/\partial z)[\bar{R}_\varphi(\lambda;z)]}{1+\bar{R}_\varphi^2(\lambda;z)}\,dz \tag{C17}$$

with

$$\bar{R}_\varphi(\lambda;z)=\langle\varphi|[I^{(N)}-(1-(z/\lambda))\mathcal{R}^N(z)]^{-1}z\mathcal{R}^N(z)|\varphi\rangle. \tag{C18}$$

If we introduce in the space $\mathcal{E}_N$ an orthonormalized basis $\{|0\rangle,|1\rangle,\ldots,|N-1\rangle\}$ with $|\varphi\rangle=|0\rangle$, we see that $\mathcal{R}^N(z)$ is given by an $N\times N$ matrix whose elements are

$$\mathcal{R}^N_{ij}(z)=\langle i|[1-zH]^{-1}|j\rangle\quad(i,j=0,1,\ldots,N-1). \tag{C19}$$

These matrix elements are, for $\mathrm{Re}z>0$, meromorphic functions of z; therefore, $\bar{R}_\varphi(\lambda;z)$ is also for $\mathrm{Re}z>0$ a meromorphic function of z, because we have

$$\bar{R}_\varphi(\lambda;z)=\frac{\lambda z}{\lambda-z}\left(\frac{\mathrm{minor}_{00}[\delta_{ij}-(1-z/\lambda)\mathcal{R}^N_{ji}(z)]}{\det[\delta_{ij}-(1-z/\lambda)\mathcal{R}^N_{ij}(z)]}-1\right) \tag{C20}$$

and therefore

$$\frac{(\partial/\partial z)[\bar{R}_\varphi(\lambda;z)]}{1+\bar{R}_\varphi^2(\lambda;z)} \tag{C21}$$

is a holomorphic function of z for $0<z\leq\lambda$, because $\bar{R}_\varphi(\lambda;z)$ is then real.

From this result we see that if we want the integral (C17) to exist, it is only necessary to see what happens to the integrand for $z\to 0^+$.

We shall suppose the elements $\langle i|[1-zH]^{-1}|j\rangle$ to be indefinitely derivable at $z=0^+$. This is certainly the case for the Padé approximations, if the moments are finite, because then the vectors $|i\rangle$ are linear combinations of $H^k|\varphi\rangle$ and

$$\frac{d^p}{dz^p}\langle i|[1-zH]^{-1}|j\rangle_{z=0^+}=p!\langle i|H^p|j\rangle. \tag{C22}$$

Therefore, $\bar{R}_\varphi(\lambda;z)$ is the ratio of two C_∞ functions at $z=0$ and (C21) is C_∞ everywhere in the closed interval $0\leq z\leq\lambda$ and the integral (C17) exists.

Let us show now that

$$\frac{\partial}{\partial z}[\bar{R}_\varphi(\lambda;z)]\geq 0\quad\text{for } 0\leq z\leq\lambda. \tag{C23}$$

We have, using (C11),

$$\bar{R}_\varphi(\lambda;z)=\langle\varphi|[1-\lambda P_NH-z(1-P_N)H]^{-1}|\varphi\rangle. \tag{C24}$$

Using

$$\frac{d}{dz}[A-zB]^{-1}=[A-zB]^{-1}B[A-zB]^{-1}, \tag{C25}$$

we get

$$\frac{\partial}{\partial z}R_\varphi(\lambda;z)=\langle 0|[1-[z+(\lambda-z)P_N]H]^{-1}\times\lambda(1-P_N)H[1-[z+(\lambda-z)P_N]H]^{-1}|\varphi\rangle. \tag{C26}$$

Using

$$H[1-[z+(\lambda-z)P_N]H]^{-1}=[1-H[z+(\lambda-z)P_N]]^{-1}H, \tag{C27}$$

we have

$$\frac{\partial}{\partial z}\bar{R}_\varphi(\lambda;z)=\langle\varphi|[1-[z+(\lambda-z)P_N]H]^{-1}\times(1-P_N)[1-H[z+(\lambda-z)P_N]]^{-1}H[z+(\lambda-z)P_N]|\varphi\rangle \tag{C28}$$

and, finally,

$$\frac{\partial}{\partial z}\bar{R}_\varphi(\lambda;z)=\langle\psi(\lambda;z)|(I-P_N)|\psi(\lambda;z)\rangle, \tag{C29}$$

where

$$|\psi(\lambda;z)\rangle=[I-H(z+(\lambda-z)P_N)]^{-1}|\varphi\rangle. \tag{C30}$$

(C29) proves (C23).

As consequence of the existence of the integral (C17) and of (C23) we see that $\eta_N(\lambda)\geq 0$. QED

APPENDIX D

We want to prove that the $[N/N]$ Padé approximation to $\lambda R_\varphi(\lambda)$ converges uniformly to an analytic function, holomorphic in λ, in a compact K of the complex λ plane in which, for $N > N_0$, there are no poles of the approximations. For $N > N_0$ we can write

$$[N/N]_{\lambda R_\varphi}(\lambda) = \lambda \sum_{i=1}^{N} \frac{\gamma_N^i}{1-\lambda\mu_i}, \tag{D1}$$

where

$$\mu_i = \lambda_i^{-1}, \quad \gamma_N^i > 0 \tag{D2}$$

and for $\lambda \in K$

$$|[N/N]_{\lambda R_\varphi}(\lambda)| \leq \sum_{i=1}^{N} \frac{\gamma_N^i}{|1/\lambda - \mu_i|} \leq \frac{\sum_{i=1}^{N} \gamma_N^i}{\inf|1/\lambda - \mu_i|}, \tag{D3}$$

$$\lambda \in K, \quad i = 1, \ldots, N,$$

but

$$\sum_{N=1}^{N} \gamma_N^i = [N-1/N]_{R_\varphi}(\lambda)\Big|_{\lambda=0} = \mu_0. \tag{D4}$$

Therefore,

$$|[N/N]_{\lambda R_\varphi}(\lambda)| \leq \frac{\mu_0}{\inf|1/\lambda - \mu_i|} = C(K), \tag{D5}$$

where $C(K)$ does not depend on N or λ but only on K.

When λ is different from a real number, we know that the Padé approximation $[N/N]_{\lambda R_\varphi}(\lambda)$ converges to an analytic function in the upper or lower λ complex plane. If the moment problem is determinate, this function is $\lambda R_\varphi(\lambda)$. Now applying the Vitali's theorem[12] to the set of uniformly bounded functions $[N/N]_{\lambda R_\varphi}(\lambda)$ which converge for complex λ to an analytic function, we see that for all λ, real or complex, $[N/N]_{\lambda R_\varphi}(\lambda)$ converges uniformly toward this analytic function in all the compact K provided there are no poles of $[N/N]_{\lambda R_\varphi}(\lambda)$ entering K, for $N > N_0$.

APPENDIX E

We want to show that if the moment problem is determinate $\lambda_i = L_i$.

This result simply derives from the fact that in this case the approximate measure tends to the exact measure. However, we shall give here an alternative proof.

We show first that $\lambda_1 = L_1$.

Let us suppose $\lambda_1 < L_1$. There are no poles of Padé approximations in the interval $0 < \lambda < L_1$ which includes λ_1. Let us apply Cauchy theorem to the function

$$R_\varphi(\lambda) - [N-1/N]_{\lambda R_\varphi}(\lambda). \tag{E1}$$

We have

$$\frac{1}{2i\pi} \oint [R_\varphi(\lambda) - [N-1/N]_{\lambda R_\varphi}(\lambda)]\, d\lambda = \gamma_1, \tag{E2}$$

where the path integral is a small circuit around λ_1 and γ_1 is the residue of $R_\varphi(\lambda)$ at the $\lambda = \lambda_1$.

On the other hand, there are no poles of the Padé approximation inside the circuit and by Theorem VI we conclude that the left-hand side integral can, for N sufficiently large, become as small as one would like. The hypothesis is absurd.

In the same way, we prove now that $L_2 = \lambda_2$, because for N sufficiently large we could find otherwise a small domain around λ_2 in which the approximations would have no poles, and apply the previous reasoning. The proof extends to $L_i = \lambda_i$.

APPENDIX F

Let us consider the interval $\lambda_i < \lambda < \lambda_{i+1}$. For N sufficiently large there are no poles of the Padé approximation in the interval $\lambda_i - \epsilon < \lambda < \lambda_{i+1}$. Therefore, by Theorem VI, in this interval $[N/N]_{\lambda R_\varphi}(\lambda)$ converges uniformly to $\lambda R_\varphi(\lambda)$. ϵ being arbitrarily small, we see that on the open interval $\lambda_i < \lambda < \lambda_{i+1}$ we have uniform convergence. We see by Theorem VII that in the closed interval $\lambda_i \leq \lambda \leq \lambda_{i+1}$ we have convergence for the arctan of $[N/N]_{\lambda R_\varphi}(\lambda)$ to arctan $\lambda R_\varphi(\lambda)$. This being true for any i is true for their union: the real positive axis.

APPENDIX G

Let us assume that $\{|\varphi_n\rangle\}$ is a complete system and H a bounded self-adjoint operator.

If we consider the difference, for $\mathrm{Im}\lambda \neq 0$,

$$\eta(\lambda) = \langle\varphi|(1-\lambda P_N H P_N)^{-1}|\varphi\rangle - \langle\varphi|(1-\lambda H)^{-1}|\varphi\rangle, \tag{G1}$$

then we can write

$$\eta(\lambda) = \langle\varphi|(1-\lambda H)(1-\lambda P_N H P_N)^{-1}|\varphi\rangle - \langle\psi|\varphi\rangle, \tag{G2}$$

where

$$|\psi\rangle = (1-\bar{\lambda}H)^{-1}|\varphi\rangle.$$

From (G2) it follows that

$$\begin{aligned}\eta(\lambda) &= \langle\psi|(P_N - \lambda H P_N)(1-\lambda P_N H P_N)^{-1}|\varphi\rangle \\ &\quad - \langle\psi|(1-\lambda P_N H P_N)(1-\lambda P_N H P_N)^{-1}|\varphi\rangle \\ &= -\lambda\langle\psi|(I-P_N)HP_N(1-\lambda P_N H P_N)^{-1}|\varphi\rangle.\end{aligned} \tag{G3}$$

Then

$$|\eta(\lambda)| \leq \frac{\||\varphi\rangle\|}{|\mathrm{Im}(1/\lambda)|}\|H\| \cdot \|(I-P_N)|\psi\rangle\|, \tag{G4}$$

where $\|H\|$ is the bound of H. We see easily that

$$\eta(\lambda) \underset{N\to\infty}{\to} 0.$$

APPENDIX H: CONNECTION OF THE PADÉ APPROXIMATION METHOD WITH THE JACOBI TRIDIAGONALIZATION METHOD AND THE LANCZOS METHOD

In the previous section the connection of the Padé approximation with the Rayleigh–Ritz method has been fully analyzed.

We recall here for completeness the connection with the Jacobi trigonalization method and the Lanczos method.

In the space $\mathcal{E}_N$ spanned by the vectors $\{|\varphi\rangle; H|\varphi\rangle; \cdots; H^{N-1}|\varphi\rangle\}$, we construct an orthonormalized basis (by the method of orthogonalization of Schmidt):

$$|0\rangle = |\varphi\rangle \quad (\langle\varphi|\varphi\rangle = 1),$$

$$|1\rangle = \bar{Q}_1(H)|\varphi\rangle$$
$$\vdots \qquad \text{(H1)}$$
$$|N-1\rangle = \bar{Q}_{N-1}(H)|\varphi\rangle,$$

where the polynomial $\bar{Q}_j(\mu)$ is simply related[9] to the polynomial $Q_j(\lambda)$ of the denominator of the Padé approximation $[N-1/N]$ to the resolvent $R_\varphi(\lambda)$ of the operator H by

$$\bar{Q}_j(t) = C(j)t^j Q_j(1/t), \qquad \text{(H2)}$$

the constant $C(j)$ being adjusted in such a way that the polynomials $\bar{Q}_j(t)$ form an orthonormalized set with respect to the spectral measure of H associated to $|\varphi\rangle$:

$$\int_{-\infty}^{+\infty} \bar{Q}_j(t)\bar{Q}_k(t)\, d\mu(t) = \delta_{jk}. \qquad \text{(H3)}$$

By using the spectral representation of H, it is evident that the set (H1) is an orthonormalized set.

From (H1), one sees immediately that in the basis (H1) the operator $H_N = P_N H P_N$ is tridiagonalised:

$$H_{jk}^{(N)} = \langle\varphi|Q_j(H)P_N H P_N Q_k(H)|\varphi\rangle = \langle\varphi|Q_j(H)HQ_k(H)|\varphi\rangle$$
$$= \int_{-\infty}^{+\infty} \bar{Q}_j(t)\bar{Q}_k(t)t\, d\mu(t). \qquad \text{(H4)}$$

Due to the orthogonality properties of the $\bar{Q}_j(t)$, we see that

$$H_{jk}^{(N)} = 0 \quad \text{except if } j=k, \text{ or } j=k-1, \text{ or } j=k+1. \qquad \text{(H5)}$$

Furthermore, all elements $H_{jk}^{(N)}$ are real: The basis (H1) enjoys the remarkable property that the restriction of H to the space $\mathcal{E}_N$ appears as a real symmetrical tridiagonal matrix (Jacobi tridiagonal matrix).

More particularly, we see that $\bar{Q}_j(t)$ fulfill the recursive relation

$$t\bar{Q}_j(t) = H_{j,j+1}^N \bar{Q}_{j+1}(t) + H_{j,j}^{(N)}\bar{Q}_j(t) + H_{j,j-1}^{(N)}\bar{Q}_{j-1}(t)$$
$$\text{with } \bar{Q}_0(t) = 1. \qquad \text{(H6)}$$

If we expand now the eigenstates $|\psi_N^i\rangle$ of H_N

$$H_N|\psi_N^i\rangle = \mu_N^i|\psi_N^i\rangle \quad (i=0,1,\ldots,N-1)$$

with $\bar{Q}_N(\mu_N^i) = 0$, on the basis (H1), we obtain

$$|\psi_N^i\rangle = \sum_{j=0}^{N-1} \alpha_j(i)\bar{Q}_j(H)|\varphi\rangle, \qquad \text{(H7)}$$

where the $\alpha_j(i)$ fulfill the relation

$$\mu_N^i \alpha_j(i) = H_{j,j+1}^{(N)}\alpha_{j+1}(i) + H_{j,j}^{(N)}\alpha_j(i) + H_{j,j-1}^{(N)}\alpha_{j-1}(i). \qquad \text{(H8)}$$

This relation is precisely the relation (H6) if we set

$$\alpha_j(i) = \bar{Q}_j(\mu_N^i). \qquad \text{(H9)}$$

Therefore, we have

$$|\psi_N^i\rangle = \sum_{j=0}^{N-1} \bar{Q}_j(\mu_N^i)\bar{Q}_j(H)|\varphi\rangle \qquad \text{(H10)}$$
$$\text{with } \bar{Q}_0 = 1 \quad \langle\varphi|\varphi\rangle = 1.$$

We see that we reproduce the results of the method of Lanczos[9] (method of minimal iterations).

Recall that we have put this here to point out another advantage of the Padé approximation method with respect to the extraction of the discrete eigenvalues embedded in the continuum, which will be discussed in the next section.

APPENDIX I: BOUNDS FOR THE RESIDUES OF THE RESOLVENT OF H IN THE DISCRETE PART OF THE SPECTRUM—EXTENSION TO THE DISCRETE POLES EMBEDDED IN THE CONTINUUM

The residue at pole $\lambda = \lambda_N^i$ of the $[N-1/N]$ Padé approximation to the resolvent of H,

$$[N-1/N]_{R_\varphi}(\lambda) = \sum_{i=1}^{N} \frac{\gamma_N^i}{1-\lambda\mu_N^i} \quad \mu_N^i = (\lambda_N^i)^{-1}, \qquad \text{(I1)}$$

is

$$\gamma_N^i = \frac{|\langle\varphi|\psi_N^i\rangle|^2}{\langle\psi_N^i|\psi_N^i\rangle}. \qquad \text{(I2)}$$

So, from (H10) we deduce

$$\gamma_N^i = 1/\sum_{j=0}^{N-1} \bar{Q}_j^2(\mu_N^i). \qquad \text{(I3)}$$

It is therefore interesting to introduce the function

$$\gamma_N(x) = \left\{\sum_{j=0}^{N-1} Q_j^2(x)\right\}^{-1}. \qquad \text{(I4)}$$

The sequence $\{\gamma_N(x)\}$ has very remarkable properties[1] which show another important aspect of the Padé approximation method. We will consider here only the case where the moment problem is determinate.

Let

$$\gamma(x) = 1/\sum_{j=0}^{\infty} \bar{Q}_j^2(x). \qquad \text{(I5)}$$

We have

$$\gamma_N(x) \geq \gamma_{N+1}(x) \geq \cdots > \gamma(x). \qquad \text{(I6)}$$

If we put

$$\langle\varphi|(1-\lambda H)^{-1}|\varphi\rangle = \int_{-\infty}^{+\infty} \frac{d\mu(t)}{1-\lambda t},$$

it can be shown that[1]

$$\mu(t+0) - \mu(t-0) = \gamma(t). \qquad \text{(I7)}$$

From (G6) it follows that

$$\mu(t+0) - \mu(t-0) < \gamma_N(t). \qquad \text{(I8)}$$

Now let us consider the case A, for definiteness. For $t > 0$, $\mu(t)$ is a nondecreasing function built up of step functions. Its discontinuities are related to the residues of the poles of $\langle\varphi|(1-\lambda H)^{-1}|\varphi\rangle$ for $\lambda > 0$. It is then clear from (I8) that one can obtain bounds on these residues by analyzing the function $\gamma_N(t)$ in some proper positive intervals of t.

Furthermore, we see from (I7) that

$$\lim_{N\to\infty} \gamma_N(t) = 0$$

for all points t which belong to the pure continuous spectrum. Therefore, if we have an eigenvalue embedded in the continuous spectrums, $\gamma_N(t)$ gives us the means to pick them out: The sequence $\gamma_N(t)$ will have its maximum points in the neighborhood of such eigenvalues.

Further, extremal properties of the function $\gamma_N(t)$ are discussed fully in Ref. 1. They give the tools, in our procedure, to obtain more information on the spectral function $\mu(t)$.

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Static cylindrically symmetric solutions of the Einstein–Maxwell equations*

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A general class of solutions of Einstein–Maxwell equations with static cylindrical symmetry is obtained. The equations are derived using canonical methods and the fields are shown to satisfy a certain Painlevé differential equation of the third transcendental type. A particular algebraic solution is studied in detail, and is found to have a certain mass and current on the axis and a helical magnetic field around it.

I. INTRODUCTION

Various classes of solutions of Einstein–Maxwell field equations in a cylindrically symmetric static spacetime have been discussed in the literature.[1,2] All these solutions assume "whole cylinder symmetry," i.e., the solutions are invariant under rotation about and translation along a symmetry axis, and under reflection in any plane containing the symmetry axis or perpendicular to it. The consequence of whole cylinder symmetry is that for time-dependent, vacuum spacetimes we obtain the Einstein–Rosen gravitational waves with only one polarization state, corresponding to a single gravitational potential function ψ. By relaxing the demand that spacetime be invariant under reflections, one obtains cylindrical gravitational waves with two polarization states.[3] Here we study cylindrical coupled grativational and electromagnetic systems which do not obey the reflection symmetry. Thus, the metric will contain two gravitational potential functions $\psi(r,t)$ and $\sigma(r,t)$. The electromagnetic field in a suitably chosen gauge will be given in terms of two electromagnetic vector potential functions $A_z(r,t)$ and $A_\phi(r,t)$. (ϕ is an azimuthal angle about the symmetry axis and z is a coordinate measured along it.)

We use the canonical methods developed by Dirac,[4] Arnowitt, Deser, and Misner[5] to cast the Einstein–Maxwell action into Hamiltonian form. The constraints in the problem are solved by Kuchař's technique[6] to obtain a reduced Hamiltonian. Hamilton's equations then give the Einstein–Maxwell equations for the gravitational and electromagnetic potentials. Next, we specialize to the static case with a view towards studying strong helical magnetic fields and their influence on the geometry of the spacetime. We find that the system of coupled Einstein–Maxwell equations can be reduced to a single second order differential equation. It turns out to be a Painlevé differential equation of the third transcendental type[7] and in general its solution is a new type of transcendental function. We take a particular algebraic solution of this equation and study its properties.

This particular solution is characterized by a single constant which is related to the presence of both the electromagnetic field and the second polarization state of the gravitational field. Test particles spiral in this geometry according to the helically symmetric nature of the fields.

II. THE EINSTEIN–MAXWELL EQUATIONS

To cast the Einstein–Maxwell field equations into canonical form we start by splitting the metric tensor of spacetime into the spatial metric tensor g_{ik}, the lapse function N, and the shift function N_i. Specializing these quantities according to the requirements of cylindrical symmetry but without the "whole cylinder symmetry," we find that the most general line element for our problem can be written in the form

$$ds^2 = -(N^2 - e^{2\psi-2\gamma}N_1^2)\,dt^2 + 2N_1\,dt\,dr + e^{2\gamma-2\psi}\,dr^2 + e^{2\psi}(dz + \sigma\,d\phi)^2 - \lambda^2 e^{-2\psi}\,d\phi^2 \tag{1}$$

where N, N_1, γ, ψ, λ, and σ are functions of t and r. The Einstein action for the gravitational field can then be written in the canonical form

$$I_g = \int dt\,d^3x(\pi_\psi\dot{\psi} + \pi_\sigma\dot{\sigma} + \pi_\lambda\dot{\lambda} + \pi_\gamma\dot{\gamma} + N\mathcal{H}_g^0 - N_1\mathcal{H}_g^1) \tag{2}$$

where dot denotes differentiation with respect to time and π_ψ, π_σ, π_λ, π_γ are momenta conjugate to ψ, σ, λ, and γ, respectively. $\mathcal{H}_g^0$ and $\mathcal{H}_g^1$ are the constraints which are given by

$$\mathcal{H}_g^0 = e^{\psi-\gamma}\left(\frac{1}{8\lambda}\pi_\psi^2 - \tfrac{1}{2}\pi_\lambda\pi_\gamma + \tfrac{1}{2}\lambda e^{-4\psi}\pi_\sigma^2 + 2\lambda'' - 2\lambda'\gamma' + 2\lambda\psi'^2 + \frac{1}{2\lambda}e^{4\psi}\sigma'^2\right), \tag{3}$$

$$\mathcal{H}_g^1 = -e^{-2\gamma+2\psi}(\pi_\gamma' - \gamma'\pi_\gamma - \lambda'\pi_\lambda - \sigma'\pi_\sigma - \psi'\pi_\psi) \tag{4}$$

and we note that the symmetries imposed on this problem result in the trivial satisfaction of the remaining constraint equations. Differentiation with respect to r is denoted by a prime. The canonical decomposition for the electromagnetic fields compatible with the requirements of cylindrical symmetry is

$$I_e = \int dt\,d^3x(\mathcal{E}^z\dot{A}_z + \mathcal{E}^\phi\dot{A}_\phi - N\mathcal{H}_e^0 - N_1\mathcal{H}_e^1) \tag{5}$$

where

$$\mathcal{H}_e^0 = e^{\psi-\gamma}\{\tfrac{1}{2}\lambda e^{-2\psi}(\mathcal{E}^{\phi 2} + A_z'^2) + \frac{1}{2\lambda}e^{2\psi}[(\mathcal{E}^z + \sigma\mathcal{E}^\phi)^2 + (A_\phi' - \sigma A_z')^2]\}, \tag{6}$$

$$\mathcal{H}_e^1 = e^{-2\gamma+2\psi}(\mathcal{E}^z A_z' + \mathcal{E}^\phi A_\phi'). \tag{7}$$

A_z, A_ϕ and $\mathcal{E}^z$, $\mathcal{E}^\phi$ which are canonically conjugate variables are the two surviving components of the vector potential and the electric field densities, respectively.

The total action which consists of the sum of I_g and I_e is thus cast into canonical form. We now impose the coordinate condition $\lambda = r$ and solve the momentum constraint equation

$$\mathcal{H}_g^1 + \mathcal{H}_e^1 = 0 \tag{8}$$

for π_λ. Next imposing the extrinsic time coordinate condition[6]

$$t = -\tfrac{1}{2}\int \pi_\gamma \, dr \tag{9}$$

we solve the Hamiltonian constraint equation

$$\mathcal{H}_g^0 + \mathcal{H}_e^0 = 0 \tag{10}$$

for the reduced Hamiltonian, which turns out to be $2\gamma'$ for the above coordinate condition. It can be shown that these coordinate conditions are equivalent to choosing the lapse and shift functions as

$$N = e^{\gamma - \psi} \tag{11}$$

and

$$N_1 = 0. \tag{12}$$

Integrating over the surface of cylinder of unit height, the action reduces to

$$I = 2\pi \int dt\, dr (\pi_\psi \dot{\psi} + \pi_\sigma \dot{\sigma} + \mathcal{E}^z \mathring{A}_z + \mathcal{E}^\phi \mathring{A}_\phi - H) \tag{13}$$

where

$$\begin{aligned} H = {} & \frac{1}{8r}\pi_\psi^2 + 2r\psi'^2 + \tfrac{1}{2}re^{-4\psi}\pi_\sigma^2 + \frac{1}{2r}e^{4\psi}\sigma'^2 \\ & + \frac{1}{2r}e^{2\psi}(\mathcal{E}^z + \sigma\mathcal{E}^\phi)^2 + \tfrac{1}{2}re^{-2\psi}A_z'^2 \\ & + \tfrac{1}{2}re^{-2\psi}\mathcal{E}^{\phi 2} + \frac{1}{2r}e^{2\psi}(A_\phi' - \sigma A_z')^2 \end{aligned} \tag{14}$$

and Hamilton's equations correspond to the Einstein–Maxwell field equations for ψ, σ, A_z, and A_ϕ.

III. STATIC SOLUTIONS

We will now specialize to the static case. Hamilton's equations are now ordinary second order differential equations for ψ, σ, A_z, and A_ϕ. They can be integrated so that only the following set of four first order ordinary differential equations remain to be solved:

$$2r\psi' = c_3\sigma - c_2\sigma A_z - \tfrac{1}{2}c_1 A_z + \tfrac{1}{2}c_2 A_\phi + c_4, \tag{15}$$

$$\frac{1}{r}e^{4\psi}\sigma' = -c_2 A_z + c_3, \tag{16}$$

$$re^{-2\psi}A_z' = c_1 + c_2\sigma, \tag{17}$$

$$re^{2\psi}A_\phi' = c_1\sigma e^{4\psi} + c_2\sigma^2 e^{4\psi} + c_2 r^2, \tag{18}$$

where c_1, c_2, c_3, c_4 are constants of integration. Once the integration of these coupled equations is effected, the remaining metric component γ can be obtained by quadrature from

$$2r\gamma' = c_2 A_\phi - c_2\sigma A_z + c_3\sigma + c_5. \tag{19}$$

While these constants c_1–c_5 are in general arbitrary, it can easily be seen that the presence of some of them does not lead to physically distinguishable states of the system and hence can be dropped without loss of generality. Alternatively, for $c_2 \neq 0$ we can use the transformations

$$\begin{aligned} \bar{\psi} &= \psi, \\ \bar{\gamma} &= \gamma, \\ \bar{\sigma} &= c_2\sigma + c_1, \\ \bar{A}_\phi &= c_2 A_\phi + c_1 A_z, \\ \bar{A}_z &= A_z - c_3/c_2, \\ \bar{r} &= c_2 r, \end{aligned} \tag{20}$$

which will accomplish the same purpose. Thus in the solution c_1 can be absorbed by a redefinition of the Killing coordinate directions and this is accounted for in the transformation law for A_ϕ. Furthermore, c_3 can be avoided by choosing the zero of the potential A_z and c_2 corresponds to a rescaling of the r coordinate. The case $c_2 = 0$ will be treated separately. Now Eqs. (15)–(18) reduce to (dropping the bars)

$$2r\psi' = \tfrac{1}{2}A_\phi - \sigma A_z + k_1, \tag{21}$$

$$\frac{1}{r}e^{4\psi}\sigma' = -A_z, \tag{22}$$

$$re^{-2\psi}A_z' = \sigma, \tag{23}$$

$$re^{2\psi}A_\phi' = r^2 + e^{4\psi}\sigma^2, \tag{24}$$

and

$$2r\gamma' = A_\phi - \sigma A_z + k_2, \tag{25}$$

where we are left with only two arbitrary constants k_1 and k_2.

We now define the variables

$$y = e^{-2\psi}, \tag{26}$$

$$x = \sigma^2/y + r^2 y, \tag{27}$$

and from Eqs. (21)–(24) obtain the following two coupled equations:

$$\frac{d}{dr}\left(\frac{1}{ry^2}\frac{d}{dr}(xy)\right) = -\frac{x}{r}, \tag{28}$$

$$\frac{d}{dr}\left(\frac{1}{ry^2}\frac{d}{dr}(\sigma)\right) = \frac{-\sigma}{ry} \tag{29}$$

For convenience we introduce an auxialiary variable f defined by the relation

$$\sigma = fxy \tag{30}$$

and see that f satisfies the differential equation

$$\frac{df}{dr} = \frac{\alpha r}{x^2} \tag{31}$$

where α is an arbitrary constant. This definition of f enables us to express y in the form

$$y = x/(f^2x^2 + r^2). \tag{32}$$

Substituting this form into the Eq. (28) and using Eq. (31), we can decouple equations (21)–(25) and obtain the second order differential equation

$$x'' = \frac{1}{x}(x')^2 - \frac{1}{r}x' + \frac{\alpha^2}{x} - \frac{x^2}{2r^2}. \tag{33}$$

This equation is not integrable in terms of classical transcendents. In fact, the transformation

$$z = r^{1/2} \tag{34}$$
$$w = x/r^{1/2}$$

brings Eq. (33) into the canonical form of Painlevé's equation of the third transcendental type.

Let us now consider the case $c_2 = 0$. In this case Eqs. (15)–(18) become

$$ryA'_z = c_1, \tag{35}$$
$$A'_\phi = \sigma A'_z, \tag{36}$$
$$\sigma' = c_3 r y^2, \tag{37}$$
$$r(y'/y) = (c_1/2)A_z - c_3\sigma - c_4 \tag{38}$$

where y is again given by Eq. (26). From these equations we find that

$$y'' = \frac{1}{y}(y')^2 - \frac{1}{r}y' + \frac{c_1^2}{2r^2} - c_3^2 y^3 \tag{39}$$

and letting $\tilde{r} = r^{1/2}$, $\tilde{y} = r^{1/2}y$ we see that one again gets a Painlevé equation of the third transcendental type.

IV. A PARTICULAR SOLUTION

In the last section we have seen that for our problem the solution of the Einstein–Maxwell equations will in general be expressed in terms of Painlevé transcendents of the third kind. In this section we shall study a particular solution which can be given in closed form in terms of algebraic functions. This solution is obtained by noting that Eq. (33) admits

$$x = (2\alpha^2)^{1/3} r^{2/3} \tag{40}$$

as a particular solution.[8] The metric and the electromagnetic fields corresponding to this solution are given by

$$ds^2 = kr^{-4/9} e^{a^2 r^{2/3}}(dr^2 - dt^2) + r^{4/3}dz^2 + r^{2/3}(d\phi + ar^{2/3}dz)^2,$$
$$A = \sqrt{2}\, ar^{2/3}d\phi + \frac{a^2}{\sqrt{2}} r^{4/3}dz \tag{41}$$

where k and a are arbitrary constants. The constant k may be absorbed by a coordinate transformation and consequently has no physical meaning for static problems. However, for convenience we shall keep it because in time dependent problems this constant will play a role in describing gravitational radiation.[9] The constant a can be expressed in terms of α as $a = 3(\alpha/16)^{1/3}$ and it is related both to the fact we have two polarization states and that electromagnetic fields are present. Obviously by setting $a = 0$ one switches off the electromagnetic fields and one of the polarization states. For the particular Einstein–Rosen solution which is obtained in this limit we find that Thorne's c-energy is given by

$$E(r) = \tfrac{1}{9}\ln r \tag{42}$$

and the corresponding Levi–Civita mass is negative. The occurrence of negative mass on the axis persists if one considers the weak field-low velocity limit when $a \neq 0$. This solution also requires the presence of currents on the axis since it is singular on the axis of symmetry.

We shall now study the motion of charged and neutral test particles in this geometry. For a test particle of charge e and mass m we have the Hamilton–Jacobi equation for the geodesics

$$g^{\mu\nu}\left(\frac{\partial S}{\partial x^\mu} - eA_\mu\right)\left(\frac{\partial S}{\partial x^\nu} - eA_\nu\right) = -m^2 \tag{43}$$

which in our case is trivially separable. So with the ansatz

$$S = -\alpha_0 t + \int^r Q(r')\,dr' + \alpha_\phi \phi + \alpha_z z, \tag{44}$$

we obtain

$$Q^2(r) = \alpha_0^2 - V(r) \tag{45}$$

where the effective potential $V(r)$ is given by

$$V(r) = ke^{a^2 r^{2/3}} \times (m_1 r^{8/9} + m_2 r^{2/9} + m_3 r^{-4/9} + m_4 r^{-10/9} + m_5 r^{-16/9}) \tag{46}$$

and for the constants m_i we have

$$\begin{aligned} m_1 &= e^2 a^4/2, \\ m_2 &= 2e^2 a^2 - \sqrt{2}ea^3\alpha_\phi, \\ m_3 &= a^2\alpha_\phi^2 + \sqrt{2}ea^2\alpha_z - 2\sqrt{2}ea\alpha_\phi + m^2, \\ m_4 &= \alpha_\phi^2 - 2a\alpha_\phi\alpha_z, \\ m_5 &= \alpha_z^2. \end{aligned} \tag{47}$$

The conditions that waves with nearly identical values of $\alpha_0, \alpha_z, \alpha_\phi$ have the same phase S for all times gives the first integrals of the motion. Explicitly, we have

$$\dot{\phi} = \frac{k}{\alpha_0} e^{a^2 r^{2/3}}\left(-\frac{ea^3}{\sqrt{2}} r^{2/9} + (\alpha_\phi a^2 - \sqrt{2}ea)r^{-4/9} + (\alpha_\phi - a\alpha_z)r^{-10/9}\right), \tag{48}$$

$$\dot{z} = \frac{k}{\alpha_0} e^{a^2 r^{2/3}}\left(\frac{ea^2}{\sqrt{2}} r^{-4/9} - a\alpha_\phi r^{-10/9} + \alpha_z r^{-16/9}\right). \tag{49}$$

From these equations it follows that in the presence of two polarization states and electromagnetic fields a charged test particle will always perform helical motion, i.e., it will always have a nonzero velocity in ϕ and z directions, even when $\alpha_\phi = \alpha_z = 0$. The presence of the constant a puts restrictions also on the motion of neutral test particles. We see that even for neutral particles circular orbits and motions parallel to the symmetry axis are not permitted. On the other hand, when both α_ϕ and α_z are zero massive neutral particles perform radial oscillations around the point $r = (\frac{2}{3})^{3/2} \times a^{-3}$ and zero rest mass particles behave as free particles.

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A spinor field theory on a seven-dimensional homogeneous space of the Poincaré group

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A field theory of half-integer spin particles is constructed on a seven-dimensional homogeneous space of the Poincaré group. The mass spectrum consists of nonparallel linear trajectories. The field theory has no spacelike or lightlike solutions. Electromagnetic form factors and structure functions of the theory are discussed.

1. INTRODUCTION

Field theories on homogeneous spaces of the Poincaré group have been studied by many authors in recent years.[1–6] Among them, the theory of the fields defined over a seven-dimensional homogeneous space of the Poincaré group[5,6] is distinguished by its connection with the construction of manifestly covariant quantum mechanical operators,[6] in particular, position operators, which require the introduction of a unit 4-vector η^μ. The dependence of the field operators on this unit vector, in addition to their dependence on space—time points x^μ, leads to consideration of the field theories defined on the seven-dimensional manifold of (x,η) points. In Refs. 5 and 6 the general theory of these fields was developed and models of fields transforming as scalars under the homogeneous Lorentz group were considered. As a result the spectrum of these models consisted of integer spin particles only. Moreover, to obtain a reasonable mass spectrum, it was necessary to consider field equations involving high order derivatives.

This paper is devoted to the study of spinor fields defined on the seven-dimensional homogeneous space of the Poincaré group. It will be seen that a simple field equation may be written which yields a reasonable mass spectrum consisting of half integer spin particles. In Sec. 2 the field equation is introduced and its mass spectrum is investigated. The spectrum consists of a set of nonparallel linear trajectories in the mass squared spin plane. The only free parameter of the theory is that of a mass scale. The spin intercepts are independent of this parameter. It is shown that due to nonunitarity of the spin representation of the Lorentz group, the theory has no spacelike solutions. Similarly, no lightlike solutions appear. In Sec. 3 a Lagrangian is written from which the generators of the Poincaré group and a conserved current are constructed. Form factors of the ground state are calculated and the structure functions are shown to scale in the Bjorken limit and to satisfy the Drell—Yan relation.

2. THE FIELD EQUATION AND ITS SOLUTIONS

We denote the fields by $\psi_\alpha(x,\eta)$, where α is the Dirac spinor index and η is a 4-vector on a unit hyperboloid $(\eta_\mu\eta^\mu=1)$, on which a unitary representation of the homogeneous Lorentz group may be built, with the inner product between two functions f and g defined by

$$(f,g)=\int_{\eta^2=1}\overline{f(\eta)}g(\eta)\frac{\vec{d}\eta}{\eta_0}\,. \tag{2.1}$$

We assume that the fields transform, under the action of the Poincaré group, as

$$U(a)\psi_\alpha(x,\eta)\,U(a)^{-1}=\psi_\alpha(x+a,\,\eta), \tag{2.2}$$

under space—time translations; and as

$$U(\Lambda)\psi_\alpha(x,\eta)U(\Lambda)^{-1}=S_{\alpha\beta}(\Lambda)\psi_\beta(\Lambda x,\,\Lambda\eta), \tag{2.3}$$

under homogeneous Lorentz transformations. $S(\Lambda)$ is the 4×4 Dirac representation of the homogeneous Lorentz group. It is trivial then, to verify that the generators of the Poincaré group behave as

$$[\psi(x,\eta),\ P_\mu]=i\partial_\mu\psi(x,\eta), \tag{2.4}$$

$$[\psi(x,\eta),\ M_{\mu\nu}]=[i(x_\mu\partial_\nu-x_\nu\partial_\mu)+i(\eta_\mu\delta_\nu-\eta_\nu\delta_\mu)+\tfrac{1}{2}\sigma_{\mu\nu}]\psi(x,\eta), \tag{2.5}$$

where $\sigma_{\mu\nu}=\frac{1}{2}i[\gamma_\mu,\gamma_\nu]$ and γ_μ are the usual Dirac matrices. Here δ_μ is simply a partial differential operator with respect to the η_μ variable, consistent with the restriction $\eta_\mu\eta^\mu=1$. In calculations, it is sufficient to remember that

$$\delta_\mu=(g_{\mu\nu}-\eta_\mu\eta_\nu)\frac{\partial}{\partial\eta_\nu}\,, \tag{2.6}$$

where $\partial/\partial\eta_\nu$ is simply the partial differential operator with respect to η_ν irrespective of the condition $\eta_\mu\eta^\mu=1$, and that in integration by parts

$$\int\overline{f(\eta)}\ \delta_\mu g(\eta)\ \frac{\vec{d}\eta}{\eta_0}=-\int\overline{[\delta_\mu f(\eta)]}g(\eta)\frac{\vec{d}\eta}{\eta_0}+\int\overline{[3\eta_\mu f(\eta)]}g(\eta)\frac{\vec{d}\eta}{\eta_0} \tag{2.7}$$

for suitably chosen functions f and g, which allow the vanishing of the surface integrals.[5] It is obvious from (2.7) that $i(\delta_\mu-\frac{3}{2}\eta_\mu)$ is an Hermitian operator on $L_2(H^3)$.

After these preliminaries we introduce our wave equation

$$[i\partial_\mu \Gamma^\mu + l_0 \partial^2]\psi(x,\eta) = 0, \tag{2.8}$$

where l_0 is a parameter and

$$\Gamma_\mu = \sigma_{\mu\nu}(\delta^\nu - \tfrac{3}{2}\eta^\nu). \tag{2.9}$$

We remark in passing that it is easily seen that the vector operator Γ_μ together with the generators of Lorentz group on the hyperboloid H^3,

$$S_{\mu\nu} = i(\eta_\mu \delta_\nu - \eta_\nu \delta_\mu),$$

satisfy the Lie algebra of $SO(4.1)$.[5]

To find solutions of Eq. (2.8) let us proceed to reduce the equation in the manner used to reduce the Dirac equation. Performing a Fourier transform on the fields,

$$\psi(x,\eta) = \frac{1}{(2\pi)^2} \int \tilde{\psi}(p,\eta) \exp(-ip\cdot x)\, dp^4,$$

we get for Eq. (2.8)

$$(p_\mu \Gamma^\mu - l_0 p^2)\tilde{\psi}(p,\eta) = 0, \tag{2.10}$$

which upon multiplication on the left by the factor $(P_\mu \Gamma^\mu + l_0 P^2)$, gives

$$[(p\cdot\Gamma)^2 - l_0^2 p^4]\tilde{\psi}(p,\eta) = 0, \tag{2.11}$$

which with a little algebra (see Appendix A), becomes

$$[p^2 D^2 - (p\cdot D)^2 + 2\Omega(p)\cdot\Sigma(p) - l_0^2 p^4]\tilde{\psi}(p,\eta) = 0, \tag{2.12}$$

where for brevity we have introduced the notation

$$\begin{aligned} D_\mu &= \delta_\mu - \tfrac{3}{2}\eta_\mu, \\ \Omega_\mu(p) &= -i\epsilon_{\mu\nu\lambda\rho}\eta^\nu \delta^\lambda p^\rho, \\ \Sigma_\mu(p) &= -\tfrac{1}{4}\epsilon_{\mu\nu\lambda\rho}\sigma^{\nu\lambda}p^\rho. \end{aligned} \tag{2.13}$$

Note that the Pauli–Lubanski operator

$$W_\mu = -\tfrac{1}{2}\epsilon_{\mu\nu\lambda\rho}M^{\nu\lambda}P^\rho$$

in the representation described by Eq. (2.4) and Eq. (2.5) is of the form

$$W_\mu(P) = \Omega_\mu(p) + \Sigma_\mu(p). \tag{2.14}$$

Note also that the most general solution of Eq. (2.11), when $p^2 \neq 0$, can be written as

$$\tilde{\psi}(p,\eta) = (p\cdot\Gamma + l_0 p^2)\tilde{\chi}(p,\eta), \tag{2.15}$$

where $\tilde{\chi}(p,\eta)$ is any solution of Eq. (2.11). To see this observe that if $\tilde{\psi}(p,\eta)$ is a solution of Eq. (2.10), then

$$\begin{aligned} \tilde{\psi}(p,\eta) &\equiv \frac{1}{2l_0 p^2}[(p\cdot\Gamma + l_0 p^2) - (p\cdot\Gamma - l_0 p^2)]\tilde{\psi}(p,\eta) \\ &= (p\cdot\Gamma + l_0 p^2)\,\frac{1}{2l_0 p^2}\,\tilde{\psi}(p,\eta), \end{aligned}$$

which proves the assertion. We will later prove that the original equation [Eq. (2.11)] has no acceptable solution for $p^2 = 0$.

A. Timelike solutions

In this case we choose $p_\mu = (m,0,0,0)$, and expand the wavefunction $\tilde{\psi}(p,\eta)$ in terms of the rotation group basis vectors

$$\tilde{\psi}(p,\eta) = \sum_{\rho,m,\epsilon} \phi_l^\epsilon(a)\, U^\epsilon_{l,m}(\theta,\phi), \quad \vec{p} = 0 \tag{2.16}$$

[see Appendix A for the definition of $U^\epsilon_{l,m}(\theta,\phi)$]. $\{a,\theta,\phi\}$ is the spherical parametrization of the hyperboloid. Then Eq. (2.12) will lead to a second order differential equation for $\phi(a)$. In particular, we have

$$(1-Z^2)f'' - (2l+3)Zf' + (\lambda - l)f = 0, \tag{2.17}$$

where

$$\phi(a) = Z^{3/2}(1-Z^2)^{l/2} f(Z), \quad Z = \frac{1}{\cosh a} = \frac{1}{\eta_0}, \tag{2.18}$$

$$\lambda = l_0^2 p^2 + \epsilon(j+\tfrac{1}{2}) - 1, \quad j = l + \epsilon\tfrac{1}{2}, \quad \epsilon = \pm 1. \tag{2.19}$$

Equation (2.17) is the differential equation for the ultraspherical harmonics $C_n^{l+1}(Z)$,[7] where n is a nonnegative integer. It is possible to verify directly that for other values of n, the Hermitian form

$$\langle \psi_1, \psi_2 \rangle = \int \frac{\vec{d\eta}}{\eta_0}\, \bar{\psi}_1 \psi_2 \tag{2.20}$$

diverges.

It must be understood that the relevant Hilbert space of field function is smaller than that defined by the Hermitian form (2.20). The requirement of convergence of the integrals appearing in the generators of the Poincaré group imposes further restriction. At this point we anticipate the result from the next section and write down the metric derived from the Lagrangian,

$$\langle \tilde{\psi}(\nu),\ \tilde{\psi}'(p')\rangle I_0 \int_{\eta^2=1} \frac{\vec{d\eta}}{\eta_0}\, \bar{\chi}(p,\eta) I_0(p,p',\eta)\chi'(p',\eta), \tag{2.21}$$

where

$$\begin{aligned} &I_0(p,p',\eta) \\ &\quad = 2l_0 p_0 (p\cdot\Gamma p\cdot\Gamma' + l_0^2 p^4) + (p\cdot\Gamma - l_0 p^2)\Gamma_0(p'\cdot p - l_0 p^2). \end{aligned}$$

A simple power counting will show that the solutions of (2.17) with odd n remain in the space defined by the metric I_0. Furthermore, using the form of the operators Γ_μ, it can be shown that solutions with even n, contribute divergently to (2.20). To see this, observe that

$$\langle \psi_1(p), \psi_2(p')\rangle = \int \frac{\vec{d\eta}}{\eta_0}\, \chi_1(-p\cdot\Gamma + l_0 p^2)(p'\cdot\Gamma + l_0 p'^2)\chi_2,$$

where

$$\frac{\vec{d\eta}}{\eta_0} = d\Omega Z^{-3}(1-Z^2)^{1/2}\, dZ,$$

$$D_0 = Z(1-Z^2)^{1/2}\,\frac{d}{dZ} - \frac{3}{2}\,\frac{1}{Z},$$

$$\vec{D} = -\hat{\mathbf{r}}(1-Z^2)^{1/2}\,\frac{d}{dZ} + (1-Z^2)^{-1/2} Z\hat{\nabla},$$

and $\hat{\mathbf{r}}$ and $\hat{\nabla}$ are the unit vector and the gradient operator on the sphere $\{\theta,\phi\}$, and $d\Omega$ is the differential element corresponding to it. Since, $C_n^{l+1}(Z)$ is odd or even according to whether n is odd or even, it may be seen that, for even n, the terms involving $\vec{D}$, make the integral (2.20) divergent.

Thus we are left with odd n, with the resultant mass spectrum

$$l_0^2 p^2 = (4N+3-\epsilon)j + 2(N+1)(2N+2-\epsilon), \quad n = 2N+1,$$

or,

$$j=\frac{l_0^2p^2}{4N+3-\epsilon}-\left(N+\frac{5-\epsilon}{4}\right),\quad \epsilon=\mp1,\quad N=0,1,2,\cdots. \tag{2.22}$$

This equation relates j and p^2 linearly. The j-intercepts are at $-(N+1)$ for $\epsilon=+1$ and $-(N+\frac{3}{2})$ for $\epsilon=-1$. The functions $\chi^{\epsilon}_{N,l,m}(\vec{p}=0,\vec{\eta})$ form a complete orthonormalizable basis for the space $L_2(H^3)\otimes D$, where H^3 denotes the hyperboloid and D the Dirac spinor space, and where

$$\chi^{\epsilon}_{N,l,m}(\vec{p}=0,\eta)=\phi_{N,l}(a)U^{\epsilon}_{l,m}(\theta,\phi).$$

The reason is that

$$C^{l+1}_{2N+1}(Z)\sim Z\,P_N^{(l+1/2,\,1/2)}(2Z^2-1),$$

where P_N are the Jacobi polynomials which satisfy[7]

$$\int_{-1}^{1}dx(1-x)^{\alpha}(1+x)^{\beta}P_N^{(\alpha,\beta)}(x)\,P_{N'}^{(\alpha,\beta)}(x)\sim\delta_{NN'}.$$

B. Spacelike momenta

When $p^2<0$, it is convenient to choose $p_\mu=(0,0,0,p_3)$. Then any solution of Eq. (2.12) may be expanded in terms of the basis functions of the principle series representation of the $O(2,1)$ group

$$\chi(\eta)=\sum_{m,\epsilon}\int dl\;\phi^{\epsilon}_{l,m}(a)U^{\epsilon}_{l,m}(b,\phi),$$

where $l=-\frac{1}{2}+i\rho$, ρ is any real number, and $\{a,b,\phi\}$ is the hyperbolic parametrization of the hyperbolid (see Appendix A). $m=\mp\frac{1}{2},\ \mp\frac{3}{2},\ \mp\frac{5}{2},\ \cdots$ and $\epsilon=\mp1$. Then Eq. (2.12) may be written as

$$(\tilde{D}^2+\Omega\cdot\textstyle\sum+l_0^2q^2)\chi(\eta)=0,\quad p^2=-q^2, \tag{2.23}$$

where $\tilde{D}^2=D_0^2-D_1^2-D_2^2$. As in the case of timelike solutions, the functions $U^{\epsilon}_{l,m}$ satisfy the eigenvalue equation

$$\Omega\cdot\textstyle\sum U^{\epsilon}_{l,m}(b,\phi)=[\epsilon(l+\frac{1}{2})-1]U^{\epsilon}_{l,m}(b,\phi). \tag{2.24}$$

Note that eigenvalues of (2.24) are nonreal for $\rho\neq0$. In that case Eq. (2.23) leads to a contradiction since $l_0^2q^2$ is real by definition and $\tilde{D}^2$ by virtue of (2.7) is a Hermitian operator on $L_2(H^3)$, in which lies $\chi(\eta)$. Consequently, eigenvalue equation (2.23) reduces to

$$\tilde{D}^2\chi^{\epsilon}_{l,m}=(1-i\epsilon\rho-l_0^2q^2)\chi^{\epsilon}_{l,m},$$

where $\chi^{\epsilon}_{l,m}=\phi^{\epsilon}_{l,m}(a)U^{\epsilon}_{l,m}(b,\phi)$, which has no solution except for $\rho=0$.

In the case $\rho=0$, the solution contributes divergently to the integral (2.20) since $U_{-1/2,m}(b,\phi)$ corresponds to the continuous spectrum of the Casimir operator of $O(2.1)$. For a convergent contribution, we would need a set of $U_{\rho,m}$'s for a continuous range of ρ to be smeared over ρ. Thus, there are no spacelike solutions to our field equations from which conserved quantities may be built.

C. Lightlike momenta

When $p^2=0$, it is convenient to work in the frame with $p_\mu=(p_0,0,0,p_0)$. Here again the solution of Eq. (2.12) may be expanded in terms of the simultaneous eigenfunctions $U^{\epsilon}_{\rho,m}(r,\phi)$ of $W^2(p)$ and $\Omega^2(p)$, where $\{a,r,\phi\}$ is the parabolic parametrization of the hyperboloid H^3. It is important to note that $\Omega(p)\cdot\sum(p)$ vanishes on $U^{\epsilon}_{\rho,m}(r,\phi)$ (see Appendix A). Therefore, the Eq. (2.12) now reads

$$(p\cdot D)^2\chi=0. \tag{2.25}$$

But as shown in Appendix A,

$$p\cdot D=-p_0\left(e^a\frac{\partial}{\partial a}+\frac{3}{2}e^a\right),$$

which turns Eq. (2.25) into

$$\left(\frac{\partial^2}{\partial a^2}+4\frac{\partial}{\partial a}+\frac{15}{4}\right)\phi_\rho(a)=0, \tag{2.26}$$

where

$$\chi(\eta)=\int_\rho\phi(a)\;U^{\epsilon}_{\rho,m}(r,\phi)\,d\rho.$$

Solutions of Eq. (2.26) are of the form $\exp[-(3/2)a]$ and $\exp[-(5/2)a]$. But because of the form of the integration measure,

$$\frac{d\vec{\eta}}{\eta_0}=\exp(2a)\,da\,r\,dr\,d\phi,$$

both of these solutions contribute divergently to the expression (2.21). The reason is that I_0 of Eq. (2.21) involves Γ_μ to third power, which contributes a factor of $\exp(3a)$ to the integrand of (2.21), making the solutions of (2.26) unacceptable. Again since (2.25) does not involve a free parameter, smearing of the solutions for the purpose of construction of finite generators of Poincaré group is not possible. Thus there are no lightlike solutions for Eq. (2.12) and consequently for the Eq. (2.10).

Quantization of the field $\psi(x,\eta)$ follows the conventional approach. The field is expanded in terms of the solutions of the field equation (2.8),

$$\psi(x,\eta)=\frac{1}{(2\pi)^3}\sum_{N,l,m,\epsilon}\int\frac{dp^3}{p^0_{N,l,t}}\,[\exp(-ip\cdot x)\times U^{\epsilon}_{N,l,m}a^{\epsilon}_{N,l,m}(\vec{p})+\exp(ip\cdot x)\,U^{\epsilon}_{N,l,m}\,b^{\dagger}_{N,l,m}(\vec{p})], \tag{2.27}$$

and coefficients are interpreted as creation and annihilation operators with

$$[a_{N,l,m}(p),\ a^{\epsilon',\dagger}_{N',l',m'}(\vec{p}')]_+=[b^{\epsilon}_{N,l,m}(\vec{p}),\ b^{\epsilon',\dagger}_{N',l',m'}(\vec{p}')]_+=(2\pi)^3\delta_{NN'}\delta_{ll'}\delta_{mm'}\delta_{\epsilon\epsilon'}\delta(\vec{p}-\vec{p}'), \tag{2.28}$$

with all the other anticommutators vanishing. We conclude this section with the observation that under parity, charge conjugation, and time reversal, field equation (2.10) is obviously invariant, with the qualification that in order to define time reversal it is necessary to allow $\eta_0\to-\eta_0$. As this entials no complications, and has been discussed in detail in Ref. 5, we refrain from pursuing it any further.

3. THE LAGRANGIAN AND CURRENTS

In this section we drive the wave equation (2.8) from a variational principle, which in turn yields the conserved quantities of the theory. In particular, energy momentum and angular momentum can be constructed

and verified to be the generators of the Poincaré group. In addition, a divergence free 4-vector current operator is obtained as a consequence of the invariance of the Lagrangian under the gauge transformation of the first kind. Finally, the matrix elements of this current operator, between the lowest lying states, are evaluated and compared with the nucleon form factors. In deriving the wave equation from a Lagrangian, we treat the *hyperplane dependence* on the same footing as the position dependence, and use a variational principle which involves variation in both *hyperplane variables* and position variables.[6] The wave equation may not be derived from a *simple* Lagrangian, though. We need to use an auxiliary field in our variational principle.[8]

The Lagrangian we use is

$$L(x,\eta)=\partial^{u}\bar{\Omega}(i\Gamma_{u}+l_{0}\partial_{u})\psi+\text{h. c.}, \tag{3.1}$$

which leads to

$$(i\partial_{u}\Gamma^{u}-l_{0}\partial^{2})\,\psi(x,\eta)=0, \tag{3.2}$$

$$(i\partial_{u}\Gamma^{u}-l_{0}\partial^{2})\,\Omega(x,\eta)=0. \tag{3.3}$$

In order to relate Ω to ψ, we use the reduced wavefunctions $\tilde{\chi}(p,\eta)$ of Eq. (2.15) and define

$$\tilde{\Omega}(p,\eta)=(l_{0}p^{2}-p\cdot\Gamma)\tilde{\chi}(p,\eta). \tag{3.4}$$

The current operator derived from (3.1) is

$$J^{u}(x)=\int d\eta\{-i[l_{0}\partial^{u}\Omega\,\psi+\bar{\psi}(i\overleftarrow{\Gamma}^{u}+l_{0}\overleftarrow{\partial^{u}})\Omega]+\text{h. c.}\}, \tag{3.5}$$

which yields for the charge operator

$$\begin{aligned}Q&=\int dx^{3}J_{0}(x)\\&=\int dx^{3}d\eta[-il_{0}(\partial^{0}\bar{\Omega}\psi+\partial^{0}\bar{\psi}\Omega)+\bar{\psi}\Gamma_{0}\Omega+\text{h. c.}].\end{aligned} \tag{3.6}$$

It is straightforward, using expansion (2.27) and definition of Ω (Eq. 3.4), to show that

$$Q=\sum_{N,l,m}\int\frac{dp^{3}}{p_{0}}\,[a^{\dagger}_{N,l,m}(\vec{p})\,a_{N,l,m}(\vec{p})+b_{N,l,m}(\vec{p})\,b^{\dagger}_{N,l,m}(\vec{p})]. \tag{3.7}$$

Next we use the anticommutation relations (2.28), and discard the vacuum contribution, to obtain the standard charge operator

$$:Q:=\sum_{N,l,m}\int\frac{dp^{3}}{p_{0}}\,[a^{\dagger}_{N,l,m}(\vec{p})\,a_{N,l,m}(\vec{p})+b^{\dagger}_{N,l,m}(\vec{p})\,b_{N,l,m}(\vec{p})], \tag{3.8}$$

The Lagrangian (3.1) will produce generators for the Poincaré group, which can easily be verified to satisfy Eqs. (2.4) and (2.5).

In the rest of this section we will discuss the electromagnetic form factors and the structure functions of the lowest lying state of the spectrum of the spinor field, using the local current (3.5). For form factors the relevant matrix elements are

$$\langle p'|J_{u}(0)|p\rangle=U_{N,l,m}(\vec{p}')J_{u}(0)\,U_{N,l,m}(\vec{p}),$$

for $N=0$, $l=0$, which becomes

$$\langle p'|J_{u}(0)|p\rangle=2l_{0}C^{2}\bar{U}(p')\int\frac{d\eta^{3}}{\eta_{0}}\,\frac{1}{(\eta p')^{5/2}}\,[P_{u}(p'\cdot\Gamma\,p\cdot\Gamma-l_{0}^{2}p^{2})-p^{2}(\Gamma_{u}p\cdot\Gamma\,p'\cdot\Gamma+\Gamma_{u})]\,\frac{1}{(\eta p)^{5/2}}\,U(p). \tag{3.9}$$

Where $U(p)$ is the Dirac wavefunction, and $P_{u}=p_{u}+p'_{u}$, and c is the normalization factor. This expression is evaluated in Appendix B. The result is

$$\langle p'|J_{u}(0)|p\rangle=\bar{U}(p')\left(F_{1}(q^{2})\gamma_{u}+F_{2}(q^{2})\,i\sigma_{u\nu}\,\frac{q^{\nu}}{m}\right)U(p), \tag{3.10}$$

with

$$\begin{aligned}F_{1}(q^{2})&=\frac{16}{27\pi}\,(1-Z)^{3/2}\\&\quad\times[(6-Z-8Z^{2})\,D(Z^{1/2})+(3-5Z-4Z^{2})C(Z^{1/2})],\end{aligned} \tag{3.11}$$

$$F_{2}(q^{2})=\frac{4}{27\pi}\,(1-Z)^{3/2}\left[\left(\frac{1}{Z}+11-2Z-16Z^{2}\right)D(Z^{1/2})+\left(-\frac{4}{Z}+10-10Z-8Z^{2}\right)C(Z^{1/2})\right], \tag{3.12}$$

where $D(Z^{1/2})$ and $C(Z^{1/2})$ are the complete elliptic functions (B6) and (B7), and

$$Z=q^{2}/(4-q^{2}),\quad q_{u}=m^{-1}(p_{u}-p'_{u}).$$

It is easily seen that, for large values of $-q^{2}$, the form factors behave as $(-q^{2})^{-3/2}$ multiplied by the logarithmic factors originating from the asymptotic behavior of the elliptic functions. Note that the singularity of F_{2} at $Z=0$ is only apparent and removable, which can be verified by inserting the series expansion of C and D, about $Z=0$, in (3.12). Using these expansions, it is found that $F_{2}(0)=0.49$, which corresponds to a magnetic dipole moment of $\mu=1.98$ nucleon magneton, to be compared with the observed magnetic moment of the proton, $\mu_{p}=2.79$ nucleon magneton.[9] Similarly, the slopes of F_{1} and F_{2} at $Z=0$ give $\langle r_{1}\rangle=0.3F$, $\langle r_{2}\rangle=0.2F$, for the change and magnetic radius of the particle, which may be compared with those of proton, $\langle r_{1}\rangle_{p}\approx\langle r_{2}\rangle_{p}\approx 0.8F$.[10]

Finally, we consider the structure functions for the ground state,[11]

$$\begin{aligned}W_{u\nu}&=\sum_{\{n\}}\delta[p'^{2}-m'^{2}_{\{n\}}]\,\langle p|J_{u}(0)|\{n\},p'\rangle\langle\{n\},p'|J_{\nu}(0)|p\rangle\\&=\left(\frac{q_{u}q_{\nu}}{q^{2}}-q_{u\nu}\right)W_{1}(q^{2},\nu)+\frac{1}{m^{2}}\left(p_{u}-\frac{p\cdot q}{q^{2}}\,q_{u}\right)\\&\quad\times\left(p_{\nu}-\frac{p\cdot q}{q^{2}}\,q_{\nu}\right)W_{2}(q^{2},\nu),\end{aligned} \tag{3.13}$$

where $\{n\}$ designates the collection of quantum numbers describing the final state in the electroproduction, and $\nu=p\cdot q/m$, $\zeta=-92/2m\nu$. Calculation of the structure functions W_{1} and W_{2} in the Bjorken limit is rather involved and the detail will be reported elsewhere. Here we simply sketch the procedure and comment on the results.

Going to the frame where $p=m(k_{0,0,0},k_{n})$, $p'=m'(1,\vec{0})$, we get

$$\frac{\nu}{m} W_2 = 2\xi[4\xi(1-\xi)W_{00} + W_{11}],$$
$$W_1 = W_{11}. \tag{3.14}$$

Calculations of the W_{11} and W_{00} in the Bjorken limit is enormously simplified by observing that the matrix elements in Eq. (3.13) reduce to matrix elements of the current between a state of rest and a state of infinite momentum. Utilizing techniques developed earlier,[12] we find that in the Bjorken limit

$$W_{11}^{n,l} \to 0,$$
$$W_{00}^{n,l} \to \left(\frac{32}{3\pi}\right)^2 \frac{k_0^3}{l_0^4 m'^2}\, \mu\Lambda\mathcal{H}\left(\tfrac{1}{2}k_0(\Lambda) - \Lambda k_0'(\Lambda) - \frac{l_0^2 mm'}{k_0}\, k(\Lambda)\right)^2. \tag{3.15}$$

Here (n, l) designates the quantum numbers of the dominant final state, $n = 2N + 1 + l$, $m'^2 = p'^2$, $k_0(\Lambda)$ is the modified Bessel function of zero order. $\mathcal{H}$, Λ, and μ are the quantum numbers of the infinite momentum states

$$\mathcal{H} = \lim_{\substack{k_0 \to \infty \\ l \to \infty}} \frac{l}{k_0}, \qquad \Lambda = \lim_{\substack{k_0 \to \infty \\ l \to \infty}} \frac{n}{k_0}, \qquad \mu = [\Lambda^2 - \mathcal{H}^2]^{1/2}.$$

Then, since the mass spectrum of the final states is discrete, we average the structure functions[11]

$$\langle W_{00}\rangle = \frac{1}{b-a}\int_a^b d\rho'^2\, W_{00}^{n,l}(p'^2)\delta(p'^2 - m'^2) = \frac{1}{\Delta m'^2}\, W_{00}^{n,l}(m'^2), \tag{3.16}$$

with $\Delta m'^2 = 2\sqrt{n^2 - l^2}/l_0^2$. We have used the fact that in the Bjorken limit only final states with finite $\mathcal{H}$, Λ, and μ contribute. In fact, the contributing states have $l_0^2 m'^2 = \mu^2 k_0^2$. It is easily seen that $\mu = 2\sqrt{3}\,(1-\xi)$.

The extra variable Λ in Eq. (3.16), is not in fact independent of μ, because it may be shown that the mass spectrum has no mass degeneracy. Therefore, Λ is a function of ξ, albeit a very discontinuous one. Finding this functional relation is a problem in number theory which we do not attempt to solve.

On the other hand, since in the experimental situation states with arbitrary Λ, but fixed μ are detected almost simultaneously, we make a second average and obtain

$$\langle\langle W_{00}\rangle\rangle = \frac{1}{2}\left(\frac{32}{3\pi}\right)^2 \frac{1}{\mu}\int_\mu^\infty \Lambda d\Lambda\, [\tfrac{1}{2}k_0(\Lambda) - \Lambda k_0'(\Lambda) - \sqrt{3}\,\mu k_0(\Lambda)]^2.$$

Here we have used the integration measure corresponding to the infinite momentum states of the form $d\mathcal{H}d\Lambda$.[12] The final result is

$$\lim_{Bj} \frac{\nu}{m} W_2 = \left(\frac{64}{3\pi}\right)^2 \xi^2(1-\xi^2) f(\xi), \tag{3.17}$$

$$\lim_{Bj} W_1 = 0,$$

where $f(\xi) = \int_1^\infty \alpha d\alpha\, [\tfrac{1}{2}k_0(\alpha\mu) - \alpha\mu k_0'(\alpha\mu) - \sqrt{3}\,\mu k_0(\alpha\mu)]^2$. It is easily seen that for threshold $\xi \approx 1$ the function $f(\xi)$ behaves as some power of logarithm of $(1-\xi)$. We see therefore that $(\nu/m)W_2$ scales in this model and its threshold behavior $(1-\xi)^2$ (logarithmic terms), compared with the $(q^2)^{-3/2}$ (log terms) behavior of the form factors [Eq. (3.11), Eq. (3.12)], agrees with the Drell–Yan relation.[13]

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APPENDIX A

In this appendix we gather some of the relations used in the text and verify some of the claims made there and refer the reader for discussions to more detailed treatments. We have designated the hyperboloid by H^3, and the space of square-integrable functions on H^3 by $L_2(H^3)$. In the case of timelike momenta it is found to be convenient to parametrize in spherical coordinates:

$$\eta_0 = \cosh a, \quad \vec{\eta} = \sinh a\,\hat{r}, \qquad \hat{r}_1 = \sin\theta\cos\phi, \quad \hat{r}_2 = \sin\theta\sin\phi, \quad \hat{r}_3 = \cos\theta. \tag{A1}$$

In this coordinate system

$$\delta_0 = -\sinh a\,\frac{\partial}{\partial a}, \quad \vec{\delta} = r\cosh a\,\frac{\partial}{\partial a} + \frac{1}{\sinh a}\,\hat{\nabla},$$
$$\hat{\nabla}_1 = \cos\theta\cos\phi\,\frac{\partial}{\partial\theta} - \frac{\sin\phi}{\sin\theta}\,\frac{\partial}{\partial\phi},$$
$$\hat{\nabla}_2 = \cos\theta\sin\phi\,\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\sin\theta}\,\frac{\partial}{\partial\phi}, \tag{A2}$$
$$\hat{\nabla}_3 = -\sin\theta\,\frac{\partial}{\partial\theta}.$$

It is important to note that the $O(3)$ group generated by $\vec{L} = i^{-1}\hat{r}\times\hat{\nabla}$, has, for its Casimir operator, $L^2 = -\hat{\nabla}^2$, with spherical harmonics as eigenfunction,

$$\hat{\nabla}^2 Y_{l,m}(\theta,\phi) = -l(l+1)\,Y_{l,m}(\theta,\phi).$$

For $\vec{p} = 0$, the invariant subgroup of $O(3.1)$ as represented on $L_2(H^3)\otimes D$ has the basis

$$U^\epsilon_{l,m}(\theta,\phi) = \left(\frac{l+\frac{1}{2}+\epsilon m}{2l+1}\right)^{1/2} Y_{l,m-1/2}(\theta,\phi)\begin{pmatrix}1\\0\end{pmatrix} + \epsilon\left(\frac{l+\frac{1}{2}-\epsilon m}{2l+1}\right)^{1/2} Y_{l,m+1/2}(\theta,\phi)\begin{pmatrix}0\\1\end{pmatrix}, \quad \epsilon = \mp 1, \tag{A3}$$

which satisfies

$$-W^2 U^\epsilon_{l,m} = p_0^2 j(j+1)\,U^\epsilon_{l,m}, \quad j = l + \epsilon\tfrac{1}{2}, \tag{A4}$$

$$\Omega \cdot \sum U^{\epsilon}_{l,m} = [\epsilon(j+\tfrac{1}{2}) - 1] U^{\epsilon}_{l,m}. \tag{A5}$$

In the case of spacelike momenta, it is convenient to choose the hyperbolic parametrization of H^3,

$$\begin{aligned} &\eta_3 = \sinh a, \quad \tilde{\eta} = \cosh a \tilde{r}, \\ &\tilde{r}_0 = \cosh b, \quad \tilde{r}_1 = \sinh b \cos\phi, \quad \tilde{r}_2 = \sinh b \sin\phi. \end{aligned} \tag{A6}$$

In this coordinate system

$$\begin{aligned} &\delta_3 = \cosh a \frac{\partial}{\partial a}, \quad \tilde{\delta} = -\tilde{r} \sinh a \frac{\partial}{\partial a} + \frac{1}{\cosh a} \tilde{\nabla}, \\ &\tilde{\nabla}_0 = -\sinh b \frac{\partial}{\partial b}, \\ &\tilde{\nabla}_1 = \cosh b \cos\phi \frac{\partial}{\partial b} - \frac{\sin\phi}{\sinh b} \frac{\partial}{\partial \phi}, \\ &\tilde{\nabla}_1 = \cosh b \sin\phi \frac{\partial}{\partial b} + \frac{\cos\phi}{\sinh b} \frac{\partial}{\partial \phi}. \end{aligned} \tag{A7}$$

It can be seen that the $O(2.1)$ group generated by $\tilde{L} = i\tilde{r} \times \tilde{\nabla}$ has, for its Casimir operator,

$$\tilde{\nabla}^2 = -\tilde{L}^2,$$

with eigenfunctions,

$$\begin{aligned} &Y_{l,m}(b, \phi), \\ &\tilde{L}^2 Y_{l,m}(b, \phi) = l(l+1) Y_{l,m}(b, \phi), \\ &\tilde{L}_0 Y_{l,m}(b, \phi) = m Y_{l,m}(b, \phi). \end{aligned} \tag{A8}$$

Here $Y_{l,m}(b, \phi)$ are simply the analytic continuation of $O(3)$ spherical harmonics, with

$$l = -\tfrac{1}{2} + i\rho, \quad \rho \text{ real}, \tag{A9}$$

forming the principle series unitary representation of $O(2.1)$ group on $L_2(H^2)$, $H^2 = \{b, \phi\}$. These functions may be used to construct a basis for the representation of $O(2.1)$ on $L_2(H^2) \otimes D$. The construction is identical to the case of $O(3)$ in Eq. (A3). In this connection recall that $O(3.1)$ is generated on D by

$$\vec{L} = \tfrac{1}{2}\vec{\sigma}, \quad \vec{N} = -i2^{-1}\vec{\sigma}, \tag{A10}$$

where $\vec{\sigma}$ are the Pauli matrices, and the Casimir operator of $O(2.1)$,

$$L_3^2 - N_1^2 - N_2^2 = -\vec{\sigma}^2 \tag{A11}$$

having the same eigenvectors $\binom{1}{0}$ and $\binom{0}{1}$ as $\vec{L}^2$. For light-like momenta it is convenient to use the parabolic parametrization of H^3,

$$\begin{aligned} &\eta_0 - \eta_3 = \exp(a), \quad \eta_i = \exp(a) x_i, \quad i = 1, 2, \\ &x_1 = r\cos\phi, \quad x_2 = r\sin\phi, \end{aligned} \tag{A12}$$

with the other coordinate determined by the condition $\eta_\mu \eta^\mu = 1$. In this coordinate system,

$$\begin{aligned} &\delta_0 + \delta_3 = -\exp(a) \frac{\partial}{\partial a}, \\ &\delta_i = \eta_i \frac{\partial}{\partial a} + \exp(-a) \frac{\partial}{\partial x_i}, \quad i = 1, 2. \end{aligned} \tag{A13}$$

The invariant subgroup of $O(3.1)$ corresponding to $p_\mu = p_0(1, 0, 0, 1)$ is an $E(2)$ group generated by

$$\begin{aligned} &L_3 = -i \frac{\partial}{\partial \phi}, \\ &E_1 = i\left(\cos\phi \frac{\partial}{\partial r} - \frac{\sin\phi}{r} \frac{\partial}{\partial \phi}\right), \\ &E_2 = i\left(\sin\phi \frac{\partial}{\partial r} + \frac{\cos\phi}{r} \frac{\partial}{\partial \phi}\right). \end{aligned} \tag{A14}$$

The Casimir operator of this group is

$$E_1^2 + E_2^2 = -\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right), \tag{A15}$$

with eigenfunction $j_m(\rho r)\exp(im\phi)$,

$$-\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) j_m(\rho r)\exp(im\phi) = \rho^2 j_m(\rho r)\exp(im\phi), \tag{A16}$$

which are the Bessel functions of integer order m. These functions may be used to construct $E(2)$ representations on $L_2(H^3) \otimes D$. But the important property, for our purposes, lies in the E_2 representation on D. Here, the Casimir operator vanishes identically as may be verified from Eq. (A10). Moreover,

$$\begin{aligned} 2\Omega \cdot \sum &= (L_3, E_1, E_2, L_3) \cdot (\sigma_3, \sigma_2 - i\sigma_1, -i\sigma_2 - \sigma_1, \sigma_3) \\ &= iE^- \sigma^\dagger = 2i \begin{pmatrix} 0 & E^- \\ 0 & 0 \end{pmatrix}, \end{aligned} \tag{A17}$$

where $E^- = E_1 - iE_2$. Now if

$$\begin{pmatrix} 0 & E^- \\ 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix},$$

then $\lambda = 0$, which proves that eigenvalues of $\Omega \cdot \sum$ vanish.

In the rest of this appendix we will carry out the details of the verification of the Eq. (2.12).

To begin with, notice that, using the definition of the Pauli—Lubanski operators for the appropriate space Eq. (2.13), it is straightforward to verify that

$$\Omega \cdot \sum = \tfrac{1}{4}[p^2 S^{\mu\nu} \sigma_{\mu\nu} - 2S^{\mu\nu} p_\nu \sigma_{\mu\lambda} p^\lambda], \tag{A18}$$

where

$$S_{\mu\nu} = i(\eta_\mu \delta_\nu - \eta_\nu \delta_\mu) = i[D_\mu, D_\nu].$$

On the other hand, from the definition of Γ_μ, it is again straightforward to obtain

$$\begin{aligned} (p \cdot \Gamma)^2 &= p^2 \Gamma^2 - (p \cdot \Gamma)^2 + [p\Gamma, p \cdot \Gamma] \\ &= p^2 \Gamma^2 - (p \cdot \Gamma)^2 - \tfrac{1}{2} p^2 \sigma_{\mu\nu} S^{\mu\nu} \\ &\quad + S_{\mu\nu} p^\nu \sigma^{\mu\lambda} p_\lambda. \end{aligned} \tag{A19}$$

Comparison of Eq. (A19) and Eq. (A18) results in Eq. (2.12).

APPENDIX B

In this appendix, the expressions for the form factors (3.10) and (3.11) are derived. We start from the equation (3.9) and after some algebra find that

$$F_1 = \frac{4}{3\pi^2}\left[\left(-3x + 10 - \frac{8}{x+1}\right) y_{5/2,5/2}(x)\right.$$

$$+\left(1-\frac{2}{x+1}\right)y_{3/2,3/2}(x)\Big], \tag{B1}$$

$$F_2=\frac{2}{3\pi^2}\left[\left(8-3x-\frac{4}{x-1}-\frac{8}{x+1}\right)y_{5/2,5/2}(x)\right.$$

$$\left.+\left(1+\frac{1}{x-1}-\frac{2}{x+2}\right)y_{3/2,3/2}(x)\right], \tag{B2}$$

where the basic functions $y_{n',n}$ are

$$y_{n',n}(x)=\int\frac{d\eta}{\eta_0}\frac{1}{(\eta k)^{n'}(\eta k)^{n}}, \quad k_\mu=\frac{1}{m}p_\mu, \tag{B3}$$

$$k'_\mu=\frac{1}{m}p'_\mu, \quad x=k\cdot k'.$$

It is possible to evaluate the above integral for the particular cases needed and obtain

$$y_{3/2,3/2}(x)=4\pi(1-z)^{3/2}D(z^{1/2}), \tag{B4}$$

$$y_{5/2,5/2}(x)=\frac{4\pi}{q}(1-z)^{5/2}[2D(z^{1/2})+C(z^{1/2})], \tag{B5}$$

where $z=(x-1)/(x+1)$, and D and C are the complete elliptic functions[12]

$$D(z^{1/2})=\int_0^{\pi/2}\frac{\sin^2\phi}{(1-z\sin^2\phi)^{1/2}}\,d\phi, \tag{B6}$$

$$C(z^{1/2})=\int_0^{\pi/2}\frac{\sin^2\phi\cos^2\phi}{(1-z\sin^2\phi)^{3/2}}\,d\phi. \tag{B7}$$

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Boundaries of spacetimes

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A review of the Schmidt technique and the Sachs technique for assigning boundary points to spacetimes is given. A modification of the Sachs process which makes it obviously identical with Schmidt's is suggested. Some simple examples are discussed.

I. INTRODUCTION

Recently two methods for assigning boundaries to spacetimes have been proposed,[1,2] both being generalizations of Geroch's[3] g-boundary technique. The boundaries defined by the above methods terminate not only incomplete geodesics but also inextendible timelike curves of bounded acceleration and finite proper length.

The central idea in both of the new approaches is to associate with a spacetime another larger manifold which by virtue of its relationship to the spacetime admits a positive-definite metric tensor. The larger manifold is then Cauchy completed (an operation undefined for spacetimes) to define its boundary. Elements of this larger boundary are grouped together by an appropriate equivalence relation to define elements of the spacetime boundary.

In this paper we give a brief review of the Schmidt process,[1] and discuss in some detail the Sachs process.[2] In particular, we suggest a natural modification of the Sachs technique and show that this modified Sachs procedure agrees with the Schmidt method. Finally, we give some simple two-dimensional examples to illustrate concepts and to demonstrate a potentially useful calculational technique.

In this paper M denotes the spacetime manifold, (assumed to be four-dimensional, connected, Hausdorff, oriented, and time-oriented), endowed with a C^∞ metric tensor g of signature $(+++-)$. The connection is the usual metric and torsion free Levi-Civita connection.[4]

II. THE SCHMIDT COMPLETION PROCESS: THE b-BOUNDARY

A. Formal considerations

Let $L(M)$ be the set of all oriented and future-pointing orthonormal frames[5] at all points of M. The proper homogeneous orthochronous Lorentz group, here denoted by L, acts on $L(M)$ without fixed points: An orthonormal frame at a point p of M is denoted

$$u=(p;X_1,X_2,X_3,X_4)\in L(M).$$

This u is mapped into $\bar{u}=(p;\bar{X}_1,\bar{X}_2,\bar{X}_3,\bar{X}_4)$ by a member Λ of L, where $\bar{X}_m=L_m{}^sX_s$, with $(L_m{}^s)$ being the matrix representative of Λ. This mapping, which preserves the point p, is denoted

$$\bar{u}=u\Lambda=R_\Lambda u$$

(both notations will be used). The action of L induces an equivalence relation on $L(M)$, and each equivalence class in $L(M)/L$ may be identified with a point of M. We denote by

$$\pi: L(M)\to M$$

the canonical projection mapping which takes u to the point p in M to which it is attached. Thus, $\pi(u\Lambda)=\pi(u)=p$. The set $\pi^{-1}(p)$ is called the fibre over p.[6] $L(M)$ is ten-dimensional.

$L(M)$ has special properties that a general manifold does not possess. First, there is a preferred class of curves in $L(M)$ called vertical curves. These are integral curves of vectors tangent to fibres of $L(M)$. At each u there is a six-dimensional subspace V_u of T_u, the full ten-dimensional tangent space, called the vertical subspace at u containing the tangents to the above curves. Specifically, the vertical vectors correspond to elements of the Lie algebra dL of L. An element Z in dL generates a one-dimensional subgroup $A(t)$ in L passing through the identity. $A(t)$ acts on $L(M)$ to create a curve $u(t)=u(0)A(t)$. The tangent to this curve Z^* is said to be induced by Z and is tangent to the fibre through $u(0)$. If we pick a particular basis $\{Z_A, A=1,\ldots,6\}$ of dL then this basis gives rise to a basis $\{Z_A^*\}$ of V_u called a fundamental basis.

Another special property of $L(M)$ is the existence of a second preferred class of curves in $L(M)$ called horizontal curves. A horizontal curve is defined if we pick a curve $q(t)$ in M through some initial point $q(0)$, pick an initial orthonormal frame $X_i(0)$ at $q(0)$, and then parallel propagate this frame along $q(t)$. The result is an orthonormal frame at each point of the curve and hence a curve in $L(M)$. We call this curve a horizontal lift of $q(t)$ or simply a horizontal curve in $L(M)$; the tangent to this curve is called the horizontal lift of the tangent to $q(t)$. Since parallel propagation is achieved by solving first order linear ordinary differential equations with well-posed initial conditions, the horizontal lift of a given curve is unique.

The tangent vectors to the family of horizontal curves through u determine a four-dimensional subspace H_u of the full tangent space T_u. This horizontal subspace is dependent on the existence of a connection in M and contains no vector (but the zero vector) which is tangent to the fibre through u. Moreover, the projection map π determines a map π_* of vectors such that $\pi_*(H_u)$ is just

the full tangent space $T_{\pi(u)}$ at the point $p=\pi(u)$ in M.[7] Similarly, the map of tangent vectors R_{A*} determined by the map R_A on $L(M)$ preserves the property of being horizontal since parallel propagation commutes with Lorentz transformations on M: $H_{uA}=R_{A*}(H_u)$.[8]

It is often convenient to choose as basis elements of H_u so-called standard horizontal vectors, B_i, $i=1, 2, 3, 4$. These vectors are defined as the unique horizontal vectors which satisfy $\pi_*(B_i)=X_i$, where B_i is in the tangent space of $u=(p; X_1, X_2, X_3, X_4)$. The integral curve of the projection of a standard horizontal vector field is a geodesic in M: It is a curve whose tangent vector is parallelly propagated along the curve. Conversely, the horizontal lift of any geodesic in M is the integral curve of some standard horizontal vector field.

Consequently, by virtue of the Lorentz group action and the Levi-Civita connection on M, it is possible to uniquely decompose the full tangent space T_u into a direct sum of vertical and horizontal parts

$$T_u=V_u+H_u.$$

In other words, any vector in T_u can be written uniquely as the sum of a vertical and horizontal part.

The fundamental vertical vectors and the standard horizontal vectors are used to define a positive-definite metric G on $L(M)$: These vectors are taken to be orthonormal. This metric is, of course, dependent on which basis is chosen. In the Schmidt procedure of defining the boundary of a spacetime, however, all metrics of this kind give the same results.[1] $L(M)$, endowed with the Riemannian metric G, is a space with a distance function $d(u, v)$, that is, a topological metric space.[9]

$L(M)$ may therefore be Cauchy completed to form $\bar{L}(M)$.[10] The process is very beautifully described by Korevaar,[11] and we briefly summarize his treatment. A subset $\{u_i\}$ of $L(M)$ is a Cauchy sequence if for every $\epsilon>0$ there is an integer N such that whenever $i, j>N$, $d(u_i, u_j)<\epsilon$. Two Cauchy sequences $\{u_i\}$, $\{v_i\}$ are said to be equivalent if the sequence of numbers $\{d(u_i, v_i)\}$ tends to zero as $i\to\infty$. Each equivalence class of Cauchy sequences as defined by this relation either converges to a point in $L(M)$ or does not converge to a point in $L(M)$.

Picture an equivalence class as a "spider." If the sequences in the class converge to a point in $L(M)$, the spider has a "heart"; otherwise it is a "heartless spider." The set of all equivalence classes, "spider space," is $\bar{L}(M)$. In $\bar{L}(M)$ a distance function $\bar{d}$ may be defined to agree with d when restricted to $L(M)$, which is identified as the subset of spiders with hearts. $L(M)$ is dense in $\bar{L}(M)$, and it is easily shown that $\bar{L}(M)$ is complete.

Schmidt[1] has shown that the action of L may be extended uniform continuously to $\bar{L}(M)$. A generalized fibre through a given point is thus defined even for points in $\bar{L}(M)$ which are not in $L(M)$: It is the orbit of L through that point. The boundary elements $\mathring{M}$ of the spacetime are then defined to be this set of generalized fibres of $\bar{L}(M)$,

$$\mathring{M}=\bar{M}-M=[\bar{L}(M)-L(M)]/L.$$

Schmidt has shown that $\mathring{M}$ is physically interesting: An incomplete geodesic or an inextendable timelike curve of bounded acceleration and finite proper length each determine elements of $\mathring{M}$ via the above construction.

B. Local expressions

It is convenient for calculations to have explicit expressions for the fundamental and standard horizontal vector fields. It is also convenient to have expressions for the 1-forms which are dual to the aforementioned vector field basis, since the 1-forms are used to display the bundle metric tensor. These forms span the dual space T_u^* at each $u\in L(M)$.

The connection 1-forms $\{\omega^A, A=1, 2, \cdots, 6\}$ are defined by

$$\mathrm{ver}Y=\omega^A(Y)E_A^*$$

where $Y\in T_u(L(M))$, ver$Y$ represents the vertical part of Y, and $\{E_A^*\}$ are the fundamental vector fields which span V_u. The canonical 1-forms are defined by

$$\pi_*(Y)_u=\theta^i(Y)X_i, \quad i=1, \cdots, 4,$$

where Y is a vector at u and u is the orthonormal frame at p, $(p; X_1, X_2, X_3, X_4)$. The canonical and connection 1-forms obey the duality conditions (where $\{B_j\}$ spans H_u):

$$\theta^i(B_j)=\delta^i{}_j, \quad \theta^i(E_A^*)=0,$$

$$\omega^A(B_j)=0, \quad \omega^A(E_B^*)=\delta^A{}_B.$$

In this section we will give local expressions for all the above quantities.

Since $L(M)$ is locally $U\times L$ where $U\subset M$, we may use (x^i, α^A) as local coordinates on $L(M)$. Here $\{x^i\}$ are local coordinates on U and $\{\alpha^A\}$ local coordinates on L. The explicit matrix which rotates an orthonormal frame at a point into another orthonormal frame at the same point is uniquely determined from the six real numbers $\{\alpha^A\}$ through the matrix exponential map:

$$L_m^n(\alpha^A)=[\exp(\alpha^A M_A)]_m{}^n.$$

The M_A are the constant matrices in dL which generate infinitesimal transformations on L.

We may take $\{X_i, \partial/\partial\alpha^A\}$ as a local basis of the tangent space at each point of $L(M)$, ($\{X_i\}$ is the orthonormal basis at $p\in M$). Then $\{\bar{\omega}^i, d\alpha^A\}$ is a local basis of the cotangent space at each point of $L(M)$ where

$$\bar{\omega}^i(X_j)=\delta_j{}^i, \quad \bar{\omega}^i\left(\frac{\partial}{\partial\alpha^B}\right)=0$$

$$d\alpha^A\left(\frac{\partial}{\partial\alpha^B}\right)=\delta_B{}^A, \quad d\alpha^A(X_j)=0.$$

We will first derive the local expression for the horizontal lift of a vector on M to $L(M)$. Let us choose a curve $\gamma(\tau):\{x^i(\tau)\}$ in M and a frame at $\gamma(0)$. We parallel propagate the frame along the curve to generate a curve $u(\tau)$ in $L(M)$. The tangent vector $\mathring{u}(\tau)$ to this curve is the horizontal lift of $\dot{\gamma}(\tau)$. Locally, we may express $\mathring{u}(\tau)$ as

$$\dot{u}(\tau) = \xi^r(\tau) X_r + \frac{d\alpha^A}{d\tau}\frac{\partial}{\partial \alpha^A}$$

where $\xi^r(\tau)$ are the frame components of $\dot{\gamma}(\tau)$. The frame at $\tau = 0$ is parallel propagated along the curve so that the parallel propagated frame is $\bar{X}_i(\tau) = L_i^s(\tau) X_s(\tau)$, $\{X_s(\tau)\}$ being the frame at the point $\gamma(\tau)$. We have that $(dL_m{}^n/d\tau)(\tau) = -\Gamma^n_{st} L_m{}^s \xi^t$ where the Γ^n_{st} are the connection coefficients on M in the orthonormal frame.[12] Since

$$\frac{dL_m{}^n}{d\tau} = \frac{\partial L_m{}^n}{\partial \alpha^A}\frac{d\alpha^A}{d\tau}$$

and since $(\partial L^n_m/\partial \alpha^A)$ is invertible [inverse being written $(\partial \alpha^A/\partial L^n_m)$], we find that

$$\frac{d\alpha^A}{d\tau} = -\frac{\partial \alpha^A}{\partial L_n{}^m}\Gamma^n_{st} L_m{}^s \xi^t.$$

Hence we may write

$$\dot{u}(\tau) = \xi^s X_s - \frac{\partial \alpha^A}{\partial L_n{}^m}\Gamma^n_{ts} L_m{}^t \xi^s \frac{\partial}{\partial \alpha^A}.$$

If we let

$$W_s = X_s - \frac{\partial \alpha^A}{\partial L_n{}^m}\Gamma^n_{ts} L_m{}^t \frac{\partial}{\partial \alpha^A},$$

$$\dot{u}(\tau) = \xi^a W_a,$$

and thus the $\{W_a\}$ span $H_{u(\tau)}$.

The standard horizontal vector fields $(B_r)_u$ are linear combinations of the W_a so to find their local expressions we need only compute the combination coefficients: $(B_r)_u = A_r{}^m W_m$. The definition of $(B_r)_u$ says that $\pi_*(B_r)_u = L_r^m X_m$. But $\pi_*(B_r)_u = \pi_*(A_r{}^m W_m) = A_r{}^m \pi_*(W_m) = A_r{}^m X_m$ and so we have that

$$(B_r)_u = L_r^m W_m.$$

By making use of the duality relation we may calculate expressions for the canonical forms θ^i:

$$\theta_i(L_r^m X_m) = L_r^m \theta^i(X_m) = \delta_r^i$$

and thus

$$\theta^i = (L_r^i)^{-1}\bar{\omega}^r.$$

The fundamental vector fields E^*_A are simply given by $E^*_A = \partial/\partial \alpha^A$, and we may calculate expressions for the connection forms ω^A by the duality relations $\omega^A(B_r) = 0$ and $\omega^A(E^*_B) = \delta^A_B$. The connection forms are readily found to be

$$\omega^A = d\alpha^A + \frac{\partial \alpha^A}{\partial L_n^p} L p^m \bar{\omega}^n_m \text{ where } \bar{\omega}^n_m = \Gamma^n_{sm}\bar{\omega}^s.$$

At this point we give an explicit representation of the positive-definite bundle metric tensor which was previously defined to be the function satisfying

$$G(B_r B_s) = \delta_{rs},$$

$$G(B_r, E^*_A) = 0,$$

$$G(E^*_A, E^*_B) = \delta_{AB}.$$

It is easily checked that the function G is given by[13]

$$G(X, Y) = \theta^i(X)\theta^i(Y) + \omega^A(X)\omega^A(Y)$$

where $X,\ Y \in T_u(L(m))$.

III. THE SACHS COMPLETION PROCESS: THE s-BOUNDARY

The Riemannian manifold which is used in the Schmidt process is the ten-dimensional proper homogeneous orthochronous Lorentz bundle, $L(M)$. The boundary which is assigned to M in this way is called the b-boundary. Instead of using $L(M)$, Sachs[2] has given a prescription for defining a Riemannian metric H on the seven-dimensional tangent sphere bundle $T'(M)$ which consists of the set of all unit timelike vectors at all points of[14] M. $T'(M)$ is Cauchy completed with respect to the distance function induced by H, and an equivalence relation is defined on $\bar{T}'(M)$. The boundary points of M are then defined to be equivalence classes of "heartless spiders" in $\bar{T}'(M)$. We will refer to the set of boundary points assigned to M by the Sachs method as the s-boundary of M. In this section we give a detailed discussion of the Sachs process. We defer the discussion of the relationships between the b-boundary and the s-boundary to the next section where we will suggest a natural modification of Sachs' procedure for defining equivalence classes.

Let M be a spacetime with metric tensor g. A unit timelike vector at $p \in M$ is a member u_p of $T_p(M)$ satisfying $g_{ij}u^i u^j = -1$. We denote by $T'(M)$ the set of all unit timelike vectors at all points of M. $T'(M)$ forms a manifold and we may label a point in $T'(M)$ by local coordinates (x^i, u^α) where x^i are local coordinates on $U \subset M$ and u^α are three independent components of the unit timelike vector field with respect to the basis $\{\partial/\partial x^i\}$ (say, the first three components of u^i, for convenience the fourth components being obtainable from u^α by use of the fact that u is unit). The tangent sphere bundle may be considered as a submanifold of the full tangent bundle defined by

$$f(x^i, u^i) = g_{ij}(x^k)u^i u^j + 1 = 0.$$

There is a projection mapping $\pi : T'(M) \to M$ whereby a unit timelike vector at a point is mapped onto the point to which it is attached. The set of points $\pi^{-1}(p)$ is diffeomorphic to a hypersurface in R^4 defined by

$$K = \{(\xi^1, \xi^2, \xi^3, \xi^4) \mid (\xi^1)^2 + (\xi^2)^2 + (\xi^3)^2 - (\xi^4)^2 = -1\}.$$

$T'(M)$ is locally diffeomorphic to $U \times K$ where U is a coordinate neighborhood of M.

A vector field W in the full tangent bundle $T(M)$ may be expressed as

$$W = W_1{}^i \frac{\partial}{\partial x^i} + W_2{}^i \frac{\partial}{\partial u^i}.$$

If W is tangent to the submanifold $f(x^i, j^i) = 0$, then we may consider it as a differential operator in either $T(M)$ or $T'(M)$. The condition that W be tangent to the submanifold $f(x^i, j^i) = 0$ is that $df(W) = 0$ where

$$df = \frac{\partial f}{\partial x^i}dx^i + \frac{\partial f}{\partial u^i}du^i.$$

In terms of local coordinates this condition is simply

$$g_{ij,a}u^i u^j W_1{}^a + 2g_{ia}u^i W_2{}^a = 0.$$

As in the case of $L(M)$ the existence of the Levi–Civita connection on M enables us to distinguish pre-

ferred curves in $T'(M)$ called horizontal curves.[15] If we take a curve $x^i(\tau)$ on M and parallel propagate an arbitrary unit timelike vector u^i along $x^i(\tau)$ then this defines a horizontal curve on $T'(M)$. In terms of local coordinates, the tangent V to this curve may be written as

$$V=\frac{dx^i}{d\tau}\frac{\partial}{\partial x^i}+\frac{du^i}{d\tau}\frac{\partial}{\partial u^i}=\frac{dx^k}{d\tau}\frac{D}{dx^k},$$

where

$$\frac{D}{dx^k}=\frac{\partial}{\partial x^k}-\Gamma^i{}_{jk}u^j\frac{\partial}{\partial u^i}$$

and Γ^i_{jk} are the connection symbols on M. The D/dx^k thus span the horizontal subspace and the vector

$$V=\frac{dx^k}{d\tau}\frac{D}{dx^k}$$

is called the horizontal lift of the tangent to $x^i(\tau)$. As can be seen by direct calculation, $df(V)=0$ and so V is tangent to $T'(M)$.

If $x^i(\tau)$ is a timelike geodesic then its tangent vector is parallel propagated along the curve and this generates a particular type of horizontal vector field L called the timelike geodesic spray vector field. In $T(M)$ L may thus be written locally as

$$L=v^i\frac{\partial}{\partial x^i}-\Gamma^a_{bc}v^bv^c\frac{\partial}{\partial v^a}$$

where v^i is the unit tangent vector to $x^i(\tau)$. L is, of course, tangent to $T'(M)$.

Since u^i are local coordinates on the fibres we may use the vectors $\{\partial/\partial u^i\}$ to span the vertical subspace in the full tangent bundle and so the $\{\partial/\partial u^\alpha\}$ span the vertical subspace in $T'(M)$ at each point. Thus taking the $\{D/dx^k\}$, $\{\partial/\partial u^\alpha\}$ together, we have a basis for the tangent space at each point of $T'(M)$. An arbitrary vector Z may then be written as

$$Z=Z^i_{\text{hor}}\frac{D}{dx^i}+Z^\alpha_{\text{ver}}\frac{\partial}{\partial u^\alpha}.$$

Since we have local coordinates (x^i, u^i) in $T(M)$, the coordinate vectors $(\partial/\partial x^i,\ \partial/\partial u^i)$ span the tangent space at each point. The 1-forms du^k, dx^k satisfy the duality conditions

$$du^k\left(\frac{\partial}{\partial u^j}\right)=\delta_j{}^k,\quad dx^k\left(\frac{\partial}{\partial u^j}\right)=0,$$

$$du^k\left(\frac{\partial}{\partial x^i}\right)=0,\quad dx^k\left(\frac{\partial}{\partial x^j}\right)=\delta_j{}^k.$$

If we define $Du^i=du^i+\Gamma^i_{jk}u^j\,dx^k$, then we may see immediately that the 1-forms Du^i, dx^j satisfy the duality conditions

$$Du^i\left(\frac{D}{dx^k}\right)=0,\quad dx^k\left(\frac{D}{dx^s}\right)=\delta_s{}^r,$$

$$Du^i\left(\frac{\partial}{\partial u^j}\right)=\delta_j{}^i,\quad dx^s\left(\frac{\partial}{\partial u^r}\right)=0.$$

Thus the 1-forms $(dx^r,\ Du^s)$ cotangent space at each point of $T(M)$ and are dual to $(D/dx^k,\ \partial/\partial u^i)$. The 1-forms $(dx^r,\ Du^s)$ are adapted to the structure induced on the tangent space at each point of $T(M)$ by the connection on M.

It is natural to define a Riemannian metric on $T(M)$ by demanding that there exist a positive-definite, bilinear, symmetric operator H which makes horizontal and vertical vectors orthogonal. Just such an operator has been defined by Sachs as $H=h_{ij}\,dx^i\otimes dx^j+h_{ij}Du^i\otimes Du^j$, where $h_{ij}=+g_{ij}+2u_iu_j$, $u_i=g_{ij}u^i$, and $Du^i=du^i+\Gamma^i{}_{jk}u^j\,dx^k$. Direct calculation shows that

$$H\left(\frac{D}{dx^m},\frac{D}{dx^n}\right)=h_{mn},$$

$$H\left(\frac{D}{dx^m},\frac{\partial}{\partial u^n}\right)=0,$$

$$H\left(\frac{\partial}{\partial u^m},\frac{\partial}{\partial u^n}\right)=h_{mn},$$

and so the expression is manifestly positive-definite. The tensor character of H is apparent from its definition in terms of the 1-forms dx^i and Du^i. It can also be verified that the components of H with respect to $(dx^i,\ du^i)$ transform like the components of a covariant tensor under a change of coordinates

$$(x^i, u^i)\to\left(\bar{X}^i, \bar{u}^i=\frac{\partial\bar{x}^i}{\partial x^j}u^j\right).$$

We note that even though H is positive-definite it directly carries information about the connection on M through the h_{ij} and the 1-forms Du^i. A Riemannian metric may now be induced on $T'(M)$ by setting $g_{ij}u^iu^j=-1$ in the expression for H. Of course in this case only three of the u^i are linearly independent (for example, this relation makes one component of u^i a function of the other three and of x^i in H).

The tangent sphere bundle endowed with the Riemannian metric is a metric space with distance function induced by the metric. Its Cauchy completion consists of the set of all equivalence classes of Cauchy sequences. An equivalence relation R may be defined on the set of all equivalence classes, both those with "hearts" and those "without hearts," and the boundary of the spacetime may be defined as $\dot{M}=\bar{M}-M$ where $\bar{M}=\bar{T}'(M)/R$. Of course, when we restrict R to the set of equivalence classes of Cauchy sequences which is isometric to $T'(M)$ we must recover M. The problem then is to define such an equivalence relation. Sachs has given one such relation; we shall give another which is more natural.

Sachs' equivalence relation is: Two equivalence classes of Cauchy sequences S_1 and S_2 are R-equivalent if there are Cauchy sequences α in S_1 and β in S_2 of the form

$$\alpha=\{(p_1, U_1),\ (p_2, U_2), \cdots\},$$

$$\beta=\{(p_1, V_1),\ (p_2, V_2), \cdots\}.$$

Two equivalence classes are thus R-equivalent if one representative Cauchy sequence in each is formed over the same sequence of points in M. R is a true equivalence relation. When R is applied to the subset of equivalence classes of Cauchy sequences which is isometric to $T'(M)$, the resulting quotient set may be identified with M itself; i.e., $T'(M)/R=M$. This technique of defining an equivalence relation on $T'(M)$, however, in a sense violates the "spirit of the game" since we are re-

quired to use information about sequences on M in order to decide when equivalence classes of Cauchy sequences in $T'(M)$ are equivalent. Furthermore, it lacks the elegance of Schmidt's technique, which uses a group operation extendable to the boundary of $L(M)$.

IV. PRINCIPAL BUNDLES AND ASSOCIATED BUNDLES

There is a natural extension of the Schmidt technique for completing M which enables us to define "tensor spaces" over boundary points of M.[16] The extension is based upon the general mathematical technique for constructing an associated bundle from a given principal fibre bundle.[17] It turns out that this construction suggests a more natural equivalence relation to be imposed upon members of the Cauchy completion of the tangent sphere bundle than has been proposed initially by Sachs.

We now briefly outline the technique for constructing an associated bundle from an arbitrary principal bundle.[17]

A differentiable manifold B is called a principal fibre bundle over a manifold M if the following conditions are satisfied:

(a) There exists a Lie group G acting freely on B to the right as a Lie transformation group, $B\times G \ni (b, g) \to b\cdot g \in B$;

(b) M is the quotient space of B by the equivalence relation induced by G, i.e., B/G may be identified with M, and there is a map $\pi: B \to M$ which is differentiable;

(c) every point p in M has a neighborhood $U \subset M$ such that $\pi^{-1}(U)$ is diffeomorphic with $U\times G$.

The manifold M is called the base space of B, G is called the structure group, π is called the canonical projection mapping, and $\pi^{-1}(p)$ is called the fibre over p. A principal fibre bundle is often denoted by $B(M, G, \pi)$ when it is desirable to emphasize its composite elements. $L(M)$, where M is a spacetime, is an example of a principal fibre bundle.

Now let F be a differentiable manifold on which G acts differentiably on the left: $G\times F \in (g, \xi) \to g^{-1}\cdot\xi$. We will construct a manifold A which is called the fibre bundle associated to B with standard fibre F.

The group action on both B and F defines a group action on the set $B\times F$ by the rule $B\times F \in (b, \xi) \to (b\cdot g, g^{-1}, \xi)$. The action of G on $B\times F$ then defines an equivalence relation on $B\times F$ and we denote the resulting set of equivalence classes by $A = (B\times F)/G$: Each equivalence class in A consists of elements of the form $(b\cdot g, g^{-1}\cdot\xi)$ where b and ξ are fixed and g varies through G. We now define a mapping ψ: $B\times F \to M$ by $(b, \xi) \to \pi(b) \in M$ where π is the projection map of B. Since $\pi(b) = \pi(b\cdot g)$ we see that $\psi(b, \xi) = \psi(b\cdot g, g^{-1}\cdot\xi) = \pi(b) \in M$. If we denote the map which takes the pair (b, ξ) into the equivalence class consisting of $(b\cdot g, g^{-1}\cdot\xi)$ where b, ξ are fixed and g ranges through G by α: $B\times F \to A$, then we see that there is an induced mapping from A to M, call it π_a, whereby each equivalence class goes to a point in M. Thus π_a is a projection mapping. Then since $\pi_a^{-1}(U)$ where $U \subset M$ is locally $U\times F$, we can easily endow A with a differentiable structure.

As explicit examples of the above construction we consider the following:[18]

(a) Take B to be a principal fibre bundle and let G act on itself by group multiplication. Then $A = (B\times G)/G = B$ and B is the bundle associated with itself with standard fibre G.

(b) Take B to be the principal fibre bundle $L(M)$ where M is a spacetime with signature $(+++-)$. Let G be L and let F be R^4. Then $A = (L(M)\times R^4)/L$ is the tangent bundle $T(M)$ of M having a standard fibre which may be identified with the tangent space $T_p(M)$ at $p \in M$. This identification is simply another way of saying that a tangent vector at a point $p \in M$ is a rule that assigns a 4-tuple of real numbers to a frame u at p such that when the frame changes by a Lorentz transformation the numbers change by the inverse of that transformation.

(c) Take B to be $L(M)$, $G = L$, and F to be the tensor product of R^4 (s times) and its dual (r times). Then A is a tensor bundle over M having a standard fibre over $p \in M$ which may be identified with the set of all tensors of valence (s, r) over p. In other words, a tensor of valence (s, r) at point $p \in M$ is a rule that assigns 4^{s+r} – tuples of real numbers to a frame u at p such that when the frame changes by a Lorentz transformation the r-numbers change by the same transformation, whereas, the s-numbers change by the inverse transformation.

(d) Take B to be $L(M)$, $G = L$, and let F be the unit hyperboloid in R^4: $K = \{(\xi^1, \xi^2, \xi^3, \xi^4) \mid +(\xi^1)^2 + (\xi^2)^2 + (\xi^3)^2 - (\xi^4)^2 = -1\}$. Then A is the tangent sphere bundle of M, $T'(M)$, having a typical fibre which may be identified with the set of all unit timelike vectors at a point $p \in M$.

The above general construction may now be used to apply the Schmidt process to the tangent bundle. First, use the fact that the Cauchy completion $\bar{L}(M)$ of $L(M)$ can be uniquely defined and that L can be extended to act upon it. Now take $F = R^4$ and note that L acts as a matrix group: for $\xi = (\xi^1, \xi^2, \xi^3, \xi^4) \in R^4$, $\bar{\xi}^m = (L_n{}^m)^{-1}\xi^n$, $L_n{}^m \in L$. Form the set $\bar{L}(M)\times R^4$, and introduce a group action on $\bar{L}(M)\times R^4$ by $[(p; X_1, X_2, X_3, X_4), (\xi^1, \xi^2, \xi^3, \xi^4)] \to [(p; \bar{X}_1, \bar{X}_2, \bar{X}_3, \bar{X}_4), (\bar{\xi}^1, \bar{\xi}^2, \bar{\xi}^3, \bar{\xi}^4)]$ where $\bar{u} = \{\bar{X}_n\}$ and $u = \{X_m\}$ are in $\bar{L}(M)$, $\bar{X}_m = L_m{}^n X_n$ and $\bar{\xi}^i = (L_j{}^i)^{-1}\xi^j$. Now take the quotient of $\bar{L}(M)\times R^4$ by the induced equivalence relation and denote the resulting set of equivalence classes as $\bar{T}(M)$.

There exists a mapping $\bar{\psi}$: $\bar{L}(M)\times R^4 \to \bar{M}$, $(u, \xi) \to \bar{\pi}(u) \in \bar{M}$, where $\bar{M}$ denotes the Schmidt completion of M and when it is applied to $L(M)$ it maps the fibre over a point onto the point itself. Since $\bar{\pi}(u) = \bar{\pi}(u\cdot g) = \bar{p} \in \bar{M}$, it follows that $\bar{\psi}(u, \xi) = \bar{\psi}(u\cdot g, g^{-1}\xi) = \bar{p} \in \bar{M}$. Thus there is an induced mapping $\bar{\pi}_t$: $\bar{T}(M) \to \bar{M}$ whereby each equivalence class in $\bar{L}(M)\times R^4$ is associated with a point in $\bar{M}$. This result may now be interpreted in two ways. Since there are as many points in $\bar{T}(M)$ as there are points in

$\bar{M}$, assuming $\bar{M}$ has been directly constructed by the Schmidt completion of M using $L(M)$, then the existence of $\bar{\pi}_t$ may be interpreted as saying that the Schmidt completion of M by using the tangent bundle is the same as the direct Schmidt completion of M using $L(M)$.

We may also regard $\bar{\pi}_t^{-1}(\bar{p})$, $\bar{p} \in \bar{M}$, as a "tangent space" associated with the point $\bar{p} \in \bar{M}$. We put tangent space in quotation marks because it may happen that the group extension to $\bar{L}(M)$ may be degenerate, owing to a degenerate configuration of the equivalence classes of Cauchy sequences and so the "dimension of the tangent space at the boundary" may be different from that at an interior point.

We can of course go back and replace R^4 by the unit hyperboloid and repeat the above construction to obtain the Schmidt completion of the tangent sphere bundle $\bar{T}'(M)$. We then obtain a map

$$\bar{\pi}_{t'}: \bar{T}'(M) = (\bar{L}(M) \times H)/L \to \bar{M}.$$

Then just as before we may interpret the map as saying that the Schmidt completion using the tangent sphere bundle is the same as the Schmidt completion using the full tangent bundle and that both of these are equivalent to the Schmidt completion of M by direct use of $L(M)$. We may also consider $\bar{\pi}_{t'}(\bar{p})$, $\bar{p} \in \bar{M}$, as a "unit tangent space" at $\bar{p}$.

The same thing may of course be done for tensors of type (s, r). We replace R^4 by a tensor product of R^4 (s times) with its dual (r times). We repeat the above construction to obtain the Schmidt completion of the tensor bundle $\bar{T}_r^s(M)$ of type (s, r). We may also consider $\bar{\pi}_T^{-1}(\bar{p})$, $\bar{p} \in \bar{M}$, as a "tensor space" at $\bar{p}$ where $\bar{\pi}_T : \bar{T}_r^s(M) \to \bar{M}$, with the same caution as above concerning its dimensional interpretation.

The possibility of attaching tensorial quantities to boundary points of a spacetime is rich in potential applications.[19] In particular, the Schmidt completion of the tangent sphere bundle suggests a natural way to modify the equivalence relation initially proposed by Sachs for identifying boundary elements in his completion of the tangent sphere bundle. Recall that two equivalence classes of Cauchy sequences in the Cauchy completion of the tangent sphere bundle with respect to the Sachs metric are defined to be R-equivalent if one representative Cauchy sequence in each class is formed over the same sequence of points in the base space. Each R-equivalence class which does not correspond to a point in M is then defined to be an s-boundary point of M.

In the Sachs procedure, it is only R-equivalence which is cumbersome and it seems desireable to seek an equivalence relation which is somewhat more natural. Just such an equivalence relation is suggested by the Schmidt completion of the tangent sphere bundle: We simply define two equivalence classes of Cauchy sequences in the Cauchy completion of the tangent sphere bundle based on the Sachs metric to be S-equivalent if they arise from sequences of unit timelike vectors which have the same limit in $\bar{T}'(M)$, as defined by Schmidt.

Thus if we keep part of the Sachs technique and only change the equivalence relation from R to S, then the modified s-boundary is in one-to-one correspondence with $\bar{M}$ as originally defined by Schmidt. Sachs has shown that the s-boundary, as he originally defined it, is in one-to-one correspondence with the b-boundary.[2]

V. THE INTERPRETATION OF THE BOUNDARY POINTS

As we have seen in the last section, the boundary points of the spacetime M correspond to equivalence classes in $\bar{T}'(M)$. In order to interpret these boundary points it is necessary to find a relation between the bundle length of a curve containing a Cauchy sequence which defines the given boundary point and the affine or proper length of the corresponding curve in M. We will show that incomplete geodesics, as well as inextendable timelike curves of bounded acceleration and finite proper length, generate curves in $T'(M)$ with finite bundle length and thus determine boundary points of M.

First, consider the case of geodesics. Let $x^i(\tau)$ be a geodesic in M of finite affine length where τ is an affine parameter, with v^i the affine tangent vector. Then $Dv^i/d\tau = 0$ by the definition of a geodesic. Once $x^i(\tau)$ is given we can always choose a unit timelike vector u^m which is parallel propagated along $x^i(\tau)$ so that $Du^m/d\tau = 0$ by construction. Then both $v_m v^m$ and $v_m u^m$ are constant along $x^i(\tau)$. Now consider the curve $(x^i(\tau), u^i(\tau))$. The tangent vector to this curve is thus

$$W = v^i(\tau)\frac{\partial}{\partial x^i} + \frac{du^i}{d\tau}\frac{\partial}{\partial u^i}.$$

The length squared of W is given by

$$H(W, W) = h_{ij}v^i v^j = +v_i v^i + 2(u_i v^i)^2 = \text{const.}$$

Thus the bundle length of the curve $(x^i(\tau), u^i(\tau))$ is finite since the affine length of $x^i(\tau)$ is assumed to be finite.

Second, let $x^i(\tau)$ be an inextendible timelike curve of finite proper length and bounded acceleration in M with unit velocity v^i. The curve $(x^i(s),\ v^i(s))$ is a curve in $T'(M)$ with tangent vector

$$W = v^i(s)\frac{\partial}{\partial x^i} + \frac{dv^i}{ds}\frac{\partial}{\partial v^i}$$

having length squared

$$H(W, W) = h_{ij}v^i v^j + h_{ij}\frac{Dv^i}{ds}\frac{Dv^j}{ds}.$$

Using the fact that $v_i(Dv^i/ds) = 0$, we find that $H(W, W) = 1 + g_{ij}A^i A^j$ where $A^i = Dv^i/ds$. Since the acceleration of $x^i(s)$ is bounded there is a finite number N_0 such that $+g_{ij}A^i A^j < N_0$. Hence the bundle length of the curve $(x^i(s), v^i(s))$ is less than $s\sqrt{1+N_0}$ where s is the proper length of $x^i(s)$. Thus the bundle length is finite.

The preceeding properties thus imply the following: If the bundle metric is complete, then the connection is geodesically complete.

VI. EXAMPLES

The Schmidt process for assigning a boundary to a spacetime involves the formidable task of Cauchy completing the bundle of orthonormal frames, a task which is only slightly less formidable in the Sachs procedure.

A technique which we have used to gain insight into what the boundary should be for simple cases consists of solving for the eigenvector corresponding to zero eigenvalue, when such exists, of the bundle metric tensor at a boundary determined from coordinate limits. The Cauchy completion of the bundle then consists of the set of all integral curves of this degenerate eigenvector (possibly with additional identifications). The boundary points of the spacetime are then constructed by identifying integral curves under the action of L.

We first consider a positive-definite example: the quadrant of R^2 with metric

$$ds^2 = dx^2 + \frac{4x^2}{(1+y^2)^2} dy^2, \quad x > 0, \quad 0 < y < \infty.$$

The "structure of the singularity" appears to be a line, but this apparent structure is deceptive. The Schmidt metric is given by

$$d\sigma^2 = \theta^i \theta^i + \omega^A \omega^A,$$

where $\theta^i = (L_j{}^i)^{-1} \bar{\omega}^j$ and

$$\omega^A = d\alpha^A + \frac{\partial \alpha^A}{\partial L_b} L_p{}^m \bar{\omega}_m{}^n.$$

(Here L_j^i is a rotation matrix.) The $\bar{\omega}_m^n$ are given by the solutions of $d\bar{\omega}^n = -\bar{\omega}_m^n \wedge \bar{\omega}^m$ with $ds^2 = \delta_{ij} \bar{\omega}^i \bar{\omega}^j$. Only one parameter is needed for the structure group (rotation group in this case) and we denote it by λ:

$$L_m^n = \begin{pmatrix} \cos\lambda & \sin\lambda \\ -\sin\lambda & \cos\lambda \end{pmatrix} \longleftrightarrow (L_m^n)^{-1} = \begin{pmatrix} \cos\lambda & -\sin\lambda \\ \sin\lambda & \cos\lambda \end{pmatrix}.$$

We write $\bar{\omega}^1 = dx$, $\bar{\omega}^2 = [2x/(1+y^2)]\, dy$ and find that

$$\bar{\omega}_1^2 = x^{-1} \bar{\omega}^2 = -\bar{\omega}_2^1.$$

With respect to the basis $\{dx, dy, d\lambda\}$ we may write the Schmidt metric as

$$G_{\alpha\beta} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \dfrac{4x^2+16}{(1+y^2)^2} & \dfrac{4}{1+y^2} \\ 0 & \dfrac{4}{1+y^2} & 1 \end{pmatrix}.$$

Here $\det G_{\alpha\beta}$ goes to zero as x goes to zero and we thus expect the boundary points to lie at the limit $x = 0$, this limit being parameterized by the two variables y, λ.

Consider the reduced matrix $G_{ab}^{(0)}$ on an $x = \text{const}$. hypersurface.

The eigenvalues $\mu^{\pm}$ of this reduced matrix are given by

$$u_{\pm} = +\tfrac{1}{2}\left[1 + \frac{4x^2}{(1+y^2)^2}\left(1 + \frac{4}{x^2}\right)\right] \pm \tfrac{1}{2}\left\{\left[1 + \frac{4x^2}{(1+y^2)^2}\left(1 + \frac{4}{x^2}\right)\right]^2 - \frac{16x^2}{(1+y^2)^2}\right\}^{1/2}.$$

Note that as $x \to 0$, $\mu_- \to 0$, while μ_+ remains finite for all values of x. The eigenvector on the "$x = 0$ hypersurface" corresponding to the zero eigenvalue of $G_{ab}^{(0)}$ corresponds to a degenerate direction. Two Cauchy sequences approaching this "$x = 0$ hypersurface" which have their separation vector coincide with this degenerate direction will determine the same boundary point.

The eigenvector $V^{(0)}$ corresponding to the zero eigenvector is given by

$$V^{(0)} = a\frac{\partial}{\partial y} - \frac{4a}{1+y^2}\frac{\partial}{\partial \lambda}, \quad a \text{ arbitrary}.$$

The integral curve $\Gamma^{(0)} : (y(\tau), \lambda(\tau))$ of $V^{(0)}$ is given by

$$\lambda = -4\tan^{-1} y + \text{const}.$$

The "singularity structure" of the bundle is thus one-dimensional. To project to the base space we identify equivalence classes with different values of λ.

Thus the b-boundary of this space is simply a point. The transformation

$$x = r, \quad y = \tan(\theta/2)$$

shows that this example is simply the plane in polar coordinates r, θ with the $r = 0$ point missing.

For another example, we consider a two-dimensional Friedmann–Robertson–Walker (FRW) type spacetime with local coordinates (x, t), $t > 0$, $-\infty < x < \infty$. The metric tensor is given by $ds^2 = +a^2(t)\, dx^2 - dt^2$, where $a(t) \to 0$ as $t \to 0$ and $a'(t) = da(t)/dt \to \infty$ as $t \to 0$. We again use λ as a coordinate on L,

$$(L_m^n) = \begin{pmatrix} \cosh\lambda & \sinh\lambda \\ \sinh\lambda & \cosh\lambda \end{pmatrix} \longleftrightarrow (L_m^n)^{-1} = \begin{pmatrix} \cosh\lambda & -\sinh\lambda \\ -\sinh\lambda & \cosh\lambda \end{pmatrix}.$$

We choose $\bar{\omega}^1 = a(t)\, dx$, $\bar{\omega}^2 = dt$ and find that the only nonzero $\bar{\omega}_m{}^n$ are $\bar{\omega}_1^2 = \bar{\omega}_2^1 = [a'(t)/a(t)]\bar{\omega}^1$. In the basis $\{dx, dt, d\lambda\}$ the determinant of the Schmidt metric $G_{\alpha\beta}$ is $a^2(t)$ and so goes to zero with t. It can be shown (e.g., by calculating bundle curvature invariants) that this apparent singular behavior is not simply a coordinate effect and we thus expect the boundary to be the "$t = 0$ hypersurface."

To determine the structure of the boundary, we solve for the eigenvalues of the reduced metric $G_{ab}^{(0)}$ on a $t = \text{const}$ hypersurface as t goes to zero. The eigenvalues of the reduced metric are given by

$$\mu_{\pm} = +\tfrac{1}{2}[1 + a^2\cosh 2\lambda + 4(a')^2] \pm \tfrac{1}{2}\{[1 + a^2\cosh 2\lambda + 4(a')^2]^2 - 4a^2\cosh 2\lambda\}^{1/2}.$$

Thus one eigenvalue goes to zero and one to infinity as t goes to zero (assuming $\cosh\lambda < \infty$). The integral curves of the eigenvector corresponding to the zero eigenvalue are given for this case by lines "parallel" to the λ axis. We thus conclude that the singularity structure of $L(M)$ is one-dimensional and that of M also one-dimensional.

The Sachs metric on $T'(M)$ is $d\sigma^2 = h_{ij}\, dx^i\, dx^j + h_{ij} Du^i Du^j$ where $h_{ij} = g_{ij} + 2u_i u_j$, $u_i = g_{ij} u^j$, $Du^j = du^k + \Gamma^i_{jk} u^j\, dx^k$, and it is understood that du^i is to be expressed in terms of $d\lambda$ and dt. For the FRW-type metric the Sachs metric becomes identical to the Schmidt metric if $t \to 2t$ in the Schmidt expression.

VII. CONCLUSIONS

It is possible to assign boundary points to a spacetime by associating with the spacetime a higher-dimensional Riemannian manifold, Cauchy completing this Rieman-

nian manifold, and then "projecting" to define the boundary points of the spacetime. Two such techniques for assigning boundary points to a spacetime are currently available: one due to Schmidt using the proper homogeneous orthochronous Lorentz bundle $L(M)$ over a spacetime, and one due to Sachs using the tangent sphere bundle $T'(M)$. We introduced a natural modification of the projection method in the Sachs technique which makes it agree rather easily with the Schmidt technique. The original Sachs technique projection is somewhat cumbersome although Sachs has shown that his original scheme gives to the same results as Schmidt' s.

Both the Schmidt process and the Sachs process are more general than the g-boundary technique formulated by Geroch. Geroch' s method of assigning boundary points to a spacetime uses only incomplete geodesics whereas both the Sachs method and the Schmidt method include not only incomplete geodesics but also other curves, such as inextendible timelike curves of finite proper length and bounded acceleration. This is an important advantage in principle but both of the new techniques are far more difficult to apply than Geroch' s. It is a formidable task to calculate either the b-boundary or the s-boundary for even the simplest spacetime models whereas Geroch' s technique is relatively straightforward in these simple cases.

We note in passing that more complex versions of the Sachs and Schmidt ideas for assigning boundary points to a spacetime have been given. Brill[20] described a process whereby long sequences of successively higher-dimensional manifolds may be defined, each but the most complicated having indefinite metrics, and only the last being Riemannian. The singularity structure of the last manifold is determined by grouping Cauchy sequences into equivalence classes. The sequence is then followed back down to arrive at the singularity structure of the original manifold M. The major unanswered question with this procedure is when or if all of the processes suggested by Brill lead to the same singularity structure for M.

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[3]R. Geroch, Ann. Phys. **48**, 526 (1968).
[4]Reference 1 treats the case of an arbitrary linear connection. We review the process here for the special case of a spacetime.
[5]An orthonormal frame u at a point $p \in M$ is an ordered tetrad of tangent vectors at p satisfying $g(X_n, X_m) = \eta_{nm}$ with $(\eta_{nm}) = \mathrm{diag}(+1, +1, +1, -1)$. The order convention we use is such that X_1, X_2, X_3 are spacelike and X_4 is timelike. X_4 is also assumed future pointing.
[6]$L(M)$ is a special case of a principal fibre bundle; see S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry* (Interscience, New York, 1963), Vol. 1, for a general discussion of fibre bundles and their properties.
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[8]A connection on a principal bundle is often defined to be a collection of subspaces satisfying $\pi_*(H_u) = T_{\pi(u)}(M)$ and $H_{uA} = (R_A)_* H_u$. We have taken the above backwards approach simply to illustrate the geometrical implications for $L(M)$ of a connection on M.
[9]The distance d from u to v in $L(M)$ is the minimum length of all curves from u to v, length being defined by use of G. See N. Hicks, *Notes on Differential Geometry* (Van Nostrand-Reinhold, New York, 1965).
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Spacetime symmetries and linearization stability of the Einstein equations. I*

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We consider the Marsden–Fischer conditions for linearization stability applied to vacuum spacetimes with compact Cauchy hypersurfaces. We show that if a vacuum spacetime S admits a Killing vector field, then the Marsden–Fischer criterion fails to be satisfied at any Cauchy surface for S. We also show that if the Marsden–Fischer criterion fails to hold on an initial surface, then there is a Cauchy development of this intial data which admits one or more Killing vectors. The number of independent Killing fields present is shown to equal the dimension of the kernel of the linear map defined by Marsden and Fischer.

I. INTRODUCTION

Fischer and Marsden[1,2] have recently proven an important theorem concerning the applicability of linear perturbation theory to problems in general relativity. They establish conditions upon an exact solution of the vacuum Einstein equations which are sufficient to ensure that all solutions to the corresponding linearized equations approximate (i.e., are tangent to) curves of exact solutions passing through the given one. If all solutions of the linearized equations do indeed approximate curves of exact solutions, then the given solution is said to be linearization stable. The importance of this idea is enhanced by examples due to Brill[3] and Brill and Deser[4] of vacuum spacetimes which are not linearization stable. For these examples some solutions of the perturbation equations are spurious and should be discarded.

In this paper we consider the Fischer—Marsden conditions for vacuum spacetimes determined by Cauchy data prescribed on a 3-manifold M which is compact and without boundary. The conditions for linearization stability (reviewed here in Sec. III) are expressed in terms of a system of linear partial differential equations defined on any Cauchy surface for the spacetime. Linearization stability holds if these equations admit only the trivial solution (i.e., the associated linear map has trivial kernel). We shall show that if a Cauchy development of the initial data admits one or more Killing vector fields then the Fischer—Marsden criterion for linearization stability fails to hold at any Cauchy surface of this development. Conversely, we shall also show that if the Fischer—Marsden conditions fail to hold on an initial surface, then there is a Cauchy development of the initial data which admits one or more Killing vector fields. The number of independent Killing vectors which occur is shown to equal the dimension of the kernel of the linear map mentioned above. As a corollary we obtain the natural result that the Fischer—Marsden criterion is independent of the choice of Cauchy surface to which it is applied and depends only upon the presence or absence of isometries of the enveloping spacetime.

When the Fischer—Marsden conditions fail to hold one can derive additional restrictions upon the perturbations which are necessary to exclude spurious solutions of the linearized equations. Special cases of these restrictions have been discussed by Brill and Deser[4] and by Fischer and Marsden who outlined a general method for deriving such constraints.[2] In a subsequent paper we shall discuss these additional constraints which are necessary (according to the arguments given here) whenever the background spacetime admits Killing vector fields. We shall show that they require that the conserved quantity associated with each independent Killing vector field must be constrained to vanish. This restriction upon the perturbations is independent of the choice of initial hypersurface at which it is imposed and is essential to exclude spurious solutions.

For the case in which M is noncompact and the spacetime asymptotically flat the Fischer—Marsden conditions are less restrictive. Nonvanishing solutions to the corresponding Fischer—Marsden equations do not violate linearization stability unless they have suitable asymptotic behavior. Thus Killing vectors (which always induce solutions to these equations) would be allowed provided they did not vanish asymptotically. In particular, as shown by Fischer and Marsden[1,2] and independently by Choquet-Bruhat and Deser,[5] Minkowski space is linearization stable. However, since the details of the general linearization stability theorem for noncompact M have not yet been published, we shall confine our attention to the compact case.

A different approach to the study of linearization stability has recently been published by O'Murchadha and York.[6] They consider both compact Cauchy surfaces and noncompact Cauchy surfaces with asymptotically flat initial data. In the latter case they conclude that any asymptotically flat initial data set for which the trace of the second fundamental form vanishes is linearization stable.

II. NOTATION AND BASIC EQUATIONS

We consider vacuum spacetimes determined by suitable Cauchy data prescribed on a compact 3-mainfold M which is orientable and without boundary. The Einstein equations determine a Lorentzian metric ${}^{(4)}g$ (signature $-+++$) on ${}^{(4)}V=(-\epsilon,\epsilon)\times M$ which is unique up to diffeomorphisms that leave the Cauchy data fixed. In coordinates for which the hypersurfaces $x^0=t=\text{const}$ are spacelike, we express the components of ${}^{(4)}g$ as[7]

$$ {}^{(4)}g_{ij}=g_{ij},\quad {}^{(4)}g_{0i}=N_i,\quad {}^{(4)}g_{00}=-N^2+g^{ij}N_iN_j \qquad (2.1) $$

where g^{ij} is the inverse of the Riemannian metric g_{ij}. N and N_i are called the lapse function and shift vector, respectively. The metric ${}^{(4)}g$ induces on each spacelike

hypersurface a second fundamental form k. In terms of k and g we define the gravitational momentum π

$$\pi^{ij} = (\det g)^{1/2}(g^{ij}\,\mathrm{tr}k - k^{ij}) \tag{2.2}$$

where $\det g$ is the determinant of g_{ij} and $\mathrm{tr}\,k = k^{ij}g_{ij}$ is the trace of k. Covariant differentiation with respect to ${}^{(4)}g$ of tensor fields defined on $({}^{(4)}V, {}^{(4)}g)$ is signified by a semicolon. Thus if ${}^{(4)}X$ is a vector field defined over ${}^{(4)}V$, we write

$$(L_{{}^{(4)}X}\,{}^{(4)}g)_{\mu\nu} = {}^{(4)}X_{\mu\,;\nu} + {}^{(4)}X_{\nu\,;\mu}, \tag{2.3}$$

where $L_{{}^{(4)}X}$ is the Lie derivative with respect to ${}^{(4)}X$. Covariant differentiation with respect to g of tensor fields defined over a hypersurface (M, g) is signified by a vertical bar. Thus we write

$$(\delta\pi)^i = \pi^{ij}{}_{|j} \tag{2.4}$$

where $\delta\pi$ is the divergence of π.

The various function spaces used in the Fischer–Marsden analysis are spaces of C^∞ tensor fields over M (in the technical proofs Sobolev spaces are used instead). Define

$\mathcal{S}_2(\mathcal{S}_2^*)$ = space of symmetric covariant second rank tensors (tensor densities) over M,

$\mathcal{S}^2(\mathcal{S}_*^2)$ = space of symmetric contravariant second rank tensors (tensor densities) over M,

$\mathcal{M}$ = space of Riemannian metrics of M,

$\mathcal{C}^\infty(\mathcal{C}_*^\infty)$ = space of scalar functions (scalar densities) over M,

$\mathcal{X}_1(\mathcal{X}_1^*)$ = space of covariant vector fields (densities) over M,

$\mathcal{X}^1(\mathcal{X}_*^1)$ = space of contravariant vector fields (densities) over M.

In addition, write $T^*\mathcal{M} \approx \mathcal{M} \times \mathcal{S}_*^2$ for the cotangent bundle of $\mathcal{M}$.

As is well known, Cauchy data (g, π) induced upon a spacelike hypersurface of a Ricci-flat spacetime satisfy the constraint equations $\mathcal{H}(g, \pi) = \delta(g, \pi) = 0$, where

$$\mathcal{H}(g, \pi) = (\det g)^{-1/2}(\pi^{ij}\pi_{ij} - 1/2(\mathrm{tr}\,\pi)^2) - (\det g)^{1/2}R, \tag{2.5}$$

$$\delta(g, \pi) = 2\pi^{ij}{}_{|j} \tag{2.6}$$

and R is the scalar of curvature of g. These constraints define a subset $\mathcal{C}$ of $T^*\mathcal{M}$:

$$\mathcal{C} = \{(g, \pi) \mid \mathcal{H}(g, \pi) = \delta(g, \pi) = 0\}. \tag{2.7}$$

The Einstein evolution equations which propagate the Cauchy data to determine a metric ${}^{(4)}g$ on $(-\epsilon, \epsilon)\times M$ are given by

$$\partial g_{ij}/\partial t = 2N(\det g)^{-1/2}(\pi_{ij} - (1/2)g_{ij}\,\mathrm{tr}\,\pi) + N_{i|j} + N_{j|i}, \tag{2.8}$$

$$\partial\pi^{ij}/\partial t = -N(\det g)^{1/2}(R^{ij} - (1/2)g^{ij}R) + (1/2)N(\det g)^{-1/2}g^{ij}(\pi^{kl}\pi_{kl} - (1/2)(\mathrm{tr}\,\pi)^2) - 2N(\det g)^{-1/2}(\pi^{ik}\pi_k{}^j - (1/2)\pi^{ij}\,\mathrm{tr}\,\pi) + (\det g)^{1/2}(N^{|ij} - g^{ij}N^{|k}{}_{|k}) + (\pi^{ij}N^k)_{|k} - N^i{}_{|k}\pi^{kj} - N^j{}_{|k}\pi^{ki} \tag{2.9}$$

where R^{ij} is the Ricci tensor of g.

We shall need some standard theorems on existence and (with suitable coordinate conditions) uniqueness of solutions of the Einstein equations and of the linearized Einstein equations. These results have been obtained by Choquet-Bruhat[8] who established the strict hyperbolicity of the Einstein equations in harmonic coordinates and by Fischer and Marsden[9] who reexpressed the equations in first order symmetric hyperbolic form. The hyperbolicity of the corresponding linearized equations may be deduced from these results provided the background exact solution is properly Lorentzian. For our purposes it will be convenient, in Secs. V and VI, to impose Gaussian normal coordinate conditions (${}^{(4)}g_{00} = -1$, ${}^{(4)}g_{0i} = 0$) on the exact solutions and Gaussian gauge conditions (i.e., vanishing perturbations of ${}^{(4)}g_{00}$ and ${}^{(4)}g_{0i}$) on the perturbation solutions. This specialization simplifies a number of the computations but limits the conclusions of these sections to those Cauchy developments on which Gaussian coordinates exist.

III. FISCHER-MARSDEN CONDITIONS FOR LINEARIZATION STABILITY

Following Fischer and Marsden[1,2] we define

$$\Phi : T^*\mathcal{M} \to \mathcal{C}_*^\infty \times \mathcal{X}_*^1, \quad (g, \pi) \mapsto (\mathcal{H}(g, \pi),\ \delta(g, \pi)) \tag{3.1}$$

and compute the derivative $D\Phi(g, \pi)$ of Φ at points $(g, \pi) \in \mathcal{C} = \Phi^{-1}(0)$. If $(h, \omega) \in \mathcal{S}_2 \times \mathcal{S}_*^2 = T_{(g,\pi)}\mathcal{M} \times \mathcal{S}_*^2$, then

$$\begin{aligned} D\Phi(g, \pi)\cdot(h, \omega) &= \{D\mathcal{H}(g, \pi)\cdot(h, \omega),\ D\delta(g, \pi)\cdot(h, \omega)\} \\ &= \{(\det g)^{-1/2}[-1/2(\pi\cdot\pi - 1/2(\mathrm{tr}\,\pi)^2)\mathrm{tr}\,h \\ &\quad + 2(\pi\cdot\omega - \tfrac{1}{2}\mathrm{tr}\,\pi\cdot\mathrm{tr}\,\omega) + 2(\pi\times\pi - \tfrac{1}{2}(\mathrm{tr}\,\pi)\pi)\cdot h] \\ &\quad - (\det g)^{1/2}[\delta\delta h - \Delta(\mathrm{tr}\,h) \\ &\quad - (\mathrm{Ric}(g) - 1/2\,gR(g))\cdot h]; \\ &\quad 2\omega^{ij}{}_{|j} + \pi^{jk}(h^i{}_{j|k} + h^i{}_{k|j} - h_{jk}{}^{|i})\}, \end{aligned} \tag{3.2}$$

where $\cdot$ signifies contraction (e.g., $\pi\cdot h = \pi^{ij}h_{ij}$) and tr signifies trace ($\mathrm{tr}\,h = g^{ij}h_{ij}$). Also, $\pi\times\pi = \pi^{ik}\pi_k{}^j$, $\delta\delta h = h_{ij}{}^{|ij}$, $\Delta(\mathrm{tr}\,h) = (\mathrm{tr}\,h)_{|i}{}^{|i}$ and $\mathrm{Ric}(g)$ is the Ricci tensor of g. Our notation, except for some sign conventions, is essentially that of Ref. 2. However, our function $\delta(g, \pi)$ has been defined, for convenience, to be minus twice that of Ref. 2.

From the implicit function theorem one knows that if $D\Phi(\cdot)$ is surjective at $(g, \pi) \in \mathcal{C}$, then

(i) $\mathcal{C}$ is a smooth submanifold of $T^*\mathcal{M}$ in a neighborhood of (g, π) and

(ii) all solutions (h, ω) of $D\Phi(g, \pi)\cdot(h, \omega) = 0$ are tangent to $\mathcal{C}$ at (g, π).

Using elliptic theory Fischer and Marsden prove that $D\Phi(g, \pi)$ is surjective if and only if the adjoint map $D\Phi(g, \pi)^*$ is injective (i.e., has trivial kernel). The adjoint, computed from (3.2) using the standard L^2 inner product, is given explicitly by

$$D\Phi(g,\pi)^*: C^\infty \times \mathcal{X}_1 \to \mathcal{S}_*^2 \times \mathcal{S}_2;\ (C,X)$$
$$\mapsto \{(\det g)^{-1/2}[-\tfrac{1}{2}(\pi\cdot\pi - \tfrac{1}{2}(\mathrm{tr}\pi)^2)g^{-1}C$$
$$+ 2(\pi\times\pi - \tfrac{1}{2}\pi(\mathrm{tr}\pi))C] - (\det g)^{1/2}[(\mathrm{Hess}C)^{-1}$$
$$- \Delta C\, g^{-1} - (\mathrm{Ric}(g) - \tfrac{1}{2}gR)^{-1}C] + L_X\pi;$$
$$2C(\det g)^{-1/2}(\pi_* - \tfrac{1}{2}(\mathrm{tr}\pi)g) - L_X g\} \tag{3.3}$$

where $\pi\times\pi = \pi^{ik}\pi_k{}^j$, Hess $C = C_{|ij}$, L_X = Lie derivative with respect to X, and where we have used $\delta(g,\pi)=0$ for $(g,\pi)\in C$. Also $\pi_* = \pi_{ij}$, the covariant form of π and $^{-1}$ indicates the contravariant form of a tensor.

The problem is thus to characterize those points $(g,\pi)\in C$ for which $D\Phi(g,\pi)^*$ has trivial kernel. In Sec. IV we show that if a Cauchy development $({}^{(4)}V, {}^{(4)}g)$ of (M,g,π) admits a Killing vector field ${}^{(4)}X$, then ${}^{(4)}X$ induces upon each Cauchy hypersurface (M,g',π') of $({}^{(4)}V, {}^{(4)}g)$ a nontrivial solution (C',X') of $D\Phi(g',\pi')^*\cdot(C',X')=0$. The scalar C' and vector X' are then the normal and tangential projections of ${}^{(4)}X$. To prove the converse, we assume in Sec. V that the adjoint map $D\Phi(g,\pi)^*$ admits a nontrivial kernel (C,X) and integrate four of Killing's equations to define a vector field ${}^{(4)}X$ on a Cauchy development $({}^{(4)}V, {}^{(4)}g)$ of (M,g,π). We then show in Sec. VI that ${}^{(4)}X$ satisfies the remaining six Killing equations on $({}^{(4)}V, {}^{(4)}g)$. With these results we shall be able to conclude that $D\Phi(g,\pi)$ is surjective if and only if the spacetime determined by the Cauchy data (g,π) admits no Killing vector fields.

By working directly with Eqs. (3.3) Fischer and Marsden derived two necessary conditions for the adjoint map to be injective:

(i) If $\pi=0$, g is not flat;

(ii) there are no nonzero vector fields X such that $L_X g=0$ and $L_X\pi=0$.

However, these conditions were not sufficient without the additional, and overly restrictive, constraint:

(iii) tr$k$ is constant on M.

Our results show that necessary and sufficient conditions for $D\Phi(\cdot)$ to be surjective are most simply expressed in terms of the 4-geometry rather than in terms of the geometry of some arbitrarily chosen hypersurface. In particular, we obtain the natural result that the dimension of the kernel of the adjoint map is independent of the choice of hypersurface at which it is evaluated, being in fact equal to the number of independent Killing vector fields of the spacetime.

IV. KILLING VECTORS AND THE KERNEL OF THE ADJOINT MAP

In this section we show that the dimension of the kernel of $D\Phi(g,\pi)^*$ is at least as large as the number of independent Killing vectors of $({}^{(4)}V, {}^{(4)}g)$. Let ${}^{(4)}X$ be an arbitrary, smooth vector field on $({}^{(4)}V, {}^{(4)}g)$ and let $\phi(e)$ [with $e\in(-\alpha,\alpha)$] be the one parameter family of diffeomorphisms generated by ${}^{(4)}X$ [with $\phi(0)=$ identity]. Write ${}^{(4)}g(e) = \phi^*(e)\,{}^{(4)}g$ for the induced family of metrics isometric to ${}^{(4)}g(0) = {}^{(4)}g$ generated by the natural action of this family of diffeomorphisms. Then, as is well known,

$${}^{(4)}h \overset{\text{def}}{=} \partial\,{}^{(4)}g(e)/\partial e\,\big|_{e=0} = L_{({}^{(4)}X)}\,{}^{(4)}g. \tag{4.1}$$

For convenience choose coordinates such that the hypersurface (M,g,π) of interest occurs as an $x^0 = t = \text{const}$ surface and define the tensor $h\in\mathcal{S}_2$ on each $t=\text{const}$ hypersurface by

$$h_{ij} = {}^{(4)}h_{ij} = {}^{(4)}X_{i;j} + {}^{(4)}X_{j;i}. \tag{4.2}$$

Reexpress h by writing out the covariant derivatives explicitly and using Eqs. (2.8) to eliminate the time derivatives of g which occur in the connection components. After a short computation the result may be written as

$$h_{ij} = -2C(\det g)^{-1/2}(\pi_{ij} - 1/2\, g_{ij}\,\mathrm{tr}\pi) + X_{i|j} + X_{j|i}, \tag{4.3}$$

where

$$C = {}^{(4)}X_\alpha\, n^\alpha = N^{-1}({}^{(4)}X_0 - g^{ij}N_i\,{}^{(4)}X_j), \tag{4.4}$$

the projection of ${}^{(4)}X$ along the unit normal n of the $t=\text{const}$ hypersurface, and where

$$X_i = {}^{(4)}X_i = t^\alpha_{(i)}\,{}^{(4)}X_\alpha, \tag{4.5}$$

the projections of ${}^{(4)}X$ along the three independent vector fields $t_{(i)} = \delta_i^\alpha\partial/\partial x^\alpha$ tangent to the $t=\text{const}$ hypersurface.

The gravitational momentum π may be expressed in terms of ${}^{(4)}g$ and its first derivatives by solving for π in Eq. (2.8). The result is equivalent to

$$\pi^{ij} = (-\det{}^{(4)}g)^{1/2}(g^{im}g^{jn} - g^{ij}g^{mn})\Gamma^0_{mn} \tag{4.6}$$

where $\Gamma^\alpha_{\beta\gamma}$ are the connection components of ${}^{(4)}g$. The family $\phi(e)$ of diffeomorphisms generated by ${}^{(4)}X$ therefore induces a family $\pi(e)$ obtained by evaluating Eq. (4.6) on ${}^{(4)}g(e)$. Define $p\in\mathcal{S}_*^2$ on each $t=\text{const}$ hypersurface by

$$p^{ij} = \partial\pi^{ij}(e)/\partial e\,\big|_{e=0} \tag{4.7}$$

and compute p explicitly using expression (4.6) and $\partial({}^{(4)}g(e)/\partial e\,|_{e=0} = L_{({}^{(4)}X)}\,{}^{(4)}g$. The resulting expression involves second derivatives of both ${}^{(4)}g$ and ${}^{(4)}X$. Eliminate the first time derivatives of g using Eqs. (2.8) and the first time derivatives of π (which arise through second time derivatives of g) using Eqs. (2.9). After a rather lengthy computation one finds that the time derivatives of the lapse function N and shift vector N_i and of ${}^{(4)}X$ cancel leaving

$$p^{ij} = \{C[(\det g)^{1/2}(R^{ij} - 1/2\, g^{ij}R)$$
$$- 1/2(\det g)^{-1/2}g^{ij}(\pi^{mn}\pi_{mn} - 1/2(\mathrm{tr}\pi)^2)$$
$$+ 2(\det g)^{-1/2}(\pi^{ik}\pi_k{}^j - 1/2\pi^{ij}\mathrm{tr}\pi)]$$
$$- (\det g)^{1/2}(C^{|ij} - g^{ij}C_{|k}{}^{|k})$$
$$+ (X^k\pi^{ij})_{|k} - X^i{}_{|k}\pi^{kj} - X^j{}_{|k}\pi^{ki}\} \tag{4.8}$$

with C and $X_i = g_{ij}X^j$ given, as before, by Eqs. (4.4) and (4.5).

Evaluating (h,p) on the $t=\text{const}$ hypersurface (M,g,π) one sees, by comparing Eqs. (4.3) and (4.8) with Eq. (3.3), that

$$(p, -h)_{(g,\pi)} = D\Phi(g,\pi)^*\cdot(C,X), \tag{4.9}$$

where C and X are the normal and tangential projections

of ${}^{(4)}X$. Now suppose that ${}^{(4)}X$ is a Killing vector field of ${}^{(4)}g$. Then from the definitions of h and p in terms of $\partial {}^{(4)}g(e)/\partial e|_{e=0} = L_{(4)X}\,{}^{(4)}g = 0$ one sees that h and p vanish on every $t = \text{const}$ hypersurface. However, since any Cauchy hypersurface of $({}^{(4)}V, {}^{(4)}g)$ can be taken as the initial $(t=0)$ surface with a suitable choice of coordinates, we obtain

Lemma 4.1: A Killing vector ${}^{(4)}X$ of ${}^{(4)}g$ induces upon every Cauchy hypersurface (M, g, π) of $({}^{(4)}V, {}^{(4)}g)$ a solution (C, X) of $D\Phi(g,\pi)^*$. $(C, X) = 0$. C and X are the projections of ${}^{(4)}X$ normal and tangential to the hypersurface, respectively.

To complete the argument we must show that Killing vectors on $({}^{(4)}V, {}^{(4)}g)$ are linearly independent if and only if their normal and tangential projections on any Cauchy surface are linearly independent. We first prove

Lemma 4.2: If ${}^{(4)}X$ is a Killing vector of $({}^{(4)}V, {}^{(4)}g)$ and ${}^{(4)}X$ vanishes on a Cauchy surface S, then ${}^{(4)}X$ vanishes on $({}^{(4)}V, {}^{(4)}g)$.

Proof: Let γ be any timelike geodesic of $({}^{(4)}V, {}^{(4)}g)$ and let t $(t^\alpha = dx^\alpha/ds)$ be the tangent to γ parametrized by proper time s. Then from Killing's equations for ${}^{(4)}X$ and the geodesic equations for t one easily shows that

$$\frac{d}{ds}(t \cdot {}^{(4)}X) = \frac{d}{ds}(t_\alpha\, {}^{(4)}X^\alpha) = 0$$

along γ. Let p be any point of ${}^{(4)}V$ not contained in S. Since S is a Cauchy surface each timelike geodesic through p intersects S precisely once. Let γ be any timelike geodesic through p and let t be the tangent to γ. Then $(t \cdot {}^{(4)}X)_p$ vanishes since $t \cdot {}^{(4)}X$ is conserved along γ and vanishes at the point at which γ intersects S (since ${}^{(4)}X$ vanishes there). Thus ${}^{(4)}X_p$ must be orthogonal to every timelike vector at p and this can happen only if ${}^{(4)}X$ vanishes at p. Thus ${}^{(4)}X$ vanishes on $({}^{(4)}V, {}^{(4)}g)$.

Now suppose ${}^{(4)}X_{(a)}$ $(a = 1, \ldots, n)$ are linearly independent Killing vectors on $({}^{(4)}V, {}^{(4)}g)$. If c_a are any real constants (not all zero), then ${}^{(4)}Y = \sum_a c_a\, {}^{(4)}X_{(a)}$ is a Killing vector on $({}^{(4)}V, {}^{(4)}g)$. Clearly, ${}^{(4)}Y$ cannot vanish on a Cauchy surface S since, by Lemma 4.2, it would therefore vanish globally, contradicting the assumption of linear independence of the ${}^{(4)}X_{(a)}$. Thus linearly independent Killing vectors induce linearly independent projections $(C_{(a)}, X_{(a)})$ on each Cauchy surface of $({}^{(4)}V, {}^{(4)}g)$. The converse is obviously also true.

Combining the results of these lemmas we obtain

Theorem 4.1: If (M, g, π) is a Cauchy surface for a vacuum spacetime $({}^{(4)}V, {}^{(4)}g)$, then the dimension of $\ker D\Phi(g,\pi)^*$, the kernel of the adjoint map at (M, g, π), is at least as large as the number of linearly independent Killing vector fields of $({}^{(4)}V, {}^{(4)}g)$.

V. INTEGRATION OF KILLING'S EQUATIONS

Assume that $(C, X) \in \mathcal{C}^\infty \times \mathcal{X}_1$ is an element of $\ker D\Phi(g,\pi)^*$. We wish to show eventually that there is a Cauchy development of (M, g, π) and a Killing vector on this development which induces (C, X) on the initial hypersurface (M, g, π) as normal and tangential projections. To do this we integrate four of Killing's equations to define a vector field on a tubular neighborhood ${}^{(4)}V = (-\epsilon, \epsilon) \times M$ of the initial hypersurface. Since this vector field is uniquely determined from (C, X), it is the only candidate for a Killing field with the given initial data. In the next section we shall show that the remaining six Killing equations are also satisfied on $({}^{(4)}V, {}^{(4)}g)$.

For simplicity we now specialize to Gaussian normal coordinates on a tubular neighborhood of the initial $(t=0)$ hypersurface (M, g, π). In these coordinates ${}^{(4)}g_{00} = -1$ and ${}^{(4)}g_{0i} = 0$, so that the line element is given by

$$ds^2 = -dt^2 + g_{ij}\, dx^i\, dx^j. \tag{5.1}$$

In Gaussian coordinates four of the components of $L_{(4)X}\,{}^{(4)}g$ are given by

$$\begin{aligned} (L_{(4)X}\,{}^{(4)}g)_{00} &= 2C_{,t} = 2\partial C/\partial t, \\ (L_{(4)X}\,{}^{(4)}g)_{0i} &= g_{ij}(X^j{}_{,t} + C_{|k} g^{kj}), \end{aligned} \tag{5.2}$$

where C and $X^i = g^{ij}X_j = g^{ij}\,{}^{(4)}X_j$ are the normal and tangential components of ${}^{(4)}X$ defined by Eqs. (4.4) and (4.5) and evaluated in Gaussian coordinates.

Given $(C, X) \in \ker D\Phi(g,\pi)^*$ we construct Gaussian coordinates on a tubular neighborhood of the initial $(t=0)$ surface (M, g, π) and define a vector field ${}^{(4)}X$ on $(-\epsilon, \epsilon) \times M$ by requiring $(L_{(4)X}\,{}^{(4)}g)_{00} = (L_{(4)X}\,{}^{(4)}g)_{0i} = 0$. The components of ${}^{(4)}X$ are thus defined on $({}^{(4)}V = (-\epsilon, \epsilon) \times M,\ {}^{(4)}g)$ by integrating

$$C_{,t} = X^j{}_{,t} + g^{jk}C_{|k} = 0. \tag{5.3}$$

These equations determine ${}^{(4)}X$ uniquely from the initial data $(C, X)_{t=0}$. Furthermore, the remaining six Killing equations $h_{ij} = (L_{(4)X}\,{}^{(4)}g)_{ij} = 0$ are satisfied at the initial surface since, by assumption, $(C, X) \in \ker D\Phi(g,\pi)^*$. This gives, in addition, $p^{ij} = 0$ at the initial surface. In the next section we shall show that $(h, p)(t)$ obey a system of evolution equations which, for vanishing initial data, have only the trivial solution $h(t) = p(t) = 0$ for $-\epsilon < t < \epsilon$. With this result we shall have $h_{ij} = (L_{(4)X}\,{}^{(4)}g)_{ij} = 0$ on $(-\epsilon, \epsilon) \times M$ and thus that $L_{(4)X}\,{}^{(4)}g = 0$ on this Cauchy development of (M, g, π).

VI. PROPAGATION EQUATIONS

In this section we suppose that the adjoint map evaluated at a hypersurface (M, g, π) has nontrivial kernel. We show that for each non-zero element of the kernel one may define a vector field on a Cauchy development of (M, g, π) which is, in fact, a Killing vector field. Linearly independent elements of the kernel correspond to linearly independent Killing fields. Combining this result with that of Sec. IV, we shall conclude that the dimension of $\ker D\Phi(g,\pi)^*$ is equal to the number of independent Killing fields existing on $(-\epsilon, \epsilon) \times M$.

From Cauchy data $(M, g, \pi) \in \mathcal{C}$, the Einstein equations (2.8), (2.9) restricted to Gaussian coordinates $(N = 1,\ N_i = 0)$ uniquely determine a metric ${}^{(4)}g$ on ${}^{(4)}V = (-\epsilon, \epsilon) \times M$. If $(C, X) \in \ker D\Phi(g,\pi)^*$ we integrate Eqs. (5.3) to define a vector field ${}^{(4)}X$ on $({}^{(4)}V, {}^{(4)}g)$ and use Eqs. (4.3) and (4.8) to define $h(t)$ and $p(t)$ for $-\epsilon < t < \epsilon$.

By assumption h and p vanish at the initial ($t=0$) surface and ${}^{(4)}X$ has been defined so that ${}^{(4)}h_{0\nu}=(L_{{}^{(4)}X}\,{}^{(4)}g)_{0\nu}=0$ on ${}^{(4)}V$. We wish to show that $h(t)=0$ and thus that ${}^{(4)}h=L_{{}^{(4)}X}\,{}^{(4)}g=0$ on ${}^{(4)}V$. The idea is to show that $(h(t),\ p(t))$ obey a system of evolution equations which, for vanishing initial data, have only the trivial solution $(h(t),p(t))=0$.

To see why $(h,p)(t)$ should satisfy a system of evolution equations at all recall that, for any vector field ${}^{(4)}X$,

$$L_{{}^{(4)}X}\mathrm{Ric}({}^{(4)}g)=D\,\mathrm{Ric}({}^{(4)}g)\cdot L_{{}^{(4)}X}\,{}^{(4)}g, \tag{6.1}$$

where $\mathrm{Ric}({}^{(4)}g)$ is the Ricci tensor of ${}^{(4)}g$. But when ${}^{(4)}g$ obeys the Einstein equations, $\mathrm{Ric}({}^{(4)}g)=0$, we have $L_{{}^{(4)}X}\mathrm{Ric}({}^{(4)}g)=0$ so that ${}^{(4)}h=L_{{}^{(4)}X}\,{}^{(4)}g$ obeys the linearized Einstein equations

$$D\,\mathrm{Ric}({}^{(4)}g)\cdot{}^{(4)}h=0. \tag{6.2}$$

This familiar result is often called the gauge invariance of the linearized Einstein equations. Recalling their definitions one sees that $h(t)$ and $p(t)$ are the gauge-like perturbations of g and π induced by the vector field ${}^{(4)}X$. Therefore, $(h,p)(t)$ should satisfy the perturbed versions of Eqs. (2.8), (2.9) and ($\Phi=0$). The perturbations of the lapse and shift functions will be found to vanish since this is implied by the equations ${}^{(4)}h_{0\nu}=(L_{{}^{(4)}X}\,{}^{(4)}g)_{0\nu}=0$ which we have already imposed.

One may derive the evolution equations for h and p directly by differentiating Eqs. (4.3) and (4.8) with respect to t. Using Eqs. (2.8) and (2.9) (restricted to Gaussian coordinates) to eliminate the time derivatives of g and π and Eqs. (5.3) to eliminate the time derivatives of C and X one finds, after a lengthy computation, that the time derivatives of h and p may be expressed as

$$\begin{aligned}\partial h_{ij}(t)/\partial t=\{&(\det g)^{-1/2}\,[2(p_{ij}-1/2\,g_{ij}\,\mathrm{tr}p)\\&-\mathrm{tr}h(\pi_{ij}-1/2\,g_{ij}\,\mathrm{tr}\pi)\\&+2(h_{ik}\pi^{k}{}_{j}+h_{jk}\pi^{k}{}_{i}-1/2h_{ij}\,\mathrm{tr}\pi\\&-1/2\,g_{ij}\,h_{mn}\pi^{mn})]\}\,(t),\end{aligned} \tag{6.3}$$

$$\begin{aligned}\partial p^{ij}(t)/\partial t=\{&(\det g)^{1/2}\,[-1/2\,\mathrm{tr}h(R^{ij}-1/2\,g^{ij}R)\\&+h^{ik}R_{k}{}^{j}+h^{jk}R_{k}{}^{i}-1/2h^{ij}R-1/2\,g^{ij}h^{mn}R_{mn}\\&+1/2((\mathrm{tr}h)^{|ij}+h^{ij|k}{}_{|k}-h^{ki|j}{}_{|k}-h^{kj|i}{}_{|k}\\&-g^{ij}(\mathrm{tr}h)^{|k}{}_{|k}+g^{ij}h_{mn}{}^{|mn})]\\&+(\det g)^{-1/2}[-1/4\ \mathrm{tr}h\,g^{ij}(\pi^{kl}\pi_{kl}-1/2(\mathrm{tr}\pi)^{2})\\&+\mathrm{tr}h(\pi^{ik}\pi_{k}{}^{j}-1/2\pi^{ij}\mathrm{tr}\pi)-1/2h^{ij}(\pi^{kl}\pi_{kl}-1/2(\mathrm{tr}\pi)^{2})\\&+g^{ij}(h_{km}\pi^{k}{}_{n}\pi^{mn}-1/2\,h_{kl}\pi^{kl}\,\mathrm{tr}\pi)\\&+g^{ij}(\pi_{kl}p^{kl}-1/2\,\mathrm{tr}p\,\mathrm{tr}\pi)\\&-2h_{kl}(\pi^{ik}\pi^{lj}-1/2\pi^{ij}\pi^{kl})\\&-2g_{kl}(p^{ik}\pi^{lj}+p^{lj}\pi^{ik}-1/2p^{ij}\,\pi^{kl}\\&-1/2\pi^{ij}p^{kl})]\}\,(t)\end{aligned} \tag{6.4}$$

with $-\epsilon<t<\epsilon$. It may be verified that Eqs. (6.3) and (6.4) are the linearized versions of (2.8) and (2.9) where the background metric is expressed in Gaussian coordinates ($N=1$, $N_i=0$) and where the perturbations of N and N_i are taken to vanish (Gaussian gauge conditions). That the perturbations of the lapse and shift functions vanish is equivalent to our requirement that ${}^{(4)}h_{0\nu}=(L_{{}^{(4)}X}\,{}^{(4)}g)_{0\nu}=0$. Thus $(h(t),p(t))$ satisfy the linearized Einstein evolution equations with Gaussian gauge conditions. One can also verify directly that they satisfy the perturbed constraint equations $D\Phi(g(t),\ \pi(t))\cdot(h(t),\ p(t))=0$ [one needs to use the exact equations, $\Phi(g(t),\pi(t))=0$, in verifying this]. However, this also follows from the observation that the perturbed constraints are satisfied initially and are conserved by the evolution equations (a consequence of the perturbed Bianchi identities).

As discussed in Sec. II the linearized Einstein equations determine solutions uniquely from initial data provided suitable gauge conditions are imposed to fix the gauge away from the initial surface. In the present case the gauge is fixed by the Gaussian gauge conditions ${}^{(4)}h_{0\nu}=0$ so that the unique solution for vanishing initial data is $(h_{ij}(t),p^{ij}(t))=0$ for $-\epsilon<t<\epsilon$. The gauge conditions together with the vanishing of $h_{ij}(t)$ give

$${}^{(4)}h_{\mu\nu}=(L_{{}^{(4)}X}\,{}^{(4)}g)_{\mu\nu}=0 \tag{6.5}$$

and thus that ${}^{(4)}X$ is a Killing field on $({}^{(4)}V,\,{}^{(4)}g)$. From this result and those of Sec. IV one sees that linearly independent elements of the kernel of $D\Phi(g,\pi)^{*}$ determine linearly independent vector fields on ${}^{(4)}V$ which are all Killing fields of ${}^{(4)}g$. Therefore, the number of linearly independent Killing vector fields of $({}^{(4)}V,\,{}^{(4)}g)$ is at least as large as the dimension of the kernel of the adjoint map evaluated at the initial hypersurface (M,g,π). However, since the converse of this result was obtained in Sec. IV, we obtain the following:

Theorem 6.1: The dimension of $\ker D\Phi(g,\pi)^{*}$ is equal to the number of linearly independent Killing vector fields of $({}^{(4)}V,\,{}^{(4)}g)$, the spacetime determined (in Gaussian coordinates) by initial data (M,g,π).

VII. DISCUSSION

According to the results obtained here, the Marsden–Fischer criterion for linearization stability (applied to vacuum spacetimes with compact, boundaryless Cauchy surfaces) fails to hold on any Cauchy hypersurface whenever the spacetime admits a Killing vector field. Conversely, if the criterion fails to hold on an initial hypersurface then there is a Cauchy development of this hypersurface which admits one or more Killing vector fields. When Killing vectors do occur one can always derive additional, nonlinear constraints upon the perturbations which are necessary to exclude spurious solutions which do not approximate any curve of exact solutions. In a subsequent paper we shall examine these additional constraints and relate them to the conserved quantities which exist by virtue of the occurence of Killing symmetries of the spacetime. We shall show that the additional constraints are equivalent to requiring that each conserved quantity must vanish.

As mentioned in the introduction, the case of open, asymptotically flat spacetimes is also covered by the Fischer–Marsden theorem though the technical details have not yet been published. There one uses function spaces with suitable asymptotic conditions. The adjoint map fails to be injective only if it admits a nontrivial

kernel within the appropriate function space. Killing vector fields would again provide solutions (C, X) to $D\Phi(g, \pi)^*$. $(C, X) = 0$ but unless (C, X) has appropriate asymptotic behavior it does not count as an element of the kernel. Thus Killing fields, such as those of Minkowski space, which do not vanish at infinity do not contribute to the kernel of the adjoint map and thus do not affect the linearization stability of a solution. A precise statement of this idea must await the full details of the general Fischer–Marsden theorem.

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Lie theory and separation of variables. 6. The equation $iU_t + \Delta_2 U = 0$

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This paper constitutes a detailed study of the nine-parameter symmetry group of the time-dependent free particle Schrödinger equation in two space dimensions. It is shown that this equation separates in exactly 26 coordinate systems and that each system corresponds to an orbit consisting of a commuting pair of first- and second-order symmetry operators. The study yields a unified treatment of the (attractive and repulsive) harmonic oscillator, linear potential and free particle Hamiltonians in a time-dependent formalism. Use of representation theory for the symmetry group permits simple derivations of addition and expansion theorems relating various solutions of the Schrödinger equation, many of which are new.

INTRODUCTION

This paper is a continuation of a series of articles studying the connection between Lie group theory and the separation of variables in the principal equations of mathematical physics.[1-5] The group theoretic method for the description of separation of variables originated from the study of the Helmholtz equation

$$\Delta\psi = \partial_\mu \partial^\mu \psi = \lambda\psi, \quad \partial_\mu = \frac{\partial}{\partial x_\mu}, \quad \mu = 1, 2, \tag{0.1}$$

in two variables for spaces of constant (or zero) curvature. Much of this original work was done by Winternitz and co-workers[6,7] with a view to describing all possible quantum mechanical operators which can be used to label bases for the "little groups" of the Poincaré group. This work used the earlier results of Olevskiĭ,[8] who classified all separable coordinate systems for (0.1) in two and three dimensions for spaces of constant (nonzero) curvature. In order to correlate separation of variables with the underlying symmetry group G of (0.1), it is found necessary to require that ψ be the eigenfunction of an additional basis operator L. This operator belongs to the factor space $T = S/S \cap C$, where C is the center of the universal enveloping algebra U of G and S is the set of all symmetric second order elements in U. There is then a one-to-one correspondence between equivalence classes of elements of T under the action of G and the various distinct orthogonal separable coordinate systems for (0.1). It is found that the operator L in many cases does not correspond to the Casimir operator of a Lie subgroup of G. The resulting type of basis has been termed a non-subgroup basis.[9] We should mention here that the case of the Helmholtz equation in the pseudo-Euclidean plane is somewhat more complicated. The reader is referred to Ref. 10 for further details. The correlation between separation of variables and the symmetry group of (0.1) in n dimensions can easily be extended from the two-dimensional case. A basis is now specified by an $(n-1)$tuple of mutually commuting operators $L_1, \ldots, L_{n-1}$. In addition to equivalence under the group action two such $(n-1)$tuples, $\{L_1, \ldots, L_{n-1}\}'$ and $\{L'_1, \ldots, L'_{n-1}\}$ are equivalent if

$$L_i = \sum_{j=1}^{n-1} a_{ij} L'_j$$

with real nonsingular matrix (a_{ij}).

For the treatment of the Helmholtz equation in a two-dimensional space of positive constant curvature [two-dimensional sphere with symmetry group $SO(3)$], see Refs. 4, 9. The corresponding problem for negative constant curvature [upper sheet of two sheeted hyperboloid with symmetry group $SO(2,1)$], see Refs. 4, 11. Some investigations have also been made for the Helmholtz equation in three dimensions in Euclidean space,[12] on the three-dimensional sphere,[13] and on the upper sheet of the two sheeted three-dimensional hyperboloid.[14]

The present paper is a continuation of Ref. 5 which will be referred to as 5 in the following. In that paper the problem of the separation of variables for the free-particle time-dependent Schrödinger equation in one space dimension was treated in detail, i.e., the equation

$$U_{xx} + iU_t = 0. \tag{0.2}$$

The corresponding symmetry group G of this equation was taken to be that generated by the largest set of first-order partial differential operators in the variables t and x [each of which is a symmetry of (0.2)]. This group is isomorphic to the semidirect product of the three-dimensional Weyl group and $SL(2,R)$. It was found in 5 that there is a correspondence between R-separable coordinate systems for (0.2) and equivalence classes of elements of the Lie algebra of G. In this paper we extend this earlier work to the case of two space dimensions.

We present a detailed study of the free-particle time-dependent Schrödinger equation

$$u_{x_1x_1} + u_{x_2x_2} + iu_t = 0. \tag{0.3}$$

Boyer[15] has classified all equations of the form

$$u_{x_1x_1} + u_{x_2x_2} - V(x_1, x_2)\, u + iu_t = 0, \tag{0.4}$$

which admit a nontrivial symmetry algebra of first order differential operators. He has shown that (1) the maximal dimension for a symmetry algebra is nine, (2) this maximum occurs only for constant, linear, and attractive or repulsive harmonic oscillator potentials, and (3) the algebras of maximal dimension are isomorphic. Furthermore, it is known, e.g., Niederer,[16] that the oscillator and linear potential equations are actually equivalent to (0.3). In this paper we will examine the equivalence explicitly and relate it to separation of variables for (0.3).

In Sec. 1 we rederive the nine-parameter symmetry group G of (0.3). Here G is a semidirect product of the five-parameter Weyl group W and $SO(2)\otimes SL(2,R)$. We determine the global action of G and compute the orbit structure of its Lie algebra $\mathcal{G}$ (the Schrödinger algebra) under the adjoint representation. We also determine the second order symmetry operators admitted by (0.3) and show that they form a 20-dimensional vector space consisting of symmetric quadratic polynomials from $\mathcal{G}$. (This last computation was carried out in Ref. 17 for the equivalent case of the harmonic oscillator, but the results are incomplete.)

In Sec. 2 we classify the 26 possible coordinate systems such that variables separate in (0.3). In Sec. 3 we show that each such system is characterized by a G-orbit of symmetry operators, an element of which consists of a commuting pair of symmetries, one first order and one second order. Our derivation of possible coordinates which permit separation and the relation to G-orbits is new. We also show that each of these orbits can be naturally associated with exactly one of the four Hamiltonians mentioned above.

In Secs. 4 and 5 we compute the eigenbasis in a two-parameter model for a representative of each G-orbit. We also calculate the basis in the three-parameter model of functions depending on variables x_1, x_2, t and determine overlap functions relating various distinct bases. Our knowledge of the G-structure of (0.3) greatly simplifies these computations and provides many expansion theorems for functions in $L_2(R_2)$, some of which are new.

Among the special functions arising as solutions of (0.3) are Bessel, Airy, Hermite, parabolic cylinder, Mathieu, Laguerre, and Ince functions. Our group theoretic approach provides deep insight into the problem of expanding one of these functions in terms of another. Unless otherwise mentioned, all special functions are defined as in the Bateman project.[18]

1. SYMMETRIES OF THE EQUATION $iu_t + \Delta_2 u = 0$

Let X be the partial differential operator

$$X = i\partial_t + \partial_{x_1x_1} + \partial_{x_2x_2} \tag{1.1}$$

acting on the space $\mathcal{J}$ of locally C^∞ functions of the real variables x_j, t. We begin by determining the maximal symmetry algebra of the free-particle Schrödinger equation

$$iu_t + u_{x_1x_1} + u_{x_2x_2} = Xu = 0, \tag{1.2}$$

i.e., we compute all linear differential operators

$$L = a(x_j,t)\,\partial_{x_1} + b(x_j,t)\,\partial_{x_2} + c(x_j,t)\,\partial_t + d(x_j,t),$$
$$a,\ldots,d \in \mathcal{J}, \tag{1.3}$$

such that Lu is a solution of (1.2) whenever u is a solution. A necessary and sufficient condition for L to be a symmetry is

$$[L,X] = r(x_j,t)X \tag{1.4}$$

for some $r \in \mathcal{J}$.[15,19,20] Equating coefficients of $\partial_{x_jx_j}, \partial_t, \partial_{x_j}$ and 1 on both sides of (1.4), we obtain a system of differential equations for $a,\ldots,d,r$, see Refs. 15, 19 for details. Solving these equations, one finds that the allowable L form a nine-dimensional complex Lie algebra $\mathcal{G}^c$ with basis

$$K_2 = -t^2\partial_t - t(x_1\partial_{x_1} + x_2\partial_{x_2}) - t + (i/4)(x_1^2 + x_2^2),\quad K_{-2} = \partial_t,$$
$$P_j = \partial_{x_j},\quad B_j = -t\partial_{x_j} + ix_j/2,\quad M = x_1\partial_{x_2} - x_2\partial_{x_1},\quad E = i,$$
$$D = x_1\partial_{x_1} + x_2\partial_{x_2} + 2t\partial_t + 1 \tag{1.5}$$

and commutation relations

$$[D,K_{\pm2}] = \pm 2K_{\pm2},\quad [D,B_j] = B_j,\quad [D,P_j] = -P_j$$
$$[D,M] = 0,\quad [M,K_{\pm2}] = 0,\quad [P_j,M] = (-1)^{j+1}P_l,$$
$$[B_j,M] = (-1)^{j+1}B_l,\quad [K_2,K_{-2}] = D,\quad [K_2,B_j] = 0,$$
$$[K_{-2},B_j] = -P_j,\quad [K_{-2},P_j] = 0,\quad [P_j,K_2] = B_j,$$
$$[P_j,B_j] = \tfrac{1}{2}E,\quad [P_j,B_l] = 0,\quad j,l = 1,2,\ j \neq l, \tag{1.6}$$

with E in the center of $\mathcal{G}^c$. In the following we will study only the real Lie algebra $\mathcal{G}$ with basis (1.5), the Schrödinger algebra.

A second useful basis for $\mathcal{G}$ is given by the operators B_j, P_j, E which generate the five-dimensional Weyl algebra $\mathcal{W}$, the operator M, and the three operators L_1, L_2, L_3, where

$$L_1 = D,\quad L_2 = K_2 + K_{-2},\quad L_3 = K_{-2} - K_2. \tag{1.7}$$

Here,

$$[L_1,L_2] = -2L_3,\quad [L_3,L_1] = 2L_2,\quad [L_2,L_3] = 2L_1 \tag{1.8}$$

so that the L_ν satisfy the commutation relations of $sl(2,R)$. It follows that $\mathcal{G}$ is the semidirect product of $sl(2,R)\oplus o(2)$ and $\mathcal{W}$. Here $o(2)$ is the one-dimensional Lie algebra spanned by M.

Using standard results from Lie theory,[21] we can exponentiate the differential operators in $\mathcal{G}$ to obtain a local Lie group G of operators acting on $\mathcal{J}$ and mapping solutions of (1.2) into solutions, the Schrödinger group. The action of the Weyl group W is given by operators

$$T(\mathbf{w},\mathbf{z},\alpha) = \exp(w_1B_1)\exp(z_1P_1)\exp(w_2B_2)\exp(z_2P_2)$$
$$\times\exp(\alpha E),$$
$$\mathbf{w} = (w_1,w_2),\quad \mathbf{z} = (z_1,z_2)$$

such that

$$T(\mathbf{w},\mathbf{z},\alpha)\,T(\mathbf{w}',\mathbf{z}',\alpha') = T(\mathbf{w}+\mathbf{w}',\mathbf{z}+\mathbf{z}',\alpha+\alpha'+\tfrac{1}{2}\mathbf{w}'\circ\mathbf{z}), \tag{1.9}$$

where

$$[T(\mathbf{w},\mathbf{z},\alpha)f](\mathbf{x},t)=\exp(i/4)(2\mathbf{x}\cdot\mathbf{w}-t\,\mathbf{w}\cdot\mathbf{w}+4\alpha)]$$
$$\times f[\mathbf{x}-t\,\mathbf{w}+\mathbf{z},t],\quad f\in\mathcal{J}.$$

The action of $SO(2)$ is given by $T(\theta)=\exp\theta M$,

$$T(\theta)\,T(\theta')=T(\theta+\theta'),$$

where

$$[T(\theta)f](\mathbf{x},t)=f(\mathbf{x}\Theta,t),$$
$$\Theta=\begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix}. \tag{1.10}$$

Finally, the action of $SL(2,R)$ is given by operators

$$[T(A)f](x,t)=\exp[i\beta(x^2+y^2)/[4(\delta+t\beta)](\delta+t\beta)^{-1}$$
$$\times f[(\delta+t\beta)^{-1}\mathbf{x},(\gamma+t\alpha)/(\delta+t\beta)],\quad f\in\mathcal{J},$$
$$A=\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}\in SL(2,R), \tag{1.11}$$

where

$$T(A)\,T(B)=T(AB),\quad A,B\in SL(2,R).$$

The one-parameter subgroups of $SL(2,R)$ generated by $K_{\pm2},L_1,L_2,L_3$, respectively, are given by expressions (1.11) in Ppaer 5. The adjoint actions of $SO(2)$ and $SL(2,R)$ on W are

$$T^{-1}(A)\,T(\mathbf{w},\mathbf{z},\alpha)\,T(A)=T(\mathbf{w}A,\mathbf{z}A,\alpha'),$$
$$\alpha'=\alpha+\tfrac{1}{4}(\mathbf{w}\circ\mathbf{z}-\mathbf{w}A\circ\mathbf{z}A), \tag{1.12}$$
$$T^{-1}(\theta)\,T(\mathbf{w},\mathbf{z},\alpha)\,T(\theta)=T(\mathbf{w}\Theta,\mathbf{z}\Theta,\alpha).$$

These identities define G as a semidirect product of $SL(2,R)\oplus SO(2)$ and W:

$$g=(A,\theta,v)\in G,\quad A\in SL(2,R),\quad \theta\in SO(2),$$
$$v=(\mathbf{w},\mathbf{z},\alpha)\in W, \tag{1.13}$$
$$T(g)=T(A)\,T(\theta)\,T(v).$$

The group G acts on the Lie algebra $\mathcal{G}$ of differential operators K via the adjoint representation

$$K\to K^g=T(g)KT^{-1}(g)$$

and this action splits $\mathcal{G}$ into G-orbits. We will classify the orbit structure of the factor algebra $\mathcal{G}'\cong\mathcal{G}/\{E\}$, where $\{E\}$ is the center of $\mathcal{G}$. Let $K\in\mathcal{G}'$ and let A_2,A_0,A_{-2} respectively, be the coefficients corresponding to K_2,D,K_{-2} in the expansion of $K\neq0$ in terms of the basis (1.5). Setting $\alpha=A_2A_{-2}+A_0^2$, we find that α is invariant under the adjoint representation.

The following list is a complete set of orbit representatives in the sense that any $K\neq0$ lies on the same G-orbit as a real multiple of exactly one of the operators in this list:

Case 1($\alpha<0$): $K_{-2}-K_2+\beta^2M$, $|\beta|\neq1$, $K_{-2}-K_2+M+\gamma B_1$;

Case 2($\alpha>0$): $D+\beta M$;

Case 3($\alpha=0$): K_2+M, K_2+P_1, K_2, M, P_1+B_2, P_1. (1.14)

We next consider the problem of determining symmetries of (1.2) which are differential operators of arbitrary finite order in x_1, x_2, and t. That is, we look for linear differential operators S of arbitrary order which map solutions of (1.2) into solutions. This is equivalent to the requirement that

$$[S,X]=RX$$

for some linear differential operator R of arbitrary finite order in x_1, x_2, and t. Since we will only apply S to solutions u of $Xu=0$, without loss of generality we can require that S contains no derivatives in t. In other words, wherever ∂_t appears in S we can replace it by $i(\partial_{x_1x_1}+\partial_{x_2x_2})$. Another way to view this is to note that if S is a symmetry operator, then so is $S'=S+QX$, where Q is an arbitrary differential operator. Moreover, $S'u=Su$ for any solution u of (1.2). There is a unique choice of Q such that S' contains no derivatives with respect to t.

With this in mind we see that only the operators P_j,B_j,E, generating the Weyl algebra and M are first order or less in the x_j. The elements $K_2=-i(B_1^2+B_2^2)$, $K_{-2}=i(P_1^2+P_2^2)$, and $D=-i(B_1P_1+P_1B_1+B_2P_2+P_2B_2)$ are second order. [These equalities are valid modulo the replacement of ∂_t by $i(\partial_{x_1x_1}+\partial_{x_2x_2})$.] More generally we can compute all symmetries S which are second order or less in x_1 and x_2:

$$S=\sum_{i,j=1}^{2}a_{ij}(x_1,x_2,t)\,\partial_{x_ix_j}$$
$$+\sum_{i=1}^{2}b_i(x_1,x_2,t)\,\partial_{x_i}+c(x_1,x_2,t).$$

A tedious computation shows that such S form a 20-dimensional vector space. A basis for this space is provided by the zeroth-order operator E, the five first-order operators P_j,B_j,M and the three second-order operators $iK_{\pm2},iD$ listed above, plus the eleven second-order operators

$$B_1^2-B_2^2,\quad B_1P_1-B_2P_2,\quad P_1^2-P_2^2,\quad B_1M+MB_1,\quad B_2M+MB_2,$$
$$P_1M+MP_1,\quad P_2M+MP_2,\quad B_1B_2,\quad P_1P_2,\quad B_1P_2+B_2P_1,\quad M^2. \tag{1.15}$$

It follows that all second-order symmetries are symmetric quadratic forms in B_j, P_j, E, and M.

2. SEPARATION OF VARIABLES FOR THE EQUATION $u_{xx}+u_{yy}+iu_t=0$

In this section we examine the problem of separation of variables for Eq. (1.2). As with the similar problem for one space dimension treated in 5, we proceed directly. Let us first make the transformation of coordinates

$$x=G(v_1,v_2,v_3)\quad y=H(v_1,v_2,v_3),\quad t=F(v_1,v_2,v_3) \tag{2.1}$$

with G, H, and F real functions of v_i $(i=1,2,3)$. Then we have for the partial derivatives

$$\partial_x=B_{11}\partial_1+B_{21}\partial_2+B_{31}\partial_3,$$
$$\partial_y=B_{12}\partial_1+B_{22}\partial_2+B_{32}\partial_3, \tag{2.2}$$
$$\partial_t=B_{13}\partial_1+B_{23}\partial_2+B_{33}\partial_3,$$

where $B_{ij}=M_{ij}/\det A$, M_{ij} being the cofactor of the matrix

$$A=\begin{bmatrix} G_1 & H_1 & F_1 \\ G_2 & H_2 & F_2 \\ G_3 & H_3 & F_3 \end{bmatrix}, \tag{2.3}$$

(subscripts on the functions G, H, and F denote differentiation with respect to the variables v_i).

Equation (1.2) can then be written in the form

$$\begin{aligned} &a_{11}\partial_{11}+a_{22}\partial_{22}+a_{33}\partial_{33}+a_{12}\partial_{12}+a_{13}\partial_{13}+a_{23}\partial_{23} \\ &\quad+a_1\partial_1+a_1\partial_2+a_3\partial_3+i(b_1\partial_1+b_2\partial_2+b_3\partial_3)=0 \end{aligned} \tag{2.4}$$

We now consider the possible cases for the coefficients a_{ij} $(i<j)$:

(i) $a_{ij}\neq 0$ for all $i<j$. In this case the only way to have a separable solution is for two of the solutions to be exponentials and all the remaining coefficients to be functions of the remaining variable.

(ii) $a_{12}=0$, $a_{13},a_{23}\neq 0$. The only possible separable solution is an exponential solution in the variable v_3. The coefficients are then functions of v_1 and v_2.

(iii) $a_{12}=0, a_{13}=0, a_{23}\neq 0$. The only possible solution is an exponential solution in the variable v_3.

(iv) $a_{ij}=0 (i<j)$.

Let us proceed to evaluate all coordinate systems which are of type (iv) and admit a separation of variables. We shall see that all the coordinate systems of interest arise in this case. We shall discuss the evaluation of cases (i)—(iii) at the end of this section. For the conditions $a_{ij}=0 (j>i)$ we must have the relations

$$\begin{aligned} &B_{11}B_{21}+B_{12}B_{22}=0, \\ &B_{21}B_{31}+B_{22}B_{32}=0, \\ &B_{11}B_{31}+B_{12}B_{32}=0. \end{aligned} \tag{2.5}$$

These conditions may be interpreted to mean that the vectors $\mathbf{b}_1=(B_{11},B_{12})$, $\mathbf{b}_2=(B_{21},B_{22})$, and $\mathbf{b}_3=(B_{31},B_{32})$ are mutually orthogonal. Therefore, there must exist a nontrivial relation of the form

$$\alpha\mathbf{b}_1+\beta\mathbf{b}_2+\gamma\mathbf{b}_3=0 \tag{2.6}$$

with $(\alpha,\beta,\gamma)\neq(0,0,0)$. Let us enumerate the possibilities for the vector (α,β,γ):

(i) α,β,γ all nonzero. This case implies B_{ij} $(j\neq 3)$ are all zero and is hence inadmissable.

(ii) $\gamma=0$, β,α nonzero. This case implies that $B_{21}=B_{31}=B_{22}=B_{32}=0$. Now, considering the conditions $B_{21}=B_{22}=0$ which can be written

$$H_1F_3-F_1H_3=G_1F_3-F_1G_3=0,$$

we see that, in order to have the partial derivative ∂_2 appear in (2.4) at all, we must have $H_1G_3-G_1H_3\neq 0$. This implies $F_1=F_3=0$; the other conditions similarly imply that $F_2=F_3=0$. The matrix A is then singular. This case is therefore inadmissable.

(iii) $\alpha,\beta=0$, γ nonzero. This case implies by reasoning as in case (ii) that $F_1=F_2=0$, so that $F=F(v_3)$ and $F\neq$ const. Accordingly we can define $F(v_3)=v_3$. For this case $\det A=G_1H_2-H_1G_2$ and we have the simplifications $M_{11}=H_2$, $M_{12}=-G_2$, $M_{21}=-H_1$, $M_{22}=G_1$. The only nontrivial constraint arising from conditions (2.5) is

(*) $H_1H_2+G_1G_2=0$.

There are two possible types of separation.

(1) There is an exponential solution in the variable v_1 and $B_{12}=0$. The conditions of separation then also require $B_{21}=0$. For a nonsingular choice of coordinates these conditions imply $H_1=0$, $G_2=0$. The condition $\partial_1(H_2/G_1)=0$ implies that $G=h(v_3)v_1+f(v_3)$. In particular the condition $\partial_1(B_{31})=0$ requires $h=$ const. We can, by suitably redefining the variable v_1, take $f=0$. The corresponding problem then is equivalent to finding all separable coordinate systems for the equation $\lambda^2+u_{yy}+iu_t=0$. The only new coordinate system is then

$$x=v_1,\quad y=v_3^{1/2}v_2,\quad t=v_3. \tag{2.7}$$

If we remove the requirement $B_{12}=0$, then the coordinates which have exponential solutions will appear in separable systems of the second type (see below).

(2) These are coordinate systems for which all B_{ij}, $(i,j=1,2)$ are nonzero.

The conditions for separation for the second derivative terms are

$$\begin{aligned} &B_{11}^2+B_{12}^2=f(v_1,v_2)/h^2(v_3) \\ &B_{21}^2+B_{22}^2=g(v_1,v_2)/h^2(v_3) \end{aligned} \tag{2.8}$$

Now for functions $G=\bar{G}h$, $H=\bar{H}h$, the corresponding reduced functions $\bar{B}_{ij}$ $(i,j=1,2)$ satisfy the constraints (2.8) without the $h^2(v_3)$ term on the right-hand side. The conditions for separation in v_1,v_2 satisfied by the $\bar{B}_{ij}$ are then exactly those conditions satisfied for separation of variables in the two-dimensional Helmholtz equation in orthogonal coordinates. Therefore, to within a Euclidean motion $\bar{G},\bar{H}$, assume one of the four standard separable forms of the Helmholtz equation in two space dimensions. We can thus write

$$\begin{aligned} &G=h[\cos\alpha\,\mathcal{F}_i-\sin\alpha\,\mathcal{H}_i]+T, \\ &H=h[\sin\alpha\,\mathcal{F}_i+\cos\alpha\,\mathcal{H}_i]+U, \end{aligned} \tag{2.9}$$

where α, T, and U can be functions of v_3. The standard separable forms will be taken as:

1) Cartesian coordinates:

$$\mathcal{F}_1=v_1,\quad \mathcal{H}_1=v_2; \tag{2.10}$$

2) polar coordinates:

$$\mathcal{F}_2=v_1\cos v_2,\quad \mathcal{H}_2=v_1\sin v_2; \tag{2.11}$$

3) parabolic coordinates:

$$\mathcal{F}_3=\tfrac{1}{2}(v_1^2-v_2^2),\quad \mathcal{H}_3=v_1v_2; \tag{2.12}$$

4) elliptic coordinates:

$$\mathcal{F}_4=\cosh v_1\cos v_2,\quad \mathcal{H}_4=\sinh v_1\sin v_2. \tag{2.13}$$

The remaining conditions for separability then become

$$B_{13}=f(v_1,v_2)/h^2,\quad B_{23}=g(v_1,v_2)/h^2. \tag{2.14}$$

The form of the functions f and g is determined by the choice of $\mathcal{F}_i$ and $\mathcal{H}_i$. It follows from the general form

(2.4) that the functions h, α, T, and U have the general form

$$h=\sqrt{bv_3+c},\quad \alpha=K\ln(bv_3+c),\qquad T=av_3,\quad U=bv_3. \tag{2.15}$$

We shall now summarize our results. In each case we give the form of the functions f and g in Eqs. (2.14) and the corresponding coordinates in reduced form.

1) Cartesian coordinates. In this case $f=f(v_1)$, $g=g(v_2)$, and $K=0$. The contributions of T and U may be transformed away by using the v_3 translation properties of the Weyl group action. This process does not affect separability. The resulting coordinate systems are then

$$x=v_3^{1/2}v_1,\quad y=v_3^{1/2},\quad t=v_3, \tag{2.16}$$

$$x=v_1,\quad y=v_2,\quad t=v_3. \tag{2.17}$$

2) Polar coordinates. In this case $f=f(v_1)$, $g=g(v_1)$, and T and U are both zero. In particular for $b\neq 0$ we have $K\neq 0$. The resulting coordinate systems are

(i) $$x=v_3^{1/2}v_1\cos(v_2+K\ln v_3),\quad t=v_3,\qquad y=v_3^{1/2}v_1\sin(v_2+K\ln v_3), \tag{2.18}$$

(ii) $$x=v_1\cos v_2,\quad y=v_1\sin v_2,\quad t=v_3. \tag{2.19}$$

3) Parabolic coordinates. In this case $f=\bar{f}(v_1)/(v_1^2+v_2^2)$ and $g=\bar{g}(v_2)/(v_1^2+v_2^2)$. This implies that K, U, T, and b are all zero. We thus have only one coordinate system, viz.,

$$x=\tfrac{1}{2}(v_1^2-v_2^2),\quad y=v_1v_2,\quad t=v_3. \tag{2.20}$$

4) Elliptic coordinates. In this case $f=\bar{f}(v_1)/(\sinh^2v_1+\cos^2v_2)$ and $g=\bar{g}(v_2)/(\sinh^2v_1+\cos^2v_2)$. This implies that K, U, T are zero. The two resulting coordinate systems are

(i) $$x=v_3^{1/2}\cosh v_1\sin v_2,\quad y=v_3^{1/2}\sinh v_1\cos v_2,\quad t=v_3, \tag{2.21}$$

(ii) $$x=\cosh v_1\sin v_2,\quad y=\sinh v_1\cos v_2,\quad t=v_3. \tag{2.22}$$

This completes the list of separable coordinate systems. In particular we note that we can essentially take $K=0$ for the angular variable in the system (2.18) by redefining the variable v_2. We now seek to classify all solutions of (1.2) which admit an R-separable solution, i.e., a solution of the form $u=\exp Q(v_1,v_2,v_3)\times A(v_1)B(v_2)C(v_3)$, where Q is not expressible as a sum of functions of each of the individual variables v_i nor is it a constant. If we extract the multiplier and write down the equation for the product, we obtain an equation of the form (2.4) with new coefficients $\bar{a}_i$ and an additional constant term a_0 on the left-hand side. The possible types of R-separation can then be classified in the same manner, i.e., types (1) and (2). For solutions of type (1) we have the R-separable solutions for the corresponding equation in one space dimension found previously in Paper 5. They are:

(i) $$x=v_1,\quad y=v_2v_3+b/v_3,\quad t=v_3,\qquad S=\tfrac{1}{4}v_2^2v_3-bv_2/2v_3; \tag{2.23}$$

(ii) $$x=v_1,\quad y=v_2+bv_3^2,\quad t=v_3,\qquad S=bv_2v_3; \tag{2.24}$$

(iii) $$x=v_1,\quad y=v_2(1+v_3^2)^{1/2},\quad t=v_3,\qquad S=\tfrac{1}{4}v_2^2v_3; \tag{2.25}$$

(iv) $$x=v_1,\quad y=v_2(1-v_3^2)^{1/2},\quad t=v_3\ (|v_3|<1),\qquad S=-\tfrac{1}{4}v_2^2v_3 \tag{2.26}$$

$$x=v_1,\quad y=v_2(v_3^2-1)^{1/2},\quad t=v_3\ (|v_3|>1),\qquad S=\tfrac{1}{4}v_2^2v_3.$$

Here we have written the multiplier function $Q=R+iS$ and $R=0$ in each case. For R-separable solutions of type (2) we again require that G and H have the form given in (2.9) with $\alpha=0$. The coefficients of the partial derivatives ∂_1 and ∂_2 are then

$$c_1=2a_{11}R_1+a_1+i(2a_{11}S_1+b_1),\qquad c_2=2a_{22}R_2+a_2+i(2a_{22}S_2+b_2), \tag{2.27}$$

respectively.

The requirement of separability implies that R is at most a sum of functions of the individual variables. We may therefore take $R=0$. We give an outline of the method for the case $\mathcal{F}=v_1$, $\mathcal{H}=v_2$ and then list the results for the remaining coordinate systems. From the requirement that $c_1=f(v_1)$, $c_2=g(v_2)$ we find that S can be written in the form

$$S=\tfrac{1}{4}hh'(v_1^2+v_2^2)+\tfrac{1}{2}h(T'v_1+U'v_2). \tag{2.28}$$

Then from the constraint

$$\begin{aligned}a_0&=a_{11}(-S_1^2+iS_{11})+a_{22}(-S_2^2+iS_{22})\\&\quad+ia_1S_1+ia_2S_2-b_1S_1-b_2S_2-b_3S_3\\&=(p(v_1)+q(v_2))/h^2+s(v_3)\end{aligned} \tag{2.29}$$

we obtain the following set of coordinate systems:

(i) $$x=v_1v_3+a/v_3,\quad y=v_2v_3+b/v_3,\quad t=v_3,\quad a,b\geq 0,\qquad S=\tfrac{1}{4}(v_1^2+v_2^2)v_3-(1/2v_3)(av_1+bv_2); \tag{2.30}$$

(ii) $$x=v_1+av_3^2,\quad y=v_2+bv_3^2,\quad t=v_3,\quad a,b\geq 0,\qquad S=(av_1+bv_2)v_3; \tag{2.31}$$

(iii) $$x=v_1(1+v_3^2)^{1/2},\quad y=v_2(1+v_3^2)^{1/2},\quad t=v_3,\qquad S=\tfrac{1}{4}(v_1^2+v_2^2)v_3; \tag{2.32}$$

(iv) $$x=v_1(1-v_3^2)^{1/2},\quad y=v_2(1-v_3^2)^{1/2},\quad t=v_3,\quad |v_3|<1,\qquad S=-\tfrac{1}{4}(v_1^2+v_2^2)v_3, \tag{2.33}$$

$$x=v_1(v_3^2-1)^{1/2},\quad y=v_2(v_3^2-1)^{1/2},\quad t=v_3,\quad |v_3|>1,\qquad S=\tfrac{1}{4}(v_1^2+v_2^2)v_3.$$

In the remaining three types of coordinate systems we have the following possibilities:

Polar coordinates:

(i) $$x=(1+v_3^2)^{1/2}v_1\cos v_2,\ y=(1+v_3^2)^{1/2}v_1\sin v_2,\quad t=v_3,\qquad S=\tfrac{1}{4}v_1^2v_3; \tag{2.34}$$

(ii) $$x=(1-v_3^2)^{1/2}v_1\cos v_2,\quad y=(1-v_3^2)^{1/2}v_1\sin v_2,\quad t=v_3,\quad |v_3|<1,\qquad S=-\tfrac{1}{4}v_1^2v_3;$$

$$x=(v_3^2-1)^{1/2}v_1\cos v_2,\quad y=(v_3^2-1)^{1/2}v_1\sin v_2,$$
$$t=v_3,\quad |v_3|>1,$$
$$S=\tfrac{1}{4}v_1^2v_3; \tag{2.35}$$

(iii) $$x=v_3v_1\cos v_2,\quad y=v_3v_1\sin v_2,\quad t=v_3$$
$$S=\tfrac{1}{4}v_1^2v_3. \tag{2.36}$$

Parabolic coordinates:

(i) $$x=\tfrac{1}{2}(v_1^2-v_2^2)v_3+a/v_3,\quad y=v_1v_2v_3,\quad t=v_3,$$
$$S=\tfrac{1}{16}(v_1^2+v_2^2)^2v_3-(a/4v_3)(v_1^2-v_2^2); \tag{2.37}$$

(ii) $$x=\tfrac{1}{2}(v_1^2-v_2^2)+av_3^2,\quad y=v_1v_2,\quad t=v_3,$$
$$S=\tfrac{1}{2}a(v_1^2-v_2^2)v_3. \tag{2.38}$$

Elliptic coordinates:

(i) $$x=(1+v_3^2)^{1/2}\cosh v_1\sin v_2,\quad y=(1+v_3^2)^{1/2}\sinh v_1\cos v_2,$$
$$t=v_3,$$
$$S=\tfrac{1}{4}v_3(\sinh^2v_1+\cos^2v_2); \tag{2.39}$$

(ii) $$x=(1-v_3^2)^{1/2}\cosh v_1\cos v_2,\quad y=(1-v_3^2)^{1/2}\sinh v_1\sin v_1,$$
$$t=v_3,\quad |v_3|<1,$$
$$S=-\tfrac{1}{4}v_3(\sinh^2v_1+\cos^2v_2);$$
$$x=(v_3^2-1)^{1/2}\cosh v_1\cos v_2,\ y=(v_3^2-1)^{1/2}\sinh v_1\sin v_2,$$
$$t=v_3,\quad |v_3|>1,$$
$$S=\tfrac{1}{4}v_3(\sinh^2v_1+\cos^2v_2); \tag{2.40}$$

(iii) $$x=v_3\cosh v_1\sin v_2,\quad y=v_3\sinh v_1\cos v_2,\quad t=v_3,$$
$$S=\tfrac{1}{4}v_3(\sinh^2v_1+\cos^2v_2). \tag{2.41}$$

This completes the list of R-separable solutions of (1.2).

At this point we comment on the separable solutions of types (i)—(iii). In defining a separable coordinate system we require that in addition to admitting a separable solution, the equation in question be equivalent to three ordinary differential equations, one in each of the separation variables. For solutions of type (i)—(iii) this is not the case as we have proven. Separable solutions of types (i)—(iii) actually correspond to a change of coordinates

$$x=a_{1j}v_j,\quad y=a_{2j}v_j,\quad t=a_{3j}v_j,$$
$$\det(a_{ij})\neq 0,\quad a_{ij}\ \text{constants}. \tag{2.42}$$

We accordingly make no further comment on these cases.

The general features of the separable systems we have classified are evident from our explicit procedure. Corresponding to each system there is always a first order operator K and a second-order operator S defining the coordinate system in question. These two operators are also symmetries of (1.2), mapping solutions into solutions. The operators K and S can accordingly be expressed as first- and second-order operators, respectively, in the generators of the Lie algebra $\mathcal{G}$. The form of these basis defining operators is discussed in the next section. The notation for the coordinate systems we have introduced in Table I requires some comment. The capital letter corresponds to the type of Hamiltonian, i.e., F ⟷ free particle, L ⟷ stark effect (linear potential), O ⟷ harmonic oscillator, and R ⟷ repulsive harmonic oscillator. The small letters indicate the type of coordinates used in each of these Hamiltonians, i.e., c ⟷ Cartesian, r ⟷ radial (polar) coordinates, p ⟷ parabolic, and e ⟷ elliptic coordinates. The superscript (i) determines the coordinate

TABLE I. Separable coordinate systems for the equation $U_{xx}+U_{yy}+iU_t=0$ $(\epsilon=\operatorname{sgn}(1-v_3^2))$.

Coordinate system	Coordinates	Multiplier e^{iS}
1) $Fc^{(1)}$	$x=v_1v_3,\ y=v_2v_3$	$S=(v_1^2+v_2^2)v_3/4$
2) $Fc^{(2)}$	$x=v_1,\ y=v_2$	0
3) $Fr^{(1)}$	$x=v_1v_3\cos v_2,\ y=v_1v_3\sin v_2$	$v_1^2v_3/4$
4) $Fr^{(2)}$	$x=v_1\cos v_2,\ y=v_1\sin v_2$	0
5) $Fp^{(1)}$	$x=v_3(v_1^2-v_2^2)/2,\ y=v_1v_2v_3$	$(v_1^2+v_2^2)^2v_3/16$
6) $Fp^{(2)}$	$x=(v_1^2-v_2^2)/2,\ y=v_1v_2$	0
7) $Fe^{(1)}$	$x=v_3\cosh v_1\cos v_2,\ y=v_3\sinh v_1\sin v_2$	$(\sinh^2v_1+\cos^2v_2)v_3/4$
8) $Fe^{(2)}$	$x=\cosh v_1\cos v_2,\ \sinh v_1\sin v_2$	0
9) $Lc^{(1)}$	$x=v_1v_3+a/v_3,\ y=v_2v_3+b/v_3$	$(v_1^2+v_2^2)v_3/4-(1/2v_3)(av_1+bv_2)$
10) $Lc^{(2)}$	$x=v_1+av_3^2,\ y=v_2+bv_3^2$	$(av_1+bv_2)v_3$
11) $Lp^{(1)}$	$x=v_3(v_1^2-v_2^2)/2+a/v_3,\ y=v_1v_2v_3$	$(v_1^2+v_2^2)^2v_3/16-(a/4v_3)(v_1^2-v_2^2)$
12) $Lp^{(2)}$	$x=(v_1^2-v_2^2)/2+av_3^2,\ y=v_1v_2$	$av_3(v_1^2-v_2^2)/2$
13) Oc	$x=v_1(1+v_3^2)^{1/2},\ y=v_2(1+v_3^2)^{1/2}$	$(v_1^2+v_2^2)v_3/4$
14) Or	$x=(1+v_3^2)^{1/2}v_1\cos v_2,\ y=(1+v_3^2)^{1/2}v_1\sin v_2$	$v_1^2v_3/4$
15) Oe	$x=(1+v_3^2)^{1/2}\cosh v_1\cos v_2,\ y=(1+v_3^2)^{1/2}\sinh v_1\sin v_2$	$(\sinh^2v_1+\cos^2v_2)v_3/4$
16) $Rc^{(1)}$	$x=v_1v_3^{1/2},\ y=v_2v_3^{1/2}$	0
17) $Rc^{(2)}$	$x=v_1(\lvert v_3^2-1\rvert)^{1/2},\ y=v_2(\lvert v_3^2-1\rvert)^{1/2}$	$\epsilon(v_1^2+v_2^2)v_3/4$
18) $Rr^{(1)}$	$x=v_1v_3^{1/2}\cos v_2,\ y=v_2v_3^{1/2}\sin v_2$	0
19) $Rr^{(2)}$	$x=(\lvert v_3^2-1\rvert)^{1/2}v_1\cos v_2,\ y=(\lvert v_3^2-1\rvert)^{1/2}v_1\sin v_2$	$\epsilon v_1^2v_3/4$
20) $Re^{(1)}$	$x=v_3^{1/2}\cosh v_1\cos v_2,\ y=v_3^{1/2},\ y=v_3^{1/2}\sinh v_1\sin v_2$	0
21) $Re^{(2)}$	$x=(\lvert v_3^2-1\rvert)^{1/2}\cosh v_1\cos v_2,\ y=(\lvert v_3^2-1\rvert)^{1/2}\sinh v_1\sin v_2$	$\epsilon(\sinh^2v_1+\cos^2v_2)v_3/4$
22) L1	$x=v_1,\ y=v_2v_3+b/v_3$	$v_3v_2^2/4-bv_2/2v_3$
23) L2	$x=v_1,\ y=v_2+av_3^2$	av_2v_3
24) O1	$x=v_1,\ y=v_2(1+v_3^2)^{1/2}$	$v_3v_1^2/4$
25) R1	$x=v_1,\ y=v_2v_3^{1/2}$	0
26) R2	$x=v_1,\ y=v_2(\lvert v_3^2-1\rvert)^{1/2}$	$\epsilon v_2^2v_3/4$

system which is the simpler of two which lie on the same orbit from the point of view of the spectral analysis in a given basis.

3. THE OPERATOR CHARACTERIZATION OF VARIABLE SEPARATION

From the method of the preceding section we see that corresponding to every separation of variables for Eq. (1.2) we can find a pair of commuting differential operators K,S such that:

1) K and S are symmetries of (1.2);
2) K is first order in x_1, x_2, t and contains a term in ∂_t (except for the subgroup coordinates);
3) S is second order in x_1, x_2 and contains no terms in ∂_t.

The separation of variables is then characterized by the simultaneous equations

$$Xu=0, \quad Ku=i\lambda u, \quad Su=\mu u. \tag{3.1}$$

In particular, the eigenvalues λ, μ are the usual separation constants.

It follows from the results of Sec. 1 that K lies in the symmetry algebra $\mathcal{G}'$ while S can be expressed as a symmetric quadratic form in B_j, P_j, E, and M. Thus the possible coordinate systems in which (1.2) separates can always be characterized by eigenfunction equations for operators at most second order in the enveloping algebra of $\mathcal{G}$. From the results of Sec. 2 it is straightforward to determine the operators K,S associated with each coordinate system. This information is listed in Table II.

TABLE II. Symmetry operators associated with variable separation

Coordinate system	1st-order symmetry K	2nd-order symmetry S
1) $\mathrm{Fc}^{(1)}$	K_2	B_1^2
2) $\mathrm{Fc}^{(2)}$	K_{-2}	P_1^2
3) $\mathrm{Fr}^{(1)}$	K_2	M^2
4) $\mathrm{Fr}^{(2)}$	K_{-2}	M^2
5) $\mathrm{Fp}^{(1)}$	K_2	B_2M+MB_2
6) $\mathrm{Fp}^{(2)}$	K_{-2}	P_2M+MP_2
7) $\mathrm{Fe}^{(1)}$	K_2	$M^2-B_2^2$
8) $\mathrm{Fe}^{(2)}$	K_{-2}	$M^2-P_2^2$
9) $\mathrm{Lc}^{(1)}$	$K_2+2aP_1+2bP_2$	$B_2^2+2bP_2E$
10) $\mathrm{Lc}^{(2)}$	$K_{-2}-2aB_1-2bB_2$	$P_1^2+2aB_1E$
11) $\mathrm{Lp}^{(1)}$	K_2+aP_1	$B_2M+MB_2+aP_2^2$
12) $\mathrm{Lp}^{(2)}$	$K_{-2}+2aB_1$	$P_2M+MP_2+2aB_2^2$
13) Oc	$K_{-2}-K_2$	$P_1^2+B_1^2$
14) Or	$K_{-2}-K_2$	M^2
15) Oe	$K_{-2}-K_2$	$M^2-P_2^2-B_2^2$
16) $\mathrm{Rc}^{(1)}$	D	$B_1P_1+P_1B_1$
17) $\mathrm{Rc}^{(2)}$	$K_{-2}+K_2$	$P_1^2-B_1^2$
18) $\mathrm{Rr}^{(1)}$	D	M^2
19) $\mathrm{Rr}^{(2)}$	$K_{-2}+K_2$	M^2
20) $\mathrm{Re}^{(1)}$	D	$M^2+(B_2P_2+P_2B_2)/2$
21) $\mathrm{Re}^{(2)}$	$K_{-2}+K_2$	$M_2-P_2^2+B_2^2$
22) Ll	P_1	$B_2^2-2bP_2E$
23) L2	P_1	$P_2^2+2aB_2E$
24) Ol	P_1	$P_2^2+B_2^2$
25) Rl	P_1	$P_2P_2+P_2B_2$
26) R2	P_1	$P_2^2-B_2^2$

The above 26 coordinate systems were classified up to equivalence under the Gallilean group $G(2)\subset G$. However, from another point of view we can regard two coordinate systems as equivalent if the first can be transformed to the second under the action of some $g\in G$. In terms of operators, the system described by K,S is equivalent to the system described by K',S' if, under the adjoint action of G on the enveloping algebra of $\mathcal{G}$, the two-dimensional space spanned by K,S can be mapped onto the two-dimensional space spanned by K',S'. Under this more general equivalence relation not all of the above coordinate systems are inequivalent. Indeed the systems denoted $\mathrm{Ab}^{(1)}$ and $\mathrm{Ab}^{(2)}$ lie on the same two-dimensional orbits so that there are only 17 equivalence classes of orbits.

We can describe these equivalences in terms of the operator $J=\exp\frac{1}{4}\pi(K_2-K_{-2})$:

$$Jf(\mathbf{x},t)=[\sqrt{2}/(1+t)]\exp[\tfrac{1}{4}i(1+t)^{-1}\mathbf{x}\circ\mathbf{x}] \times f[\sqrt{2}(1+t)^{-1}\mathbf{x},(t-1)/(1+t)], \quad f\in\mathcal{F}. \tag{3.2}$$

Note that $J^2=\exp\frac{1}{2}\pi(K_2-K_{-2})$, and

$$\begin{aligned} J^2f(\mathbf{x},t)&=t^{-1}\exp[(i/4t)\mathbf{x}\circ\mathbf{x}]f(t^{-1}\mathbf{x},-t^{-1}),\\ J^4f(\mathbf{x},t)&=-f(-\mathbf{x},t),\\ J^8f(\mathbf{x},t)&=f(\mathbf{x},t). \end{aligned} \tag{3.3}$$

It is easy to show that $J(K_{-2}+K_2)J^{-1}=D$, and, checking the adjoint action of J on second-order operators, we can verify that the three coordinate systems $\mathrm{Rc}^{(2)}$, $\mathrm{Rr}^{(2)}$, $\mathrm{Re}^{(2)}$ are equivalent under J to the three systems $\mathrm{Rc}^{(1)}$, $\mathrm{Rr}^{(1)}$, $\mathrm{Re}^{(1)}$ respectively.

Denoting the adjoint action of J^2 on $K\in\mathcal{G}$ by $K'=J^2KJ^{-2}$, we find $P_j'=-B_j$, $B_j'=P_j$, $K_{-2}'=-K_2$, $K_2'=-K_{-2}$, $D'=-D$, $M'=M$, $E'=E$ so that the six pairs of the form $\mathrm{Fa}^{(1)}$, $\mathrm{Fa}^{(2)}$ or $\mathrm{La}^{(1)}$, $\mathrm{La}^{(2)}$ are equivalent under J^2.

4. TWO- AND THREE-VARIABLE MODELS

We next demonstrate that the operators (1.5) can be interpreted as a Lie algebra of skew-Hermitian operators on the Hilbert space $L_2(R_2)$ of complex-valued Lebesgue square-integrable functions on the real line. This is accomplished by considering t as a fixed parameter and replacing ∂_t by $i(\partial_{x_1x_1}+\partial_{x_2x_2})$ in expressions (1.5). It is then clear that the resulting operators multiplied by i and restricted to the domain of C^∞-functions on R_2 with compact support are essentially self-adjoint. In fact these operators are real linear combinations of the operators

$$\begin{aligned} &K_2=\tfrac{1}{4}i(x_1^2+x_2^2), \quad K_{-2}=i(\partial_{x_1x_1}+\partial_{x_2x_2}), \quad P_j=\partial_{x_j},\\ &B_j=\tfrac{1}{2}ix_j, \quad M=x_1\partial x_2-x_2\partial_{x_1}, \quad \mathcal{E}=i,\\ &D=x_1\partial_{x_1}+x_2\partial_{x_2}+1, \end{aligned} \tag{4.1}$$

which are well known to be essentially skew-adjoint. Note that when the parameter $t=0$ the operators (1.5) reduce to (4.1). Thus the script operators (4.1) satisfy the same commutation relations (1.6) as do the block operators (1.5). More specifically we have the identities

$$(\exp tK_{-2})P_j[\exp(-tK_{-2})]=P_j,$$
$$(\exp tK_{-2})B_j[\exp(-tK_{-2})]=B_j, \tag{4.2}$$

with similar expressions relating the other script and block operators.

If $f\in L_2(R_2)$, then $u(t)=(\exp tK_{-2})f$ satisfies $u_t=K_{-2}u$ or $iu_t=-\Delta_2 u$ (for almost every t) wherever f is in the domain of K_{-2}, and $u(0)=f$. Also the unitary operators $\exp\alpha K=\exp(tK_{-2})(\exp\alpha K)\exp(-tK_{-2})$ map u into $v=(\exp\alpha K)u$ which also satisfies $v_t=K_{-2}v$ for each linear combination K of the operators (4.1). Thus the operators $\exp\alpha K$ are symmetries of (1.2).

We will see later that the operators (4.1) generate a global unitary irreducible representation of the group G on $L_2(R_2)$. Assuming this here, we let $U(g)$, $g\in G$, be the corresponding unitary operators and set $T(g)=(\exp tK_{-2})U(g)[\exp(-tK_{-2})]$. It is then easy to show that the $T(g)$ are unitary symmetries of (1.2) with associated infinitesimal operators $K=(\exp tK_{-2})K\times[\exp(-tK_{-2})]$.

Next consider the operator $L_3=K_{-2}-K_2=i(\Delta_2-\frac{1}{4}(x_1^2+x_2^2))\in\mathcal{G}$. If $f\in L_2(R_2)$, then $u(t)=(\exp tL_3)f$ satisfies $u_t=L_3u$ or

$$iu_t=-\Delta_2 u+\tfrac{1}{4}(x_1^2+x_2^2)u \tag{4.3}$$

and $u(0)=f$. Similarly the unitary operators $V(g)=(\exp tL_3)U(g)[\exp(-tL_3)]$ are symmetries of (4.3), the Schrödinger equation for the harmonic oscillator, and the associated infinitesimal operators $(\exp tL_3)K[\exp(-tL_3)]$ can be expressed as first-order differential operators in t and x. Analogous statements hold for the operator $L_2=K_{-2}+K_2=i(\Delta_2+\frac{1}{2}(x_1^2+x_2^2))$ with associated equation $u_t=L_2u$,

$$iu_t=-\Delta_2 u-\tfrac{1}{4}(x_1^2+x_2^2)u, \tag{4.4}$$

(Schrödinger equation for the repulsive oscillator) and the operator $K_{-2}-B_1=i(\Delta_2-x_1/2)$ with associated equation $u_t=(K_{-2}-B_1)u$,

$$iu_t=-\Delta_2 u+\tfrac{1}{2}x_1u \tag{4.5}$$

(linear potential).

These remarks show explicitly the equivalence of equations (1.2), (4.3)—(4.5). Through we have chosen to start with Eq. (1.2) in this paper, an analysis of any of the other equations would have led us to the same results.

From Table II we see that, except for the subgroup coordinates (22)—(26) which were essentially discussed in 5, every separable coordinate system corresponds to a G-orbit which contains exactly one of the Hamiltonian operators iK_{-2}, iL_3, iL_2, or $i(K_{-2}-B_1)$. Thus each coordinate system is naturally associated with one of these four Hamiltonians.

Consider a pair of commuting self-adjoint operators iK, S, where $K\in\mathcal{G}$ and S is a symmetric quadratic operator in the enveloping algebra of $\mathcal{G}$. These operators have a common spectral resolution, i.e., there is a complete set of (generalized) eigenvectors $f_{\lambda,\mu}(\mathbf{x})$ in $L_2(R_2)$ with

$$iKf_{\lambda,\mu}=\lambda f_{\lambda,\mu},\quad Sf_{\lambda,\mu}=\mu f_{\lambda,\mu},\quad (f_{\lambda,\mu},f_{\lambda',\mu'})=\delta_{\lambda\lambda'}\delta_{\mu\mu'}, \tag{4.6}$$

where

$$(h_1,h_2)=\int_{-\infty}^{\infty}\!\!\int h_1(\mathbf{x})\bar{h}_2(\mathbf{x})\,dx_1\,dx_2,\quad h_j\in L_2(R_2). \tag{4.7}$$

Now suppose iK', S' are another pair of commuting self-adjoint operators on the same G-orbit as iK, S. Then by renormalizing these operators if necessary, it follows that there is a $g\in G$ such that

$$K'=U(g)KU(g^{-1}),\quad S'=U(g)SU(g^{-1}).$$

Thus the spectral resolution of the primed pair is identical to that for the unprimed pair. Indeed for $f'_{\lambda,\mu}=U(g)f_{\lambda,\mu}$ we have

$$iK'f'_{\lambda,\mu}=\lambda f'_{\lambda,\mu},\quad Sf'_{\lambda,\mu}=\mu f'_{\lambda,\mu}$$
$$(f'_{\lambda,\mu},f'_{\lambda',\mu'})=\delta_{\lambda\lambda'}\delta_{\mu\mu'} \tag{4.8}$$

and the $f'_{\lambda,\mu}$ form a complete ON set in $L_2(R_2)$.

In the following we will frequently need the spectral resolution of a pair iK, S, where iK is one of the four Hamiltonians listed above. However, in many cases we will be able to use the unitary symmetry operators $U(g)$ to construct an equivalent pair iK', S' whose spectral resolution is much simpler to compute. This information will then provide the spectral resolution of the original pair.

As a special case of these remarks consider the operator $K_{-2}=i\Delta_2$. If $\{f_{\lambda,\mu}\}$ is the basis (4.6) of generalized eigenvectors for the pair K, S, then $\{f'_{\lambda,\mu}(t)=[\exp(tK-2)]f_\lambda\}$ is the corresponding basis of generalized eigenvectors for the block operators $K=(\exp tK_{-2})K[\exp(-tK_{-2})]$, $S=(\exp tK_{-2})S[\exp(-tK_{-2})]$ and the $f'_{\lambda,\mu}(t)$ satisfy Eq. (1.2). Similar remarks hold for the other Hamiltonians. This clarifies the relationship between the two- and three-variable models of $\mathcal{G}$.

We now explicitly compute the spectral resolutions of the pairs of commuting operators listed in Table II. We being with the Oc orbit, i.e., by determining the spectral resolution of the pair $L_3=K_{-2}-K_2, P_1^2+B_1^2$. Equations (4.6) are

$$[-\Delta_2+\tfrac{1}{4}(x_1^2+x_2^2)]f=\lambda f,\quad (\partial_{x_1x_1}-\tfrac{1}{4}x_1^2)f=\mu f,$$

and the well-known normalized eigenfunctions are

$$f_{\lambda,\mu}=\mathrm{oc}_{n,m}(\mathbf{x})=(2^{m+n}\pi n!\,m!)^{-1/2}\exp[-(x_1^2+x_2^2)/4]$$
$$\times H_n(x_1/\sqrt{2})H_m(x_2/\sqrt{2}),$$
$$\mu=-n-\tfrac{1}{2},\quad \lambda+\mu=m+\tfrac{1}{2}. \tag{4.9}$$
$$(\mathrm{oc}_{n',m'},\mathrm{oc}_{n,m})=\delta_{nn'}\delta_{mm'},$$

where $H_n(x)$ is a Hermite polynomial.

At this point one can easily show in a manner analogous to that presented in 5, Sec. 3, that the operators (4.1) exponentiate to yield a global unitary irreducible representation of G. Indeed from the known recurrence formulas for the Hermite polynomials one can see that the operators L_1, L_2, L_3 acting on the oc-basis define a unitary representation of $sl(2,R)$ which is a direct sum of representations from the discrete series, and the W-operators define a unitary irreducible representation of W. As follows from the work of Bargmann,[22,23] this

Lie algebra representation extends to a global representation of G, irreducible since its restriction to W is already irreducible.

We now compute the unitary operators $U(g)$ on $L_2(R_2)$. The operators

$$U(\mathbf{w},\mathbf{z},\alpha)=\exp(w_1\beta_1)\exp(z_1\rho_1)\exp(w_2\beta_2)\exp(z_2\rho_2)\times\exp(\alpha\mathcal{E})$$

defining the irreducible representation of W are

$$[U(\mathbf{w},\mathbf{z},\alpha)f](\mathbf{x})=\exp[i(\alpha+\tfrac{1}{2}\mathbf{w}\cdot\mathbf{x})f(\mathbf{x}+\mathbf{z})],\quad f\in L_2(R_2). \tag{4.10}$$

The operator $U(\theta)=\exp(\theta/\mathcal{H})$ is

$$[U(\theta)f](\mathbf{x})=f(\mathbf{x}\Theta)$$

where Θ is given by (1.10). The operators $U(A)$, $A\in SL(2,R)$, are more difficult. From Ref. 24, we find

$$(\exp aK_{-2})f(\mathbf{x})=\text{l.i.m.}\ \frac{1}{4\pi i a}\times\int_{-\infty}^{\infty}\int\exp[-(\mathbf{x}-\mathbf{y})^2/4ia]\,f(\mathbf{y})\,dy_1\,dy_2. \tag{4.11}$$

(In the following we will drop the l.i.m. symbol.)

Also

$$(\exp bK_2)f(\mathbf{x})=\exp(ib\,\mathbf{x}\cdot\mathbf{x}/4)\,f(\mathbf{x}),\qquad(\exp c\partial)f(\mathbf{x})=e^c f(e^c\mathbf{x}). \tag{4.12}$$

Using group multiplication in $SL(2,R)$, we find

$$\exp\phi L_2=\exp(\tanh\phi K_2)\exp(\sinh\phi\cosh\phi K_{-2})\times\exp[-\ln(\cosh\phi)K_3]$$

so that

$$(\exp\phi L_2)f(\mathbf{x})=\frac{\exp(i\coth\phi\mathbf{x}\cdot\mathbf{x}/4)}{4\pi i\sinh\phi}\int_{-\infty}^{\infty}\int\times\exp\frac{i}{4}\left(-\frac{2}{\sinh\phi}\mathbf{x}\cdot\mathbf{y}+\cosh\phi\mathbf{y}\cdot\mathbf{y}\right)\times f(\mathbf{y})\,dy_1\,dy_2. \tag{4.13}$$

Similar computations yield

$$(\exp\theta L_3)f(\mathbf{x})=\frac{\exp(i\cot\theta\mathbf{x}\cdot\mathbf{x}/4)}{4\pi i\sin\theta}\times\int_{-\infty}^{\infty}\int\exp\frac{i}{4}\left(-\frac{2}{\sin\theta}\mathbf{x}\cdot\mathbf{y}+\cot\theta\mathbf{y}\cdot\mathbf{y}\right)\times f(y)\,dy_1\,dy_1, \tag{4.14}$$

$$\exp\rho(K_{-2}+a\beta_1)f(\mathbf{x})=\exp i\,\frac{(a\rho x_1/2-a^2\rho^3/12)}{4\pi i}\times\int_{-\infty}^{\infty}\int\exp\frac{i}{4\rho}\left[(x_1-a\rho^2-y_1)^2+(x_2-y_2)^2\right]f(\mathbf{y})\,dy_1\,dy_2. \tag{4.15}$$

From (4.11) it follows that the basis functions $\mathrm{oc}_{n,m}(\mathbf{x})$ map to the ON basis functions $\mathrm{Oc}_{n,m}(\mathbf{x},t)=\exp tK_{-2})\,\mathrm{oc}_{n,m}(\mathbf{x})$ or

$$\mathrm{Oc}_{n,m}(x,t)=(2^{m+n+1}\pi n!\,m!)^{-1/2}\exp[i\pi(m+n-1)/2]\times\exp[-\tfrac{1}{4}(v_1^2+v_2^2)(1-iv_3)]\left(\frac{v_3+i}{v_3-i}\right)^{(m+n)/2}\times(v_3-i)^{-1}H_m(v_1/\sqrt{2})H_n(v_2/\sqrt{2}), \tag{4.16}$$

where

$$x_1=v_1(1+v_3^2)^{1/2},\quad x_2=v_2(1+v_3^2)^{1/2},\quad t=v_3.$$

The functions (4.16) are those corresponding to the separable coordinate system Oc in Table I.

Next we compute the spectral resolution for the system Or:

$$i(K_{-2}-K_2)f=\lambda f,\quad \mathcal{H}^2 f=\mu f.$$

The basis of eigenvectors is

$$\mathrm{or}^{+}_{n,m}(\mathbf{x})=[m!/2^m\pi(n+m)!]^{1/2}\exp(-r^2/4)\,r^m L_n^m(\tfrac{1}{2}r^2)\times\cos m\theta,$$
$$\mathrm{or}^{-}_{n,m}(\mathbf{x})=\tan m\theta\,\mathrm{or}^{+}_{n,m}(\mathbf{x}), \tag{4.17}$$

where $m\geq 1, n\geq 0$ and $x_1=r\cos\theta$, $x_2=r\sin\theta$. The eigenvalues λ,μ are related to m,n via $\mu=-m^2$, $\lambda=2n+m+1$. For $m=0$ we get

$$\mathrm{or}^{+}_{n,0}(\mathbf{x})=(2/\pi n!)^{1/2}\exp(-r^2/4)\,L_n(\tfrac{1}{2}r^2),$$

where $L_n^{\alpha}(r)$ is a generalized Laguerre polynomial. The orthogonality relations are

$$(\mathrm{or}^{\epsilon'}_{n',m'},\mathrm{or}^{\epsilon}_{n,m})=\delta_{\epsilon\epsilon'}\delta_{n'n}\delta_{m'm},\quad \epsilon,\epsilon'=\pm.$$

The three-variable basis functions $\mathrm{Or}_{n,m}(\mathbf{x},t)=(\exp tK_{-2})\,\mathrm{or}_{n,m}(\mathbf{x})$ are

$$\mathrm{Or}^{+}_{n,m}(\mathbf{x},t)=K\left(\frac{m!}{\pi^3 2^m(n+m)!}\right)^{1/2}\frac{(-1)^{m+n}}{2^{2m}}\,\frac{(v_3+i)^{m/2+n}}{(v_3-i)^{m/2+n+1}}\times\exp[\tfrac{1}{4}v_1^2(it-1)]L_n^m(\tfrac{1}{2}v_1^2)\cos mv_2, \tag{4.18}$$

$$\mathrm{Or}^{-}_{n,m}(\mathbf{x},t)=\tan mv_2\,\mathrm{Or}^{+}_{n,m}(\mathbf{x},t),\quad m\geq 1$$

for $m=0$, $K=\sqrt{2}$; otherwise $K=1$. Also $x_1=(1+v_3^2)^{1/2}v_1\cos v_2$, $x_2=(1+v_3^2)^{1/2}v_1\sin v_2$, $t=v_3$.

For the system Oe,

$$i(K_{-2}-K_2)f=\lambda f,\quad (\mathcal{H}^2-\rho_2^2-\beta_2^2)f=\mu f,$$

we obtain the ON basis

$$\mathrm{oe}^{+}_{n,m}(\mathbf{x})=(1/\pi)\,\mathrm{hc}_p^m(i\xi,\tfrac{1}{2})\,\mathrm{hc}_p^m(\eta,\tfrac{1}{2}),$$
$$\mathrm{oe}^{-}_{n,m}(\mathbf{x})=(1/\pi)\,\mathrm{hs}_p^m(i\xi,\tfrac{1}{2})\,\mathrm{hs}_p^m(\eta,\tfrac{1}{2}), \tag{4.19}$$

where

$$\mathrm{hc}_p^m(\eta,\tfrac{1}{2})=\exp(-\cos 2\eta/8)\,C_p^m(\eta,\tfrac{1}{2}),$$
$$\mathrm{hs}_p^m(\eta,\tfrac{1}{2})=\exp(-\cos 2\eta/8)\,S_p^m(\eta,\tfrac{1}{2}),$$
$$0\leq m\leq p<\infty,\ (-1)^{m-p}=1,$$
$$x_1=\cosh\xi\cos\eta,\quad x_2=\sinh\xi\sin\eta.$$

The eigenvalues λ and μ are related to p and m via $\lambda=p+1$, $\mu=\tfrac{1}{2}\lambda+a_p^m(\tfrac{1}{2})$ or $\mu=\tfrac{1}{2}\lambda+b_p^m(\tfrac{1}{2})$.

The orthogonality relations are

$$(\mathrm{oe}^{\epsilon'}_{n'm'},\mathrm{oe}^{\epsilon}_{nm})=\delta_{\epsilon\epsilon'}\delta_{n'n}\delta_{m'm},\quad \epsilon,\epsilon'=\pm.$$

The functions $C_p^m(\eta,\xi), S_p^m(\eta,\xi)$ are Ince polynomials.[25,26] They are polynomial solutions of period 2π of the Whittaker—Hill equation. This equation has been investi-

gated in detail by Arscott,[26] and it is his notation for the solutions and eigenvalues that we use. The three-variable basis functions $\mathrm{Oe}_{n,m}(\mathbf{x},t)=(\exp tK_{-2})\,\mathrm{oe}_{n,m}(\mathbf{x})$ are

$$\mathrm{Oe}^{+}_{n,m}(\mathbf{x},t)=(\lambda^{m+}_{p}/\pi)\exp[(i/4)\,v_3(\sinh^2 v_1+\cos^2 v_2)]\times(v_3-i)^{p/2+1}(v_3+i)^{-p/2}\,\mathrm{hc}^{m}_{p}(iv_1,\tfrac{1}{2})\,\mathrm{hc}^{m}_{p}(v_2,\tfrac{1}{2}) \tag{4.20}$$

where

$$x_1=(1+v_3^2)^{1/2}\cosh v_1\cos v_2,\quad x_2=(1+v_3^2)^{1/2}\times\sinh v_1\sin v_2,\quad t=v_3.$$

The expression for $\mathrm{Oe}^{-}_{n,m}(\mathbf{x},t)$ is as above except that we now have a new constant of modulus unity λ^{m-}_{p} and the functions $\mathrm{hc}^{m}_{p}(\eta,\xi)$ are replaced by $\mathrm{hs}^{m}_{p}(\eta,\xi)$. The constants $\lambda^{m\pm}_{p}$ are in principle calculable from a knowledge of the explicit form of the Ince polynomials. They can always be calculated by inserting special values of the parameters v_i. Accordingly we make no further comment on their determination.

In the remaining cases there are always two coordinate systems associated with each orbit. For simplicity we shall always treat the coordinate system with superscript (1). The corresponding results for system (2) follow immediately upon application of the operators J or J^2, (3.2), (3.3).

The Fc system is defined by equations

$$iK_2 f=-\tfrac{1}{4}\gamma^2 f,\quad \beta_1 f=\tfrac{1}{2}i\gamma\cos\alpha\, f$$

and has a basis of generalized eigenvectors

$$\mathrm{fc}_{\gamma,\alpha}(\mathbf{x})=[\delta(r-\gamma)/\sqrt{r}\,]\,\delta(\theta-\alpha),\quad(\mathrm{fc}_{\gamma,\alpha},\mathrm{fc}_{\gamma',\alpha'})=\delta(\gamma-\gamma')\,\delta(\alpha-\alpha'),$$

$$x_1=r\cos\theta,\quad x_2=r\sin\theta,\quad 0\le\alpha<2\pi,\ 0\le\gamma. \tag{4.21}$$

The basis functions $\mathrm{Fc}_{\gamma,\alpha}(\mathbf{x},t)=(\exp tK_{-2})\,\mathrm{fc}_{\gamma,\alpha}(x)$ are

$$\mathrm{Fc}_{\gamma,\alpha}(\mathbf{x},t)=\frac{\sqrt{\gamma}}{4\pi it}\exp\frac{i}{4t}\left[(x_1-\gamma\cos\alpha)^2+(x_2-\gamma\sin\alpha)^2\right]. \tag{4.22}$$

The Fr system is defined by

$$iK_2 f=-\tfrac{1}{4}\gamma^2 f,\quad i\mathcal{H}f=-mf$$

with basis

$$\mathrm{fr}_{\gamma,m}(\mathbf{x})=\frac{\delta(r-\gamma)}{\sqrt{r}}\,\frac{\exp(im\theta)}{\sqrt{2\pi}},\quad(\mathrm{fr}_{\gamma,m},\mathrm{fr}_{\gamma',m'})=\delta(\gamma-\gamma')\,\delta_{mm'}. \tag{4.23}$$

Here $0\le\gamma$, $m=0,\pm1,\ldots$, and r,θ are polar coordinates. The three-variable basis functions are

$$\mathrm{Fr}_{\gamma,m}(\mathbf{x},t)=\left(\frac{\gamma}{2\pi}\right)^{1/2}\exp\frac{i}{4t}(r^2+\gamma^2)\,\frac{i^{m-1}}{2t}\times\exp(im\theta)\,J_m\left(\frac{-r\gamma}{2t}\right), \tag{4.24}$$

where $J_m(z)$ is a Bessel function.

The Fp system is determined by equations

$$iK_2 f=-\tfrac{1}{4}\gamma^2 f,\quad(\beta_2\mathcal{H}+\mathcal{H}\beta_2)f=-\mu f$$

with basis

$$\mathrm{fp}^{+}_{\gamma,\mu}(\mathbf{x})=(1/\sqrt{2\pi})(1+\cos\theta)^{i\mu/2-1/4}(1-\cos\theta)^{i\mu/2-1/4}\times[\delta(r-\gamma)/\sqrt{r}\,],\quad -\pi\le\theta<0,$$

$$0,\quad 0\le\theta\le\pi,$$

$$\mathrm{fp}^{-}_{\gamma,\mu}(\mathbf{x})=\mathrm{fp}^{-}_{\gamma,\mu}(r,\theta)=\mathrm{fp}^{+}_{\gamma,\mu}(r,-\theta). \tag{4.25}$$

Here r,θ are polar coordinates, $0\le\gamma,-\infty<\mu<\infty$, and the spectrum is continuous of multiplicity two.[1] The orthogonality relations are

$$(\mathrm{fp}^{\pm}_{\gamma,\mu},\mathrm{fp}^{\pm}_{\gamma',\mu'})=\delta(\gamma-\gamma')\,\delta(\mu-\mu'),\quad(\mathrm{fp}^{\pm}_{\gamma,\mu},\mathrm{fp}^{\mp}_{\gamma',\mu'})=0.$$

The three-variable basis functions are

$$\mathrm{Fp}^{\pm}_{\gamma,\mu}(\mathbf{x},t)=\frac{i\sqrt{\gamma}\exp(i\gamma^2/4t)}{2^3\pi t\cos(i\mu\pi)}\exp\left(\frac{i}{16t}(\xi^2+\eta^2)^2\right)\times\left[D_{-iu/2-1/2}\left(\frac{\sigma\xi}{\sqrt{t}}\right)\times D_{i\mu/2-1/2}\left(\frac{\sigma\eta}{\sqrt{t}}\right)+D_{-i\mu/2-1/2}\left(\frac{-\sigma\xi}{\sqrt{t}}\right)D_{-i\mu/2-1/2}\left(\frac{-\sigma\eta}{\sqrt{t}}\right)\right],$$

$$\mathrm{Fp}^{-}_{\gamma,\mu}(x_1,x_2,t)=\mathrm{Fp}^{+}_{\gamma,\mu}(x_1,-x_2,t), \tag{4.26}$$

where $\sigma=\exp(i\pi/4)\sqrt{\gamma}$ and ξ,η are parabolic coordinates

$$2x_1=\xi^2-\eta^2,\quad x_2=\xi\eta.$$

The Fe system is defined by equations

$$iK_2 f=-\gamma^2 f,\quad(\mathcal{H}^2+4\beta_1^2-4\beta_2^2)f=-\mu f,$$

[equivalent to (7) in Table II]. The basis functions are

$$\mathrm{fe}_{\gamma,n}(\mathbf{x})=\frac{\delta(r-\gamma)}{\sqrt{r\pi}}\begin{cases}\mathrm{ce}_n(\theta,\gamma^2/2), & n=0,1,2,\ldots,\\ \mathrm{se}_{-n}(\theta,\gamma^2/2), & n=-1,-2,\ldots,\end{cases} \tag{4.27}$$

$$0\le\gamma,\quad(\mathrm{fe}_{\gamma,n},\mathrm{fe}_{\gamma',n'})=\delta(\gamma-\gamma')\,\delta_{nn'},$$

where $\mathrm{ce}_n(\theta,q),\mathrm{se}_n(\theta,q)$ are the periodic Mathieu functions of integral order and r,θ are polar coordinates. The eigenvalues $\mu=\mu_n$ are discrete and all of multiplicity one. The basis functions

$$\mathrm{Fe}_{\gamma,n}(\mathbf{x},t)=(\exp tK_{-2})\,\mathrm{fe}_{\gamma,n}(\mathbf{x})$$

are

$$\mathrm{Fe}_{\gamma,n}(\mathbf{x},t)=\frac{A_{\gamma,n}}{4\pi i\tau}\left(\frac{\gamma}{\pi}\right)^{1/2}\exp[i\tau(\cos^2\sigma+\sinh^2\rho+\gamma^2)]\times\begin{cases}\mathrm{ce}_n(\sigma,\gamma^2/2)\,\mathrm{Ce}_n(\rho,\gamma^2/2), & n=0,1,2,\ldots,\\ \mathrm{se}_{-n}(\sigma,\gamma^2/2)\,\mathrm{Se}_n(\rho,\gamma^2/2), & n=-1,-2,\ldots,\end{cases} \tag{4.28}$$

where $A_{\gamma,n}$ is a normalization constant, $\mathrm{Se}_n(\rho,q)$ and $\mathrm{Ce}_n(\rho,q)$ are modified Mathieu functions, and

$$x_1=-2\tau\cosh\rho\cos\sigma,\quad x_2=-2\tau\sinh\rho\sin\sigma,\quad t=\tau.$$

The Lc system (transformed so that $b=0$) can be defined by equations

$$i(K_2+a\beta_1)f=\lambda f,\quad \beta_2^2 f=-\tfrac{1}{4}\rho^2 f$$

with basis functions

$$\mathrm{lc}_{\lambda,\rho'}(\mathbf{x})=\frac{\delta(x_2-\rho)}{\sqrt{2\pi|a|}}\exp\left[-\frac{i}{a}\left(\lambda x_1+\frac{\rho^2}{4}x_1+\frac{x_1^2}{12}\right)\right],$$

$$(\mathrm{lc}_{\lambda,\rho},\mathrm{lc}_{\lambda',\rho'})=\delta(\lambda-\lambda')\,\delta(\rho-\rho'),\quad -\infty<\lambda,\rho<\infty. \tag{4.29}$$

The three-variable basis functions are

$$\mathrm{Lc}_{\lambda,\rho}(\mathbf{x},t)=\frac{(9a)^{-1/3}}{8iv_3\sqrt{2\pi|a|}}\exp\left[i\left((v_1^2+v_2^2)\frac{v_3}{4}-\frac{av_1}{v_3}-\rho\frac{v_2}{2}-\frac{a^2}{3v_3^3}-\frac{\lambda}{v_3}\right)\right]\mathrm{Ai}\left[(36a)^{-1/3}\left(\frac{v_1}{a}+\frac{\lambda}{a}+\frac{\rho^2}{4a}\right)\right], \tag{4.30}$$

where $\mathrm{Ai}(z)$ is an Airy function. Here,

$$x_1=v_1v_3+a/v_3,\quad x_2=v_2v_3,\quad t=v_3.$$

The Lp system is defined by

$$i(\mathcal{K}_2+a\mathcal{P}_1)f=\lambda f,\quad (\beta_2\mathcal{H}+\mathcal{H}\beta_2+a\mathcal{P}_2^2)f=\mu f$$

with basis functions

$$\mathrm{lp}_{\lambda,n}(\mathbf{x})=(1/\sqrt{2\pi|a|})\,h_n(x_2)\exp[-(i/a)(\lambda x_1+\tfrac{1}{4}x_1x_2^2+\tfrac{1}{12}x_1^3)],$$
$$-\infty<\lambda<\infty, n=0,1,2,\ldots,$$
$$(\mathrm{lp}_{\lambda,n},\mathrm{lp}_{\lambda',n'})=\delta(\lambda-\lambda')\delta_{nn'}. \tag{4.31}$$

Here $h_n(x)$ is a solution of

$$h''-\left(\frac{\mu}{a}+\frac{\lambda x^2}{a^2}+\frac{x^4}{4a^2}\right)h=0 \tag{4.32}$$

such that

$$\int_{-\infty}^{\infty}|h_n(x)|^2dx=1. \tag{4.33}$$

The eigenvalues $\mu=\mu_n$ of (4.32) subject to condition (4.33) are discrete,[27] with multiplicity one, and we assume them ordered so that $\mu_0<\mu_1<\mu_2<\cdots$. Here $h_n(x)$ is either even or odd for each value of n.

Denote a general solution of (4.32) by $h_{\mu,\lambda,a}(x)$. Then it is straightforward to show that the basis functions $\mathrm{Lp}_{\lambda,n}(\mathbf{x},t)=(\exp t\mathcal{K}_{-2})\,\mathrm{lp}_{\lambda,n}(\mathbf{x})$ are

$$\mathrm{Lp}_{\lambda,n}(\mathbf{x},t)=\frac{C_{\lambda,n}}{v_3}\times\exp\left[i\left((v_1^2+v_2^2)^2\frac{v_3}{16}-\frac{a}{4v_3}(v_1^2-v_2^2)\frac{a^2}{12v_3^2}-\frac{\lambda}{v_3}\right)\right]\times h_{2\mu_n,\lambda,a/2}(v_1)\,h_{2\mu_n,\lambda,a/2}(iv_2), \tag{4.34}$$

where the two h functions have the same parity as $h_n(x)$ and $C_{\lambda,n}$ is a normalization constant. Also

$$x_1=(v_1^2-v_2^2)\frac{v_3}{2}+\frac{a}{v_3},\quad x_2=v_1v_2v_3,\quad t=v_3.$$

The Rc system is defined by the equations

$$\mathcal{D}f=\rho f,\quad (\beta_1\mathcal{P}_1+\mathcal{P}_1\beta_1)f=\mu f$$

with basis functions

$$\mathrm{rc}_{\lambda\mu}^{\epsilon\epsilon'}(\mathbf{x})=\frac{1}{2\pi}\,x_{1\epsilon}^{-i\lambda-1/2}x_{2\epsilon'}^{-i\mu-1/2}$$

$$-\infty<\lambda<\infty,\quad -\infty<\mu<\infty,\ \epsilon,\epsilon'=\pm,\quad \lambda=\rho-\mu$$

where

$$x_\pm^\lambda=\begin{cases}x^\lambda, & x>0\\ 0, & x<0\end{cases},\quad \lambda=\rho-\mu, \tag{4.35}$$

and similarly for x_-^λ. The orthogonality relations are

$$(\mathrm{rc}_{\lambda'\mu'}^{\bar\epsilon\bar\epsilon'},\mathrm{rc}_{\lambda\mu}^{\epsilon\epsilon'})=\delta_{\bar\epsilon\epsilon}\delta_{\bar\epsilon'\epsilon'}\delta(\lambda'-\lambda)\delta(\mu'-\mu).$$

The three-variable basis functions are

$$\mathrm{Rc}_{\lambda\mu}^{++}=\frac{1}{8\pi^2iv_3}\,[\exp(i\pi/4)\sqrt{2v_3}\,]^{-i(\lambda+\mu)+1}\Gamma(-i\lambda+\tfrac{1}{2})\,\Gamma(-i\mu+\tfrac{1}{2})\times\exp[i(v_1^2+v_2^2)/8]D_{i\lambda-1/2}(-v_1/\sqrt{2i})\,D_{i\mu-1/2}(-v_2/\sqrt{2i}), \tag{4.36a}$$

where $x_1=v_3^{1/2}v_1$, $x_1=v_3^{1/2}v_2$, $t=v_3$. The remaining three-variable basis functions are given by

$$\begin{aligned}\mathrm{Rc}_{\lambda\mu}^{++}(v_1,v_2)&=(-1)^{1-i(\lambda+\mu)}\mathrm{Rc}_{\lambda\mu}^{--}(-v_1,-v_2)\\&=(-1)^{1/2-i\lambda}\mathrm{Rc}_{\lambda\mu}^{-+}(-v_1,v_2)\\&=(-1)^{1/2-i\mu}\mathrm{Rc}_{\lambda\mu}^{+-}(v_1,-v_2).\end{aligned} \tag{4.36b}$$

The Rr system is defined by the equations

$$\mathcal{D}f=\rho f,\quad \mathcal{H}f=imf.$$

The eigenfunctions are then

$$\mathrm{rr}_{\rho m}(\mathbf{x})=(1/2\pi)\,r^{i\rho-1}\exp(im\theta), \tag{4.37}$$
$$-\infty<\rho<\infty,\quad m=0,\pm1,\cdots,\quad x_1=r\cos\theta,\quad x_2=r\sin\theta,$$

satisfying the orthogonality relations

$$(\mathrm{rr}_{\rho'm'},\mathrm{rr}_{\rho m})=\delta_{m'm}\delta(\rho'-\rho).$$

The three variable basis functions are

$$\mathrm{Rr}_{\rho m}(\mathbf{x},t)=\frac{2}{i\pi\sqrt{v_3}}(2\sqrt{iv_3})^{1+i\rho}\frac{\Gamma(m/2+(1+i\rho)/2)}{m!}\times v_1^{-1}\exp(iv_1^2/8)\,M_{i\rho/2,m/2}(iv_1^2/4)\exp(imv_2), \tag{4.38}$$

where $M_{v,\mu}(z)$ is a solution of Whittaker's equation and $x_1=v_3^{1/2}v_1\cos v_2$, $x_2=v_3^{1/2}v_1\sin v_2$, $t=v_3$.

The Re system is defined by the equations

$$\mathcal{D}f=i\lambda f,\quad [\mathcal{H}^2+\tfrac{1}{2}(\beta_2\mathcal{P}_2+\mathcal{P}_2\beta_2)]f=\mu f.$$

The orthonormalized eigenfunctions are then

$$\begin{aligned}\mathrm{re}_{\lambda m}^{+}(\mathbf{x})&=(1/\sqrt{2\pi})\,r^{i\lambda-1}\mathrm{Gc}_m(\theta,\tfrac{1}{4},-\lambda),\\ \mathrm{re}_{\lambda m}^{-}(\mathbf{x})&=(1/\sqrt{2\pi})\,r^{i\lambda-1}\mathrm{Gs}_m(\theta,\tfrac{1}{4},-\lambda),\end{aligned} \tag{4.39}$$

$x_1=r\cos\theta$, $x_2=r\sin\theta$. Here we have introduced the notation

$$\begin{aligned}\mathrm{Gc}_m(\theta,\tfrac{1}{4},-\lambda)&=\exp[i\cos(2\theta)/16]\,\mathrm{gc}_m(\theta,\tfrac{1}{4},-\lambda),\\ \mathrm{Gs}_m(\theta,\tfrac{1}{4},-\lambda)&=\exp[i\cos(2\theta)/16]\,\mathrm{gs}_m(\theta,\tfrac{1}{4},-\lambda).\end{aligned} \tag{4.40}$$

The functions $\mathrm{gc}_m(\theta,\alpha,\beta)$ and $\mathrm{gs}_m(\theta,\alpha,\beta)$ are nonpolynomial solutions of the Whittaker—Hill equation and the subscript m (the number of zeros in the interval $[0,2\pi]$) labels the discrete eigenvalues of the operator $\mathcal{H}^2+\frac{1}{2}(\beta_2\mathcal{P}_2+\mathcal{P}_2\beta_2)$, i.e., $\mu=\mu_m$. This notation is due to Arscott and Urwin.[28] Each of the solutions $\mathrm{Gc}_m(\theta,\alpha,\beta)$ or $\mathrm{Gs}_m(\theta,\alpha,\beta)$ can be written as an infinite series in trignometric functions which converges for the discrete eigenvalues μ_m. For further details see Ref. 28. The three-variable basis functions are

$$\begin{aligned}\mathrm{Re}_{\lambda m}^{+}(\mathbf{x},t)&=K_m^{\lambda+}v_3^{(i\lambda-1)/2}\mathrm{Gc}_m(iv_1,\tfrac{1}{4},-\lambda)\,\mathrm{Gc}_m(v_2,\tfrac{1}{4},-\lambda),\\ \mathrm{Re}_{\lambda m}^{-}(\mathbf{x},t)&=\bar K_m^{\lambda-}v_3^{(i\lambda-1)/2}\mathrm{Gs}_m(iv_1,\tfrac{1}{4},-\lambda)\,\mathrm{Gs}_m(v_2,\tfrac{1}{4},-\lambda),\end{aligned}$$

where

$$x_1=v_3^{1/2}\cosh v_1\cos v_2,\quad x_2=v_3^{1/2}\sinh v_1\sin v_2,\quad t=v_3.$$

The constants $\bar{K}_m^{\lambda\pm}$ are in principle calculable by choosing special values of the parameters v_i. In fact in the process of calculating the functions $\mathrm{Re}^{\pm}$ we get relations which to our knowledge are new, viz.,

$$K_m^{\lambda+}\,\mathrm{Gc}(iv_1,\tfrac{1}{4},-\lambda)\,\mathrm{Gc}(v_2,\tfrac{1}{4},-\lambda)$$
$$=\exp[\tfrac{1}{4}i(\sinh^2 v_1+\cos^2 v_2)]\int_{-\pi}^{\pi}d\theta\,\mathrm{Gc}_m(\theta,\tfrac{1}{4},-\lambda)$$
$$\times\exp[-\tfrac{1}{8}i(\cosh v_1\cos v_2\cos\theta+\sinh v_1\sin v_2\sin\theta)^2]$$
$$\times D_{i\lambda-1}(-(\cosh v_1\cos v_2\cos\theta+\sinh v_1\sin v_2\sin\theta/\sqrt{2i})$$

with a similar relation holding for the functions $\mathrm{Gs}_m(\theta,\frac{1}{4},-\lambda)$. The constants $K_m^{\lambda\pm}$ can be calculated for particular values of the arguments v_i, e.g., $\mathrm{Gc}_m(\theta,\frac{1}{4},-\lambda)=\sum_{r=0}^{\infty}A_r^m\cos 2r\theta$. Then

$$K_m^{\lambda+}=\frac{2\pi D_{i\lambda-1}(0)\,A_0^m}{\mathrm{Gc}_m(\frac{1}{2}\pi,\frac{1}{4},-\lambda)\,\mathrm{Gc}_m(0,\frac{1}{4},-\lambda)}.$$

Similar expressions may be obtained for the other constants. Passage to the three-variable model in this basis allows us to derive a set of orthogonal basis functions as products of two Gc or Gs functions from a knowledge of the orthogonality of single functions.

5. OVERLAP FUNCTIONS

Exactly as in Sec. 3 of 5 one can show that our results lead to a number of Hilbert space expansion theorems. Indeed if $\{f_{\lambda\mu}\}$ is an ON basis for $L_2(R_2)$, then $\{U(g)f_{\lambda\mu}\}$ for any $g\in G$ is also an ON basis. In particular, each of the three-variable models constructued in Sec. 4 provides a basis for $L_2(R_2)$. Furthermore, exactly as in (3.21) of Paper 5 we can derive discrete and continuous generating functions for each of our bases.

Now we compute overlap functions $(Aa_{\lambda\mu},Bb_{\lambda'\mu'})$ which allow us to expand eigenfunctions $Aa_{\lambda\mu}$ in terms of eigenfunctions $Bb_{\lambda'\mu'}$. The utility of these formulas is that they are invariant under the action of G so the same expressions allow us to expand $U(g)Aa_{\lambda\mu}$ in terms of $U(g)Bb_{\lambda'\mu'}$, where the results may be much less obvious. In the following we use the two-variable bases to compute some overlaps of interest. Because of G-invariance, identical results hold for the three-variable bases.

In the present paper we omit the overlaps between the three discrete bases Oc, Or, Oe, which will be treated in a forthcoming work. (However, the Oc—Or overlap is well-known.[29,30] For most of the other bases we give an overlap with either of the discrete bases Oc or Or. The principle behind these computations is obvious and the interested reader can derive for himself any of the other overlaps:

$$(\mathrm{fc}_{\gamma,\alpha},\mathrm{or}^{\pm}_{n,m})=\gamma^{1/2}\,\mathrm{or}^{\pm}_{n,m}(\gamma\cos\alpha,\gamma\sin\alpha); \tag{5.1}$$

$$(\mathrm{fr}_{\gamma,p},\mathrm{or}_{n,m})=\begin{cases}0 & \text{if } p\neq\pm m,\\ [m!\,\gamma/2^{m+1}(n+m)!\,]^{1/2}\,e^{-\gamma^2/4}\gamma^m L_n^m(\frac{1}{2}\gamma^2) & \text{if } +\text{and } p=\pm m\neq 0,\\ (p/m)i\,[m!\,\gamma/2^{m+1}(n+m)!\,]^{1/2}\,e^{-\gamma^2/4}\gamma^m L_n^m(\frac{1}{2}\gamma^2) & \text{if } -\text{and } p=\pm m\neq 0,\\ (4\gamma/n!)^{1/2}\,e^{-\gamma^2/4}L_n(\frac{1}{2}\gamma^2) & \text{if } p=m=0,\end{cases} \tag{5.2}$$

$$(\mathrm{fp}^{+}_{\gamma,\mu},\mathrm{or}^{\pm}_{n,m})$$
$$=[m!\,\gamma/2^m\pi(n+m)!\,]^{1/2}\exp(-\gamma^2/4)\gamma^m L_n^m(\tfrac{1}{2}\gamma^2)$$
$$\times\exp[-\pi i(1\mp 1)/4]\,(a_m\pm a_{-m}), \tag{5.3}$$

$$(\mathrm{fp}^{-}_{\gamma,\mu},\mathrm{or}^{\pm}_{n,m})=(\mathrm{fp}^{+}_{\gamma,\mu},\mathrm{or}^{\pm}_{n,-m}), \tag{5.4}$$

where

$$a_m=\exp[\pi(i/2-\mu)/2]\,\Gamma(m+\tfrac{1}{2})\left[\frac{(-1)^m\,\Gamma(i\mu+\frac{1}{2})}{\Gamma(i\mu+m+\frac{1}{2})}\right.$$
$$\times{}_2F_1\left(\begin{matrix}i\mu+\frac{1}{2},m+\frac{1}{2}\\ i\mu+m+1\end{matrix}\,\middle|-1\right)-\frac{i\Gamma(-i\mu+\frac{1}{2})}{\Gamma(-i\mu+m+1)}$$
$$\left.\times{}_2F_1\left(\begin{matrix}-i\mu+\frac{1}{2},m+\frac{1}{2}\\ -i\mu+m+1\end{matrix}\,\middle|-1\right)\right),$$

$$(\mathrm{fe}_{\gamma n'},\mathrm{or}^{+}_{mn})=\theta(n')\,(\gamma/\pi)^{1/2}\tfrac{1}{2}(1+(-1)^{m-n'})A_m^{n'}$$
$$\times[m!/2^m\pi(n+m)!\,]^{1/2}\exp(-\gamma^2/4)\,\gamma^m L_n^m(\tfrac{1}{2}\gamma^2), \tag{5.5}$$

where $\theta(x)=1$ for $x\geq 0$, and zero otherwise. A similar expression for $(\mathrm{fe}_{\gamma n'},\mathrm{or}^{-}_{mn})$ can be obtained by replacing $\theta(n')$ by $\theta(-n')$ and $A_m^{n'}$ by $B_n^{n'}$ in the above equation. $A_m^{n'}$, $B_m^{n'}$ are the coefficeints in the trigonometric expansions of the even and odd Mathieu functions, respectively. All other overlaps are zero. Also,

$$(\mathrm{lc}_{\lambda,\rho},\mathrm{oc}_{n,m})=\frac{\exp(-\rho^2/4)}{(2^{m-1}\pi m!)^{1/2}}\,H_m(\rho/\sqrt{2})\,C_n, \tag{5.6}$$

where

$$2^{2/3}\exp[-i(\tfrac{1}{6}+\lambda+\rho^2/4+\sqrt{2y})]\,\mathrm{Ai}[2^{2/3}(\tfrac{1}{4}-i\lambda-i\rho^2/4-i\sqrt{2y})]$$
$$=\sum_{n=0}^{\infty}[(\sqrt{2i}\,y)^n/n!\,]\,C_n,$$

and we have normalized so that $a=-1$,

$$(\mathrm{lc}_{\lambda,\rho},\mathrm{lp}_{\mu,n})=\frac{1}{2\pi|a|}\,\bar{h}_n(\rho)\,\delta\left(\frac{\lambda-\mu}{a}\right), \tag{5.7}$$

$$(\mathrm{rc}^{++}_{\lambda\mu},\mathrm{oc}_{nm})=\pi^{-2}(2^{m+n+3}n!\,m!\,)^{-1/2}\,\mathcal{L}_m^{\lambda}\mathcal{L}_n^{\mu} \tag{5.8}$$

where

$$\mathcal{L}_m^{\lambda}=2^{m+i\lambda-1/2}\,\Gamma(i\lambda/2+\tfrac{1}{4})\,\Gamma((m+1)/2)$$
$$\times{}_2F_1(-m/2,i\lambda/2+\tfrac{1}{4};\tfrac{1}{2};2)$$
$$\text{for } m \text{ even},$$
$$=2^{m+1+i\lambda}\,\Gamma(i\lambda/2+\tfrac{1}{4})\,\Gamma(m/2)\,{}_2F_1((1-m)/2,i\lambda/2+\tfrac{3}{4};\tfrac{3}{2};2)$$
$$\text{for } m \text{ odd}.$$

The remaining overlaps for $\mathrm{rc}^{+-},\mathrm{rc}^{-+}$, and rc^{--} can be calculated by using relations (4.36b):

$$(\mathrm{rr}^{+}_{\lambda m},\mathrm{or}_{nm'})=\delta_{mm'}(2/n!)^{m/2-i\lambda}$$
$$\times[(m+n)!/m!\,]^{1/2}\,\Gamma((m+1-i\lambda)/2)$$
$$\times{}_2F_1(-n,(m+1-i\lambda)/2;m+1;2), \tag{5.9}$$

$$(\mathrm{rr}^{-}_{\lambda m},\mathrm{or}_{nm'})=-i(-1)^{\mathrm{sgn}\,m}(\mathrm{rr}^{+}_{\lambda m},\mathrm{or}_{nm'}), \tag{5.10}$$

$$(\mathrm{rr}^{+}_{\lambda 0},\mathrm{or}_{nm'})=\delta_{0m'}(2^{-1/2-i\lambda}/\sqrt{n!}\,)\,\Gamma((1-i\lambda)/2)$$
$$\times{}_2F_1(-n,(1-i\lambda)/2;1;2). \tag{5.11}$$

For the basis Re we have

$$(\mathrm{re}^{+}_{\lambda m},\mathrm{or}^{+}_{nm'})=\tfrac{1}{2}(1+(-1)^{m-m'})\,\bar{A}_m^m,\sqrt{2\pi}\,(\mathrm{rr}^{+}_{\lambda m'},\mathrm{or}_{nm'}) \tag{5.12}$$

$$(\mathrm{re}^{-}_{\lambda m}, \mathrm{or}^{-}_{nm'}) = \tfrac{1}{2}(1 + (-1)^{m-m'}) \times \bar{B}^{m}_{m'} \sqrt{2\pi}\, i(-1)^{\mathrm{sgn}\, m'} (\mathrm{rr}^{-}_{\lambda m'}, \mathrm{or}_{nm'}) \qquad (5.13)$$

where $\bar{A}^{m}_{m'}$ and $\bar{B}^{m}_{m'}$ are the coefficients for the expansion of the functions $\mathrm{Gc}_m(\theta, \frac{1}{4}, -\lambda)$ and $\mathrm{Gs}_m(\theta, \frac{1}{4}, -\lambda)$, respectively, in trigonometric series.[28]

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Lie theory and separation of variables. 7. The harmonic oscillator in elliptic coordinates and Ince polynomials

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As a continuation of Paper 6 we study the separable basis eigenfunctions and their relationships for the harmonic oscillator Hamiltonian in two space variables with special emphasis on products of Ince polynomials, the eigenfunctions obtained when one separates variables in elliptic coordinates. The overlaps connecting this basis to the polar and Cartesian coordinate bases are obtained by computing in a simpler Bargmann Hilbert space model of the problem. We also show that Ince polynomials are intimately connected with the representation theory of $SU(2)$, the group responsible for the eigenvalue degeneracy of the oscillator Hamiltonian.

INTRODUCTION

In Ref. 1 (hereafter referred to as 6) the authors gave a detailed investigation of the nine-parameter symmetry group G (the Schrödinger group) of the equation

$$iU_t + \Delta_2 U = 0. \qquad (*)$$

It was found that (*) separates in 26 coordinate systems and that with each coordinate system is associated an orbit under the action of the Galilean subgroup $G(2) \subset G$ consisting of a pair of commuting operators (K, S), where $K \in \mathcal{G}$ the Lie algebra of G and S is a second-order element in the universal enveloping algebra of $\mathcal{G}$. It was further shown that in all except five cases (which are subgroup coordinates) the first-order symmetry operator K corresponds to an orbit which can be associated with one of four types of potentials: the free particle, the attractive and repulsive harmonic oscillator, and the linear potential.

The Schrödinger equation for the attractive harmonic oscillator in two space variables separates in exactly three orthogonal coordinate systems: Cartesian, polar, and elliptic. The corresponding eigenfunctions in the three systems are a product of two Hermite polynomials, a Laguerre polynomial times an exponential function, and a product of two Ince polynomials, respectively. In this paper we examine these bases and compute the overlap functions relating different bases, with special emphasis on the Ince polynomial case. Due to the equivalence of the free particle Schrödinger equation (*) and the (time dependent) harmonic oscillator equation we have chosen to present our eigenfunctions as solutions of (*). However, all our results translate immediately to the harmonic oscillator problem.

It can be seen from Table II of 6 that to each type of potential and corresponding symmetry S *except the attractive harmonic oscillator* there correspond two coordinate systems equivalent under G though not under $G(2)$. In one of these equivalent coordinate systems labeled by superscript (1), the eigenfunctions and corresponding calculations are quite simple, while the other system affords the close connection with one of the physical potentials mentioned above. It was the existence of the "simple" systems which made the computations in 6 so easy. Now it is a remarkable fact that for the attractive harmonic oscillator, the analog of the coordinate systems of type (1) is the realization of the harmonic oscillator given several years ago by Bargmann.[2] Note that although the Bargmann transform is not a member of G, it is a member of the complexification G^c of G.[3] It is the purpose of this work to explore fully this analogy, especially in the case of elliptic coordinates where almost all of the developments presented are new.

It is well known that the eigenvalues of the harmonic oscillator Hamiltonian are degenerate and that the group responsible for the degeneracy is $SU(2)$. In Sec. 3 we discuss the relationship between this group and the elliptic basis, developing the connection between Ince polynomials and the representation theory of $SU(2)$ in analogy to the connection between Lamé polynomials and $SU(2)$ as discussed in Ref. 4.

1. PRELIMINARIES

First we give explicitly the Lie algebra $\mathcal{G}$ of the symmetry group G, as well as the spectral resolutions of the pairs corresponding to the oscillator coordinates mentioned above. For further details the reader is referred to 6. The real Lie algebra $\mathcal{G}$ is spanned by the differential operators

$$K_2 = -t^2\partial_t - t(x_1\partial_{x_1} + x_2\partial_{x_2}) - t + \tfrac{1}{4}i(x_1^2 + x_2^2), \quad K_{-2} = \partial_t,$$
$$P_i = \partial_{xi}, B_i = -t\partial_{xi} + ix_i/2, \quad i = 1, 2, \quad M = x_1\partial_{x_2} - x_2\partial_{x_1},$$
$$D = x_1\partial_{x_1} + x_2\partial_{x_2} + 2t\partial_t + 1, \quad E = i. \qquad (1.1)$$

The coordinate systems related to the attractive harmonic oscillator are written as Oc, Or, and Oe [corresponding to cartesian, radial (polar), and elliptic coordinates respectively], and are presented in Table I of 6. The associated pairs of operators are $(K_{-2} - K_2, P_1^2 + B_1^2)$, $(K_{-2} - K_2, M^2)$, and $(K_{-2} - K_2, M^2 - P_2^2 - B_2^2)$ respectively, as listed in Table II of 6.

The spectral resolutions of these pairs as given in 6 with $L_3 = K_{-2} - K_2$ are

Oc: $(iL_3, P_1^2+B_1^2)$ with eigenvalues (λ,μ) and basis functions

$$\mathrm{Oc}_{n_1n_2}(\mathbf{x},t)$$
$$=(2^{n_1+n_2}\pi n_1!n_2!)^{-1/2}\exp[i\pi(n_1+n_2+1)]^{1/2}$$
$$\exp[-\tfrac{1}{4}(x_1^2+x_2^2)(1-it)]\left(\frac{t+i}{t-i}\right)^{(n_1+n_2)/2} \quad (1.2)$$
$$\times(t-i)^{-1}H_{n_1}(x_1/[2(1+t^2)]^{1/2})H_{n_2}(x_2H_n[2/(1+t^2)]^{1/2}),$$

where $\lambda=n_1+n_2+1$, $\mu=-n_1-\frac{1}{2}$, and $H_n(x)$ are Hermite polynomials.

Or: (iL_3, M^2) with eigenvalues (λ,μ) and basis functions

$$\mathrm{Or}^+_{n,m}(\mathbf{x},t)=K\left(\frac{m!}{\pi^3 2^m(n+m)!}\right)^{1/2}\frac{(-1)^{m+n}}{2^{2m}}\frac{(t+i)^{n+m/2}}{(t-i)^{n+m/2+1}}$$
$$\times\exp\left(\frac{r^2(it-1)}{4(1+t^2)}\right)L_n^m\left(\frac{r^2}{2(1+t^2)}\right)\cos m\theta \quad (1.3)$$

$$\mathrm{Or}^-_{n,m}(\mathbf{x},t)=\tan m\theta\,\mathrm{Or}^+_{n,m}(\mathbf{x},t)\quad m=1,2,\cdots,$$

where $L_n^m(r)$ are Laguerre polynomials, $K=\sqrt{2}$ for $m=0$ and 1 otherwise, $x=r\cos\theta$, $y=r\sin\theta$, $\lambda=2n+m+1$, and $\mu=-m^2$.

Oe: $(iL_3,\ M^2-P_2^2-B_2^2)$ with eigenvalues (λ,μ) and basis functions

$$\mathrm{Oe}^+(\mathbf{x},t)=\frac{\lambda_p^{m^+}}{\pi}\exp[(i/4)t(\sinh^2v_1+\cos^2v_2)]$$
$$\times(t-i)^{p/2+1}(t+1)^{-p/2}\,\mathrm{hc}_p^m(iv_1,\tfrac{1}{2})\,\mathrm{hc}_p^m(v_2,\tfrac{1}{2}), \quad (1.4)$$

where $x_1=(1+t^2)^{1/2}\cosh v_1\cos v_2$, $x_2=(1+x^2)^{1/2}\times\sinh v_1\sin v_2$, $\lambda=p+1$, $\mu^+=\frac{1}{2}\lambda+a_p^m(\frac{1}{2})$, and the functions $\mathrm{hc}_p^m(v,\xi)$ are periodic solutions of the Whittaker–Hill[5] equation and are related to the even-parity Ince polynomials through

$$\mathrm{hc}_p^m(v,\xi)=\exp[-\xi\cos(2v)/4]C_p^m(v,\xi). \quad (1.5)$$

The numbers $a_p^m(\xi)$ denote the characteristic values for the even Ince polynomials. The functions $\mathrm{Oe}^-(\mathbf{x},t)$ are obtained by replacing the even Ince polynomials by odd-parity Ince polynomials with corresponding characteristic values denoted by $b_p^m(\xi)$. These functions are thus denoted

$$\mathrm{hs}_p^m(v,\xi)=\exp[-\xi\cos(2v)/4]C_p^m(v,\xi). \quad (1.6)$$

We mention here that for our purposes it is *not* convenient to normalize the Ince polynomials as done by Arscott.[5] A full discussion of our normalization is given in Sec. 3, where it is also seen that much information about Ince polynomials follows from the representation theory of $SU(2)$. Once our normalization is fixed the constants $\lambda_p^{m\pm}$ can be determined.

To conclude this section, we give the unitary mapping which describes the time evolution of the solutions of (*), viz.,

$$\exp(tK_{-2})f(\mathbf{x})=\text{l.i.m.}\,\frac{1}{4it}\int_{-\infty}^{\infty}\int dy_1dy_2$$
$$\times\exp[-(\mathbf{x}-\mathbf{y})^2/4it]f(\mathbf{y}), \quad (1.7)$$

where $K_{-2}=i(\partial_{x_1x_1}+\partial_{x_2x_2})$. We note that $\exp(-tK_{-2})$ applied to any of the basis functions (1.2), (1.3), or (1.4) will give the same functions evaluated at $t=0$. In the next section we compose (1.7) with Bargmann's transform to relate the basis states in Bargmann Hilbert space to the solutions (1.2), (1.3), and (1.4) of the free particle Schrödinger equation (*).

2. BARGMANN'S REALIZATION

Bargmann's transformation[2] (we consider only the case of two spatial dimensions) is a unitary mapping of $L_2(R_2)$ onto the Hilbert space $\mathcal{J}(\mathbf{z})$ of functions f of two complex variables $\mathbf{z}=(z_1,z_2)$ completed with the norm $\|f\|$ induced by the inner product

$$(g,f)=\int_{R_4}d\mu(\mathbf{z})\bar{g}(\mathbf{z})f(\mathbf{z}) \quad (2.1)$$

with $d\mu(\mathbf{z})=\pi^{-2}\exp(-\bar{\mathbf{z}}\cdot\mathbf{z})d^2\mathrm{Re}z\,d^2\mathrm{Im}z$, and $\|f\|=(f,f)^{1/2}$. The mapping is given by

$$f(\mathbf{z})=(\mathbf{A}\psi)(\mathbf{z})\equiv\text{l.i.m.}\int_{R_2}d^2xA(\mathbf{z},\mathbf{x})\psi(\mathbf{x}), \quad (2.2)$$

where $\psi(\mathbf{x})\in L_2(R_2)$ and

$$A(\mathbf{z},\mathbf{x})=\pi^{-1/2}\exp[-\tfrac{1}{2}(\mathbf{z}^2+\mathbf{x}^2)+\sqrt{2}\mathbf{z}\cdot\mathbf{x}]. \quad (2.3)$$

The inverse mapping $\mathbf{A}^{-1}$ is given by

$$\psi(\mathbf{x})=(\mathbf{A}^{-1}f)(\mathbf{x})=\text{l.i.m.}\int_{R_4}d\mu(\mathbf{z})\bar{A}(\mathbf{z},\mathbf{x})g(\mathbf{z}) \quad (2.4)$$

for any $a\in\mathcal{J}_2$.

The composition of the two unitary maps $\exp(tK_{-2})$ and $\mathbf{A}^{-1}$ will then map entire functions $f\in\mathcal{J}_2$ onto $L_2(R_2)$ functions which are solutions of (*). This mapping is given by

$$[\exp(tK_{-2})\mathbf{A}^{-1}g](\mathbf{x},t)=\int_{R_4}d\mu(\mathbf{z})\overline{K_t(\mathbf{z},\mathbf{x})}g(\mathbf{z}), \quad (2.5)$$

where

$$\overline{K_t(\mathbf{z},\mathbf{x})}=\frac{1}{(1+2it)\sqrt{\pi}}\exp\left(\frac{-\frac{1}{2}(1-2it)\bar{\mathbf{z}}^2-\frac{1}{2}\mathbf{x}^2+\sqrt{2}\bar{\mathbf{z}}\cdot\mathbf{x}}{1+2it}\right). \quad (2.6)$$

Notice that when $t\to 0$, we recover Bargmann's mapping (2.4) as we must. The inverse map $\mathbf{A}\exp(-tK_{-2})$ with the kernel $K_t(\mathbf{z},\mathbf{x})$ is then obtained by complex conjugation of (2.6), viz.,

$$[A\exp(-tK_{-2})\psi](\mathbf{z})=\int_{R_2}d^2x\,K_t(\mathbf{z},\mathbf{x})\psi(\mathbf{x},t). \quad (2.7)$$

Thus we have established the one-to-one correspondence between Bargmann's Hilbert space of entire functions $\mathcal{J}_2$ with the $L_2(R_2)$ solution[6] of the free particle Schrödinger equation (*). One can also use (2.7) to construct the Lie algebra $\mathcal{G}$ in the Bargmann realization; however, it is easier to evaluate the generators (1.1) at $t=0$ and make the replacement $\partial_t\to -K_{-2}$ as done in 6 and then pass to Bargmann's realization by replacing the annilihation operator $\frac{1}{2}x_i-\partial_{x_i}$ by its analytic representation z_i. In this way the generators of $\mathcal{G}$ take the form

$$\mathcal{L}_3=-i(z_1\partial_{z_1}+z_2\partial_{z_2}+1),$$
$$\mathcal{L}_2=\tfrac{1}{2}(\partial_{z_1z_1}+\partial_{z_2z_2}+z_1^2+z_2^2),$$
$$\mathcal{D}=\tfrac{1}{2}(\partial_{z_1z_1}+\partial_{z_2z_2}-z_1^2-z_2^2),\quad \mathcal{B}_i=\tfrac{1}{2}i(z_i+\partial_{z_i}), \quad (2.8)$$
$$\mathcal{P}_i=-\tfrac{1}{2}(z_i-\partial_{z_i}),\quad \mathcal{M}=(z_1\partial_{z_2}-z_2\partial_{z_1}),\quad \mathcal{E}=i,$$

where the script letters correspond to the block letters in (1.1) and we have used, instead of K_{-2} and K_2, the combinations $\mathcal{L}_3=K_{-2}-K_2$ and $\mathcal{L}_2=K_{-2}+K_2$, which take a simpler form in the (z_1,z_2) formalism. Indeed the harmonic oscillator Hamiltonian $i\mathcal{L}_3$ now appears as a

dilatation operator making its spectral resolution in $\mathcal{J}_2$ very simple. As well we can give the integrated group action of (2.8) as done in 6. However, as we use only (2.5) and (2.7), we omit this.

Now the second order operator $\mathcal{P}_1^2+\mathcal{B}_1^2$ for the oc system takes the form

$$\mathcal{P}_1^2+\mathcal{B}_1^2=-(z_1\partial_{z_1}+1)$$

and, hence, the normalized eigenfunctions of the pair $(i\mathcal{L}_3, \mathcal{P}_1^2+\mathcal{B}_1^2)$ with eigenvalues (λ,μ) yield Bargmann's well-known result

$$gc_{\lambda,\mu}(\mathbf{z})=z_1^{n_1}z_2^{n_2}/\sqrt{n_1!n_2!}, \tag{2.9}$$

where $\mu=-n_1-\frac{1}{2}$, $\lambda=n_1+n_2+1$. These functions form an ON basis in $\mathcal{J}_2$ and map onto the Oc functions (1.2) via the unitary map (2.5).

In order to treat the systems or and oe it is expedient to introduce the complex polar coordinates[7]

$$\begin{aligned} &z_1=\rho\cos\zeta, \quad 0\leq \mathrm{Re}\rho<\infty, \quad -\infty<\mathrm{Im}\rho<\infty \\ &z_2=\rho\sin\zeta, \quad -\pi<\mathrm{Re}\zeta<\pi, \quad -\infty<\mathrm{Im}\zeta<\infty. \end{aligned} \tag{2.10}$$

In these coordinates the operators $i\mathcal{L}_3$ and $\mathcal{M}$ take the simple form

$$i\mathcal{L}_3=\rho\partial\rho+1, \quad \mathcal{M}=\partial_\zeta,$$

and hence the spectral resolution of the pair $(i\mathcal{L}_3/\mathcal{M}^2)$ with eigenvalues (λ,μ) yields the eigen functions

$$\mathrm{gr}^+_{n,m}(\mathbf{z})=K[2^{2n+m-1}n!\,\Gamma(n+m+1)]^{-1/2}\rho^{2n+m}\cos m\zeta, \tag{2.11a}$$

$$\mathrm{gr}^-_{n,m}(\mathbf{z})=\tan m\zeta\,\mathrm{gr}^+_{n,m}(\mathbf{z}), \tag{2.11b}$$

where K, n, m are as in (1.3). These basis functions form an ON basis in $\mathcal{J}_2$ which map onto the Or functions (1.3) by (2.5).

For the elliptic system oe we consider the spectral resolution of the pair $(i\mathcal{L}_3, \mathcal{M}^2-\mathcal{P}_2^2-\mathcal{B}_2^2)$ with eigenvalues (λ,μ). It is easy to see that the second of these operators gives the differential equation for Ince functions in the complex variable ζ, which we discuss in more detail in the next section. Suffice it now to write down the eigenfunctions (S_p^m is an odd-parity Ince polynomial)

$$\mathrm{ge}^+_{p,m}(\mathbf{z})=2^{-p/2}\rho^p\mathrm{C}_p^m(\zeta), \tag{2.12a}$$

$$\mathrm{ge}^-_{p,m}(\mathbf{z})=2^{-p/2}\rho^p\mathrm{S}_p^m(\zeta), \tag{2.12b}$$

where the notation follows from (1.4) and (1.5). The functions (2.12) form an ON basis in $\mathcal{J}_2$ which map onto the functions (1.4) through the unitary map (2.5).

3. INCE POLYNOMIALS AND $SU(2)$

As is well known[7] the degeneracy group for the harmonic oscillator in two spatial dimensions is $SU(2)$. Although $SU(2)$ is not a subgroup of G, a representation of its Lie algebra appears as a subalgebra of the 20-dimensional vector space of second-order elements in the enveloping algebra of $\mathcal{G}$. Rather than give immediately the representations of the Lie algebra $SU(2)$ in terms of these operators, we prefer to develop the abstract formalism along the lines presented by Patera and Winternitz[4] for Lamé polynomials, establishing the connection with the preceding section at the end.

A. The algebraic approach

Denote by $\mathcal{U}$ the universal enveloping algebra of the Lie algebra $\mathcal{L}$ [here $\mathcal{L}=SU(2)$], $\mathcal{C}$ the center of $\mathcal{U}$, $\mathcal{U}_2$ the symmetric second-order elements of $\mathcal{U}$, and define $\mathcal{U}^{(2)}=\mathcal{L}+\mathcal{U}_2$. Let $J_i, i=1,2,3$, be the standard basis for $SU(2)$. Then a general element of $\mathcal{U}^{(2)}$ can be written as $a_{ij}(J_iJ_j+J_jJ_i)+a_iJ_i$, $a_{ij}, a_i\in R$. Note that for $SU(2)$, $\mathcal{C}\subset\mathcal{U}_2$. It suffices to consider only elements of the factor algebra $\mathcal{U}^{(2)}/\mathcal{C}$. Now an arbitrary element of $\mathcal{U}^{(2)}/\mathcal{C}$ can be brought to the form $J_3^2+rJ_1^2+a_iJ_i$ through an inner automorphism of $SU(2)$. The symmetric second order elements $\mathcal{U}_2/\mathcal{C}$ have been studied by Patera and Winternitz,[4] and they have shown the one-to-one correspondence between the two $SU(2)$ orbits and separation of variables on the sphere S^2. In any case a general element of $\mathcal{U}^{(2)}/\mathcal{C}$ describes an eigenvalue problem with four free parameters giving rise to special functions which have as limiting cases both Lamé polynomials and polynomials arising from the element $J_3^2+aJ_2$, which we will show to be Ince polynomials.

The Lie algebra $SU(2)$ with the basis of Hermitian generators J_i takes the form

$$[J_i,J_j]=i\epsilon_{ijk}J_k. \tag{3.1}$$

The canonical basis for the representation space is defined by

$$\begin{aligned} &J_\pm\psi_{jr}=[(j\mp r)(j\pm r+1)]^{1/2}\psi_{jr\pm1} \\ &J_3\psi_{jr}=r\psi_{jr} \end{aligned} \tag{3.2}$$

with $J_\pm=J_1\pm iJ_2$, where we employ Vilenkin's[8] phase convention

$$\exp(i\pi J_1)\psi_{jr}=\exp(i\pi j)\psi_{j-r}.$$

We are interested in the eigenvalue problem defined by the operator

$$E=J_3^2+aJ_2, \tag{3.3}$$

with eigenvalue taken for later convenience to be $\frac{1}{4}\eta$, viz.,

$$E\psi_{j\eta}=\tfrac{1}{4}\eta\psi_{j\eta}. \tag{3.4}$$

First we consider some symmetries of E in the group of automorphisms of $SU(2)$. Now any such symmetry must map $J_2\to J_2$ and $J_3\to\pm J_3$. It is not difficult to see that any transformation R of this type necessarily takes one of two possible forms:

(i) $R^+=\alpha I$, $\alpha\in\mathbb{C}$, $I=$identity in $SU(2)$,

(ii) $R^-=\beta\exp(-i\pi J_2)$, $\beta\in\mathbb{C}$.

From the existence of R^- and Schur's lemma it is clear that the functions $\psi_{j\eta}$ do not completely specify a basis for an irreducible representation of $SU(2)$. We can define a complete basis by further specifying the eigenvalues of R^-. Furthermore, since $(R^-)^2$ is a multiple of the identity, we can take these eigenvalues to be ±1 which then determines β to be $\exp(i\pi j)$. We hereafter drop the minus supercript on R and write

$$R\psi^\pm_{j\eta}=\pm\psi^\pm_{j\eta}, \tag{3.5}$$

where $R=\exp(i\pi j)\exp(-i\pi J_2)$. The hermiticity of E and R then guarantees the orthogonality conditions

$$(\psi^{\epsilon'}_{j\eta'},\ \psi^{\epsilon}_{j\eta})=\delta_{\eta\eta'}\delta_{\epsilon\epsilon'}, \tag{3.6}$$

where we have properly normalized $\psi^{\epsilon}_{j\eta}$.

The determination of $\psi^{\pm}_{j\eta}$ is then tantamount to the determination of the overlap functions $(\psi_{jr},\ \psi^{\pm}_{j\eta})$. From (3.5) we find

$$(\psi_{jr},\psi^{\pm}_{j\eta})=\pm\exp(-i\pi r)(\psi_{j-r},\psi^{\pm}_{j\eta}) \tag{3.7}$$

and from (3.2), (3.3), and (3.4) we obtain the three-term recursion formula

$$\begin{aligned}&-(a/2i)[(j-r)(j+r+1)]^{1/2}(\psi_{jr+1},\psi^{\pm}_{j\eta})\\&+(a/2i)[(j+r)(j-r+1)]^{1/2}(\psi_{jr-1},\psi^{\pm}_{j\eta})=(r^2-\tfrac{1}{4}\eta)(\psi_{jr},\psi^{\pm}_{j\eta}).\end{aligned} \tag{3.8}$$

It is now convenient to introduce new coefficients $A^{\pm}_r$ as

$$\begin{aligned}A^{\pm}_r&=\frac{\exp[i\pi(j-r)/2](\psi_{jr},\psi^{\pm}_{j\eta})}{\sqrt{(j-r)!\,(j+r)!}},\quad 0<m\leq j,\\A^{\pm}_0&=\frac{\exp(i\pi j/2)}{2(j!)}(\psi_{j0},\psi^{\pm}_{j\eta}),\end{aligned} \tag{3.9}$$

while from (3.7) $A^{\pm}_r$ can be defined for negative r as

$$A^{\pm}_{-r}=\pm A^{\pm}_r.$$

We see immediately that $A^{-}_0=0$. Upon substituting into (3.8) our recursion formula takes precisely the form given by Arscott[5] for Ince polynomials with j integer, viz.,

$$\xi(j+r+2)A^{\pm}_{r+2}+(4r^2+4-\eta)A^{\pm}_{r+1}+\xi(j-r)A^{\pm}_r=0,\quad r>0, \tag{3.10a}$$

$$\xi(j+2)A^{\pm}_2+(4-\eta)A^{\pm}_1+2\xi jA^{\pm}_0=0, \tag{3.10b}$$

$$\xi(j+1)A^{\pm}_1-\eta A^{\pm}_0=0, \tag{3.10c}$$

$$(4j^2-\eta)A^{\pm}_j+\xi A^{\pm}_{j-1}=0, \tag{3.10d}$$

where $\xi=-2a$ and we have identified A^{+}_r and A^{-}_r with Arscott's trigonometric coefficients A_r and B_r, respectively, up to normalization. Notice also that our r takes on both integer and half-integer values. Now for j half-integer we merely delete Eqs. (3.10b, c). Moreover, Arscott's parameter p is identified with our $2j$ ($p=2j$). Thus even p corresponds to integer IR's (irreducible representations) of $SU(2)$ and odd p to half-integer IR's.

Following Arscott, we denote the characteristic values η by $a^m_j(\xi)$ and $b^m_j(\xi)$ for $\psi^{\pm}_{j\eta}$ respectively. Now the dimension of an IR is $(2j+1)$, and from (3.10) we conclude that for integer j there are $j+1$ even parity characteristic values $a^m_j(\xi)$ and j odd parity characteristic values $b^m_j(\xi)$, whereas for half-integer j there are $(j+\frac{1}{2})$ of each type.

From the structure of the operator E in (3.3), there is a further interesting symmetry property noticed by Arscott. Putting $a=-2\xi$ and writing the ξ dependence explicity, i.e., $E(\xi)=J^2_3-2\xi J_2$, we notice that

$$\exp(i\pi\,\mathrm{Ad}J_1)E(\xi)=E(-\xi) \tag{3.11}$$

and a similar relation is obtained by replacing J_1 by J_3. It follows from (3.11) that if $a^m_j(\xi)$ or $b^m_j(\xi)$ are characteristic values for $E(\xi)$, then $a^m_j(-\xi)$ and $b^m_j(-\xi)$ are also characteristic values for $E(\xi)$. Furthermore, a short computation demonstrates that

$$\begin{aligned}&\exp(i\pi\,\mathrm{Ad}J_1)R=R\ \text{ for integer } j,\\&\exp(i\pi\,\mathrm{Ad}J_1)R=-R\ \text{ for half-integer } j.\end{aligned} \tag{3.12}$$

Hence, it follows that for half-integer j the set $\{b^m_j(\xi)\}$ is given by the set $\{a^m_j(-\xi)\}$, whereas for j integer $a^m_j(-\xi)\in\{a^m_j(\xi)\}$ and $b^m_j(-\xi)\in\{b^m_j(\xi)\}$.

The expansion of the $\psi^{\pm}_{j\eta}$ basis in terms of the canonical basis is readily obtained:

$$\begin{aligned}\psi^{\pm}_{j\eta}=&\sum_r\sqrt{(j-r)!\,(j+r)!}\exp[-i\pi(j-r)/2]\\&\times A^{\pm}_r(\eta)(\psi_{jr}\pm\exp(-i\pi r)\psi_{j-r}),\end{aligned} \tag{3.13}$$

where the sum over r runs $r=0,\ldots,j$ for j integer and $r=\frac{1}{2},\frac{3}{2},\ldots,j$ for j half-integer. From the orthonormalization condition (3.6), we find

$$\begin{aligned}&4(j!)\overline{A^{\epsilon'}_0(\eta')}A^{\epsilon}_0(\eta)+2\sum_{r=1}^{j}(j-r)!\,(j+r)!\,\overline{A^{\epsilon'}_r(\eta')}A^{\epsilon}_r(\eta)\\&\quad=\delta_{\eta'\eta}\delta_{\epsilon'\epsilon}\quad(j=\text{integer})\end{aligned} \tag{3.14a}$$

$$\begin{aligned}&2\sum_{r=1/2}^{j}(j-r)!\,(j+r)!\,\overline{A^{\epsilon'}_r(\eta')}A^{\epsilon}_r(\eta)\\&\quad=\delta_{\eta'\eta}\delta_{\epsilon'\epsilon}\quad(j=\tfrac{1}{2}\text{integer}).\end{aligned} \tag{3.14b}$$

Notice that our normalization for $A^{\epsilon}_r(\eta)$ is different from that of Arscott. The inverse expansion is easily obtained from (3.13):

$$\begin{aligned}\psi_{jr}&=\exp[i\pi(j-r)/2]\sqrt{(j-r)(j+r)!}\sum_{\eta,\epsilon}\overline{A^{\epsilon}_r(\eta)}\psi^{\epsilon}_{j\eta},\quad r\neq 0,\\\psi_{j0}&=2(j!)\exp(i\pi j/2)\sum_{\eta}\overline{A^{+}_0(\eta)}\psi^{+}_{j\eta}.\end{aligned} \tag{3.15}$$

From the orthonormality of the ψ_{jr}'s we find

$$\begin{aligned}&\sum_{\eta,\epsilon}A^{\epsilon}_r(\eta)\\&\quad=(j-r)!\,(j+r)!\,\delta_{rr'}\quad(r\text{ and }r'\text{ not both }0),\end{aligned} \tag{3.16a}$$

$$\sum_{\eta}\overline{A^{+}_0(\eta)}A^{+}_0(\eta)=\tfrac{1}{2}(j!)^2 \tag{3.16b}$$

B. One variable model

A well-known[8] model of $SU(2)$ on the space of polynomials of degree $2j$ in one complex variable is given by the realization

$$J'_+=\frac{d}{dz},\quad J'_-=2jz-z^2\frac{d}{dz},\quad J'_3=j-z\frac{d}{dz}. \tag{3.17}$$

The canonical basis states are then realized as

$$\psi'_{jr}(z)=z^{j-r}/\sqrt{(j-r)!\,(j+r)!}\ . \tag{3.18}$$

In this realization the operator E [Eq. (3.3)] takes the form

$$E=z\frac{d^2}{dz^2}+\left(\frac{a}{2i}(z^2+1)-(2j-1)z\right)\frac{d}{dz}+j(j+iaz). \tag{3.19}$$

However, for our purposes it is more convenient to consider another one variable model of $SU(2)$ obtained from (3.17) by a similarity transformation. Set $z=\exp(i\pi/2)\exp(2i\xi)$ and consider the operators $J_i=z^{-j}\times J'_i z^j$. In the new variable ξ the generators J_3, $J_\pm$ take the form

$$J_3=\frac{i}{2}\frac{d}{d\xi},\quad J_\pm=-\exp(2i\xi)\left(\frac{1}{2i}\frac{d}{d\xi}\pm j\right) \tag{3.20}$$

and the canonical basis states are

$$\psi_{j,r}(\zeta)=\exp(i\pi(j-r)/2)\exp(-2ir\zeta)/\sqrt{(j-r)!\,(j+r)!}. \quad (3.21)$$

It is easy to check that the operators (3.20) satisfy the relations (3.2) on the states (3.21). Furthermore, the operator E takes the form

$$E=\frac{1}{4}\frac{d^2}{d\zeta^2}-\frac{a}{2}\sin 2\zeta\frac{d}{d\zeta}+ja\cos 2\zeta \quad (3.22)$$

and the eigenvalue equation (3.4) becomes

$$\psi''+\xi\sin 2\zeta\,\psi'+(\eta-2j\xi\cos 2\zeta)\psi=0, \quad (3.23)$$

which is precisely what Arscott[4] calls Ince's equation with $2j$ identified with Arscott's p.

We construct a realization for the scalar product (3.6) which covers the complex ζ plane once and for which (3.21) forms an orthonormal basis for each integer or half-integer j, viz.

$$(f,g)_j=\frac{\Gamma(2j+2)}{2^{2j+1}\pi}\int_{-\infty}^{\infty}d\zeta_2(\cosh 2\zeta_2)^{-2j-2}\int_{-\pi}^{\pi}d\zeta_1 f(\bar{\zeta})\,g(\zeta), \quad (3.24)$$

where $\zeta=\zeta_1+i\zeta_2$, $\zeta_1,\ \zeta_2\in R$. Writing the expansion formula (3.13) explicitly with the state (3.21), we obtain

$$\psi^{+}_{j\eta}(\zeta)=2\sum_r A^{+}_r(\eta)\cos 2r\zeta=2\,\mathrm{C}^m_{2j}(\xi,\xi) \quad (3.25a)$$

$$\psi^{-}_{j\eta}(\zeta)=-2i\sum_r A^{-}_r(\eta)\sin 2r\zeta=-2i\,\mathrm{S}^m_{2j}(\xi,\xi). \quad (3.25b)$$

It is readily verified by substitution that the solutions (3.24) satisfy the differential equation (3.23) with the recursion formulas (3.10).

It is now a simple task to make the connection of our model in this section with the previous section. It can be seen that the spectral resolution of the operator $J^2-J_2^2-\beta_2^2$ of Sec. 2 gives exactly the differential equation (3.23) with the identification $p=\lambda-1=2j$, $\frac{1}{2}-\mu+\frac{1}{2}p=\eta$, and $\xi=-\frac{1}{2}$.

Now the Lie algebra model (3.17) has been integrated to the group $SU(2)$ by Vilenkin,[8] and it is a simple task to express his representation in terms of our functions $\psi(\zeta)$. In so doing we can express the cross-basis matrix elements of $\exp(-i\theta J_1)$ in terms of a finite sum of Jacobi polynomials.

4. OVERLAP FUNCTIONS

In this section we calculate the overlap functions between the bases oc, or, and oe, respectively. However, since these functions are invariant under the unitary transformations of G as well as Bargmann's transformation **A**, they also apply to the bases Oc, Or, and Oe in Sec. 1. Thus we obtain expansion formulas for each one of these functions in terms of the others. Those expansions involving the Oe basis are probably new.

The overlap function for oc—or systems has been calculated for the case of three-dimensions.[9] In the two-dimensional case here we find

$$(\mathrm{gc}_{n_1,n_2},\mathrm{gr}^{\pm}_{nm})=K\delta_{n_1+n_2,2n+m}\,i^{n_1}\left(\frac{n_2!}{n_1!}2^{2n+m+1}n!\,(n+m)!\right)^{1/2}$$
$$\times\left(\frac{1}{-i}\right)^m\left(\frac{i^m\,{}_2F_1(-n_1,1-(n_1+n_2+m)/2;(n_2-n_1-m)/2;-1)}{\Gamma((n_1+n_2-m)/2)\Gamma((n_2-n_1+m)/2)}\right.$$
$$\left.\pm\frac{i^{-m}\,{}_2F_1(-n_1,1-(n_1+n_2-m)/2;(n_2-n_1+m)/2;-1)}{\Gamma((n_1+n_2-m)/2)\Gamma((n_2-n_1+m)/2)}\right) \quad (4.1)$$

These coefficients allow us to expand[10] the Hermite functions (1.2) in terms of the Laguerre functions (1.3) and vice-versa.

The overlap functions for the system or$^{\pm}$—oe$^{\pm}$ are even easier to calculate, viz.,

$$(\mathrm{gr}^{\pm}_{n,m'},\mathrm{ge}^{\pm}_{p,m})=K\delta_{p,2n+m'}\,2^{n+(m'-s-1)/2}[\Gamma(n+m'+1)n!]^{1/2}$$
$$\times A^{\pm}_{m'/2}(\eta_m), \quad (4.2)$$

whereas the overlap between different parity states vanishes. These coefficients allow us to expand the functions (1.3) in terms of the functions (1.4) and vice-versa. The composition of (4.1) and (4.2) gives us the overlap functions as an infinite series

$$(\mathrm{gc}_{n_1n_2},\mathrm{ge}^{\pm}_{p,m})=\sum_n(\mathrm{gc}_{n_1n_2},\mathrm{gr}^{\pm}_{n,p-2n})(\mathrm{gr}^{\pm}_{n,p-2n},\mathrm{ge}^{\pm}_{nm}). \quad (4.3)$$

Furthermore, we can combine the above results with those of 6 to obtain further overlap functions. However, we present here only those which can be readily obtained in close form and were not given in 6, viz., for the free particle radial coordinates and harmonic oscillator elliptic coordinates:

$$(\mathrm{fr}^{\pm}_{\gamma,m'},\mathrm{oe}^{\pm}_{p,m})=2^{1-m'/2}K^2\sqrt{n!\,m'!}\,A^{\pm}_{m'/2}(\eta_m)\gamma^{m'+1/2}$$
$$\times\exp(-\gamma^2/4)L^{m'}_{(p-m')/2}(\tfrac{1}{2}\gamma^2). \quad (4.4)$$

These functions allow us to expand the Bessel functions given by Eq. (4.24) in 6 in terms of the Ince polynomials (1.4) and conversely to write the functions (1.4) as an integral and sum of Bessel functions.

Similarly, for the repulsive oscillator, radial coordinates, and the harmonic oscillator, elliptic coordinates,

$$(\mathrm{rr}^{+}_{\lambda m'},\mathrm{oe}^{+}_{pm})=K^2A_{m'/2}(\eta_m)\left(\frac{2}{[(p-m')/2]!}\right)^{(m'-1)/2-i\lambda}$$
$$\times\frac{\Gamma((m'+1-i\lambda)/2)}{\sqrt{m'!}}\,{}_2F_1(-(p-m')/2,(m'+1-i\lambda)/2,$$
$$\times m'+1;2), \quad (4.5a)$$

whereas for the negative parity solutions we have

$$(\mathrm{rr}^{-}_{\lambda,m'},\mathrm{oe}^{-}_{pm})=-i(\mathrm{rr}^{+}_{\lambda m'},\mathrm{oe}^{+}_{pm}). \quad (4.5b)$$

Accordingly these coefficients allow us to expand the Whittaker functions, Eq. (4.38) of 6, in terms of the Ince polynomials (1.4) and conversely to express the Ince polynomials as an integral and sum over Whittaker functions.

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Stationary electrovacuum spacetimes with bifurcate horizons

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General features of all stationary electrovacuum solutions of Einstein–Maxwell equations which contain regular bifurcate horizons are studied. A certain set of invariant quantities is found in whose values the full information about the solutions is recorded. The quantities have a simple physical meaning and generalize directly the "local invariants" defined for the axially symmetric case in the previous paper [J. Math. Phys. **15**, 1554 (1974)]. A necessary condition that the solutions represent a neighborhood of a black hole in an asymptotically flat spacetime is given. The condition has the form of an inequality which places an upper bound on the magnitudes of the gravimagnetic, electric, and magnetic fields at the horizon. In the case of axial symmetry, the inequality reduces to that derived in the previous paper.

1. INTRODUCTION

Properties of the axisymmetric, stationary, electrovacuum spacetimes containing bifurcate horizons have been studied in Ref. 1. In the present paper, we drop the assumption of axial symmetry and generalize most of the results of Ref. 1 in the corresponding way. For the sake of brevity, let us call these more general spaces C-spacetimes (for the exact definition, see Sec. 2).

The characteristic initial data for Einstein–Maxwell equations prescribed at the bifurcate horizon of a C-spacetime are symmetric under a transformation group acting along the horizon—the so-called "collineation group C."[2] In Sec. 2, we find all solutions of the characteristic initial data constraints admitting this type of symmetry. We also introduce invariant quantities which generalize the "local invariants" of Ref. 1. The found solutions can be classified by the values of these quantities. Moreover, we show that the metric and electromagnetic field of the C-spacetime in which such a horizon is embedded is uniquely determined by these quantities.

In Sec. 3, we look for relations between our C-spacetimes and the Hawking and Ellis' "stationary regular predictable spaces" (SRPS).[3] We generalize slightly the SRPS to allow for stationary matter shells, rings, and disks whose material need not obey "well-behaved hyperbolic equations" (gas disks, solid constructions, etc.) and which surround the black hole. Such spacetimes provide the simplest possible model for the study of black hole reactions to outside influences—the fields originating in the surrounding matter (cf. Ref. 4). It is, therefore, of some use to investigate the C-spacetimes contained in SRPS as those neighborhoods of the horizons which do not intersect the matter shells, rings, or disks. The first step is to look for conditions on a C-spacetime to be a subspace of an SRPS. We use the necessary condition proved by Hawking,[3] namely that there may not be any outer trapped surfaces in an SRPS. In case of C-spacetimes, this condition implies an inequality for the invariant quantities introduced in Sec. 2. It should be mentioned that Newman and his collaborators, in a series of papers on trapped surfaces,[5] have also obtained some inequality, but this does not seem to be invariant.

2. STRUCTURE OF C-SPACETIMES

Let us introduce some conventions.

Definition 1: $(\mathcal{M},g,F)$ is an electrovacuum spacetime with metric g_{ij} and electromagnetic field F_{ij}, if

(1) g_{ij} is a symmetric covariant tensor field on $\mathcal{M}$ of signature -2 such that the spacetime $(\mathcal{M},g)$ is time-orientable;

(2) F_{ij} is an antisymmetric covariant tensor field on $\mathcal{M}$;

(3) g_{ij} and F_{ij} satisfy the Einstein–Maxwell equations

$$R_{ij}-(1/2)g_{ij}R=-2(F_{ik}F^{k}_{j}+(1/4)g_{ij}F_{kl}F^{kl}),$$
$$F_{[ij;k]}=0,$$
$$F^{ij}{}_{;j}=0,$$

everywhere in $\mathcal{M}$. R_{ij} is the Ricci tensor and R the Ricci scalar as defined by g_{ij} according to conventions written down in Ref. 1.

Our definition of the field F_{ij} as a covariant tensor is in agreement with any textbook on general relativity (cf. Ref. 6). On the other hand, under a Lorentz transformation $\Lambda_i{}^j$, F_{ij} transforms as (see, e.g., Ref. 7, Sec. 5.4)

$$F'_{ij}=\mathrm{sgn}(\Lambda_0{}^0)\Lambda_i{}^k\Lambda_j{}^l F_{kl}.$$

Such a transformation law cannot be carried over to general relativity, where any regular matrix must be allowed to replace $\Lambda_i{}^j$, because the question whether such a matrix preserves or changes time orientation makes no sense. A possible way out of this difficulty is to express the fact that the electric field does not change sign under time inversion whereas the magnetic field does by the rules relating the "physical components" in of F_{ij} (i.e., the components in an orthonormal frame) to the electric and magnetic field 3-vectors, and to let F_{ij} be a tensor. In $\mathcal{M}$, a time orientation must be chosen as positive and the rules must contain an extra minus sign if the frame has negative orientation. Accordingly, the isometry of the usual spacetimes must be generalized for the electrovacuum spacetimes to the so-called (g,F)-map as follows:

Definition 2: The map φ: $(\mathcal{M}_1,g_1,F_1)\to(\mathcal{M}_2,g_2,F_2)$ is called (g,F)-map, if

(1) φ is a diffeomorphism of $\mathcal{M}_1$ onto $\mathcal{M}_2$,

(2) $\varphi_*(g_1)=g_2$,

(3) $\varphi_*(F_1)=\pm F_2$,

where the plus sign holds when φ maps the time orientation of $\mathcal{M}_1$ onto the time orientation of $\mathcal{M}_2$, the minus sign holds in the opposite case and φ_* is the differential of φ (see, e.g. Ref. 3, p. 24).

A group of (g,F)-maps φ: $(\mathcal{M},g,F)\to(\mathcal{M},g,F)$ is called a (g,F)-group of the electrovacuum spacetime $(\mathcal{M},g,F)$.

Definition 3: Let $(\mathcal{M},g,F)$ be an electrovacuum spacetime admitting a one-dimensional (g,F)-group $\mathcal{G}$ and containing a perfect horizon H such that

(1) H is invariant under $\mathcal{G}$,

(2) the restriction of $\mathcal{G}$ to H is a collineation symmetry group on H.[2]

Then, $(\mathcal{M},g,F)$ is called a C-spacetime.

The group $\mathcal{G}$ and the horizon H need not be uniquely determined in a given C-spacetime. A drastic example of such a situation is the Robinson–Bertotti spacetime [Ref. 8, Eq. (9)]. Another example is the Kerr–Newman spacetime with $m^2>a^2+e^2$ (Ref. 9), where the group $\mathcal{G}$ is unique, but the horizon H is not: There are two intersecting perfect horizons satisfying the conditions of Definition 3. The reader will observe that $\mathcal{G}$ is not identical with the group generated by $\partial/\partial t$ in this case, because the latter is spacelike at H.

Our next task is to find an invariant description of the structure of C-spacetimes, which were analogous to, or even a direct generalization of, the local invariants introduced in Ref. 1 for axisymmetric spacetimes. Let us choose an arbitrary C-spacetime $(\mathcal{M},g,F)$ with a horizon H and a group $\mathcal{G}$ satisfying the conditions of Definition 3. As the first step, we introduce some canonical coordinates and tetrad fields along H.

The points of H invariant under $\mathcal{G}$ form a submanifold S, diffeomorphic to the two-sphere (see, e.g. Ref. 10), which is embedded in $(\mathcal{M},g)$ as a totally geodesic spacelike surface (see Lemma 6 of Ref. 2). Let α be an affine coordinate along H increasing in the future direction and equal to zero at S. α is determined up to a transformation

$$\alpha\to\eta\cdot\alpha, \tag{1}$$

where η is an arbitrary real positive function on H constant along the (null) rays. Let x^A, $A=1,2$, be arbitrary coordinates on S.[11] The functions x^A can be extended to the whole of H by demanding that they be constant along the rays. Then, the coordinates y^i, $i=0,1,2,3$, can be introduced in a neighborhood of H in $\mathcal{M}$ such that, at H, $y^0=\alpha$, $y^1=x^1$, $y^2=x^2$, $y^3=0$. We will often use such a system below, denoting by capital letters the indices 1,2, if they have to be distinguished from the rest.

Let l^i, n^i, m^i, $\bar m^i$ be a pseudo-orthonormal tetrad field along H obeying (2) of Ref. 1 together with the relations

$$\alpha_{,i}l^i=1 \quad \alpha_{,i}m^i\big|_S=0, \tag{2}$$

and satisfying the following orientation convention. l^i has been chosen tangential to the rays and future oriented. The relation $n^i l_i=1$ requires n^i to be future oriented, as well. Define e_0^i and e_1^i by

$$e_0^i=(1/\sqrt{2})\,(l^i+n^i),\quad e_1^i=(1/\sqrt{2})\,(l^i-n^i) \tag{3}$$

and choose e_2^i, e_3^i such that the triad e_1^i, e_2^i, e_3^i is right-handed. m^i is defined by the relation

$$m^k=(1/\sqrt{2})(e_2^k-ie_3^k) \tag{4}$$

up to a rotation

$$m^k\to e^{i\varphi}m^k,$$

where φ is an arbitrary real function on H which is constant along the rays.

According to (2), the complex vector field m^i is tangential to S. As S is totally geodetic, we have

$$m^i{}_{;j}m^j\big|_S=-\Gamma m^i,\quad \bar m^i{}_{;j}m^j\big|_S=\Gamma\bar m^i, \tag{5}$$

or

$$\lambda\big|_S=\mu\big|_S=0,$$

where Γ, Ω, λ, μ are the rotation coefficients defined by the triad l^i, m^i, $\bar m^i$ and (2) of Ref. 1.

As the second step, we solve the equations (14)–(16) of Ref. 2 (which are implied by Einstein–Maxwell equations and Bianchi identities along H) together with the additional conditions which follow from the existence of the (g,F)-group $\mathcal{G}$. Equation (14) of Ref. 2 implies

$$\frac{\partial\Gamma}{\partial\alpha}=\frac{\partial\Omega}{\partial\alpha}=\lambda=0,\quad \mu=\Psi_2\cdot\alpha. \tag{6}$$

For the Maxwell and Weyl spinor fields Φ_a, Ψ_a, the $\mathcal{G}$-symmetry requires that if a frame field l'^i, n'^i, m'^i, $\bar m'^i$ is $\mathcal{G}$-propagated along H, then the corresponding components Φ'_a, Ψ'_a must not depend on α. Such a frame is, e.g., given by

$$l'^i=\alpha l^i,\quad n'^i=\frac{1}{\alpha}n^i,\quad m'^i=m^i,\quad \bar m'^i=\bar m^i.$$

The transformation rules (28) of Ref. 8 for the components Φ_a, Ψ_a, yield

$$\Phi_2=\alpha\Phi'_2,\quad \Psi_3=\alpha\Psi'_3,\quad \Psi_4=\alpha^2\Psi'_4.$$

Substituting this in (14) of Ref. 2, we obtain

$$\begin{aligned}
&\Phi_0=0,\quad \frac{\partial\Phi_1}{\partial\alpha}=0,\quad \Phi_2=(\bar M\Phi_1)\cdot\alpha,\\
&\Psi_0=\Psi_1=0,\quad \frac{\partial\Psi_2}{\partial\alpha}=0,\\
&\Psi_3=(\bar M\Psi_2+2\bar\Phi_1\bar M\Phi_1)\cdot\alpha,\\
&\Psi_4=\big((\bar M+\bar\Gamma)(\bar M\Psi_2+2\bar\Phi_1\bar M\Phi_1)+2\bar\Phi_1(\bar M+\bar\Gamma)\bar M\Phi_1\big)\cdot\tfrac12\alpha^2,
\end{aligned} \tag{7}$$

where the differential operator M is defined by

$$Mx=x_{,i}m^i,$$

for any function x on H. With (6) and (7), (14), and (16) of Ref. 2 are fulfilled identically, the only independent quantities being Γ, Ω, Φ_1, and Ψ_2. These must be chosen so as to satisfy (15) of Ref. 2.

Let us write the complex function Φ_1 in terms of two real functions E and H as in Ref. 1:

$$E=F_{ab}l^a n^b,\quad H=-lF_{ab}m^a\bar m^b, \tag{8}$$

$$\Phi_1 = (1/2)(E - iH) \tag{9}$$

(see Ref. 12). According to this definition, E and H are independent of the choice of canonical coordinates and tetrads. On the other hand, using the relations (3) and (4), we find that E and H are e_1-components of the electric and magnetic vectors, respectively, as calculated in the frame e_0, e_1, e_2, e_3.

Let the line element ds^2 on $\mathcal{H}$ be given by

$$ds^2 = -\gamma_{AB}dx^A dx^B \tag{10}$$

in the canonical coordinates α, x^A, and let the metric covariant derivative on the Riemann manifold $(S, +\gamma_{AB})$ be denoted by ";". We may use the same notation as for the derivative on $(\mathcal{M}, g_{ij})$, because both affine connections coincide on S (S is totally geodesic). Relation (5) implies, then, that Γ is uniquely determined by m^A and γ_{AB}. By means of the Gauss curvature K of (S, γ) and the functions E and H, the first equation of (15) of Ref. 2 can be written as follows [see (20) of Ref. 2]

$$\mathrm{Re}\Psi_2 = (1/2)(E^2 + H^2 - K). \tag{11}$$

The vector m^i is tangential to S, so its only nonzero components at S are m^A. Hence, the complex scalar field Ω determines a real vector field Ω^A on S by

$$\Omega^A = \Omega\bar{m}^A + \bar{\Omega}m^A. \tag{12}$$

The direct meaning of Ω^A is clear from the relation [cf. (2) of Ref. 1]

$$l^i{}_{;A} = l^i\Omega_A, \quad \Omega_A = \gamma_{AB}\Omega^B. \tag{13}$$

Under the transformation (1), Ω_A behaves, therefore, as follows:

$$\Omega'_A = \Omega_A + (\log\eta)_{,A}. \tag{14}$$

The second equation of (15) of Ref. 2 is equivalent to [see (23) of Ref. 2]

$$\mathrm{Im}\Psi_2 = -i|\gamma|^{-1/2}(\Omega_{2;3} - \Omega_{3;2}). \tag{15}$$

where $|\gamma|$ is the determinant of γ_{AB}. In such a way, the vector field Ω_A together with the metric γ_{AB} determines $\mathrm{Im}\Psi_2$ uniquely. On the other hand, Ω^A is not well-defined. Equation (14) implies that any two vector fields Ω'^A and Ω^A on S correspond to the same horizon structure, if they differ by a gradient of a smooth function on S. For a given horizon $\mathcal{H}$, we obtain, therefore, a whole class of fields Ω^A on S. If we can choose a representant in a unique, invariant way from each such class, a great simplification would result. An elegant choice, which will turn out to be advantageous in more aspects later, is provided by a corollary to the Theorem of Hodge (see, e.g., Ref. 13, p.152, Corollary 1.4.4.). According to it, there is a unique divergenceless vector field

$$\Omega^A{}_{;A} = (\Omega^A\sqrt{|\gamma|})_{,A} = 0 \tag{16}$$

in each class given by the relation (14) on any compact Riemann manifold without boundary. From now on, we allow only such affine coordinates α, for which the field Ω^A satisfies (16). Any two such α's are still related by (1), but η is a real constant now.

It is still possible to express the information contained in γ and Ω by means of invariant functions, e.g., the Gauss curvature K of γ and $\mathrm{Im}\Psi_2$. But some of our formulas are not expressible by means of K and $\mathrm{Im}\Psi_2$, because the quantities appearing in them can be obtained only by solving partial differential equations with coefficients depending on K and $\mathrm{Im}\Psi_2$. On the other hand, from γ and Ω, everything is obtained by simple algebra and differentiation. In addition, γ and Ω, together with E and H, form a quadruple of quantities which enter formulas in a nice coherent way. Moreover, we shall see that γ and Ω generalize directly the invariants R, $A(\vartheta)$, $B(\vartheta)$ which are so useful in the axially symmetric case.[1] These are the reasons leading to the following definition.

Definition 4: A C-structure (γ, Ω, E, H) consists of a Riemann metric γ_{AB} on S, a divergenceless vector field Ω^A on S, and two real functions E and H on S, where S is the two-sphere. We have, therefore, proved the following.

Theorem 1: Let $(\mathcal{M}, g, F)$ be a C-spacetime and $\mathcal{H}$ a horizon satisfying the conditions of Definition 3. Then, a unique C-structure (γ, Ω, E, H) is determined by the relations (8), (9), (13), and (16). Let an arbitrary C^2 C-structure (γ, Ω, E, H) be given. Then, a unique perfect horizon $\mathcal{H}$ together with Maxwell and Weyl spinor fields along it is determined by the relations (5), (6), (2) of Ref. 1, (7), (8), (10), (11), and (15). The structures along $\mathcal{H}$ obtained in such a way satisfy the Eqs. (14)–(16) of Ref. 2 identically and are invariant under a collineation group.

Suppose that the C-spacetime $(\mathcal{M}, g, F)$ together with the horizon $\mathcal{H}$ is axisymmetric. Then, a C-structure (γ, Ω, E, H) is determined by Theorem 1, and, on the other hand, the local invariants R, $A(\vartheta)$, $B(\vartheta)$, $E(\vartheta)$ and $H(\vartheta)$ are well defined, too (see Ref. 1). What is the relation between the two in such a case? The axial symmetry allows us to choose the coordinates ϑ, φ on S such that

$$\gamma_{\vartheta\vartheta} = R^2, \quad \gamma_{\varphi\varphi} = R^2A^2(\vartheta), \quad \gamma_{\vartheta\varphi} = 0. \tag{17}$$

In this coordinate system, the rest of the C-structure quantities is denoted by $\Omega^\vartheta(\vartheta, \varphi)$, $\Omega^\vartheta(\vartheta, \varphi)$, $E(\vartheta, \varphi)$, $H(\vartheta, \varphi)$. The axial symmetry implies

$$\frac{\partial}{\partial\varphi}\Omega^\vartheta(\vartheta,\varphi) = \frac{\partial}{\partial\varphi}\Omega^\varphi(\vartheta,\varphi) = \frac{\partial}{\partial\varphi}E(\vartheta,\varphi) = \frac{\partial}{\partial\varphi}H(\vartheta,\varphi) = 0.$$

Thus, we have

$$E(\vartheta,\varphi) = E(\vartheta), \quad H(\vartheta,\varphi) = H(\vartheta). \tag{18}$$

Ω^A will be divergenceless and at the same time well defined at the poles $\vartheta = 0$, π only if

$$\Omega^\vartheta(\vartheta,\varphi) = 0.$$

The corresponding affine coordinate α is obtained by the construction described in Ref. 8, p.63, and is, therefore, exactly the same as that used in Ref. 8 to define $B(\vartheta)$; so we obtain from (31), (40) of Ref. 8 and our relation (12)

$$\Omega_\varphi(\vartheta,\varphi) = -B(\vartheta). \tag{19}$$

Up to now, we have found the structure of all possible C-horizons. But we can do more: in analogy to Ref. 1, we can determine the structure of all possible C-space-

times. With the same tools as in Ref. 8, one can establish the following lemmas.

Lemma 1: Let $(\mathcal{M},g,F)$ be a C-spacetime with a group $\mathcal{G}$ and a horizon H^+ as required by Definition 3. Then, there is another perfect horizon, H^-, say, in $\mathcal{M}$ satisfying the conditions of Definition 3 together with $\mathcal{G}$. The intersection $\mathcal{S}=H^+\cap H^-$ is identical with the set of all points of H^+ (and H^-) invariant under $\mathcal{G}$. The two C-structures $(\gamma^\pm,\Omega^\pm,E^\pm,H^\pm)$ given in a common coordinate system x^A on $\mathcal{S}$ are related as follows:

$$\gamma^+_{AB}=\gamma^-_{AB},\quad \Omega^+_A=-\Omega^-_A,\quad E^+=-E^-,\quad H^+=-H^-.$$

Definition 5: Two C-structures $(\gamma^\pm,\Omega^\pm,E^\pm,H^\pm)$ are called conjugate, if there is a diffeomorphism $\varphi:\mathcal{S}\to\mathcal{S}$ such that

$$\varphi_*(\gamma^+)=\gamma^-,\quad \varphi_*(\Omega^+)=-\Omega^-,\quad \varphi_*(E^+)=-E^-,\quad \varphi_*(H^+)=-H^-.$$

Lemma 2: Let the conditions of Lemma 1 be satisfied. Then, the characteristic initial data for Einstein–Maxwell equations obeying the corresponding constraints and prescribed along the two intersecting null hypersurfaces H^+ and H^- (this all abbreviated by "CID") determines a C-structure up to a conjugation. Any C^4 C-structure determines a unique CID.

Hence, we have as in Ref. 1:

Theorem 2: Let (γ,Ω,E,H) be a C^4 C-structure. Then, there is at most one C-spacetime $(\mathcal{M},g,F)$ determining (γ,Ω,E,H) as in the first half of Theorem 1. The uniqueness of $(\mathcal{M},g,F)$ is understood up to extensions and restrictions. Two conjugated C-structures determine the same C-spacetime in this way.

In proving Theorem 2, we have used the method of Ref. 14, where the uniqueness of the development of the characteristic initial data for Einstein vacuum equations has been shown, under the condition that such a development exists. The existence remains problematic, but it is very likely, at least if some differentiability conditions are assumed. We will try to deal with this problem in future. On the other hand, only the Einstein vacuum equations were considered in Sachs' paper,[14] not the Einstein–Maxwell equations, and the characteristic initial data was defined without using the Newman–Penrose quantities. These two points represent small technical difficulties which are easy to overcome, as anyone writing down the corresponding Newman–Penrose system of equations can see.

3. BLACK HOLE C-SPACETIMES

In Ref. 3, a very general class of stationary spacetimes containing black holes was investigated, the so-called stationary regular predictable spaces (SRPS). Every SRPS contains a perfect horizon (Proposition 9.3.1 of Ref. 3), but this need not be bifurcate. Either it is of C-type but geodesically incomplete (some sort of directional singularity being present at $\mathcal{S}$) or it is of T-type.[2] The singularity at $\mathcal{S}$ is very unlikely and the conjecture that the T-horizons (as, e.g., the extreme Kerr–Newman) are not interesting for black hole physics seems very plausible (cf. Ref. 4). More investigations on the singularity and on the T-horizons will, of course, be necessary before one can exclude them with some certainty. In any case, the C-spacetimes are less general than SRPS in that they can contain only bifurcate horizons.

On the other hand, the C-spacetimes are more general than SRPS in several aspects. They need not be asymptotically flat, can possess singularities on both sides of their horizons, need not develop from partial Cauchy surfaces, etc. But some of these points can represent mathematical pathologies rather than physically interesting generalizations, and another of them would lead to nonnecessary complications of the theory. The only point at which one really wishes to generalize the SRPS is the condition (3) on p. 323 of Ref. 3. This condition excludes stationary rings, disks, or shells surrounding the black hole and consisting of the ideal fluid or of some other material that does not obey a "well-behaved hyperbolic equation." The reason for such a wish is that stationary systems with black holes and nonhyperbolic matter can, first, be good approximations to some phenomena in astrophysics and, second, they provide the simplest theoretical model of the interaction between black holes and some independent outside agents (cf. Ref. 4, where nonhyperbolic matter was allowed in axially symmetric spacetimes that were vacuum outside the matter). Let us, therefore, replace the condition (3) of Hawking and Ellis by the following points:

(3a) The region $\mathcal{T}$ in $\mathcal{M}$, where the matter does not obey well-behaved hyperbolic equations, has a compact spacelike section.

(3b) The energy-momentum tensor T_{ij} satisfies the strong energy condition in $\mathcal{T}$.[3]

(3c) $\mathcal{M}-\mathcal{T}$ consists of one or more electrovacuum spacetimes.

The immediate consequence of these conditions is that the region $\mathcal{T}$ cannot intersect the horizon H, because there are no timelike stationary trajectories for the matter at H (strong energy condition!). As $\mathcal{T}$ is compact, H will have an open electrovacuum neighborhood $\mathcal{U}$ in $\mathcal{M}$. H must admit a symmetry group acting along its rays, because $\mathcal{M}$ is stationary (see Ref. 3). Let H be bifurcate. Then, $\mathcal{U}$ is a C-spacetime.

Definition 6: Such spacetimes $\mathcal{U}$ are called black hole C-spacetimes.

The reader will notice that the maximal analytic extension of a black hole C-spacetime will in general contain a singularity outside of the horizon. These singularities are not serious in the sense that they can be "smoothed up" by some reasonable, stationary matter filling. (Here, we suppose that a stationary electrovacuum spacetime must be analytic in analogy to vacuum stationary spacetimes.[15])

Theorem 3: Let $(\mathcal{U},g,F)$ be a black hole C-spacetime in a generalized SRPS $\mathcal{M}$. Then, the C-structures $(\gamma^\pm,\Omega^\pm,E^\pm,H^\pm)$ corresponding to its bifurcate horizon $H^+\cup H^-$, where H^+ is the event horizon in $\mathcal{M}$, must satisfy the inequality

$$\int_{\mathcal{S}}(\Omega^2+E^2+H^+)\sqrt{|\gamma|}\,d^2x<4\pi, \tag{20}$$

where $\Omega^2=\gamma_{AB}\Omega^A\Omega^B$.

Proof: Let us choose an arbitrary family of compact spacelike sections S' of the lower half of $\mathcal{H}^-$ which is symmetric under the group $\mathcal{G}$ and compute the convergence μ of the outside null normals to S'. Transformations similar to those performed in Ref. 1 lead, now, to

$$\begin{aligned}\mu=&\tfrac{1}{2}(\Psi_2+\bar{\Psi}_2+\bar{\Omega}_{,B}m^B+\Omega_{,B}\bar{m}^B-\bar{\Gamma}\Omega-\bar{\Gamma}\Omega)\\&+(\xi_{,A}\bar{m}^A)_{,B}m^B-\Gamma\xi_{,A}\bar{m}^A\\&+(\Omega+\xi_{,A}m^A)(\bar{\Omega}+\xi_{,A}\bar{m}^A),\end{aligned}\tag{21}$$

where Ψ_2, Γ, and Ω are the complex quantities corresponding to $\mathcal{H}^-$ and to a canonical tetrad along it. ξ is a smooth function on S such that the family of surfaces S' is given by

$$\alpha\circ e^{-\xi}=\text{const}$$

for all negative constants and a fixed canonical affine coordinate α. We rewrite the right-hand side of (21) from the complex into the component form using Eqs. (5), (12), and the identity

$$\gamma^{AB}=\bar{m}^Am^B+m^A\bar{m}^B.$$

Then,

$$\begin{aligned}&\bar{\Omega}_{,A}m^A+\Omega_{,A}\bar{m}^A-\Gamma\bar{\Omega}-\bar{\Gamma}\Omega=\Omega^A{}_{;A}=0,\\&(\xi_{,A}\bar{m}^A)_{,B}m^B-\Gamma\xi_{,A}m^A=\tfrac{1}{2}\gamma^{AB}\xi_{;AB}=\tfrac{1}{2}\Delta\xi\\&(\Omega+\xi_{,A}m_A)(\bar{\Omega}+\xi_{,A}\bar{m}^A)=\tfrac{1}{2}\Omega^2+\Omega^A\xi_{,A}+\tfrac{1}{2}(\text{grad}\,\xi)^2.\end{aligned}\tag{22}$$

Relation (11) together with (22) yields

$$\mu=\tfrac{1}{2}(\Delta\xi+2\Omega^A\xi_{,A}+E^2+H^2+\Omega^2-K)+\tfrac{1}{2}(\text{grad}\,\xi)^2.\tag{23}$$

Now, according to a theorem of Hodge,[16] ξ can be chosen such that the first term on the right-hand side of (23) is a constant real number, $\frac{1}{2}k$, say:

$$k=\Delta\xi+2\Omega^A\xi_{,A}+E^2+H^2+\Omega^2-K.\tag{24}$$

Integrating this equality on S, we obtain

$$k\circ\int_S\sqrt{|\gamma|}\,d^2x=\int_S(E^2+H^2+\Omega^2-K)\sqrt{|\gamma|}\,d^2x,\tag{25}$$

because

$$\int_S(\Delta\xi+2\Omega^A\xi_{,A})\sqrt{|\gamma|}\,d^2x=0,$$

as it easily follows from (13). If $k\geq 0$, then (24) and (23) give $\mu\geq 0$ everywhere on S' and we have an outer trapped surface in $\mathcal{M}$ (Ref. 3, p. 319), which is impossible. Thus, k must be negative, in which case (25) implies (20). QED

In the axially symmetric case, we obtain (11) of Ref. 1 setting (17), (18), and (19) for γ_{AB}, Ω_A, E, and H into (20). Thus, (20) is a direct generalization of (11) of Ref. 1. The physical meaning of the functions E and H is the same as in Ref. 1; in the subsequent paper, it will be shown that Ω^A is the gravimagnetic field at the horizon. Hence, (20) sets an upper limit on the magnitudes of the electric, magnetic and gravimagnetic fields at the horizon exactly as (11) of Ref. 1 did.

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Static electrovacuum spacetimes with bifurcate horizons

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We prove a necessary and sufficient condition for a stationary electrovacuum spacetime with a bifurcate horizon to be static. The condition is expressed by means of the invariant quantities introduced in the preceding paper.

1. INTRODUCTION

Properties of stationary electrovacuum spacetimes containing regular bifurcate horizons (called C-spacetimes) have been studied in Ref. 1. It has been shown, in particular, that all C-spacetimes can be classified by values of four invariant quantities—a symmetric tensor field γ_{AB}, a divergenceless vector field Ω^A, and two functions E and H, all defined on the two-sphere. The tensor γ_{AB} is the metric of any spacelike section of the horizon. The vector Ω^A is built from two rotation coefficients in a special tetrad field and is, therefore, a part of the specetime affine connection at the horizon. The function E is the electric and H the magnetic field component as measured by an observer at the point where his trajectory cuts the horizon and in the direction considered by him as normal to the surface of the "black hole."

In the present paper, we show that $\Omega^A = 0$ and $H = 0$, if and only if the corresponding spacetime is static. Loosely speaking, this means that the source of the gravitational force represented by Ω^A is either some stationary matter current or the rotation of the black hole, and that Ω^A embodies the totality of such a force, because its vanishing implies nonexistence of stationary movements. Ω^A is, therefore, tentatively called gravimagnetic field.

The plan of the paper is as follows. In Sec. 2, we study some discrete symmetries of the characteristic initial data for Einstein—Maxwell equations along a pair of intersecting horizons. It turns out that each of the three fields Ω^A, E, and H possesses "its own" symmetry—a reflection-like transformation of C-spacetimes. The transformation keeps "its" field invariant, but changes sign of the remaining two. The properties of one of these symmetries are used in Sec. 3, where the proof of the necessary and sufficient condition for staticity of C-spacetimes is given.

The notation and conventions are taken over from Ref. 1.

2. SYMMETRIES OF BIFURCATE HORIZONS

Let $(\mathcal{M}, g, F)$ be a C-spacetime with the group $\mathcal{G}$ and the pair of horizons $\mathcal{H}^+$ and $\mathcal{H}^-$ (see Ref. 1). The subset $\mathcal{H}^+ \cup \mathcal{H}^-$ of $\mathcal{M}$ is not a manifold, because no neighborhood of any point of $\mathcal{S} = \mathcal{H}^+ \cap \mathcal{H}^-$ is diffeomorphic to R^3. We describe the status of these points more explicitly.

Let $p \in \mathcal{S}$ and let $\tilde{p}^+$ and $\tilde{p}^-$ be the (null) rays through p lying in $\mathcal{H}^+$ and $\mathcal{H}^-$, respectively. Then, the vector spaces $T_p(\tilde{p}^+)$, $T_p(\tilde{p}^-)$, $T_p(\mathcal{S})$, $T_p(\mathcal{H}^+)$, $T_p(\mathcal{H}^-)$, $T_p(\mathcal{M})$ are well defined and satisfy the following relations [$T_x(Y)$ is the tangential space to manifold Y in point x]:

$$\begin{aligned} T_p(\mathcal{M}) &= T_p(p^+) \oplus T_p(\tilde{p}^-) \oplus T_p(\mathcal{S}), \\ T_p(\mathcal{H}^+) &= T_p(\tilde{p}^+) \oplus T_p(\mathcal{S}), \\ T_p(\mathcal{H}^-) &= T_p(\tilde{p}^-) \oplus T_p(\mathcal{S}), \end{aligned} \tag{1}$$

where $\oplus$ denotes the direct sum of vector spaces. Any tensor t on $T(\mathcal{M})$ defines multilinear pairings of the spaces $T_p(\tilde{p}^+)$, $T_p(\tilde{p}^-)$, $T_p(\mathcal{S})$, as well as multilinear forms on them from which, in turn, t can be reconstructed. The most important example is given by the metric g which defines the following structures:

(a) the bilinear pairing g_1: $T_p(\tilde{p}^+) \otimes T_p(\tilde{p}^-) \to R^1$:

$$g_1(x, y) = g_{ij}(p) x^i y^j, \quad x \in T_p(\tilde{p}^+), \quad y \in T_p(\tilde{p}^-); \tag{2}$$

(b) the bilinear form g_2: $T_p(\mathcal{S}) \otimes T_p(\mathcal{S}) \to R^1$:

$$g_2(x, y) = g_{ij}(p) x^i y^j, \quad x \in T_p(\mathcal{S}), \quad y \in T_p(\mathcal{S}).$$

By means of relation (1), $T_p(\mathcal{M})$ can be built up from $T_p(\tilde{p}^+)$, $T_p(\tilde{p}^-)$, and $T_p(\mathcal{S})$. Let x, y be arbitrary vectors from $T_p(\mathcal{M})$. Then, they can be written in a unique way as

$$x = x_1 + x_2 + x_3, \quad y = y_1 + y_2 + y_3, \tag{3}$$

where x_1 and y_1 lie in $T_p(\tilde{p}^+)$, x_2 and y_2 in $T_p(\tilde{p}^-)$, x_3 and y_3 in $T_p(\mathcal{S})$. Then,

$$g_{ij}(p) x^i y^j = g_1(x_1, y_2) + g_1(y_1, x_2) + g_2(x_3, y_3).$$

The reader will notice that g_2 is a metric induced by that of $\mathcal{H}^+$ or $\mathcal{H}^-$ being thus a part of the structure of, e.g., $\mathcal{H}^+$ alone, but g_1 makes sense only on bifurcate horizons.

We can regard $\mathcal{H}^+ \cup \mathcal{H}^-$ as a sort of geometrical space equipped with the following structures:

(i) The subsets $\mathcal{H}^+$ and $\mathcal{H}^-$ of $\mathcal{H}^+ \cup \mathcal{H}^-$ are perfect horizons ($S^2 \times R^1$ as manifolds, bearing a degenerate metric and an affine connection compatible with it, see Ref. 2) along which the Weyl and Maxwell spinor fields are prescribed. If the C-structure[1] of $\mathcal{H}^+$ is (γ, Ω, E, H), then the C-structure of $\mathcal{H}^-$ is $(\gamma, -\Omega, -E, -H)$.

(ii) At all points p of $\mathcal{S} = \mathcal{H}^+ \cap \mathcal{H}^-$, a bilinear pairing g_1: $T_p(\tilde{p}^+) \otimes T_p(\tilde{p}^-) \to R^1$ is given such that

$$g_1(x, y) > 0,$$

if x and y are both future oriented.

We call such spaces "bifurcate horizons." A symmetry of a bifurcate horizon $\mathcal{H}^+ \cup \mathcal{H}^-$ is a map of $\mathcal{H}^+ \cup \mathcal{H}^-$ onto itself which preserves all the structures given under (i) and (ii). Let us investigate some of these maps.

To describe the action of various transformations on $\mathcal{H}^+ \cup \mathcal{H}^-$, it is convenient to introduce coordinates along it as follows. Let x^A be some coordinates on $\mathcal{S}$ and let us extend the functions x^1, x^2 to the whole of $\mathcal{H}^+ \cup \mathcal{H}^-$ by demanding them to be constant along rays of both $\mathcal{H}^+$ and

$\mathcal{H}^-$. Let α^+ be a canonical affine coordinate along $\mathcal{H}^+$, α^- an affine coordinate along $\mathcal{H}^-$, l^i a null vector field tangential to $\mathcal{H}^+$ and n^i a null vector field tangential to $\mathcal{H}^-$ satisfying the conditions

$$\alpha^+{}_{,i}\, l^i = 1 \qquad \text{on } \mathcal{H}^+,$$
$$\alpha^-{}_{,i}\, n^i = 1 \qquad \text{on } \mathcal{H}^-,$$
$$g_1(l^i, n) = 1, \quad \bar{\alpha} = 0 \quad \text{on } \mathcal{S}. \tag{4}$$

It is easy to show that α^- is canonical along $\mathcal{H}^-(\Omega^A{}_{;A} = 0$, see Ref. 1). The functions α^+, α^- are uniquely determined up to a transformation

$$\alpha^+ \to \eta\alpha^+, \quad \alpha^- \to \eta^{-1}\alpha^-, \tag{5}$$

where η is a positive constant.

Choose a possible pair α^+, α^-. Any element φ^+ from the component of the identity in the collineation group C^+ of $\mathcal{H}^+$ defines a positive number k such that, for any $p \in \mathcal{H}^+$, we have (cf. Ref. 2)

$$\alpha^+(\varphi^+(p)) = k\alpha^+(p), \quad x^A(\varphi^+(p)) = x^A(p). \tag{6}$$

In turn, k determines a unique collineation φ^- on $\mathcal{H}^-$ by

$$\alpha^-(\varphi^-(p)) = k^{-1}\alpha^-(p), \quad x^A(\varphi^-(p)) = x^A(p) \tag{7}$$

for any $p \in \mathcal{H}^-$. The map φ: $(\mathcal{H}^+ \cup \mathcal{H}^-) \to (\mathcal{H}^+ \cup \mathcal{H}^-)$ defined by

$$\varphi|_{\mathcal{H}^+} = \varphi^+, \quad \varphi|_{\mathcal{H}^-} = \varphi^-$$

is a symmetry of the bifurcate horizon $\mathcal{H}^+ \cup \mathcal{H}^-$, because φ preserves the structures (i) along $\mathcal{H}^+$ and along $\mathcal{H}^-$ as well as the pairing g_1. From (5), it follows that, given a fixed pair α_1^+, α_1^-, then any other possible pair α_2^+, α_2^- can be obtained by

$$\alpha_2^+ = \varphi^*(\alpha_1^+), \quad \alpha_2^- = \varphi^*(\alpha^-) \tag{8}$$

for some φ (for the definition of φ^*, see, e.g., Ref. 3, p. 22). We observe that the existence of the pairing g_1 restricts essentially the number of symmetries on $\mathcal{H}^+ \cup \mathcal{H}^-$ which can be constructed from those of $\mathcal{H}^+$ and of $\mathcal{H}^-$.

Useful and intrinsically new types of symmetry which can be admitted by a bifurcate horizon are certain transformations which "permute" the "branches" of the horizon leaving $\mathcal{S}$ pointwise invariant. The exact definitions and properties are as follows.

The time inversion τ is defined by the relations

$$\tau^*(x^A) = x^A, \quad A = 1, 2, \quad \tau^*(\alpha^-) = -\alpha^+, \quad \tau^*(\alpha^+) = -\alpha^-. \tag{9}$$

τ depends on the pair α^+, α^- chosen. If α_1^+, α_1^- and α_2^+, α_2^- are two different pairs related by (8), then the corresponding time inversions τ_1 and τ_2 satisfy

$$\tau_2 = \varphi^{-1} \circ \tau_1 \circ \varphi.$$

τ does not commute with φ, because (6), (7), and (9) imply

$$\alpha^-(\varphi^{-1}(\tau(\varphi(p)))) = +k\,\alpha^-(\tau(\varphi(p))) = -k\alpha^+(\varphi(p)) = -k^2\alpha^+(p).$$

But we notice that

$$\varphi \circ \tau \circ \varphi = \tau \tag{10}$$

for any φ and τ. From the definition of τ it follows that $\mathcal{S}$ is pointwise invariant under τ. Let us find $\tau_*: T_p(\mathcal{H}) \to T_p(\mathcal{H})$ at a point $p \in \mathcal{S}$ [$T_p(\mathcal{H})$ is defined by (1)]. If α^+, α^-, l^i, and n^i satisfy (4), m^i and $\bar{m}^i$ are tangential to $\mathcal{S}$, $g_2(m, \bar{m}) = -1$, $g_2(m, m) = 0$, and τ is defined by (9), then

$$\tau_*(l) = -n, \quad \tau_*(n) = -l, \quad \tau_*(m) = m, \quad \tau_*(\bar{m}) = \bar{m}. \tag{11}$$

The orthonormal tetrad e_0, e_1, e_2, e_3 associated with $l, n, m, \bar{m}$ is given by

$$e_0 = (1/\sqrt{2})(l + n), \quad e_1 = (1/\sqrt{2})(l - n),$$
$$e_2 = (1/\sqrt{2})(m + \bar{m}), \quad e_3 = (1/\sqrt{2})(\bar{m} - m). \tag{12}$$

Relation (11) and the linearity of τ_* yield

$$\tau_*(e_0) = -e_0, \quad \tau_*(e_1) = e_1, \quad \tau_*(e_2) = e_2, \quad \tau_*(e_3) = e_3. \tag{13}$$

The relation (13) justifies the name "time inversion" for τ.

The space reflection ρ is defined by

$$\rho^*(x^A) = x^A, \quad A = 1, 2, \quad \rho^*(\alpha^-) = \alpha^+, \quad \rho^*(\alpha^+) = \alpha^-, \tag{14}$$

where α^+, α^- is an allowed pair of affine coordinates. Exactly as for τ, we obtain the following results: There is a number of ρ's, each of them defined by a different pair α^+, α^-. Any two ρ_1, ρ_2 are related by

$$\rho_2 = \varphi^{-1} \circ \rho_1 \circ \varphi$$

for some φ. In general, ρ and φ do not commute, but we find

$$\rho = \varphi \circ \rho \circ \varphi$$

for any φ and ρ. $\mathcal{S}$ is pointwise invariant under ρ and we have

$$\rho_*(e_0) = e_0, \quad \rho_*(e_1) = -e_1, \quad \rho_*(e_2) = e_2, \quad \rho_*(e_3) = e_3,$$

where e_0, e_1, e_2, e_3 are associated to $l, n, m, \bar{m}$ by (12) and l, n are related to α^+, α^- used in the definition (14) of ρ by Eq. (4).

From (9) and (14), we obtain

$$\rho \circ \tau = \tau \circ \rho,$$

if both ρ and τ are defined by means of the same pair α^+, α^-. Setting

$$\omega = \rho \circ \tau,$$

we have

$$\omega^*(x^A) = x^A, \quad A = 1, 2, \quad \omega^*(\alpha^+) = -\alpha^+, \quad \omega^*(\alpha^-) = -\alpha^-. \tag{15}$$

Thus, ω restricted to the horizon $\mathcal{H}^+(\mathcal{H}^-)$ is the "discrete" element of the collineation group of $\mathcal{H}^+(\mathcal{H}^-)$ (cf. 2). ω commutes with any φ,

$$\omega \circ \varphi = \varphi \circ \omega,$$

hence, ω is uniquely determined, independently of the pair α^+, α^- used in (15). In general

$$\omega \neq \varphi \circ \omega \circ \varphi.$$

Define τ, ρ, and ω by (9), (14), and (15) using a fixed pair α^+, α^-. Then, τ, ρ, ω commute with each other and

$$\tau^2=\rho^2=\omega^2=\mathrm{II}, \quad \omega\circ\tau=\rho, \quad \omega\circ\rho=\tau.$$

Hence, the quadruple $\{\mathrm{II}, \tau, \rho, \omega\}$ forms the well-known Abelian group of four roots of identity. We notice that II, τ, ρ, and ω are the only permutations of the branches of the bifurcate horizon $\mathcal{H}^+\cup\mathcal{H}^-$ which, restricted to $\mathcal{H}^+$ or $\mathcal{H}^-$, are diffeomorphisms; they also preserve the pairing g_1. On the other hand, they will not, in general, preserve the structures under (i). But we have

Lemma 1: Let $\mathcal{H}^+\cup\mathcal{H}^-$ be a bifurcate horizon. Let the C-structure of $\mathcal{H}^\pm$ be $(\gamma^\pm, \Omega^\pm, E^\pm, H^\pm)$. Then, the invariance of $\mathcal{H}^+\cup\mathcal{H}^-$ under τ is equivalent to

$$\Omega^\pm=0, \quad H^\pm=0,$$

the invariance of $\mathcal{H}^+\cup\mathcal{H}^-$ under ρ is equivalent to

$$\Omega^\pm=0, \quad E^\pm=0,$$

and the invariance of $\mathcal{H}^+\cup\mathcal{H}^-$ under ω is equivalent to

$$E^\pm=0, \quad H^\pm=0.$$

Proof: If the C-structures are given, then all of the data under (i) can be reconstructed uniquely along $\mathcal{H}^+\cup\mathcal{H}^-$, and vice versa (see Ref. 1). It is, therefore, sufficient, to investigate the transformation properties of γ_{AB}, Ω^A, E, H. These are, in turn, defined by the relations (10), (13), and (8) of Ref. 1 in terms of a pseudo-orthonormal tetrad field $l, n, m, \bar{m}$ along $\mathcal{S}$. The symmetry under a map ψ means that the quantities calculated according to the rules (10), (13), (8) of Ref. 1 in terms of the tetrad $\psi_*(l)$, $\psi_*(n)$, $\psi_*(m)$, and $\psi_*(\bar{m})$ are numerically equal to the original ones. Let $\psi=\tau, \rho, \omega$ be defined by a fixed pair α^+, α^- and let $l, n, m, \bar{m}$ be chosen so as to satisfy Eq. (4) with α^+, α^-. As $\mathcal{S}$ is pointwise invariant under any of the maps $\tau, \rho, \omega, \gamma_{AB}$ is always invariant. Ω_A is defined by

$$\Omega_A=n_i l^i{}_{;A}=-l_i n^i{}_{;A}.$$

Using (11) and the analogous relations for ρ and ω, we obtain

under τ: $\Omega_A\to-\Omega_A$,

under ρ: $\Omega_A\to-\Omega_A$,

under ω: $\Omega_A\to\Omega_A$.

E and H are defined by

$$E=+(1/2)F_{kl}l^k n^l, \quad H=-(i/2)F_{kl}m^k\bar{m}^l,$$

if e_0 is future oriented; otherwise (cf. Ref. 1)

$$E=-(1/2)F_{kl}l^k n^l, \quad H=+(i/2)F_{kl}m^k\bar{m}^l.$$

The original tetrad is future-oriented, but τ and ω change the time orientation, so we have

under τ: $E\to E$, $H\to-H$,

under ρ: $E\to-E$, $H\to H$,

under ω: $E\to-E$, $H\to-H$, QED

We observe that γ_{AB} can be arbitrary for τ-, ρ-, or ω-symmetric bifurcate horizons. If other reflections are admissible as symmetries, γ_{AB} must have a special form. A typical example is an axially symmetric bifurcate horizon. γ_{AB} allows, then, the transformation of the axisymmetry group parameter $\varphi\to-\varphi$. Under this φ-reflection, the quantities go over in (see Ref. 1)

$$\gamma_{AB}\to\gamma_{AB}, \quad \Omega_A\to-\Omega_A, \quad E\to E, \quad H\to-H.$$

Thus, the axially symmetric bifurcate horizons are always symmetric under φ-reflection times τ—the so-called (t,φ)-inversion.[1] This is a nontrivial result, if combined with the next lemma. It means that in axisymmetric stationary disks, rings, or shells around a black hole, there cannot exist any "convective" currents (cf. Ref. 4).

Lemma 2: Let $\mathcal{H}^+\cup\mathcal{H}^-$ be a bifurcate horizon symmetric under a map ψ. Let the electrovacuum spacetime $(\mathcal{M}, g, F)$ contain $\mathcal{H}^+\cup\mathcal{H}^-$. Then, there is a unique (g,F)-map ψ': $(\mathcal{M}, g, F)\to(\mathcal{M}, g, F)$ such that

$$\psi'\big|_{\mathcal{H}^+\cup\mathcal{H}^-}=\psi. \tag{16}$$

The proof is rather trivial. Observe that the bifurcate horizon represents a complete characteristic initial data for the Einstein–Maxwell equations.[1] The development of such data is unique.[1] Thus, there is a ψ' satisfying relation (16). There cannot be two different ψ'_1, ψ'_2, because $\psi'_1\circ(\psi'_2)^{-1}$ is a map preserving the hypersurfaces $\mathcal{H}^+$ and $\mathcal{H}^-$ and so a pseudo-orthonormal triad field along it. But $\psi'_1\circ(\psi'_2)^{-1}$ is an isometry, so it preserves even a pseudo-orthonormal tetrad field along $\mathcal{H}^+$ and $\mathcal{H}^-$. Hence, $\psi'_1\circ(\psi'_2)^{-1}$ is the identity.

3. STATIC C-SPACETIMES

A stationary—or time-independent—vacuum spacetime is usually defined as a spacetime which admits a timelike Killing field (infinitesimal isometry) in a neighborhood of any of its points (see, e.g., Ref. 5, p. 274). One often requires more: There should be a one-dimensional isometry group whose trajectories are everywhere timelike. Such a spacetime can rather be called globally stationary. For example, the portion of Kerr spacetime outside the horizon is just stationary but not globally stationary. A stationary vacuum spacetime is called static, if the "stationarity" Killing field is hypersurface orthogonal (Ref. 5, p. 274).

There is an analogous difference between the stationary and static electromagnetic field within the special relativity. If an inertial frame exists in which the electric and magnetic fields are time-independent, the field is called stationary. If, in addition, the magnetic field vanishes in such a frame, the field is static (cf. Ref. 6, Chap. 5). A natural generalization of these notions for electrovacuum spacetimes is given by

Definition 1: The electrovacuum spacetime $(\mathcal{M}, g, F)$ is called stationary, if it admits a timelike infinitesimal (g, F)-map in a neighborhood of any of its points [infinitesimal (g,F)-map is a vector field ξ such that

$$\mathcal{L}_\xi g=0, \quad \mathcal{L}_\xi F=0,$$

where $\mathcal{L}_\xi$ is the Lie derivative with respect to ξ].

The electrovacuum spacetime $(\mathcal{M}, g, F)$ is called static, if it satisfies the following conditions:

(a) There is a timelike infinitesimal (g,F)-map ξ in

a neighborhood of any point of $(\mathcal{M}, g, F)$ which is hypersurface-orthogonal.

(b) The magnetic field vanishes in any orthonormal frame whose timelike vector is directed along ξ.

We show the following

Theorem: Let $(\mathcal{M}, g, F)$ be a C-spacetime with group $\mathcal{G}$ and the corresponding pair of horizons $\mathcal{H}^+, \mathcal{H}^-$. Then, the following two statements are equivalent:

(a) There is a neighborhood $\mathcal{U}$ of $\mathcal{H}^+ \cup \mathcal{H}^-$ in $\mathcal{M}$ such that the subspace $(\mathcal{U} \cap I^+(\mathcal{H}^-) \cap I^-(\mathcal{H}^+), g, F)$ of $(\mathcal{M}, g, F)$ is static.[5]

(b) The C-structure (γ, Ω, E, H) of $\mathcal{H}^+$ satisfies

$$\Omega^A = 0, \quad H = 0.$$

Proof $(a) \Rightarrow (b)$: The plan of the proof is the following. We construct a totally geodesic spacelike hypersurface Σ in $\mathcal{M}$ which intersects $\mathcal{H}^+$ in $\mathcal{S}$. If such a hypersurface exists, then its unit future-directed normal vector field e_0^i is parallelly propagated along any curve in Σ_t, in particular along any curve of $\mathcal{S}$. Define still another vector e_1^i at any point of $\mathcal{S}$ by demanding that e_1^i be unit, tangential to Σ, orthogonal to $\mathcal{S}$ and oriented in such a way that

$$l^i = (1/\sqrt{2})(e_0^i + e_1^i)$$

be tangential to $\mathcal{H}^+$. Such a field e_1^i is also parallelly propagated along any curve in $\mathcal{S}$, because $\mathcal{S}$ is itself a totally geodesic surface in $\mathcal{M}$. But then, we must have

$$l^i{}_{;A} = 0.$$

Hence, for α chosen such that $\alpha_{,i} l^i = 1$, the corresponding Ω^A is zero. As this Ω^A is already divergenceless, the first part of the statement (b) would follow.

If, in addition, Σ is orthogonal to the trajectories of $\mathcal{G}$, then there is no magnetic field in the space $\Sigma \cap I^-(\mathcal{H}^+) \cap \mathcal{U}$. As F_{ij} is continuous, the magnetic field is zero even at $\mathcal{S}$, and the second part of (b) would follow.

For the construction of Σ, we need

Lemma 3: Let the conditions of Lemma 1 in Ref. 1 be satisfied. Then, any point p of $\mathcal{S}$ has an open normal neighborhood (see, e.g., Ref. 3) $\mathcal{V}$ such that

(1) The set $\mathcal{V} - (\mathcal{H}^+ \cup \mathcal{H}^-)$ consists of four components, C_1, C_2, C_3, C_4, say, defined as follows:

$$C_1 = I^+(\mathcal{H}^+, \mathcal{V}) \cap I^+(\mathcal{H}^-, \mathcal{V}),$$
$$C_2 = I^-(\mathcal{H}^+, \mathcal{V}) \cap I^+(\mathcal{H}^-, \mathcal{V}),$$
$$C_3 = I^-(\mathcal{H}^+, \mathcal{V}) \cap I^-(\mathcal{H}^-, \mathcal{V}),$$
$$C_4 = I^+(\mathcal{H}^+, \mathcal{V}) \cap I^-(\mathcal{H}^-, \mathcal{V}).$$

(2) The trajectories of $\mathcal{G}$ are timelike in C_2 and C_4 and spacelike in C_1 and C_3.

Proof of the Lemma: Let ξ be a Killing vector field of $\mathcal{G}$. At any point $q \in \mathcal{S} \cap \mathcal{V}$, $\xi^i(q) = 0$, and we obtain subsequently

$$\xi^i \xi_i = 0,$$
$$(\xi^i \xi_i)_{ij} x^j = 0,$$
$$(\xi^i \xi_i)_{ijk} x^j x^k = 2 \xi^i{}_{;j}\, \xi_{i;k} x^j x^k$$

for any vector x^i at q. $\xi^i{}_{;j}(q)$ is the matrix of a generator of the group in $T_q(\mathcal{M})$ induced by $\mathcal{G}$, so it must satisfy

$$\xi^i{}_{;j}(q)\, l^j = \kappa l^i,$$
$$\xi^i{}_{;j}(q)\, n^j = -\kappa n^i,$$
$$\xi^i{}_{;j}(q)\, m^j = 0, \tag{17}$$

where κ is a nonzero real number, l^i is tangential to $\mathcal{H}^+$, n^i to $\mathcal{H}^-$ and the tetrad $l^i, n^i, m^i, \bar{m}^i$ is pseudo-orthonormal. Writing x^i as

$$x^i = a l^i + b n^i + \bar{c} m^i + c \bar{m}^i$$

we obtain

$$x^j \xi^i{}_{;j} = a l^i - b n^i,$$

hence

$$(\xi^i \xi_i)_{;jk} x^j x^k = -2\kappa^2 ab.$$

Clearly, if $a > 0$, $b > 0$ or $a < 0$, $b < 0$, then $(\xi^i \xi_i)_{;jk} x^j x^k < 0$, if $a > 0$, $b < 0$ or $a < 0$, $b > 0$, then $(\xi^i \xi_i)_{;jk} x^j x^k > 0$, proving the lemma.

Let $p \in \mathcal{S}$ and $\mathcal{V}$ be a neighborhood of p with the properties as in Lemma 3. $\mathcal{V}$ is convex (any two points of $\mathcal{V}$ can be joined by a unique geodesic segment lying in $\mathcal{V}$). Chose an arbitrary point $r \in C_2$ and define Γ as the family of geodesics joining r with all points of $\mathcal{V} \cap \mathcal{S}$ and inextendible in $\mathcal{V}$. Let us denote by Σ the hypersurface formed by all points which lie on the geodesics of Γ. We show that Σ is orthogonal to ξ at any of its points.

Let u^i be the unit vector field at Σ tangential to geodesics of Γ and pointing, say, from $\mathcal{S}$ to r. We have

$$u^i \xi_i = 0, \tag{18}$$

because $u^i \xi_i = \text{const}$ along any geodesic and $u^i \xi_i = 0$ at $\mathcal{S}$. Choose an arbitrary Jacobi field [3] v^i of Γ along a geodesic c of Γ. Thus, v^i must satisfy

$$u_{i;j} v^j = v_{i;j} u^j. \tag{19}$$

Also,

$$v^i \xi_i = 0 \quad \text{at } \mathcal{S} \cap c \text{ and at } r. \tag{20}$$

ξ is a hypersurface-orthogonal Killing field, therefore,

$$\xi_{i;j} = -\xi_{j;i}, \quad \eta^{ijkl} \xi_j \xi_{k;l} = 0, \tag{21}$$

where η^{ijkl} is the Levi–Civita tensor. From the last relation of (21), it follows that

$$\eta^{ijkl} \xi_j \xi_{kl} \eta_{ipqs} \xi^p u^r v^s = 0.$$

Writing out $\eta^{ijkl} \eta_{ipqs}$ and using (18), we obtain

$$-2(\xi^i \xi_i) \xi_{k;l} u^k v^l = (\xi^j v_j)(\xi^i \xi_i)_{,k} u^k. \tag{22}$$

The relations (19), (18), (21), and (22) imply

$$(v^i \xi_i)_{,j} u^j = [(\xi^j \xi_j)^{-1} (\xi^j \xi_j)_{,k} u^k] \cdot (v^i \xi_i).$$

This is an ordinary differential equation for $v^i \xi_i$ along c which has the integral

$$v^i \xi_i / \xi^i \xi_i = \text{const}.$$

But $\xi^i \xi_i > 0$ in $C_2 \cup C_4$ and $v^i \xi_i = 0$ at $r \in C_2$, so

$$v^i \xi_i = 0 \quad \text{along } c.$$

Now, the claim follows easily, because we can pick out two Jacobi fields v_1^i and v_2^i along c in such a way that u^i, v_1^i, and v_2^i are linearly independent showing that ξ is orthogonal to Σ along c—that is to say everywhere, because c was arbitrary. Such a Σ must be totally geodesic.

Proof (b)⇒(a): If (b) holds, then Lemma 1 implies that the bifurcate horizon $\mathcal{H}^+ \cup \mathcal{H}^-$ is invariant under τ. According to Lemma 2, there is a (g, F)-map $\tau'\colon (\mathcal{M}, g, F) \to (\mathcal{M}, g, F)$ such that

$$\tau'|_{\mathcal{H}^+ \cup \mathcal{H}^-} = \tau.$$

In particular, τ' is an isometry in $(\mathcal{M}, g)$. We show that

$$\varphi' \circ \tau' \circ \varphi' = \tau' \quad \text{for any } \varphi' \in \mathcal{G}, \tag{23}$$

$$\tau'(\mathcal{G}(p)) = \mathcal{G}(p) \quad \text{for any } p \in I^+(\mathcal{H}^-) \cap I^-(\mathcal{H}^+), \tag{24}$$

where $\mathcal{G}(p)$ is the trajectory of the group $\mathcal{G}$ through p. Then, the two conditions of Theorem 4 in Ref. 7 are satisfied and $\mathcal{G}$ must be hypersurface-orthogonal.

Equation (23) follows immediately from Lemma 2 and (10). The proof of (24) is performed in two steps. As τ' is an isometry, it must map the trajectories of $\mathcal{G}$ onto trajectories of some one-dimensional isometry group, $\mathcal{G}_1$, say. First, we show that $\mathcal{G}_1 = \mathcal{G}$, second that there is a fixed point of τ' in any trajectory of $\mathcal{G}$.

Let ξ be a Killing vector field of $\mathcal{G}$ and ξ_1 the Killing vector field of $\mathcal{G}$, which satisfies

$$\xi_1 = \tau'_*(\xi).$$

Then,

$$\xi_{1i;j} = \tau'_*(\xi_{i;j}), \tag{25}$$

because τ' is an isometry. Let $p \in \mathcal{S}$. The only nonzero component of $\xi_{i;j}(p)$ in the frame $l^i, n^i, m^i, \overline{m}^i$ is

$$\xi_{i;j}(p)\, l^i n^j = \kappa$$

[see (17)]. From (25), it follows that

$$\xi_{1i;j}(p)\,(\tau'_*(l))^i\,(\tau'_*(n))^j = \kappa,$$

all other components of $\xi_{1i;j}$ in the frame $\tau'_*(l)$, $\tau'_*(n)$, $\tau'_*(m)$, $\tau'_*(\overline{m})$ being zero. Relation (11) and the antisymmetry of $\xi_{1i;j}$ now imply,

$$\xi_{1i;j}(p) = -\xi_{i;j}(p). \tag{26}$$

We also have $\xi_1^i(p) = 0$ because of $\xi^i(p) = 0$, or

$$\xi_1^i(p) = -\xi^i(p). \tag{27}$$

But prescribing the value of a Killing field at a point together with its first covariant derivatives determines the Killing field in a neighborhood of the point uniquely. The relations (26) and (27) show, therefore, that

$$\xi_1^i = -\xi^i$$

at all points of $\mathcal{M}$ which can be connected to p by an arc. It follows that $\mathcal{G}_1 = \mathcal{G}$.

Let us consider the geodesic given by the initial data $(p, e_1^i(p))$, $p \in \mathcal{S}$, e_1^i given by (12). This data is not changed by τ', because $\mathcal{S}$ is pointwise invariant and (13) holds. As p moves though $\mathcal{S}$, the corresponding geodesics span a hypersurface Σ, which must be pointwise invariant under τ', too. In a neighborhood $\mathcal{V}$ of p that was introduced in Lemma 3, Σ is well defined and spacelike; hence, Σ intersects C_2 and C_4, where the trajectories of $\mathcal{G}$ are timelike. Every such trajectory must intersect Σ and contain, in such a way, a fixed point of τ'.

We have shown that $\mathcal{G}$ is orthogonally transitive in C_2 and C_4. It remains to be shown that there cannot be any magnetic field in a frame whose timelike vector is directed along ξ. But this is easy, because τ' invertes the orientation of ξ being, at the same time, a (g, F)-map. In the time-inverted frame, the magnetic field is just the opposite of the field in the original frame. In a (g, F)-mapped frame, it must be the same, so the only allowed value is zero. QED

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Algebraic identities among $U(n)$ infinitesimal generators

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Some algebraic identities among infinitesimal generators of the n-dimensional unitary group $U(n)$ have been found. They satisfy a simple quadratic equation for degenerate representations. A generalization of Holstein–Primakoff boson realization for the $U(n)$ group is also given.

1. SUMMARY OF PRINCIPAL RESULTS

The n-dimensional unitary group $U(n)$ is very important for studies[1,2] of the $SU(3)$ and $SU(6)$ symmetries in the particle physics as well for the nuclear physics.[3]

Louck and Biedenharn[4] have established various fundamental theorems on properties of infinitesimal generators of the $U(n)$ group. However, many of their results are rather involved with content being often implicit. The main purpose of the present note is to find some explicit identities among these generators by a simpler method. We shall see that we can express them into surprisingly simple forms which are suitable for various physical applications. Also, all vector operators are expressible as a linear combination of powers of the generators.

The infinitesimal generators A^μ_ν of the $U(n)$ group satisfy the Lie commutation relations[5]

$$[A^\mu_\nu, A^\alpha_\beta] = \delta^\mu_\beta A^\alpha_\nu - \delta^\alpha_\nu A^\mu_\beta. \tag{1.1}$$

Hereafter, all Greek indices assume n values $1,2,\ldots,n$. In case we are interested in the $SU(n)$ subgroup, we have only to replace A^μ_ν by its traceless tensor

$$B^\mu_\nu = A^\mu_\nu - \frac{1}{n}\delta^\mu_\nu \sum_{\lambda=1}^{n} A^\lambda_\lambda.$$

As is well known,[6] irreducible representations of the $U(n)$ group are characterized by n integers satisfying

$$f_1 \geq f_2 \geq \cdots \geq f_n. \tag{1.2}$$

It is sometimes more convenient to use

$$l_\lambda = f_\lambda + n - \lambda, \quad n \geq \lambda \geq 1, \tag{1.3}$$

which satisfy a strictly decreasing inequality

$$l_1 > l_2 > \cdots > l_n. \tag{1.4}$$

Then, the dimension N of the irreducible representation (hereafter referred to as IR) characterized by the signature $(1,2)$ is given by the Weyl's formula[6]

$$N = \frac{\prod_{\mu<\nu}^{n}(l_\mu - l_\nu)}{1!2!\cdots(n-1)!}. \tag{1.5}$$

Hereafter, we restrict ourselves in the given IR specified by the signature $(1,2)$ so that n^2 infinitesimal generators A^μ_ν represent their $N\times N$ matrix representations, though all results are also valid for more abstract vector operators acting on the IR space of the signature (1.2). Since any representation of the $U(n)$ group is known to be equivalent to a unitary one, we can hereafter impose an additional hermiticity condition

$$(A^\mu_\nu)^* = A^\nu_\mu \tag{1.6}$$

without loss of generality.

Now, $N\times N$ matrices T^μ_ν $(\mu,\nu=1,2,\ldots,n)$ will be called a vector operator, if they satisfy

$$[A^\mu_\nu, T^\alpha_\beta] = \delta^\mu_\beta T^\alpha_\nu - \delta^\alpha_\nu T^\mu_\beta. \tag{1.7}$$

Comparing (1.7) to (1.1), we see that A^μ_ν itself is a vector operator. Although we can define[4,7] more general tensor operators, they are beyond the scope of the present note. Suppose that we have two vector operators S^μ_ν and T^μ_ν. Then, we can define a product vector operator[5] R^μ_ν by

$$R^\mu_\nu = \sum_{\lambda=1}^{n} S^\lambda_\nu T^\mu_\lambda. \tag{1.8}$$

We may easily verify that R^μ_ν satisfies the required commutation relation (1.7) of vector operator. Hereafter, we often suppress tensor indices μ and ν and write (1.8) simply as

$$R = ST. \tag{1.8'}$$

We notice that a product defined in this way is associative, i.e., we have

$$(ST)U = S(TU) \tag{1.9}$$

for products of three vector operators S^μ_ν, T^μ_ν, and U^μ_ν. Moreover, the unit vector operator I is a $N\times N$ matrix

$$I^\mu_\nu = \delta^\mu_\nu E, \tag{1.10}$$

where E is the $N\times N$ identity matrix.

We can define the jth power A^j by the recursion relation

$$A^0 = I, \quad A^{j+1} = AA^j. \tag{1.11}$$

These are vector operators. For example,

$$(A^3)^\mu_\nu = \sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} A^\alpha_\nu A^\beta_\alpha A^\mu_\beta.$$

As we shall prove at the end of this paper that any vector operator is expressible as a linear combination of $I, A, \ldots, A^{n-1}$. Hence, our vector product is automatically Abelian, i.e., we have

$$ST = TS \tag{1.12}$$

for any two vector operators, since (1.12) is obvious for any linear combinations of A^j.

Next, for any vector operator T^μ_ν, we can assign a scalar $\langle T\rangle$ by the formula

$$\sum_{\lambda=1}^{n} T^\lambda_\lambda = \langle T\rangle E. \tag{1.13}$$

This is so because (1.7) leads to

$$[A^\mu_\nu, \sum_{\lambda=1}^{n} T^\lambda_\lambda] = 0,$$

and hence by the Schur's lemma $\sum_{\lambda=1}^{n} T^\lambda_\lambda$ is a multiple of the unit matrix E. Especially, we set

$$M_j = \langle A^j\rangle, \quad j=0,\ 1,\ 2,\ \cdots, \tag{1.14}$$

which are eigenvalues of generalized Casimir operators (or Gel'fand invariants) of the $U(n)$ group. Its explicit value has been computed by Louck and Biedenharn[4] to be

$$M_j = \sum_{\lambda=1}^{n} (l_\lambda)^j \prod_{\nu=1}^{n}{}' \frac{1+l_\nu - l_\lambda}{l_\nu - l_\lambda}, \tag{1.15}$$

where the product on ν omits the singular point $\nu=\lambda$. We shall also give an alternative derivation of this formula in the next section. We may remark[4] that M_j is a symmetric polynomial of $l_1, l_2, \ldots, l_n$ of the degree j. Therefore, n constants M_j $(j=1,2,3,\ldots,n)$ can be also used to characterize the IR instead of the original n integers $f_1, f_2, \ldots, f_n$.

Louck and Biedenharn also proved[4] that we can express A^n in terms of a linear combination of $I, A, \ldots, A^{n-1}$. For the special case $n=3$, this fact is well known and basic to derive the $SU(3)$ mass formula.[5] We shall show that we can express this linear dependence in a very simple form of

$$A(l_1)A(l_2)\cdots A(l_n) = 0. \tag{1.16}$$

Here, we have set for simplicity

$$A(l) = A - lI, \tag{1.17}$$

and the product in (1.16) is meant to be the vector product defined as in (1.8′) and (1.9).

Second, it may happen that two values of f_μ and f_ν for $\mu\neq\nu$ may coincide. In such a case, we can have a stronger identity. To be more precise, let us suppose that we have

$$f_k > f_{k+1} = f_{k+2} = \cdots = f_{k+p} > f_{k+p+1}.$$

We shall call all factors $A(l_j)$ with $k+1 \leq j < k+p$ redundant factors. Then, our prescription is to omit all redundant factors in (1.16). As an illustration, let us consider a specific case $n=8$ with

$$f_1 = f_2 = f_3 > f_4 = f_5 > f_6 > f_7 = f_8. \tag{1.18}$$

Now, all factors $A(l_1)$, $A(l_2)$, $A(l_4)$, and $A(l_7)$ are redundant, and we have a stronger identity

$$A(l_3)A(l_5)A(l_6)A(l_8) = 0 \tag{1.19}$$

instead of (1.16) with $n=8$. Of course, the validity of (1.19) implies that of (1.16). We shall prove that equations of the type (1.19) are the minimal polynomial equations among A^j.

Let us call an IR degenerate if we have an integer j such that

$$f_1 = f_2 = \cdots = f_j \geq f_{j+1} = f_{j+2} = \cdots = f_n. \tag{1.20}$$

Then, the above rule implies the validity of

$$(A - l_j I)(A - l_n I) = 0 \tag{1.21}$$

or equivalently of

$$\sum_{\lambda=1}^{n} A^\lambda_\nu A^\mu_\lambda = (l_j + l_n)A^\mu_\nu - l_j l_n \delta^\mu_\nu E. \tag{1.22}$$

Conversely, we can prove that (1.21) or (1.22) is also sufficient for the representation to be degenerate. This fact is previously known[8,9] for the special case $n=3$ and answers positively a conjecture stated elsewhere.[10]

Returning to the general case, let us define a Hermitian conjugate vector operator $\bar{S}^\mu_\nu$ of S^μ_ν by

$$(\bar{S})^\mu_\nu = (S^\nu_\mu)^*. \tag{1.23}$$

It is easy to verify the fact that $\bar{S}$ is indeed a vector operator, because of (1.7) and (1.6). Next, we can introduce an inner product (S,T) for two vector operators by

$$(S,T) = \langle \bar{S}T\rangle. \tag{1.24}$$

Then, it is obvious that

$$(S,S) \geq 0 \tag{1.25}$$

and, moreover, $(S,S)=0$ if and only if we have $S^\mu_\nu = 0$ identically. Therefore, with this inner product, all vector operators form a finite-dimensional Hilbert space which we denote by $\mathcal{H}$. Similarly, a linear subspace of $\mathcal{H}$ spanned by all linear combinations of A^j $(j=0,1,2,\cdots)$ form the subHilbert space $\mathcal{H}_0$. Actually, we can prove that $\mathcal{H}=\mathcal{H}_0$, i.e., all vector operators are linear combinations of A^j. Also, (1.16) or (1.19) assures us that the dimension of $\mathcal{H}$ is at most n. More precisely, it is equal to the number of nonredundant values of f_μ. We may regard any vector operator S as a linear transformation in $\mathcal{H}$ by assigning a mapping of a vector operator T into ST. Then, all vector operators of the $U(n)$ group form a commutative Hilbert algebra with dimension less than or equal to n. We can rephrase our identity (1.16) or (1.19) as follows. The linear operator A in our Hilbert space can have exactly n integer eigenvalues, l_μ $(\mu=1,2,\ldots,n)$ if all f_μ are distinct. However, in case that we have $f_\mu = f_\nu$ for some pair, μ and ν, with $\mu\neq\nu$, then A can assume only those values of l_μ corresponding to nonredundant values of f_μ.

From (1.24), we have

$$(A^j, A^k) = M_{j+k}, \tag{1.26}$$

since the hermiticity condition (1.6) implies $\bar{A}=A$. Therefore, if c_j $(j=0,1,2,\cdots)$ are arbitrary complex numbers, then (1.26) and (1.25) lead to

$$\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} C_j C_k^* M_{j+k} \geq 0. \tag{1.27}$$

Especially, this gives

$$\begin{aligned} &M_{2j} \geq 0, \quad M_{2j}M_{2k} \geq (M_{j+k})^2, \\ &\det(A^j, A^k) = \det M_{j+k} \geq 0. \end{aligned} \tag{1.28}$$

Now, a linear independence among p operators $I, A, \ldots, A^{p-1}$ is equivalent to have nonzero Gram determinant $\det m_{jk} \neq 0$ for $p\times p$ matrix, $m_{jk} = (A^j, A^k) = M_{j+k}$, $j, k = 0,1,2,\ldots,p-1$. This quantity has been studied in

great detail by Louck and Biedenharn.[4] Their result is indeed that the maximal number of the linearly independent operators among A^J is precisely equal to the number of nonredundant f_μ. We shall prove the same fact in a different way.

We have noted that any degenerate representation leads to the validity of (1.22). One particularly interesting example is that of the completely symmetric IR with signature $f_2=f_3=\cdots=f_n=0$. After setting $f_1\equiv f$, then (1.22) is rewritten as

$$\sum_{\lambda=1}^{n} A^\lambda_\nu A^\mu_\lambda = (f+n-1)A^\mu_\nu. \tag{1.29}$$

An interesting fact is that for completely symmetric case, we can have the following additional relations,[11]

$$A^\mu_\nu A^\alpha_\beta - A^\mu_\beta A^\alpha_\nu = \delta^\mu_\beta A^\alpha_\nu - \delta^\mu_\nu A^\alpha_\beta, \tag{1.30}$$

as we shall show in the next section. If we note $M_1=f$, then (1.30) immediately gives (1.29) by setting $\mu=\beta$ and summing over μ. Other identities of this kind can be found in Ref. 10. One simple way[11] proving the validity of (1.30) is to utilize n creation (a^+_μ) and annihilation (a_μ) boson operators satisfying the standard canonical commutation relations:

$$\begin{aligned}&[a_\mu, a^+_\nu]=\delta_{\mu\nu},\\ &[a_\mu, a_\nu]=[a^+_\mu, a^+_\nu]=0.\end{aligned} \tag{1.31}$$

Then, if we set

$$A^\mu_\nu = a^+_\nu a_\mu, \tag{1.32}$$

it is easy to see that A^μ_ν satisfy the $U(n)$ Lie algebra (1.1) as well as the special relations (1.29) and (1.30). Actually, these operators are defined in a dense subset of the whole boson Fock space which will reduce into a direct sum of finite dimensional IR's of the $U(n)$ group. The subspace consisting exactly of f bosons gives the desired completely symmetric IR. In this construction, we have utilized all of n boson operators. However, we could find a slightly more economical realization in which we use only $n-1$ bosons as follows. Let us set

$$\theta(f) = (f-\sum_{\lambda=1}^{n-1} a^+_\lambda a_\lambda)^{1/2}. \tag{1.33}$$

For any positive integer f, this operator has a well-defined meaning in a boson Fock subspace satisfying

$$f \geq \sum_{\lambda=1}^{n-1} a^+_\lambda a_\lambda \geq 0. \tag{1.34}$$

When we define

$$\begin{aligned}&A^\mu_\nu = a^+_\nu a_\mu, \quad \mu\neq n,\ \nu\neq n\\ &A^n_\nu = a^+_\nu \theta(f), \quad \mu=n,\ \nu\neq n,\\ &A^\mu_n = \theta(f) a_\mu, \quad \mu\neq n,\ \nu=n,\\ &A^n_n = \theta(f)\theta(f), \quad \mu=n,\ \nu=n,\end{aligned} \tag{1.35}$$

then we can prove that these n^2 operators A^μ_ν obey (1.1), (1.29), and (1.30), if we notice

$$\begin{aligned}&\theta(f)a^+_\mu = a^+_\mu\theta(f-1),\\ &\theta(f)a_\mu = a_\mu\theta(f+1),\\ &\theta(f+1)\theta(f+1)-\theta(f)\theta(f)=1.\end{aligned}$$

Comparing (1.35) with (1.32), we see that the former can be obtainable from the latter by a formal substitution

$$a_n \to \theta(f), \quad a^+_n \to \theta(f)$$

of a_n and a^+_n by the same Hermitian operator $\theta(f)$. Of course, we have to be careful of the order of the operators involved in this substitution. At any rate, this fact justifies the usual boson approximation used for treatment of dilute boson gas problems,[12] if we take care of the order of operators.

The special case $n=2$ in (1.35) is especially interesting. If we set

$$\begin{aligned}&J_1+iJ_2=A^2_1, \quad J_1-iJ_2=A^1_2,\\ &J_3=\tfrac{1}{2}(A^1_1-A^2_2),\end{aligned}$$

then J_1, J_2 and J_3 are infinitesimal generators of the three-dimensional orthogonal group $O(3)$, or more precisely of the $SU(2)$. Then, (1.35) becomes

$$\begin{aligned}&J_1+iJ_2 = a^+(f-a^+a)^{1/2},\\ &J_1-iJ_2 = (f-a^+a)^{1/2}a,\\ &J_3 = a^+a-\tfrac{1}{2}f,\end{aligned} \tag{1.36}$$

where we have set $a_1\equiv a$. This is precisely the formula of Holstein and Primakoff,[13] and we may regard (1.35) as its generalization. We can easily verify an identity

$$\mathbf{J}^2 = J_1^2+J_2^2+J_3^2 = \tfrac{1}{2}f(\tfrac{1}{2}f+1)$$

so that $f/2$ corresponds to the total angular momentum. The Holstein–Primakoff realization (1.36) has been used by Tanabe and Sugawara-Tanabe[14] for study of some deformed rotating nuclei. Also, it has been utilized by Pang, Klein, and Dreizler[15] for an analysis of an exactly solvable nuclear model. For the special case $n=3$, Li, Klein, and Dreizler[16] previously discovered an asymptotic form of (1.35) for large values of f. Also, the special conditions (1.29) and (1.30) for completely symmetric representations have been successfully applied[9] to simplify electromagnetic mass formulas of the baryon decuplet in the $SU(3)$ symmetry. Also, their validity explains the reason why the $SU(3)$ mass formula for the decuplet states becomes so simple.[1] Further applications of the present identities will be given elsewhere.

2. DERIVATION OF IDENTITIES

In this section we shall prove various statements made in the previous section. Before going into details, let us briefly recapitulate some basic facts of the representation theory of the $U(n)$ group. Setting

$$H_\mu = A^\mu_\mu, \quad \mu=1,2,\ldots,n, \tag{2.1}$$

then the n operators H_μ form a maximal Abelian subalgebra of our Lie ring. Consider a simultaneous eigenvector χ satisfying

$$H_\mu\chi = h_\mu\chi.$$

Then, the n eigenvalues h_μ ($\mu=1,2,\ldots,n$) are called a weight. We introduce a partial ordering relation for two weights h_μ and k_μ as follows. If we have an integer j, such that

$$h_1=k_1,\quad h_2=k_2,\ldots,\quad h_j=k_j,$$

but $h_{j+1}>k_{j+1}$, then we say that the weight h_μ is higher than k_μ. Any irreducible representation is specified by its highest weight. In particular, the irreducible representation with signature (1.2) is characterized by the highest weight vector ϕ satisfying

$$H_\mu\phi=f_\mu\phi,\quad \mu=1,2,\ldots,n. \tag{2.2}$$

Hereafter, ϕ always refers to the highest weight state with the highest weight f_μ. Then, the standard argument immediately leads to

$$A^\mu_\nu\phi=0,\quad \mu>\nu. \tag{2.3}$$

However, if we have a special situation $f_\mu=f_\nu$ for some μ and ν with $\mu\neq\nu$, then we find an additional condition

$$A^\mu_\nu\phi=\delta^\mu_\nu f_\mu\phi,\quad f_\mu=f_\nu \tag{2.4}$$

including the case $\mu<\nu$. To prove this last statement, we notice that (1.1) and (2.2) give us

$$[A^\mu_\nu,A^\nu_\mu]\phi=(A^\nu_\nu-A^\mu_\mu)\phi=(f_\nu-f_\mu)\phi.$$

Suppose that we have $\mu<\nu$ since otherwise (2.4) is valid always in view of (2.2) and (2.3). If we have $f_\mu=f_\nu$, the above relation leads to

$$A^\nu_\mu A^\mu_\nu\phi=0,$$

where we used the fact $A^\nu_\mu\phi=0$ because we assumed $\nu>\mu$. Using the hermiticity condition (1.6), we can rewrite this as

$$(A^\mu_\nu)^*A^\mu_\nu\phi=0.$$

Since the matrix $(A^\mu_\nu)^*A^\mu_\nu$ multiplying ϕ is nonnegative, this is possible only if we have $A^\mu_\nu\phi=0$, and this proves (2.4).

Now, we shall proceed to prove validities of our main results, identity (1.16) and the redundant factor rule illustrated by (1.19). For this purpose, let us introduce n new vector operators $D^\mu_\nu(\alpha)$, $(n\geq\alpha\geq1)$ by

$$D^\mu_\nu(\alpha)=[\prod_{j=\alpha}^{n}A(l_j)]^\mu_\nu. \tag{2.5}$$

For a fixed value of α, $D^\mu_\nu(\alpha)$ is obviously a vector operator, i.e., it satisfies

$$[A^\tau_\lambda,D^\mu_\nu(\alpha)]=\delta^\tau_\nu D^\mu_\lambda(\alpha)-\delta^\mu_\lambda D^\tau_\nu(\alpha). \tag{2.6}$$

Now, we shall prove the following lemma.

Lemma 1: We have

$$D^\mu_\nu(\alpha)\phi=0\quad\text{for}\quad \mu\geq\alpha\ \text{and}\ \nu=1,2,\ldots,n. \tag{2.7}$$

The proof is by induction on decreasing values of α. First, for the highest possible value $\alpha=n$, we see

$$D^\mu_\nu(n)=[A(l_n)]^\mu_\nu=A^\mu_\nu-l_n\delta^\mu_\nu E$$

so that

$$D^\mu_\nu(n)\phi=A^\mu_\nu\phi-f_n\delta^\mu_\nu\phi.$$

However, $\mu\geq\alpha$ implies $\mu=n$ in this case. Therefore, $D^n_\nu(n)\phi=0$ is the result of (2.2) and (2.3), and the lemma is valid for $\alpha=n$. Next, suppose that the lemma holds for $\alpha=\beta+1$, i.e., we have

$$D^\mu_\nu(\beta+1)\phi=0\quad\text{for}\quad \mu\geq\beta+1. \tag{2.8}$$

Then, we proceed to show the validity of

$$D^\mu_\nu(\beta)\phi=0\quad\text{for}\quad \mu\geq\beta. \tag{2.9}$$

First, we notice

$$D^\mu_\nu(\beta)=[D(\beta+1)A(l_\beta)]^\mu_\nu=[A(l_\beta)D(\beta+1)]^\mu_\nu \tag{2.10}$$

from the Abelian nature of the product involving A^j. For $\mu\geq\beta+1$, we use the second form of (2.10) to find

$$D^\mu_\nu(\beta)\phi=\sum_{\lambda=1}^{n}[A(l_\beta)]^\lambda_\nu D^\mu_\lambda(\beta+1)\phi=0$$

because of the induction hypothesis (2.8). Hence, we have only to prove (2.9) for the case $\mu=\beta$. Using now the first form of (2.10), we compute

$$D^\beta_\nu(\beta)\phi=\sum_{\lambda=1}^{n}D^\lambda_\nu(\beta+1)[A^\beta_\lambda-l_\beta\delta^\beta_\lambda E]\phi.$$

Because of (2.2), (2.3), and (2.6), we can rewrite this as

$$D^\beta_\nu(\beta)\phi=\sum_{\lambda>\beta}\{A^\beta_\lambda D^\lambda_\nu(\beta+1)-\delta^\beta_\nu D^\lambda_\lambda(\beta+1)+\delta^\lambda_\lambda D^\beta_\nu(\beta+1)\}\phi$$
$$+(f_\beta-l_\beta)D^\beta_\nu(\beta+1)\phi.$$

The first and second terms in the above expression are zero in view of the induction hypothesis (2.8) since the summation over λ runs only for $\lambda\geq\beta+1$. Therefore, we finally find

$$D^\beta_\nu(\beta)\phi=(n-\beta+f_\beta-l_\beta)D^\beta_\nu(\beta+1)\phi,$$

which is identically zero if we note Eq. (1.3), i.e., $l_\beta=f_\beta+n-\beta$. This completes the proof of (2.9) so that, by induction, we have proved Lemma 1.

By setting $\alpha=1$, the lemma implies

$$D^\mu_\nu(1)\phi=0$$

for all values of μ and ν since the condition $\mu\geq1$ is trivially satisfied. Then, as we shall see shortly, this gives

$$D^\mu_\nu(1)=0$$

identically, which proves the validity of (1.16). Now, in the above argument, we utilize the following lemma.

Lemma 2: If a vector operator T^μ_ν satisfies

$$T^\mu_\nu\phi=0$$

for all values of μ and ν, then T^μ_ν is identically zero.

This can be shown as follows. Multiplying A^α_β on this equation and noting (1.7), this gives

$$T^\mu_\nu A^\alpha_\beta\phi=0.$$

Repeating the same procedure, we find

$$T^\mu_\nu F(A)\phi=0,$$

where $F(A)$ is an arbitrary polynomial of generators A^α_β. Since we are dealing with an irreducible representation, any state is cyclic, so that all states of the form $F(A)\phi$ generate the whole irreducible representation space. Hence, $T^\mu_\nu=0$ follows immediately.

So far, in our derivation of the Lemma 1, we used only the basic condition (2.3). However, if we have $f_\mu=f_\nu$ for some values of μ and ν with $\mu\neq\nu$, then we can utilize the additional condition (2.4) so that we can make

a stronger statement. In that case, we can simply omit all redundant factors $A(l_\mu)$ in $D(\alpha)$ as has been explained in Sec. 1. To be more precise, let us suppose that we have

$$f_\gamma > f_{\gamma+1} = f_{\gamma+2} = \cdots = f_\beta > f_{\beta+1}, \quad \beta \geq \gamma+1. \tag{2.11}$$

Then, we omit all redundant $A(l_\mu)$ $(\gamma+1 \leq \mu \leq \beta-1)$ in the definition of $D(\gamma+1)$. This implies that instead of (2.10), we now define $\tilde{D}(\gamma+1)$ by

$$\tilde{D}^\mu_\nu(\gamma+1) = [A(l_\beta)\tilde{D}(\beta+1)]^\mu_\nu = [\tilde{D}(\beta+1)A(l_\beta)]^\mu_\nu. \tag{2.12}$$

Also, suppose that we have

$$f_\tau > f_{\tau+1} = f_{\tau+2} = \cdots = f_n \tag{2.13}$$

at the extreme right end, and set

$$\tilde{D}^\mu_\nu(\tau+1) = [A(l_n)]^\mu_\nu = A^\mu_\nu - l_n\delta^\mu_\nu E. \tag{2.14}$$

Now, (2.12) and (2.14) define $\tilde{D}^\mu_\nu(\alpha)$ recursively and we can still prove the validity of the Lemma 1 for this new $\tilde{D}^\mu_\nu(\alpha+1)$, if we use (2.4) in addition to (2.3). Indeed, we can repeat essentially the same argument, word by word. For example, we have, to begin with

$$\tilde{D}^\mu_\nu(\tau+1)\phi = 0 \quad \text{for} \quad n \geq \mu \geq \tau+1$$

from (2.4) and (2.14) if we notice $f_\mu = f_n$. Next, suppose that we have (2.8) for $D \to \tilde{D}$. Then, we can easily prove the validity of

$$\tilde{D}^\mu_\nu(\gamma+1)\phi = 0 \quad \text{for} \quad \mu \geq \gamma+1,$$

which now replaces (2.9). This implies that the same induction method proceeds exactly in the same way for $\tilde{D}(\alpha)$. Therefore, the identities such as (1.19) and (1.21) are valid. Especially, this shows that (1.22) is a necessary condition for the degenerate representation. Actually, we can prove the following stronger converse statement. Suppose that we have

$$\sum_{\lambda=1}^{n}(A^\lambda_\nu - b\delta^\lambda_\nu E)(A^\mu_\lambda - c\delta^\mu_\lambda E) = 0 \tag{2.15}$$

for some complex numbers b and c. Then, we can show that the IR is degenerate and that one of b and c must coincide with l_n. Moreover, unless the IR is one-dimensional with $f_1 = f_2 = \cdots = f_n$, we find an integer j such that $f_1 = f_2 = \cdots = f_j > f_{j+1} = \cdots = f_n$, with $b = l_j$ and $c = l_n$. Note that, for the one-dimensional case, only one of b and c must be equal to l_n but the other can assume any complex number. To prove this statement, let z be a complex variable and consider a polynomial of z, given by

$$g(z) = \prod_{\lambda=1}^{n}(z - l_\lambda).$$

Using the standard algorithm, we can find another polynomial $h(z)$ and constants d_0 and d_1 such that

$$g(z) = (z-b)(z-c)h(z) + d_0 z + d_1.$$

Since the vector product involving A^j is Abelian, we can replace z and 1 by $N\times N$ matrices A and I in the above. For any irreducible representation, A satisfies (1.16), so that we must have

$$d_0 A^\mu_\nu + d_1\delta^\mu_\nu E = 0$$

if the IR satisfies (2.15). This implies that the representation is one-dimensional if $d_0 \neq 0$. In that case, we repeat essentially the same argument to show that both $g(z)$ and $(z-b)(z-c)$ must be divisible by $d_0 z + d_1$. In this way, we establish the first part of our assertion. On the other hand, if $d_0 = 0$, we must have $d_1 = 0$ also, and $(z-b)(z-c)$ must divide the polynomial $g(z)$. Therefore, b and c must coincide with l_μ and l_ν for some values of μ and ν with $\mu \neq \nu$. However, as we shall prove shortly, identities such as (1.19) or (1.21) are minimal so that the IR under consideration must be necessarily degenerate with $l_\mu = l_j$ and $l_\nu = l_n$.

As we mentioned in Sec. I, we can obtain a stronger relation (1.30) for the completely symmetric IR. This is due to the following fact. Because of (2.4), we have now

$$A^\mu_\nu\phi = 0 \quad \text{for} \quad \mu \neq 1.$$

Then, we can easily verify

$$(A^\mu_\nu A^\alpha_\beta - A^\mu_\beta A^\alpha_\nu - \delta^\mu_\beta A^\alpha_\nu + \delta^\mu_\nu A^\alpha_\beta)\phi = 0$$

if we use (1.1). Now, the same reasoning which led to Lemma 2 is applicable to prove the validity of (1.30).

We have assigned a scalar $\langle T\rangle$ for any vector operator T^μ_ν. However, we can make a stronger statement by assigning n scalars $\sigma_\lambda(T)$ $(\lambda = 1,2,\ldots,n)$ by

$$T^\lambda_\lambda\phi = \sigma_\lambda(T)\phi. \tag{2.16}$$

The reason for the validity of (2.16) is due to the fact that the state $T^\lambda_\lambda\phi$, for a fixed value of λ, has exactly the same highest weight f_μ, as we may verify easily. Therefore, $\langle T\rangle$ is given by

$$\langle T\rangle = \sum_{\lambda=1}^{n}\sigma_\lambda(T). \tag{2.17}$$

Also, we can show the validity of

$$T^\mu_\nu\phi = \delta^\mu_\nu\sigma_\mu(T)\phi \quad \text{for} \quad \mu \geq \nu. \tag{2.18}$$

Moreover, if we have $f_\mu = f_\nu$ for some values of μ and ν, then (2.18) is also applicable for such pairs of μ and ν even though we may have $\mu < \nu$. This is a simple consequence of (2.3) and (2.4) since we have

$$T^\mu_\nu\phi = [A^\mu_\nu, T^\mu_\mu]\phi = \{\sigma_\mu(T) - T^\mu_\mu\}A^\mu_\nu\phi = 0$$

in view of (2.3) or (2.4) for $\mu \neq \nu$.

Lemma 3: Suppose that T^μ_ν is a vector operator, then we have first

$$AT = TA, \quad \text{i.e.,} \quad (AT)^\mu_\nu = (TA)^\mu_\nu \tag{2.19}$$

and second

$$\sigma_\mu(AT) = \sum_{\nu=1}^{n}K_{\mu\nu}\sigma_\nu(T), \tag{2.20}$$

where $K_{\mu\nu}$ $(\mu,\nu = 1,2,\ldots,n)$ is defined by

$$\begin{aligned} &K_{\mu\nu} = 0, \quad \mu > \nu, \\ &K_{\mu\mu} = l_\mu, \quad \mu = \nu, \\ &K_{\mu\nu} = -1, \quad \mu < \nu. \end{aligned} \tag{2.21}$$

In the matrix form, K is an $n\times n$ matrix of the form

$$K = \begin{pmatrix} l_1 & & & -1 \\ & l_2 & & \\ & & \ddots & \\ 0 & & & l_n \end{pmatrix}.$$

First, Eq. (2.19) can be proven by computing

$$[\sum_{\lambda=1}^{n}(AA)_{\lambda}^{\lambda},\ T_{\nu}^{\mu}]=2(AT)_{\nu}^{\mu}-2(TA)_{\nu}^{\mu}$$

and noting the fact that the Casimir operator $\sum_{\lambda=1}^{n}(AA)_{\lambda}^{\lambda}$ is a multiple of the unit matrix E.

Next, we compute

$$(AT)_{\mu}^{\mu}\phi=\sum_{\lambda=1}^{n}A_{\mu}^{\lambda}T_{\lambda}^{\mu}\phi=\sum_{\lambda\geqslant\mu}^{n}A_{\mu}^{\lambda}T_{\lambda}^{\mu}\phi$$

$$=f_{\mu}\sigma_{\mu}(T)\phi+\sum_{\lambda>\mu}^{n}A_{\mu}^{\lambda}T_{\lambda}^{\mu}\phi,$$

where we used (2.18). However, the second term is

$$\sum_{\lambda>\mu}^{n}A_{\mu}^{\lambda}T_{\lambda}^{\mu}\phi=\sum_{\lambda>\mu}^{n}(T_{\lambda}^{\mu}A_{\mu}^{\lambda}+\delta_{\lambda}^{\lambda}T_{\mu}^{\mu}-\delta_{\mu}^{\mu}T_{\lambda}^{\lambda})\phi$$

$$=(n-\mu)\sigma_{\mu}(T)\phi-\sum_{\lambda>\mu}^{n}\sigma_{\lambda}(T)\phi$$

since the first term is zero because of (2.3). These are rewritten as (2.20) with (2.21).

Now, replacing the vector operator T by AT in (2.20) with repeated uses of (2.20), we obtain

$$\sigma_{\mu}(A^{j}T)=\sum_{\nu=1}^{n}(K^{j})_{\mu\nu}\sigma_{\nu}(T) \tag{2.22}$$

where K^{j} is the jth power of the $n\times n$ matrix K (*not* the $N\times N$ matrix!!). Especially, if we set $T=I$ in (2.22) and sum over μ, then we compute

$$M_{j}=\sum_{\mu=1}^{n}\sum_{\nu=1}^{n}(K^{j})_{\mu\nu}. \tag{2.23}$$

We can diagonalize the $n\times n$ matrix K easily as

$$(R^{-1}KR)_{\mu\nu}=l_{\mu}\delta_{\mu\nu}, \tag{2.24}$$

where the explicit form of the diagonalizing matrix R is given by

$$R_{\mu\nu}=\begin{cases}0, & \mu>\nu,\\ \prod_{j=1}^{\mu-1}(l_{j}-l_{\nu})\prod_{k=\mu+1}^{\nu}(1+l_{k}-l_{\nu}), & \mu\leqslant\nu,\end{cases} \tag{2.25}$$

$$(R^{-1})_{\mu\nu}=\begin{cases}0, & \mu>\nu;\\ \prod_{j=\mu}^{\nu-1}(1+l_{j}-l_{\mu})\prod_{k=1}^{\nu}{}'(l_{k}-l_{\mu})^{-1}, & \mu\leqslant\nu.\end{cases} \tag{2.26}$$

In (2.25) and (2.26), we interpret the product such as $\prod_{j=\mu}^{\nu-1}$ for $\nu-1<\mu$ and $\prod_{k=\mu+1}^{\nu}$ for the case $\mu+1>\nu$ to be one. Also, in (2.26), the product on k omits the singular point $k=\mu$. From (2.23), (2.24), (2.25), and (2.26), we can derive the formula (1.15) if we note identities

$$\sum_{\mu=1}^{n}R_{\mu\nu}=\prod_{j=1}^{\nu}(1+l_{j}-l_{\nu}),$$

$$\sum_{\nu=1}^{n}(R^{-1})_{\mu\nu}=\prod_{j=\mu}^{n}(1+l_{j}-l_{\mu})\prod_{k=1}^{n}{}'(l_{k}-l_{\mu})^{-1}. \tag{2.27}$$

Again in (2.27), the product on k omits the singular point $k=\mu$.

We are now in a position to prove that the identities derived in the present section is the minimal one. Suppose that $f(z)$ is a polynomial of a complex variable z

$$f(z)=\sum_{j=0}^{\infty}c_{j}z^{j}.$$

Then we can define a vector operator $f(A)$ by

$$[f(A)]_{\nu}^{\mu}=\sum_{j=0}^{\infty}C_{j}(A^{j})_{\nu}^{\mu}.$$

From (2.22) and (2.24), we compute

$$\sigma_{\mu}[f(A)T]=\sum_{\lambda=1}^{n}\sum_{\nu=1}^{n}R_{\mu\lambda}f(l_{\lambda})(R^{-1})_{\lambda\nu}\sigma_{\nu}(T). \tag{2.28}$$

Suppose that we have $f(A)=0$ identically. Then, this gives $\sigma_{\mu}[f(A)]=0$. By setting $T=I$ in (2.28) and noting (2.25) and (2.27), this leads to

$$0=\sum_{\lambda=\mu}^{n}f(l_{\lambda})\prod_{j=\mu+1}^{n}(1+l_{j}-l_{\lambda})\prod_{k=\mu}^{n}{}'(l_{k}-l_{\lambda})^{-1}$$

for all $\mu=1,2,\ldots,n$. First let us set $\mu=n$, which gives $f(l_{n})=0$. Next, we choose $\mu=n-1$ and find $f(l_{n-1})=0$ unless $l_{n-1}=l_{n}+1$, i.e., $f_{n-1}=f_{n}$. Continuing, we discover $f(l_{j})=0$ always unless we have $f_{j}=f_{j+1}$. Therefore, we have $f(l_{\mu})=0$ for nonredundant values of f_{μ}. This proves that (1.16) is the minimal polynomial if all f_{μ} are distinct. Similarly, for the special case (1.18), Eq. (1.19) is the minimal polynomial for which A satisfies.

Finally, we shall show that any vector operator must be a linear combination of A^{j}. To this end, we prove the following lemma.

Lemma 4: Let T_{ν}^{μ} be a vector operator. Then the following three statements are equivalent:

(i) $T_{\nu}^{\mu}=0$ identically,

(ii) $\sigma_{\mu}(T)=0$ for all $\mu=1,2,\ldots,n$,

(iii) $\langle A^{j}T\rangle=0$ for all $j=0,1,2,\cdots$.

Obviously (i) leads to (ii) trivially, while (iii) follows from (ii) because of (2.22) and (2.17). Conversely, suppose that (iii) is valid. Then, this implies that we have $\langle f(A)T\rangle=0$ for arbitrary polynomial $f(z)$. Hence, by summing (2.28) over $\mu=1,2,\ldots,n$ and noting (2.27), this gives

$$\sum_{\lambda=1}^{n}\prod_{j=1}^{\lambda}(1+l_{j}-l_{\lambda})\,f(l_{\lambda})\sum_{\nu=1}^{n}(R^{-1})_{\lambda\nu}\sigma_{\nu}(T)=0$$

for an arbitrary polynomial $f(z)$. We can always find a polynomial $f(z)$ such that $f(l_{\lambda})=0$ for all $\lambda\neq\mu$ but $f(l_{\mu})=1$ for any given value of μ. Then, it is easy to check that this leads to (ii). Now, we come to the most difficult part that (ii) implies (i). First of all, we note that (ii) leads immediately to

$$\sigma_{\mu}[f(A)T]=0,\quad \langle f(A)T\rangle=0 \tag{2.29}$$

for an arbitrary polynomial $f(z)$ if we use (2.28). Then, we can prove that T_{ν}^{μ} satisfies

$$(A-l_{1})(A-l_{2})\cdots(A-l_{n-1})T=0, \tag{2.30}$$

where we have for simplicity omitted the presence of the unit matrix I in front of l_{μ}'s. Note that in compari-

son to (1.16) this simply replaces the last factor $A - l_n$ by T. Moreover, if we have $f_\mu = f_\nu$ for some pair μ and ν with $\mu \neq \nu$, we can omit all those redundant factors as in (1.19).

To prove (2.30), we shall define vector operators $T^\mu_\nu(\alpha)$ by

$$T(n) = T, \quad \alpha = n,$$
$$T(\alpha) = (A - l_\alpha)(A - l_{\alpha-1}) \cdots (A - l_{n-1})T, \quad \alpha < n.$$

Then, we can prove by induction on decreasing values of α,

$$T^\mu_\nu(\alpha)\,\phi = 0, \quad \text{for } \mu \geq \alpha.$$

The proof is exactly the same as in the Lemma 1, if we note (2.18), (2.19), and (2.29). Then, setting $\alpha = 1$, we find (2.30) because of the Lemma 2. For the case that we have $f_\mu = f_\nu$, we can omit redundant factors by the same reasoning.

Next, we shall show that T also satisfies another identity

$$(A - 1 - l_2)(A - 1 - l_3) \cdots (A - 1 - l_n)T = 0. \tag{2.31}$$

Again, we can omit all redundant factors in (2.31), if two of f_μ and f_ν coincide. The proof of (2.31) is slightly more complicated. To this end, we define a new vector product $S \circ T$ for two vector operators S^μ_ν and T^μ_ν by

$$(S \circ T)^\mu_\nu = \sum_{\lambda=1}^{n} S^\mu_\lambda T^\lambda_\nu. \tag{2.32}$$

Then setting

$$\tilde{T}(1) = T, \quad \alpha = 1,$$
$$\tilde{T}(\alpha) = (A + 1 - f_2) \circ (A + 2 - f_3) \circ \cdots \circ (A + \alpha - 1 - f_2) \circ T, \quad \alpha > 1, \tag{2.33}$$

we can now prove by induction on increasing values of α

$$\tilde{T}^\mu_\nu(\alpha)\,\phi = 0 \quad \text{for } \alpha \geq \nu. \tag{2.34}$$

Setting $\alpha = n$ and using the Lemma 2, this gives

$$\tilde{T}^\mu_\nu(n) = 0. \tag{2.35}$$

Now, we can rewrite the product (2.32) in terms of the old product (1.8). By noting (2.29), then this leads to (2.31). Another way of proving (2.35) is to use

$$\tilde{A}^\mu_\nu = -A^{n-\nu+1}_{n-\mu+1}, \quad \tilde{T}^\mu_\nu = -T^{n-\nu+1}_{n-\mu+1},$$
$$\tilde{f}_\mu = -f_{n-\mu+1}, \quad \tilde{l}_\mu = \tilde{f}_\mu + n - \mu. \tag{2.36}$$

Then,[6] $\tilde{A}^\mu_\nu$ is the generator of the complex conjugate representation with signature $(\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_n)$. Hence, we must have

$$(\tilde{A} - \tilde{l}_1)(\tilde{A} - \tilde{l}_2) \cdots (\tilde{A} - \tilde{l}_{n-1})\tilde{T} = 0$$

in analogy to (2.30). This is noting but the relation (2.35).

Now, since T satisfies both Eqs. (2.30) and (2.31), there must be a minimal polynomial $f(A)$ satisfying

$$f(A)T = 0.$$

Then, using the standard algorithm, we conclude that $f(z)$ must divide two polynomials

$$g_1(z) = (z - l_1)(z - l_2) \cdots (z - l_{n-1}),$$
$$g_2(z) = (z - 1 - l_2)(z - 1 - l_3) \cdots (z - 1 - l_n).$$

However, $g_1(z)$ and $g_2(z)$ have no common factor, noting that $l_j - l_k$ can never assume values ± 1. This is because in reality we can omit all redundant factors in both $g_1(z)$ and $g_2(z)$ if we have $f_\mu = f_\nu$. Therefore, we conclude that $f(z)$ must be a constant and we have $T^\mu_\nu = 0$ identically. This proves (i).

Our Lemma 4 implies that the subspace of the Hilbert space $\mathcal{H}$ orthogonal to $\mathcal{H}_0$ is identically null. Hence, we find $\mathcal{H} = \mathcal{H}_0$ as we stated in Sec. 1. In other words, all vector operators are linear combinations of A^j. This fact is important in deriving the $SU(3)$ mass formula.[5]

We remark that by means of the new vector product, we can derive an identity

$$(A + n - 1 - l_1) \circ (A + n - 1 - l_2) \circ \cdots \circ (A + n - 1 - l_n) = 0. \tag{2.37}$$

This must coincide with (1.16) if we convert the new product into the old one. We can explicitly verify this fact for the case $n = 3$. Of course, our formulas (1.16) and (2.37) agree with the result of the Ref. 5 for the special case $n = 3$.

The present method may be applicable for more general Lie algebras. We may note that an analog of (1.29) exists also for the n-dimensional orthogonal group $O(n)$ where its generators $J_{\mu\nu}$ satisfy

$$J_{\mu\nu} = -J_{\nu\mu},$$
$$[J_{\mu\nu}, J_{\alpha\beta}] = \delta_{\nu\alpha}J_{\mu\beta} - \delta_{\nu\beta}J_{\mu\alpha} + \delta_{\mu\alpha}J_{\beta\nu} - \delta_{\mu\beta}J_{\alpha\nu}. \tag{2.38}$$

For the spinor representation of the $O(n)$ group, we can easily verify a special relation

$$\sum_{\lambda=1}^{n} (J_{\mu\lambda}J_{\lambda\nu} + J_{\nu\lambda}J_{\lambda\mu}) = \tfrac{1}{2}(n-1)\,\delta_{\mu\nu}. \tag{2.39}$$

As a matter of fact, this relation is related to various identities[17] found for the nuclear boson expansion method where the relevant Lie algebra is B_n, corresponding to the $O(2n+1)$ group. Also some interesting identities among $O(n)$ generators are noticed by several authors.[18]

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Wave propagation with stochastically coupled propagating and evanescent modes

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The problem of electromagnetic wave propagation in a randomly perturbed waveguide is analyzed in the forward scattering approximation. Both propagating and evanescent modes are taken into account. Coupled power equations are derived in the asymptotic limit of long guide length and small perturbations. More generally, a diffusion equation is derived which governs the evolution of functions of the process in this same asymptotic limit. The resulting dynamical equations characterize the evolution of the propagating modes; the evanescent modes affect this propagation through their modification of the parameters in these equations. However, in the presence of evanescent modes, the forward scattering approximation leads to nonconservative coupled power equations; energy is apparently exchanged with the neglected backward waves through their coupling to the evanescent modes.

INTRODUCTION

We shall consider the propagation of electromagnetic waves in a randomly perturbed cylindrical metallic waveguide. Such perturbations, arise from geometric imperfections and variations in the constitutive parameters of the material filling the waveguide and are typically small. However, the distances over which propagation takes place are usually long. Therefore, we shall analyze the problem in the asymptotic limit of small random perturbations and long waveguides. A number of authors, including those cited in Refs. 1—17, have studied electromagnetic propagation problems in this context. For the waveguide problem, interest has centered mainly upon obtaining statistical information about the flow of energy in the guide and upon the derivation of coupled power equations for the expected values of the modal powers.

The electromagnetic fields in a cylindrical metallic guide can be represented by a countably infinite superposition of modes. At any given frequency of operation, a finite number of these modes will propagate along the guide while the remainder will be evanescent modes, exponentially damped in the direction of propagation. The entire collection of modes, propagating and evanescent, will in general be excited at an obstacle, imperfection, or any other deviation of the guide from its homogeneous cylindrical configuration.

Most studies of propagation in the randomly perturbed guide have dealt with a mathematical model which ignores the evanescent modes. Clearly, such modes cannot transport energy. Nevertheless, the small random imperfections couple the propagating modes to the evanescent modes and this modal interaction is sustained over long guide lengths. Consequently, although the nonpropagating modes do not in themselves transport energy, we shall show that they make their presence felt by modifying the parameters governing the evolution of the propagating modal powers.

In Sec. I we adapt the stochastic perturbation theory of Papanicolaou and Keller[5] to the problem being considered and derive coupled power equations. These equations form a linear constant coefficient, first order system of ordinary differential equations. In the absence of evanescent modes, they reduce to the equations derived by Papanicolaou.[6] In Sec. II we apply these coupled power equations to an example studied by Matveev[18] and recover in a mean square sense a relation which he has shown to hold almost surely. In Sec. III we further use the perturbation theory of Ref. 5 to derive a partial differential equation of diffusion type which is satisfied by expectations of functions of the process. In an appendix we use the local uniform modes introduced by Snyder[17,19,20] to derive the coupled equations for the modal expansion coefficients which are used as our basic mathematical model.

Throughout this work we use the forward scattering approximation, wherein the transfer of energy to backward travelling waves is neglected. Such an approximation has been used by a number of authors[4,6,11,13]; it significantly simplifies the mathematical model since it replaces a two-point boundary value problem with a more tractable initial value problem. It is a reasonably good approximation at high frequencies, although its precise impact remains to be assessed. The need for an ultimate treatment of the full boundary value problem is pointed out in Sec. I by the fact that when evanescent modes are included, the forward scattering approximation ceases to be conservative. Energy can be either gained or lost by the propagating modes, presumably to the neglected backward-travelling waves, through their coupling to the evanescent modes.

The mathematics will be developed in a formal manner. This approach leads one quickly to the important results and, within the context of the forward scattering approximation, embodies the relevant physics. Previous applications of the formalism have been rigorously justified.[21,22] Moreover, G.C. Papanicolaou and the author[23] have developed a stochastic limit theorem which (at least for the case of a finite number of evanescent modes) rigorously justifies the application of the formalism to the problem considered in this paper.

I. DERIVATION OF COUPLED POWER EQUATIONS

Let us consider the infinite-dimensional stochastic initial value problem:

$$\frac{d}{dz}X(z,\omega,\epsilon)=[-iD_p-D_e+\epsilon B(z,\omega)]X(z,\omega,\epsilon),$$

$$X(0,\omega,\epsilon)=X_0, \tag{1}$$

where

$$D_p\equiv\operatorname{diag}\{\beta_1,\beta_2,\cdots,\beta_N\}\oplus O_\infty,\quad 0<\beta_1\leq\beta_1\leq\cdots\leq\beta_N.$$
$$D_e\equiv O_N\oplus\operatorname{diag}\{\kappa_{N+1},\kappa_{N+2},\cdots\},\quad 0<\kappa_{N+1}\leq\kappa_{N+2}\leq\cdots \tag{2}$$

The symbol $\oplus$ denotes a direct sum of matrices while the subscripts N and ∞ indicate square matrices which are $N\times N$ and infinite dimensional, respectively. We assume that $\omega\in\Omega$, where $(\Omega,\mathcal{J},P)$ denotes an underlying probability space, and that ϵ is a small real parameter. $B(z,\omega)$ is a square infinite matrix-valued stochastic process which couples the components of X. The generally complex-valued elements of B will be denoted by $b_{ij}(z,\omega)$. The process $B(z,\omega)$ will be assumed to be centered and wide-sense stationary, i.e.,

$$\begin{aligned}&\langle b_{ij}(z,\omega)\rangle=0,\\ &\langle b_{ij}(z+s,\omega)b_{kl}(z,\omega)\rangle\equiv\rho_{ij,kl}(s),\\ &\langle b_{ij}(z+s,\omega)b^*_{kl}(z,\omega)\rangle\equiv\hat{\rho}_{ij,kl}(s),\end{aligned} \tag{3}$$

where the brackets denote expected or mean values and the star denotes complex conjugation. The initial condition X_0 in (1) is a nonrandom constant vector.

In an appendix, we shall derive coupled equations for the modal expansion coefficients of the electromagnetic waves propagating in a (nominally) cylindrical metallic waveguide. We assume that both the geometry and the constitutive parameters of the medium filling the guide are subjected to small random perturbations. Thus, the modal expansion coefficients are not constants but rather random functions of distance along the guide. We shall show that (1) models a system of N propagating modes, with propagation constants $\beta_1,\cdots,\beta_N$, and a countably infinite set of nonpropagating or evanescent modes in the forward-scattering approximation, wherein the backward travelling waves are neglected. This model also assumes a harmonic time dependence $\exp(i2\pi ft)$ which is not shown.

In the context of this model, the quantities $|x_i(z,\omega,\epsilon)|^2$, $i=1,\cdots,N$ (where x_i is the ith component of X), represent the power content of the N propagating modes at location z along the guide. In this section, we shall use a modification of the stochastic perturbation method of Papanicolaou and Keller[5] to derive a system of N equations for $\langle|x_i(z,\omega,\epsilon)|^2\rangle$, $i=1,\cdots,N$, which are valid in an appropriate asymptotic limit as ϵ goes to zero and z goes to infinity. This system of equations generalizes those derived by Papanicolaou[6] since it accounts for the presence of the evanescent modes. We obtain, on the one hand, a drastic reduction in the dimensionality of the system from the denumerably infinite coupled mode description to the N-dimensional coupled power description. On the other hand, the nonpropagating modes make their presence felt by modifying the coefficients governing the propagation and interaction of the N propagating modal powers.

We begin by defining a change of dependent variable which removes the rapid phase variations. Let

$$Y(z)\equiv\exp(iD_pz)X(z),$$

$$\exp(iD_pz)=\operatorname{diag}\{\exp(i\beta_1z),\cdots,\exp(i\beta_Nz)\}\oplus I_\infty, \tag{4}$$

where we no longer explicitly indicate dependence upon all the variables. Then

$$\frac{d}{dz}Y(z)=-D_eY(z)+\epsilon C(z,\omega)Y(z),\quad Y(0)=X_0, \tag{5}$$

where

$$C(z,\omega)\equiv\exp(iD_pz)B(z,\omega)\exp(-iD_pz). \tag{6}$$

We now define the Kronecker product

$$U(z)\equiv Y(z)\otimes Y^\dagger(z), \tag{7}$$

where $\dagger$ denotes complex conjugate transpose. From (5) and (6)

$$\frac{d}{dz}U=-D_eU-UD_e+\epsilon(CU+UC^\dagger),\quad U(0)=X_0\otimes X_0^\dagger. \tag{8}$$

We shall now develop the two-timing perturbation analysis of initial value problem (8). Observe that $u_{ii}=|x_i|^2$, $i=1,2,\cdots$. We first define a "slow variable" ξ; since the process $C(z,\omega)$ is centered, the appropriate choice is $\xi\equiv\epsilon^2z$. Next we shall assume that $U\equiv U(z,\xi,\epsilon)$ so that differential equation (8) may be written as

$$\frac{\partial}{\partial z}U+\epsilon^2\frac{\partial}{\partial\xi}U=-D_eU-UD_e+\epsilon(CU+UC^\dagger). \tag{9}$$

Let

$$U=U(z,\xi,\epsilon)=\sum_{k=0}^{\infty}\epsilon^kU_k(z,\xi). \tag{10}$$

Substituting (10) into (9) and equating coefficients of powers of ϵ, we obtain

$$\begin{aligned}&\frac{\partial}{\partial z}U_k+\frac{\partial}{\partial\xi}U_{k-2}=-D_eU_k-U_kD_e+CU_{k-1}+U_{k-1}C^\dagger,\\ &k=0,1,2,\cdots,\\ &U_0(0,0)=X_0\otimes X_0^\dagger;\quad U_k(0,0)=0,\quad k=1,2,\cdots.\end{aligned} \tag{11}$$

The stochastic perturbation theory that will be applied essentially involves the following two assumptions:

(i) The "fast" and "slow" variables, i.e., z and ξ respectively, will be treated as two independent distance variables. Such an assumption underlies all multiscale procedures.

(ii) Stochastic processes evolving at the "fast" spatial rate will be assumed to be statistically independent of those evolving at the "slow" rate. In other words, random functions of z alone will be assumed statistically independent of functions of ξ alone.

This second assumption can be justified for a rather general class of stochastic processes known as strongly mixing processes.[21-23] Such processes are characterized, roughly speaking, by the fact that random variables formed by sampling the process become asymptotically independent as the distance between sampling points becomes infinite.

Equations (11) can be recast into the following system of integral equations:

$$U_k(z,\xi)=\exp(-D_ez)U_k(0,\xi)\exp(-D_ez)+\int_0^z\exp[-D_e(z-s)]$$

$$\times\Big(C(s)\,U_{k-1}(s,\xi)+U_{k-1}(s,\xi)C^{\dagger}(s)$$
$$-\frac{\partial}{\partial\xi}U_{k-2}(s,\xi)\Big)\exp[-D_e(z-s)]\,ds,\quad k=0,1,2,\cdots. \tag{12}$$

We shall now iteratively solve for U_1 and U_2 in terms of U_0 and take expected values. For brevity, define

$$\langle U_0(0,\xi)\rangle \equiv W(\xi)\equiv[w_{ij}(\xi)] \tag{13}$$

$$V_{z,s}[A]\equiv\exp[-D_e(z-s)][C(s)A+A^{\dagger}C^{\dagger}(s)]\exp[-D_e(z-s)]. \tag{14}$$

Then

$$U_0(z,\xi)=\exp(-D_ez)U_0(0,\xi)\exp(-D_ez),$$
$$U_1(z,\xi)=\exp(-D_ez)U_1(0,\xi)\exp(-D_ez)$$
$$+\int_0^z V_{z,s}[U_0(s,\xi)]\,ds, \tag{15}$$
$$U_2(z,\xi)=\exp(-D_ez)U_2(0,\xi)\exp(-D_ez)$$
$$+\int_0^z\Big(V_{z,s}[U_1(s,\xi)]-\exp[-D_e(z-s)]$$
$$\times\frac{\partial}{\partial\xi}U_0(s,\xi)\exp[-D_e(z-s)]\Big)ds.$$

Observe that the random behavior in $U_0(z,\xi)$ and $U_1(0,\xi)$ depends on ξ alone while $V_{z,s}[\cdot]$ is a centered random operator whose random behavior depends upon s. Using the two assumptions, we obtain

$$\langle U_0(z,\xi)\rangle=\exp(-D_ez)W(\xi)\exp(-D_ez),$$
$$\langle U_1(z,\xi)\rangle=\exp(-D_ez)\langle U_1(0,\xi)\rangle\exp(-D_ez), \tag{16}$$
$$\langle U_2(z,\xi)\rangle=\exp(-D_ez)\langle U_2(0,\xi)\rangle\exp(-D_ez)$$
$$+\int_0^z\int_0^s\langle V_{z,s}\circ V_{s,t}\rangle$$
$$[\exp(-D_et)\,W(\xi)\exp(-D_et)]\,dt\,ds$$
$$-\exp(-D_ez)z\frac{d}{d\xi}W(\xi)\exp(-D_ez),$$

where $V_{z,s}\circ V_{s,t}$ denotes composition.

The basic strategy of the two-timing procedure involves the development of equations for the unknown functions of the "slow" variable, i.e., $w_{ij}(\xi)$, in such a way as to suppress secular growth of the terms in $\langle U_2(z,\xi)\rangle$ as $z\to\infty$. Noting (2), we see that the principal $N\times N$ submatrix of the third term grows linearly with z while all other terms are exponentially decaying. Let the matrix subscript $N\times N$ be used to denote principal $N\times N$ submatrix. Then, the strategy of suppressing secularity in the third of Eqs. (16) leads to the equation

$$\frac{d}{d\xi}W_{N\times N}(\xi)=\lim_{z\to\infty}\frac{1}{z}$$
$$\Big[\int_0^z\int_0^s\langle V_{z,s}\circ V_{s,t}\rangle$$
$$[\exp(-D_et)W(\xi)\exp(-D_et)]\,dt\,ds\Big]_{N\times N},$$
$$W_{N\times N}(0)=[X_0\otimes X_0^{\dagger}]_{N\times N} \tag{17}$$

One can show that (17) is actually a well-defined initial value problem, i.e., that the right side of the differential equation involves only the N^2 elements $w_{ij}(\xi)$, $1\le i,\ j\le N$. For brevity of notation, let

$$\Delta\beta_{kl}\equiv\beta_k-\beta_l. \tag{18}$$

A development of the right side of (17) and an application of the limit leads to the system of equations

$$\frac{d}{d\xi}w_{ij}=\sum_{\substack{1\le l\le N\\ \Delta\beta_{jl}=0}}(\alpha_{il}w_{lj}+\alpha^{*}_{jl}w_{il})$$
$$+\sum_{\substack{1\le k,\,l\le N\\ \Delta\beta_{kl}=\Delta\beta_{ij}}}(\hat{\alpha}_{ikjl}w_{kl}+\hat{\alpha}^{*}_{jkil}w_{lk}) \tag{19}$$
$$w_{ij}(0)=x_{0_i}x^{*}_{0_j},\quad 1\le i,j\le N,$$

where

$$\alpha_{jl}\equiv\sum_{k=1}^{N}\int_0^{\infty}\rho_{jk,kl}(u)\exp(i\Delta\beta_{jk}u)\,du$$
$$+\sum_{k=N+1}^{\infty}\int_0^{\infty}\rho_{jk,kl}(u)\exp(-\kappa_ku+i\beta_ju)\,du, \tag{20}$$
$$\hat{\alpha}_{ikjl}\equiv\int_0^{\infty}\hat{\rho}_{ikjl}(u)\exp(i\Delta\beta_{ik}u)\,du.$$

In the special case of nondegenerate propagating modes, i.e., $k=l$ if $\beta_k=\beta_l$, the diagonal terms w_{ii}, $i=1,\cdots,N$, decouple from the remaining terms and we obtain the following system of coupled power equations:

$$\frac{d}{d\xi}w_{ii}=2\mathrm{Re}\{\alpha_{ii}\}w_{ii}+2\sum_{k=1}^{N}\mathrm{Re}\{\hat{\alpha}_{ikik}\}w_{kk},$$
$$w_{ii}(0)=|x_{0_i}|^2,\quad i=1,\cdots,N. \tag{21}$$

Let the infinite matrix B be partitioned as follows:

$$B\equiv\begin{pmatrix}B_{11}&B_{12}\\ \hline B_{21}&B_{22}\end{pmatrix},\quad B_{11}\text{ is }N\times N. \tag{22}$$

In the Appendix we show that, for the general lossless waveguide problem, B_{11} is skew-Hermitian. Therefore, $\rho_{ij,ji}=-\hat{\rho}_{ijij}$ for $1\le i,\ j\le N$ and Eqs. (21) can be written in the form:

$$\frac{d}{d\xi}w_{ii}=\sum_{k=1}^{N}(Q_{ki}w_{ii}-Q_{ik}w_{kk})+\tilde{Q}_iw_{ii},\quad i=1,\cdots N$$
$$Q_{ki}=Q_{ik}\equiv2\mathrm{Re}\Big[\int_0^{\infty}\rho_{ik,ki}(u)\exp(i\Delta\beta_{ik}u)\,du\Big] \tag{23}$$
$$\tilde{Q}_i\equiv2\sum_{k=N+1}^{\infty}\mathrm{Re}\Big[\int_0^{\infty}\rho_{ik,ki}(u)\exp(-\kappa_ku+i\beta_iu)\,du\Big]$$

In the absence of evanescent modes (i.e., $\tilde{Q}_i=0$) we obtain

$$\sum_{i=1}^{N}w_{ii}=\text{const}. \tag{24}$$

This conservation relation, derived in Ref. 6, is somewhat surprising since the backward travelling waves are ignored.

In the Appendix we show that if the geometric and material imperfections form statistically independent random processes, we obtain the following simple relation:

$$Q_{ki} = -\int_0^\infty [R_{ik}^{(g)}(u) + R_{ik}^{(m)}(u)] \cos\Delta\beta_{ik} u \, du \leq 0, \tag{25}$$

where $R_{ik}^{(g)}$ and $R_{ik}^{(m)}$ are (real) correlation functions associated with the geometric and material fluctuation processes, respectively. The inequality in (25) follows from the fact that the cosine transform of a correlation function is nonnegative.

In the presence of evanescent modes, $\tilde{Q}_i$ must be taken into account. Conservation relation (24) no longer holds. For the general waveguide problem, no simple transformation relates the submatrices B_{12} and B_{21}. This is apparent from Eq. (A9) since the matrix ϵB is simply an appropriate arrangement of the C_{mn} coefficients. When one of the modes is nonpropagating, its characteristic impedance and admittance become imaginary. For the simple case of a single propagating H-mode, ideal geometry, and random lossless fluctuations in the dielectric constant, it follows from (23) and (A14) that

$$w_{11}(\xi) = w_{11}(0)\exp(\tilde{Q}_1 \xi), \tag{26}$$

$$\tilde{Q}_1 = \sum_{k=2}^{\infty} \int_0^\infty [R_{1n}^{hh}(u)\exp(-\kappa_n'' u) - R_{1n}^{he}(u)\exp(-\kappa_n' u)] \sin\beta_1'' u \, du,$$

where R_{1n}^{hh} and R_{1n}^{he} represent real correlations of the random coupling of the propagating H-mode to evanescent H-modes and E-modes, respectively. The single and double prime superscripts indicate quantities associated with E-modes and H-modes, respectively. This gain or loss of energy apparently represents an interaction with the neglected backward travelling waves through their mutual coupling to the evanescent modes.

This lack of energy conservation arises from the forward scattering assumption rather than any shortcoming of the perturbation theory. This claim is based on the fact that the perturbation formalism gives the same results as a rigorous treatment.[23] Also, in Sec. II, we study a system considered by Matveev[18] and recover his result.

II. EXAMPLE OF MATVEEV

We shall apply the formalism of Sec. I to the following example considered by Matveev[18]:

$$\frac{d}{dz}E_l(z) = -\gamma_l E_l(z) + \sum_{k\neq l} \epsilon\eta_{kl}(z)E_l(z), \quad k, l = 1, \cdots, M, \tag{27}$$

where $\eta_{kl}(z)$ is a real stochastic process, $\epsilon \geq 0$, $\gamma_l = \alpha_l + i\beta_l$, and

$$0 < \alpha_1 < \alpha_2 \leq \cdots \leq \alpha_M, \qquad \eta_{kl}(z) = -\eta_{lk}(z). \tag{28}$$

We shall assume that the process $(\eta_{kl}(z))$ is centered and wide-sense stationary. This assumption differs somewhat from those made by Matveev since he studied the problem in the context of almost sure convergence while our results hold in a mean square sense. By means of the change of dependent variable,

$$x_1(z) = \exp(\alpha_1 z)E_1(z), \quad x_k(z) = \exp[(\alpha_1 + i\beta_k)z]E_k(z), \quad k = 2, \cdots, N, \tag{29}$$

we recast (27) into the form

$$\frac{d}{dz}x_1 = -i\beta_1 x_1 + \epsilon\sum_{k=2}^{M}(\eta_{1k}(z)\exp(-i\beta_k z))x_k(z), \tag{30}$$

$$\frac{d}{dz}x_l = -(\alpha_l - \alpha_1)x_l + \epsilon\sum_{k\neq l}^{M}(\eta_{lk}(z)\exp(i\Delta\beta_{lk}z))x_k(z). \tag{31}$$

From (20) and (21) we obtain

$$w_{11}(\xi) = |E_1(0)|^2 \exp[2\mathrm{Re}(\alpha_{11} + \hat{\alpha}_{11,11})\xi]. \tag{32}$$

However, $\hat{\alpha}_{11,11} = 0$ since $\eta_{11} \equiv 0$. From (20), (28), and (29), it follows that

$$\langle |E_1^2(z)| \rangle = |E_1(0)|^2 \exp\left[-2\alpha_1 z - 2\epsilon^2 z \times \left(\sum_{k=2}^{M}\int_0^\infty \exp[-(\alpha_k - \alpha_1)u]\cos\Delta\beta_{k1}u\,\langle\eta_{1k}(u)\eta_{1k}(0)\rangle\,du\right)\right]. \tag{33}$$

The decay constant in (33) is that obtained by Matveev in the context of almost sure convergence.

III. DERIVATION OF DIFFUSION EQUATION

In this section, we extend our considerations from the specific case of the second moments of the process to general functions of the process. The formal perturbation procedure of Sec. I will be used to derive partial differential equations of diffusion type that are satisfied by the expected value of such functions. The collapse in the dimensionality of the system that characterized the special case of Sec. I will again occur. For the case of N propagating modes, the limiting diffusion process will evolve in a $2N$-dimensional (real) coordinate space.

We begin by recasting (5) into a real system. Let

$$Y_j(z) \equiv Y_j^{(1)}(z) + iY_j^{(2)}(z), \qquad b_{jk}(z) \equiv b_{jk}^{(1)}(z) + ib_{jk}^{(2)}(z), \quad j, k = 1, 2, \cdots, \tag{34}$$

Then, (5) is equivalent to the system

$$\begin{aligned}
\frac{d}{dz}Y_k^{(1)} &= -d_k Y_k^{(1)} + \epsilon\sum_{l=1}^{\infty}[(b_{kl}^{(1)}(z)\cos\Delta\beta_{kl}z - b_{kl}^{(2)}(z) \times \sin\Delta\beta_{kl}z)Y_l^{(1)} - (b_{kl}^{(2)}(z)\cos\Delta\beta_{kl}z \\
&\quad + b_{kl}^{(1)}(z)\sin\Delta\beta_{kl}z)Y_l^{(2)}], \\
\frac{d}{dz}Y_k^{(2)} &= -d_k Y_k^{(2)} + \epsilon\sum_{l=1}^{\infty}[(b_{kl}^{(2)}(z)\cos\Delta\beta_{kl}z \\
&\quad + b_{kl}^{(1)}(z)\sin\Delta\beta_{kl}z)Y_l^{(1)} \\
&\quad + (b_{kl}^{(1)}(z)\cos\Delta\beta_{kl}z - b_{kl}^{(2)}(z)\sin\Delta\beta_{kl}z)Y_l^{(2)}]
\end{aligned} \tag{35}$$

$$Y_k^{(j)}(0) \equiv X_{0_k}^{(j)}, \quad j = 1, 2, \quad X_0 \equiv X_0^{(1)} + iX_0^{(2)},$$

$$d_k \equiv \begin{cases} 0, & 1 \leq k \leq N, \\ \kappa_k, & k \geq N+1, \end{cases} \qquad \beta_k \equiv 0 \text{ if } k > N.$$

By making the obvious redefinitions, we shall continue to use the notation of (5) to denote the real system (35).

Let us now consider the composition $f(Y(z,\omega,\epsilon))$. The basic equation to be used is the chain rule development:

$$\frac{df}{dz}=\nabla f\cdot\frac{d}{dz}Y, \tag{36}$$

where ∇ represents an infinite-dimensional gradient. We assume that

$$f=\sum_{k=0}^{\infty}\epsilon^k f_k[z,\xi,\exp(-D_e z)X_0],\quad Y=\sum_{k=0}^{\infty}\epsilon^k Y_k(z). \tag{37}$$

Substitution of these expansions into (36) leads to the following equations:

$$\frac{\partial}{\partial z}f_k+\frac{\partial}{\partial\xi}f_{k-2}-\nabla f_k\cdot D_e\exp(-D_e z)X_0$$
$$=\sum_{l=0}^{k}\nabla f_l\cdot\frac{d}{dz}Y_{k-l},\quad k=0,1,2,\cdots. \tag{38}$$

From (5), moreover, we have

$$Y_0(z)=\exp(-D_e z)X_0,$$
$$Y_k(z)=\int_0^z\exp[-D_e(z-s)],$$
$$C(s)Y_{k-1}(s)\,ds,\quad k=1,2,\cdots. \tag{39}$$

Therefore,

$$\frac{\partial}{\partial z}f_0=0,\quad\text{i.e.,}\quad f_0=f_0(\xi,\exp(-D_e z)X_0),$$
$$\frac{\partial}{\partial z}f_1=\nabla f_0\cdot(-D_e Y_1+CY_0), \tag{40}$$
$$\frac{\partial}{\partial z}f_2=\nabla f_1\cdot(-D_e Y_1+CY_0)+\nabla f_0\cdot(-D_e Y_2+CY_1)-\frac{\partial f_0}{\partial\xi}.$$

We shall now integrate Eqs. (40) with respect to z and take expected values, using the two assumptions of Sec. I. Note in particular that the randomness in f_0 is a function of ξ alone. From (39) and (40)

$$f_1[z,\xi,\exp(-D_e z)X_0]=f_1(0,\xi,X_0)+\int_0^z\nabla f_0[\xi,\exp(-D_e s)X_0]$$
$$\cdot\left(-D_e\int_0^s\exp[-D_e(s-\lambda)]C(\lambda)\right.$$
$$\left.\times\exp(-D_e\lambda)X_0\,d\lambda+C(s)\exp(-D_e s)X_0\right)ds \tag{41}$$

$$f_2[z,\xi,\exp(-D_e z)X_0]$$
$$=f_2(0,\xi,X_0)+\int_0^z\nabla f_1[s,\xi,\exp(-D_e s)X_0]$$
$$\cdot\left(-D_e\int_0^s\exp[-D_e(s-\lambda)]C(\lambda)\exp(-D_e\lambda)X_0\,d\lambda\right.$$
$$\left.+C(s)\exp(-D_e s)X_0\right)ds+\int_0^z\nabla f_0[\xi,\exp(-D_e s)X_0]$$
$$\times\left(-D_e^2\int_0^s\int_0^\lambda\exp[-D_e(s-\lambda)]C(\lambda)\exp[-D_e(\lambda-\sigma)]C(\sigma)\right.$$
$$\left.\times\exp(-D_e\sigma)X_0\,d\sigma\,d\lambda+\int_0^s C(s)\exp[-D_e(s-\lambda)]\,C(\lambda)\right.$$
$$\left.\times\exp(-D_e\lambda)X_0\,d\lambda\right)ds-\int_0^z\frac{\partial}{\partial\xi}f_0[\xi,\exp(-D_e s)X_0]\,ds.$$

When expected values are taken, no secular terms appear in $\langle f_1\rangle$. The diffusion equation will result from the suppression of secular growth in the expression for $\langle f_2\rangle$. We define

$$w(\xi;x_1^{(1)},x_1^{(2)},\cdots,x_N^{(1)},x_N^{(2)})\equiv\lim_{z\to\infty}\langle f_0[\xi,\exp(-D_e z)X_0]\rangle, \tag{42}$$

where the coordinates of X_0 are now denoted by $x_k^{(i)}$. Note that the difference f_0-w consists of terms that are exponentially decaying in z. The strategy of suppressing secular growth leads to the relation

$$\frac{\partial}{\partial\xi}w\equiv\lim\frac{1}{z}\int_0^z\left[\int_0^s\left\langle\left(-D_e\int_0^\lambda\exp[-D_e(\lambda-\sigma)]\right.\right.\right.$$
$$\left.\times C(\sigma)\exp(-D_e\sigma)X_0\,d\sigma+C(\lambda)\exp(-D_e\lambda)X_0\right)$$
$$\cdot\nabla\nabla\langle f_0[\xi,\exp(-D_e\lambda)X_0]\rangle\cdot\left(-D_e\int_0^s\exp[-D_e(s-\eta)]\right.$$
$$\left.\times C(\eta)\exp(-D_e\eta)X_0\,d\eta+C(s)\exp(-D_e s)X_0\right)\Big\rangle\,d\lambda\,ds$$
$$+\nabla\langle f_0[\xi,\exp(-D_e s)X_0]\rangle\cdot\left(-D_e\int_0^s\int_0^\lambda\exp[-D_e(s-\lambda)]\right.$$
$$\left.\times\langle C(\lambda)\exp[-D_e(\lambda-\sigma)]C(\sigma)\rangle\exp(-D_e\sigma)X_0\,d\sigma\,d\lambda\right.$$
$$\left.\left.+\int_0^s\langle C(s)\exp[-D_e(s-\lambda)]C(\lambda)\rangle\exp(-D_e\lambda)X_0\,d\lambda\right)\right]ds. \tag{43}$$

The limit in (43) exists and yields a second order (possibly degenerate) elliptic differential operator in the $2N$ variables $x_k^{(i)}$, $i=1,2$, $k=1,\cdots,N$, which we shall denote by $\bar{V}$. Since

$$w(0,x_1^{(1)},\cdots,x_N^{(2)})=f(x_1^{(1)},\cdots,x_N^{(2)},0,0,\cdots), \tag{44}$$

we are led to the initial value problem

$$\frac{\partial}{\partial\xi}w=\bar{V}w,\quad w(0)=f(x_1^{(1)},\cdots,x_N^{(2)},0,0,\cdots). \tag{45}$$

For the general case of more than one propagating mode, the expression for the infinitesimal generator $\bar{V}$ is cumbersome since one must account for possible special relations among the propagation constant increments. Modes for which $\Delta\beta_{ij}=\pm\Delta\beta_{kl}$ or $\Delta\beta_{ij}=0$ will interact so as to contribute to the limit in (43). For the case of a single propagating mode, however, the expression for $\bar{V}$ is straightforward. Let

$$\rho_k^{(ij)}(s)\equiv\langle b_{1k}^{(i)}(s+\lambda)b_{k1}^{(j)}(\lambda)\rangle,$$
$$\gamma^{(ij)}\equiv\int_0^\infty\rho_1^{(ij)}(u)\,du,\quad i,j=1,2,\ k=1,2,\cdots,$$
$$\begin{pmatrix}\lambda^{(1)}\\ \lambda^{(2)}\end{pmatrix}\equiv\sum_{k=1}^{\infty}\int_0^\infty\exp(-d_k u)\left[(\rho_k^{(11)}(u)-\rho_k^{(22)}(u))\begin{pmatrix}\cos\Delta\beta_{1k}u\\ \sin\Delta\beta_{1k}u\end{pmatrix}\right.$$
$$\left.+(\rho_k^{(12)}(u)+\rho_k^{(21)}(u))\begin{pmatrix}-\sin\Delta\beta_{1k}u\\ \cos\Delta\beta_{1k}u\end{pmatrix}\right]du. \tag{46}$$

Then, for the case of a single propagating mode we obtain

$$\bar{V}=[\gamma^{(11)}x^2-(\gamma^{(12)}+\gamma^{(21)})xy+\gamma^{(22)}y^2]\frac{\partial^2}{\partial x^2}$$
$$+[(\gamma^{(12)}+\gamma^{(21)})(x^2-y^2)+2(\lambda^{(11)}-\lambda^{(22)})xy]\frac{\partial^2}{\partial x\partial y}$$
$$+[\gamma^{(22)}x^2+(\gamma^{(12)}+\gamma^{(21)})xy+\gamma^{(11)}y^2]\frac{\partial^2}{\partial y^2}$$
$$+(\lambda^{(1)}x-\lambda^{(2)}y)\frac{\partial}{\partial x}+(\lambda^{(2)}x+\lambda^{(1)}y)\frac{\partial}{\partial y}, \tag{47}$$

where x and y have been used instead of $x_1^{(1)}$ and $x_1^{(2)}$, respectively.

Note that the function x^2+y^2 is an eigenfunction of $\bar{V}$ with eigenvalue $2(\gamma^{(11)}+\gamma^{(22)}+\lambda^{(1)})$. Therefore, the solution of (45) with $w(0)=x^2+y^2$ is

$$w(\xi)=w(0)\exp[2(\gamma^{(11)}+\gamma^{(22)}+\lambda^{(1)})\xi]\,. \tag{48}$$

This expression, which is asymptotically equal to the power content of the single propagating mode, agrees with the solution of (21) in the case $N=1$.

In polar coordinates the operator $\bar{V}$ becomes

$$\bar{V}=\gamma^{(11)}r^2\frac{\partial^2}{\partial r^2}+(\gamma^{(22)}+\lambda^{(1)})\,r\frac{\partial}{\partial r}+\gamma^{(22)}\frac{\partial^2}{\partial\theta^2}$$
$$-(\gamma^{(12)}+\gamma^{(21)}-\lambda^{(2)})\frac{\partial}{\partial\theta}+[\gamma^{(12)}+\gamma^{(21)}]\,r\frac{\partial^2}{\partial r\partial\theta}\,. \tag{49}$$

Note that r^n is an eigenfunction of $\bar{V}$ with eigenvalue $n[(n-1)\gamma^{(11)}+\gamma^{(22)}+\lambda^{(1)}]$. Therefore, one can very easily compute all the moments of the power flowing in the propagating mode. In particular, the mean and variance are

$$\langle|x_1(\xi/\epsilon^2,\omega)|^2\rangle=|x_{0_1}|^2\exp[2(\gamma^{(11)}+\gamma^{(22)}+\lambda^{(1)})\xi]\,,$$
$$|\langle|x_1(\xi/\epsilon^2,\omega)|^4\rangle-(\langle|x_1(\xi/\epsilon^2,\omega)|^2\rangle)^2]^{1/2}$$
$$=|x_{0_1}|^2\exp[2(\gamma^{(11)}+\gamma^{(22)}+\lambda^{(1)})\xi]\,[\exp(8\gamma^{(11)}\xi)-1]^{1/2}. \tag{50}$$

For the example of Matveev discussed in Sec. II, $\rho_1^{(ij)}=0$, $i,j=1,2$. Therefore, the infinitesimal generator in this case is completely degenerate, i.e.,

$$\bar{V}=(\lambda^{(1)}x-\lambda^{(2)}y)\frac{\partial}{\partial x}+(\lambda^{(2)}x+\lambda^{(1)}y)\frac{\partial}{\partial y}\,. \tag{51}$$

The asymptotic behavior, therefore, is that of drift alone and not of diffusion.

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APPENDIX: DERIVATION OF COUPLED MODE EQUATIONS

We shall consider a metallic waveguide which, in the absence of random imperfections, is cylindrical and filled with homogeneous isotropic material. The guide cross section is assumed to lie in the xy plane with propagation occurring along the z axis. The following two assumptions will be made regarding the randomly perturbed guide:

(i) The dielectric constant and permeability of the material filling the guide can each be represented as the sum of a constant and a zero mean inhomogeneous random perturbation, i.e.,

$$\epsilon=\epsilon_0+\epsilon_1(x,y,z,\omega),\quad \mu=\mu_0+\mu_1(x,y,z,\omega),$$
$$\langle\epsilon_1\rangle=\langle\mu_1\rangle=0. \tag{A1}$$

(ii) The perfectly conducting waveguide walls have random geometric imperfections. However, we assume that the average cross section is independent of z. Thus, if $\{\mathbf{\Gamma}(\theta,z,\omega):0\le\theta<2\pi,\ -\infty<z<\infty,\ \omega\in\Omega\}$ represents the guide boundary in vector parametric form, we shall assume that $\langle\mathbf{\Gamma}(\theta,z,\omega)\rangle$ is independent of z.

The transverse and longitudinal field decomposition (cf. Ref. 24) becomes

$$-\frac{\partial}{\partial z}\mathbf{E}_t=i\omega_0\mu(\mathbf{H}_t\times\mathbf{z}_0)+\frac{i}{\omega_0}\nabla_t\epsilon^{-1}\nabla_t\cdot(\mathbf{H}_t\times\mathbf{z}_0),$$
$$-\frac{\partial}{\partial z}\mathbf{H}_t=i\omega_0(z_0\times\mathbf{E}_t)+\frac{i}{\omega_0}\nabla_t\mu^{-1}\nabla_t\cdot(\mathbf{z}_0\times\mathbf{E}_t), \tag{A2}$$
$$H_z=\frac{-i}{\omega_0\mu}\nabla_t\cdot(z_0\times\mathbf{E}_t),\quad E_z=\frac{-i}{\omega_0\epsilon}\epsilon\nabla_t\cdot(\mathbf{H}_t\times\mathbf{z}_0),$$

where the zero subscript denotes unit vectors, the t subscript denotes transverse vectors and operators ($\mathbf{E}_t\equiv\mathbf{E}-\mathbf{z}_0\mathbf{E}_z$, $\nabla_t\equiv\nabla-\mathbf{z}_0\partial/\partial z$), and $\omega_0\equiv2\pi f$ is used to denoted radian frequency. (The sample space Ω remains indexed by the variable ω.)

At each point z and for each realization ω, the transverse fields will be expanded in a complete set of local normal modes. These modes, introduced by Snyder,[19,20] will correspond to a fictitious cylindrical guide having constitutive parameters ϵ_0, u_0 and cross section defined by $\mathbf{\Gamma}(\theta,z,\omega)$. Note therefore that the local mode set will be both z-dependent and random since they are implicit functions of the random guide boundary. However, they have the obvious advantage of conforming exactly to the guide cross section at each value of z and for each realization ω.

Let $S(z,\omega)$ denote the guide cross section at point z and for realization ω. The derivation of the mode functions is well known (Ref. 24). We obtain the representation

$$\mathbf{E}_t(x,y,z,\omega)=\sum_n V_n'(z,\omega)\mathbf{e}_n'(x,y,z,\omega)+\sum_n V_n''(z,\omega)\mathbf{e}_n''(x,y,z,\omega),$$
$$\mathbf{H}_t(x,y,z,\omega)=\sum_n I_n'(z,\omega)\mathbf{h}_n'(x,y,z,\omega)+\sum_n I_n''(z,\omega)\mathbf{h}_n''(x,y,z,\omega), \tag{A3}$$

where the primed and double-primed quantities refer to E-modes (TM modes) and H-modes (TE modes) respectively. Moreover, $\mathbf{h}=z_0\times\mathbf{e}$. The following normalization is assumed:

$$\int_S\int_{(z,\omega)}\mathbf{e}_m(x,y,z,\omega)\cdot\mathbf{e}_n(x,y,z,\omega)\,dx\,dy=\delta_{mn} \tag{A4}$$

for both E- and H-modes while the right side of (A4) is identically zero if the integrand is the scalar product of an E-mode and an H-mode function.

We obtain coupled mode equations for the modal voltages and currents by inserting (A3) into (A2) and using orthornormality relation (A4). We define:

(i) $k_{t_n}^{\prime(\prime\prime)}(z,\omega) \equiv$ the transverse wavenumber associated with the nth $E(H)$ local mode function at point z and for realization ω.

(ii) $\hat{k}_{t_n}^{\prime(\prime\prime)} \equiv$ the transverse wavenumber associated with the nth $E(H)$ mode function for a cylindrical guide having the mean cross section defined by $\langle\Gamma\rangle$.

(iii) $\beta_n^{\prime(\prime\prime)} \equiv (\omega_0^2\mu_0\epsilon_0 - \hat{k}_{t_n}^{\prime(\prime\prime)2})^{1/2}$.

(iv) $Z_n' \equiv \beta_n'/\omega_0\epsilon_0, \quad Z_n'' \equiv \omega_0\mu_0/\beta_n'', \quad Y_n^{\prime(\prime\prime)} \equiv 1/Z_n^{\prime(\prime\prime)}$.

(v) $\xi_n'(z,\omega) \equiv [\hat{k}_{t_n}'^2 - k_{t_n}'^2(z,\omega)]/\omega_0\epsilon_0$,

$\eta_n''(z,\omega) \equiv [\hat{k}_{t_n}''^2 - k_{t_n}''^2(z,\omega)]/\omega_0\mu_0$.

(vi) $T_{mn}^{ee}(z,\omega) \equiv \int_S\int \mathbf{e}_m' \cdot \frac{\partial}{\partial z}\mathbf{e}_n'$,

$T_{mn}^{eh}(z,\omega) \equiv \int_S\int \mathbf{e}_m' \cdot \frac{\partial}{\partial z}\mathbf{e}_n'' = -T_{nm}^{he}$,

$T_{mn}^{hh}(z,\omega) \equiv \int_S\int \mathbf{e}_m'' \cdot \frac{\partial}{\partial z}\mathbf{e}_n''$.

(vii) $Z_{mn}^{ee}(z,\omega) \equiv i\omega_0\int_S\int \mu_1\mathbf{e}_m' \cdot \mathbf{e}_n'$

$-\frac{1}{\omega_0}\int_S\int [\epsilon^{-1} - \epsilon_0^{-1}]\nabla_t \cdot \mathbf{e}_m' \nabla_t \cdot \mathbf{e}_n'$,

$Z_{mn}^{eh}(z,\omega) \equiv i\omega_0\int_S\int \mu_1\mathbf{e}_m' \cdot \mathbf{e}_n'' = Z_{nm}^{he}(z,\omega)$,

$Z_{mn}^{hh}(z,\omega) = i\omega_0\int_S\int \mu_1\mathbf{e}_m'' \cdot \mathbf{e}_n''$.

(viii) $Y_{mn}^{ee}(z,\omega) \equiv i\omega_0\int_S\int \epsilon_1\mathbf{h}_m' \cdot \mathbf{h}_n'$,

$Y_{mn}^{eh}(z,\omega) = i\omega_0\int_S\int \epsilon_1\mathbf{h}_m' \cdot \mathbf{h}_n'' = Y_{nm}^{he}(z,\omega)$,

$Y_{mn}^{hh}(z,\omega) = i\omega_0\int_S\int \epsilon_1\mathbf{h}_m'' \cdot \mathbf{h}_n''$

$-\frac{i}{\omega_0}\int_S\int [\mu^{-1} - \mu_0^{-1}]\nabla_t \cdot \mathbf{h}_m''\nabla_t \cdot \mathbf{h}_n''$. (A5)

In terms of these quantities, the following set of equations are obtained:

$$
\begin{aligned}
-\frac{d}{dz}V_m' &= i\beta_m'Z_m'I_m' + i\xi_m'I_m' \\
&\quad + \sum_n [T_{mn}^{ee}V_n' + T_{mn}^{eh}V_n'' + Z_{mn}^{ee}I_n' + Z_{mn}^{eh}I_n''], \\
-\frac{d}{dz}V_m'' &= i\beta_m''Z_m''I_m'' \\
&\quad + \sum_n [T_{mn}^{he}V_n' + T_{mn}^{hh}V_n'' + Z_{mn}^{he}I_n' + Z_{mn}^{hh}I_n''], \\
-\frac{d}{dz}I_m' &= i\beta_m'Y_m'V_m' \\
&\quad + \sum_n [T_{mn}^{ee}I_n' + T_{mn}^{eh}I_n'' + Y_{mn}^{ee}V_n' + Y_{mn}^{eh}V_n''], \\
-\frac{d}{dz}I_m'' &= i\beta_m''Y_m''V_m'' + i\eta_m''V_m'' \\
&\quad + \sum_n [T_{mn}^{he}I_n' + T_{mn}^{hh}I_n'' + Y_{mn}^{he}V_n' + Y_{mn}^{hh}V_n''], \\
&\qquad m = 1, 2, \cdots.
\end{aligned}
\tag{A6}
$$

Note that the coefficients T_{mn} ξ_m', and η_m'' represent coupling due to geometric imperfections while the coefficients Z_{mn} and Y_{mn} represent coupling due to imperfections in the medium.

To obtain the type of equation considered in Sec. I, we define the following scattering coefficients:

$$
a_m \equiv \tfrac{1}{2}[Y_m^{1/2}V_m + Z_m^{1/2}I_m], \quad b_m \equiv \tfrac{1}{2}[Y_m^{1/2}V_m - Z_m^{1/2}I_m],
$$

$$
m = 1, 2, \cdots, \tag{A7}
$$

for both E and H modes. We then recast (A6) into an equivalent system in terms of these scattering coefficients. The forward scattering approximation disregards the backward travelling waves. We set $b_m' = b_m'' = 0$ for all m; the resulting equations are

$$
\begin{aligned}
\frac{d}{dz}a_m' &= -i\beta_m'a_m' + \sum_{n=1}^{\infty}[C_{mn}^{ee}a_n' + C_{mn}^{eh}a_n''], \\
\frac{d}{dz}a_m'' &= -i\beta_m''a_m'' + \sum_{n=1}^{\infty}[C_{mn}^{he}a_n' + C_{mn}^{hh}a_n''],
\end{aligned}
\tag{A8}
$$

where

$$
\begin{aligned}
C_{mn}^{ee} &\equiv -(i/2)\xi_m'Y_m'\delta_{mn} - \tfrac{1}{2}T_{mn}^{ee}(Z_m'^{1/2}Y_n'^{1/2} + Y_m'^{1/2}Z_n'^{1/2}) \\
&\quad - \tfrac{1}{2}(Z_{mn}^{ee}Y_m'^{1/2}Y_n'^{1/2} + Y_{mn}^{ee}Z_m'^{1/2}Z_n'^{1/2}) \\
C_{mn}^{eh} &\equiv -\tfrac{1}{2}T_{mn}^{eh}(Y_m'^{1/2}Z_n''^{1/2} + Z_m'^{1/2}Y_n''^{1/2}) \\
&\quad - \tfrac{1}{2}(Z_{mn}^{eh}Y_m'^{1/2}Y_n''^{1/2} + Y_{mn}^{eh}Z_m'^{1/2}Z_n''^{1/2}) \\
C_{mn}^{he} &\equiv -\tfrac{1}{2}T_{mn}^{he}(Y_m''^{1/2}Z_n'^{1/2} + Z_m''^{1/2}Y_n'^{1/2}) \\
&\quad - \tfrac{1}{2}(Z_{mn}^{he}Y_m''^{1/2}Y_n'^{1/2} + Y_{mn}^{he}Z_m''^{1/2}Z_n'^{1/2}) \\
C_{mn}^{hh} &\equiv -(i/2)\eta_m''Z_m''\delta_{mn} - \tfrac{1}{2}T_{mn}^{hh}(Z_m''^{1/2}Y_n''^{1/2} + Y_m''^{1/2}Z_n''^{1/2}) \\
&\quad - \tfrac{1}{2}(Z_{mn}^{hh}Y_m''^{1/2}Y_n''^{1/2} + Y_{mn}^{hh}Z_m''^{1/2}Z_n''^{1/2}),
\end{aligned}
\tag{A9}
$$

and δ_{mn} denotes the Kronecker delta.

Observe that the transition from propagating to evanescent mode occurs when m is such that $\hat{k}_{t_m}$ exceeds $\omega_0^2\mu_0\epsilon_0$; in this case $\beta_m \to i\kappa_m$. The model adopted in Sec. I basically assumes that the random coefficients in (A6) [and therefore in (A9)] are zero mean wide sense stationary processes whose amplitudes are scaled by a common small parameter. The vector X in (1) of Sec. I represents a suitable arrangement of the scattering coefficients a_m', a_m'' in an infinite column array; the matrix ϵB is the corresponding square array of the C_{mn} coefficients determined by (A8) and the definition of X.

We can assume without loss of generality that the local uniform mode functions are random vectors with real components. Then the T_{mn} are real functions, while if ϵ_1 and μ_1 are real (i.e., lossless) random perturbations, the Z_{mn} and Y_{mn} are imaginary functions. More-

over, the following identities hold:

$$T^{ee}_{mn} = -T^{ee}_{nm}, \quad T^{hh}_{mn} = -T^{hh}_{nm}, \quad T^{eh}_{mn} = -T^{he}_{nm},$$

$$Z^{ee}_{mn} = Z^{ee}_{nm}, \quad Y^{ee}_{mn} = Y^{ee}_{nm}, \quad Z^{hh}_{mn} = Z^{hh}_{nm}, \quad Y^{hh}_{mn} = Y^{hh}_{nm}, \tag{A10}$$

$$Z^{eh}_{mn} = Z^{he}_{nm}, \quad Y^{eh}_{mn} = Y^{he}_{nm}.$$

When both m and n index propagating modes, the modal impedances and admittances (i.e., Z_m, Z_n, Y_m and Y_n) are positive real constants. In this case the C_{mn} coefficients satisfy the following skew-Hermitian relations:

$$C^{ee}_{mn} = -C^{ee*}_{nm}, \quad C^{hh}_{mn} = -C^{hh*}_{nm}, \quad C^{eh}_{mn} = -C^{he*}_{nm}. \tag{A11}$$

In general these coefficients are complex. Geometric imperfections contribute a complex diagonal term (i.e., $m = n$) and real off-diagonal terms ($m \neq n$); material imperfections contribute imaginary terms.

Since these coefficients comprise the principal $N \times N$ minor of the infinite matrix ϵB, we have

$$\rho_{ij,ji}(s) = -\hat{\rho}_{ij,ij}(s), \quad 1 \leq i, j \leq N. \tag{A12}$$

Moreover, if we assume that the geometric imperfections and material imperfections are statistically independent processes, it follows that $\rho_{ij,ji}$ can be written in the form

$$\rho_{ij,ji}(s) = -R^{(g)}_{ij}(s) - R^{(m)}_{ij}(s), \quad 1 \leq i, j \leq N, \tag{A13}$$

where $R^{(g)}_{ij}$ and $R^{(m)}_{ij}$ are real correlation functions characterizing the geometry and material, respectively.

When one index, say m, refers to a propagating mode while n indexes an evanescent mode, this skew-Hermitian property no longer holds. Z_n and Y_n become imaginary in this case, and their square roots are consequently complex. For the simple case of a single propagating H-mode in a guide with ideal geometry and only dielectric constant fluctuations, we obtain

$$C^{hh}_{1n} = -[(1+i)/2\sqrt{2}]\, Y^{hh}_{1n} Z_1'^{1/2} |Z_n'|^{1/2},$$

$$C^{he}_{1n} = -[(1+i)/2\sqrt{2}]\, Y^{he}_{1n} Z_1'^{1/2} |Z_n'|^{1/2} = C^{eh}_{n1}. \tag{A14}$$

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Some remarks on the evolution of a Schrödinger particle in an attractive $1/r^2$ potential*

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Comparing the different solutions of Case and Nelson for the evolution operators of a Schrödinger particle in the potential $V(r) = -1/r^2$, we show that Nelson's nonunitary solution is a simple average, over a physical parameter related to a boundary condition at the singularity, of Case's family of solutions.

1. INTRODUCTION

In two well-known papers, Case[1] and Nelson[2] have used different approaches, and arrived at different conclusions, in calculating the evolution operators for a Schrödinger particle in the presence of the singular, attractive potential $V(r) = -1/r^2$. The most striking difference is that Case finds the operators to be unitary but not unique, whereas Nelson finds them to be unique but not unitary.

As the potential is not physical (see, however, Ref. 3, esp. Secs. V, VI), we do not try to justify one solution or the other on physical grounds. All we attempt to do is clarify the relationship between the two; we show that Nelson's nonunitary solution is a simple (time independent) average over Case's family of unitary solutions.

We choose units so that Planck's constant, $\hbar$, has magnitude 1, and for complex numbers z and w we define

$$z^w \equiv \exp[w(\ln|z| + i\arg z)],$$

where $-\pi \leq \arg z < \pi$.

2. THE TWO SOLUTIONS

We consider the Schrödinger equation in three space dimensions:

$$\frac{\partial\psi}{\partial t} = i\left(\frac{1}{2m}\Delta + \frac{1}{r^2}\right)\psi, \quad \psi(\cdot, t) \in L_2(\mathbf{R}^3), \ \forall\, t. \tag{1}$$

In spherical coordinates the Laplace operator is

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{J^2}{r^2},$$

where J^2, the square of the angular momentum operator, is

$$J^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right].$$

The natural identification of $\mathbf{R}^3$ with $S\times\mathbf{R}^+$, where S is the unit sphere in $\mathbf{R}^3$, induces a Hilbert space isomorphism $L_2(\mathbf{R}^3) \cong L_2(S)\otimes L_2(0,\infty)$. We associate with the formal differential operator J^2, in the standard way, a self-adjoint operator (also denoted J^2) on $L_2(S)$ whose spectrum is purely discrete, with eigenspaces $\mathcal{L}_j$ and eigenvalues $j(j+1)$, where $j = 0, 1, 2, \cdots$. Finally we decompose in the natural manner

$$\mathcal{H} \equiv L_2(\mathbf{R}^3) \cong \bigoplus_{j=0}^{\infty}[\mathcal{L}_j \otimes L_2(0,\infty)] \equiv \bigoplus_{j=0}^{\infty}\mathcal{H}_j.$$

As the potential $V = -1/r^2$ is spherically symmetric, we will only consider solutions U^t for (1) which commute with $J^2\otimes I_2$ [where I_2 is the identity operator on $L_2(0,\infty)$], so that U^t can be decomposed as $U^t = \oplus U^t(j)$, where $U^t(j)$ is of the form $I_1\otimes X^t(j)$ with I_1 the identity operator on $\mathcal{L}_j$ and $X^t(j)$ an operator on $L_2(0,\infty)$. [By an abuse of notation we will no longer distinguish $U^t(j)$ and $X^t(j)$]. We will usually be considering evolution operators U^t be means of their "restrictions" $U^t(j)$ to an arbitrary but fixed $\mathcal{H}_j$.

Assume that ψ is a separable solution of (1) in $\mathcal{H}_j$, with radial part ψ_ρ, and let $u(r) = r\psi_\rho(r)$. Then (1) becomes

$$\frac{\partial u}{\partial t} = \frac{1}{2mi}\left(-\frac{\partial^2}{\partial r^2}u + \frac{(\nu^2 - \frac{1}{4})}{r^2}u\right) \equiv \frac{1}{2mi}Hu, \tag{2}$$

where $\nu^2 = \frac{1}{4} + [j(j+1) - 2m]$ and $u(\cdot, t)$ is in $L_2(0,\infty)$ for each fixed time t. Our problem now is to determine evolution operators $U^t(j)$ on $L_2(0,\infty)$ for (2) whose generator is appropriately related to the formal differential operator $(2mi)^{-1}H$, which we will consider to be an operator on $L_2(0,\infty)$ with domain C_0^∞, the (equivalence classes of) infinitely differentiable functions with compact support in the open interval $(0,\infty)$. We seek a generator which is an extension of $(2mi)^{-1}H$, which is not, itself, a generator.

Nelson in Ref. 2 defines such evolution operators $U_N{}^t(j)$, $t \geq 0$, of (2) with Laplace transform

$$Q_N(\lambda)u = \int_0^\infty \exp(-\lambda t)U_N{}^t(j)u\,dt, \quad \mathrm{Re}\lambda > 0,$$

and shows that

$$[Q_N(\lambda)u](x) = \int_0^\infty G_N(x,y;\lambda)u(y)\,dy$$

with

$$G_N(x,y;\lambda) = \begin{cases} x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x]f(y), & x > y, \\ x^{1/2}J_\nu[(2mi\lambda)^{1/2}x]g(y), & x < y, \end{cases}$$

where J_ν and H_ν^1 are the usual Bessel functions as defined in Ref. 4, f and g are unknown, and $\nu = (\nu^2)^{1/2}$; he also shows that $U_N{}^t(j)$ is not unitary for $\nu^2 < 0$ but is unitary for $\nu^2 \geq 0$. Thus his solutions $U_N{}^t$ for (1) are nonunitary if and only if $m > 1/8$, the only range of mass we will consider henceforth. From his definition of $U_N{}^t(j)$ it follows easily that $Q_N(\lambda) = K[Q_N(\lambda)]^*K$ [where K is the complex conjugation operator on $L_2(0,\infty)$ and * denotes operator adjoint] and then that $G_N(x,y;\lambda) = G_N(y,x;\lambda)$ so that

$$G_N(x,y;\lambda)=n(\lambda)$$
$$\times\begin{cases}x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x](y)^{1/2}J_\nu[(2mi\lambda)^{1/2}y], & x>y,\\ x^{1/2}J_\nu[(2mi\lambda)^{1/2}x](y)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}y], & x<y,\end{cases}\tag{3}$$

where $n(\lambda)$ is independent of x and y but as yet undetermined.

An alternative approach to the problem was put forth by Case in Ref. 1, and consists of determining all possible *unitary* evolution operators $U^t(j)$ for (2) whose generators extend $(2mi)^{-1}H$. Rather than use Case's method of carrying out this approach, we will use the method of von Neumann as described in Ref. 5, which has the advantages of being of very general character, widely known, and most importantly, of leading directly to quantities that we need to calculate. We will discuss separately the cases $\nu^2\geq 0$ and $\nu^2<0$.

For $\nu^2>0$, Nelson's solution is, as he indicates, the commonly accepted one corresponding to a Friedrichs extension of H. The case $\nu=0$ is slightly more complicated, but as we show in Sec. 4 it turns out that for $\nu^2\geq 0$ Nelson's solution can be "justified" by a regularization procedure if necessary (except possibly for the $j=0$ restriction). Therefore, the only part of Nelson's solution that can be regarded as unusual is that for $\nu^2<0$, the nonunitary restrictions.

A straightforward application of Theorem 10.20 of Ref. 5, most of which is explicitly exhibited in Ref. 6, shows that for $\nu^2<0$ there is a one-parameter family of unitary solutions $U_\theta{}^t(j)$, $-\infty<t<\infty$, $0\leq\theta<2\pi$, whose Laplace transforms $Q_\theta(\lambda)$ have kernels

$$G_\theta(x,y;\lambda)=m\pi/[1-\eta^4(2mi\lambda)^\nu L(\theta)]$$
$$\times\begin{cases}x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x](y)^{1/2}\{J_\nu[(2mi\lambda)^{1/2}y]\\ \quad-(2mi\lambda)^\nu L(\theta)J_{-\nu}[(2mi\lambda)^{1/2}y]\}, & x>y,\\ x^{1/2}\{J_\nu[(2mi\lambda)^{1/2}x]-(2mi\lambda)^\nu L(\theta)\\ \quad\times J_{-\nu}[(2mi\lambda)^{1/2}x]\}(y)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}y], & x<y,\end{cases}\tag{4}$$

for $\mathrm{Re}\lambda>0$, where $\eta=\exp(-i\nu\pi/4)$ and

$$L(\theta)=\exp(-i\theta)\left(\frac{\exp(i\theta)+\eta^2}{\exp(-i\theta)+\eta^2}\right).$$

We emphasize that this is a complete list of the unitary solutions for $\nu^2<0$ and that the parameter θ is directly related to a boundary condition at the singular point $r=0$; for the relation see Refs. 5 and 7. The parameter s for the corresponding evolution operators $U_s{}^t$ on $\mathcal{H}=\oplus\mathcal{H}_j$ is a variable in $[0,2\pi)^N$; we emphasize that $j\subset\mathbf{N}$ and $\theta\in[0,2\pi)$ are independent parameters, and $U_\theta{}^t(j)\equiv U_N{}^t(j)$ if $\nu\geq 0$.

3. COMPARISON OF SOLUTIONS FOR $\nu^2<0$

Since $L(\theta)$, defined above, is of absolute value 1, we can simplify the form of $G_\theta(x,y;\lambda)$ by defining $\chi(\theta)=\arg L(\theta)+\pi$. From

$$\frac{d\chi}{d\theta}=\frac{1-\eta^4}{|\exp(i\theta)+\eta^2|^2}>0$$

we see that $\chi(\theta)$ increases monotonically from 0 to 2π with θ, and has an inverse function $\theta(\chi)$. Defining the average

$$\langle G_\theta(x,y;\lambda)\rangle=\frac{1}{2\pi}\int_0^{2\pi}G_{\theta(\chi)}(x,y;\lambda)\,d\chi$$
$$=\frac{1}{2\pi}\int_0^{2\pi}G_\theta(x,y;\lambda)\frac{d\chi}{d\theta}\,d\theta,$$

and replacing $\exp(i\chi)$ by the complex variable z and using Cauchy's integral formula, we find for $\mathrm{Re}\lambda>0$

$$\langle G_\theta(x,y;\lambda)\rangle=m\pi\begin{cases}x^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x](y)^{1/2}J_\nu[(2mi\lambda)^{1/2}y], & x>y,\\ x^{1/2}J_\nu[(2mi\lambda)^{1/2}x](y)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}y], & x<y.\end{cases}\tag{5}$$

From (3) and (4) we see that for $\mathrm{Re}\lambda>0$ the bounded operator $Q_\theta(\lambda)$ is the sum of two bounded operators

$$Q_\theta(\lambda)=h(\theta)Q^1(\lambda)+k(\theta)Q^2(\lambda)$$

with the numerical coefficients h and k carrying all the θ dependence. Clearly $Q_\theta(\lambda)$, as a function of θ, is continuous in the operator norm topology, and the average operator

$$\langle Q_\theta(\lambda)\rangle u\equiv\frac{1}{2\pi}\int_0^{2\pi}Q_{\theta(\chi)}(\lambda)u\,d\chi$$

is an integral operator with kernel $\langle G_\theta(x,y;\lambda)\rangle$.

From Theorem 11.5.2 of Ref. 8.

$$Q_N(\lambda)=2mi(2mi\lambda-H_N)^{-1},\quad Q_\theta(\lambda)=2mi(2mi\lambda-H_\theta)^{-1},$$

where $(2mi)^{-1}H_N$ [resp. $(2mi)^{-1}H_\theta$] is the generator of $U_N{}^t(j)$ [resp. $U_\theta{}^t(j)$]. Let u be a nonzero function in C_0^∞, and therefore in the domain of H, H_N and H_θ. Then $H_Nu=H_\theta u$, and $v\equiv(2mi\lambda-H_N)u=(2mi\lambda-H_\theta)u$ is nonzero since H_θ is self-adjoint. Therefore, $2miu=Q_N(\lambda)v=Q_\theta(\lambda)v=\langle Q_\theta(\lambda)\rangle v$, which implies that $n(\lambda)=m\pi$ in (3), and $Q_N(\lambda)=\langle Q_\theta(\lambda)\rangle$.

From Theorem 11.6.2 of Ref. 8, if $\mathrm{Re}q>0$ we have

$$\frac{1}{2mi}\lim_{s\to\infty}\int_0^s dp\int_{q-ip}^{q+ip}\exp(\lambda t)Q_\theta(\lambda)u\,d\lambda=\begin{cases}U_\theta{}^t(j)u, & t>0,\\ u/2, & t=0,\end{cases}\tag{6}$$

with a similar equation for $U_N{}^t(j)$. Defining

$$\langle U_\theta{}^t(j)\rangle u=\frac{1}{2\pi}\int_0^{2\pi}U_{\theta(\chi)}{}^t(j)u\,d\chi,$$

we note that the limit in (6) is uniform in θ so that for $\mathrm{Re}q>0$,

$$\frac{1}{2\pi i}\lim_{s\to\infty}\int_0^s dp\int_{q-ip}^{q+ip}\exp(\lambda t)\langle Q_\theta(\lambda)\rangle u\,d\lambda$$

$$= \begin{cases} U_\theta{}^t(j)u, & t>0, \\ u/2, & t=0, \end{cases}$$

which proves that $U_N{}^t(j) = \langle U_\theta{}^t(j)\rangle$ for $t \geq 0$.

4. REGULARIZING THE POTENTIAL

In this section we consider the possibility of regularizing the potential $V = -1/r^2$, that is, altering it in a region of the origin so as to be nonsingular, calculating the associated evolution operators as a function of the region of regularization, and then looking for limits as we allow the region of regularization to become arbitrarily small while keeping all other parameters, in particular t, fixed. (A similar program is carried out in Sec. 5 of Ref. 6, but there even the centrifugal potential term is regularized, which we prefer not to do.)

Thus we consider the differential operator

$$\tilde{H}_R = -\frac{d^2}{dr^2} + \frac{\mu^2 - \frac{1}{4}}{r^2} + \tilde{V}_R,$$

where

$$\tilde{V}_R(r) = \begin{cases} -2m/r^2, & r>R, \\ -2m/R^2, & r \leq R, \end{cases}$$

where $R>0$, and $\mu = [\frac{1}{4} + j(j+1)]^{1/2}$. If $j \geq 1$, $\tilde{H}_R$, with domain C_0^∞, is essentially self-adjoint as we see by applying Theorem 10.21 of Ref. 5. We will postpone discussion of the case $j=0$ to the end of the section.

Assuming $j \geq 1$ and denoting by H_R the closure of $\tilde{H}_R$, we wish to study its behavior as R approaches 0. We will discuss separately the cases where ν is, or is not, an integer.

A straightforward calculation using Theorem 10.21 of Ref. 5 shows that if $\mathrm{Re}\lambda > 0$ and ν is not an integer, $Q_R(\lambda)$ defined as $2mi(2mi\lambda - H_R)^{-1}$ is a bounded integral operator will kernel

$$G_R(x,y;\lambda) = \begin{cases} w_1(x)w_2(y)/W, & x>y, \\ w_2(x)w_1(y)/W, & x<y, \end{cases}$$

where

$$w_1(x) = \begin{cases} a_R(x)^{1/2}H_\nu^1[(2mi\lambda)^{1/2}x], & x>R, \\ x^{1/2}\{J_\mu[(2mi\lambda + 2m/R^2)^{1/2}x] \\ + b_R J_{-\mu}[(2mi\lambda + 2m/R^2)^{1/2}x]\}, & x \leq R, \end{cases}$$

$$w_2(x) = \begin{cases} x^{1/2}\{J_\nu[(2mi\lambda)^{1/2}x] + d_R J_{-\nu}[(2mi\lambda)^{1/2}x]\}, & x>R, \\ c_R(x)^{1/2}J_\mu[(2mi\lambda + 2m/R^2)^{1/2}x], & x \leq R, \end{cases}$$

$$a_R = \frac{J_\mu[(2mi\lambda + 2m/R^2)^{1/2}R] + b_R J_{-\mu}[(2mi\lambda + 2m/R^2)^{1/2}R]}{H_\nu^1[(2mi\lambda)^{1/2}R]},$$

$$c_R = \frac{J_\nu[(2mi\lambda)^{1/2}R] + d_R J_{-\nu}[(2mi\lambda)^{1/2}R]}{J_\mu[(2mi\lambda + 2m/R^2)^{1/2}R]},$$

$$\tilde{b}_R = \frac{\Gamma(1-\mu)}{\Gamma(1+\mu)}\left(\frac{2mi\lambda R^2 + 2m}{4}\right)^\mu$$

$$\times\left(\frac{(-\mu-\nu)[(2mi\lambda)^{1/2}/2]^{-\nu}\Gamma(1+\nu) + R^{2\nu}(\mu-\nu)[(2mi\lambda)^{1/2}/2]^{\nu}\exp(-\nu\pi i)\Gamma(1-\nu)}{(-\mu+\nu)[(2mi\lambda)^{1/2}/2]^{-\nu}\Gamma(1+\nu) + R^{2\nu}(\mu+\nu)[(2mi\lambda)^{1/2}/2]\exp(-\nu\pi i)\,\Gamma(1-\nu)}\right),$$

$$\tilde{d}_R = -R^{2\nu}\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}\left(\frac{2mi\lambda}{4}\right)^\nu\left(\frac{\mu-\nu}{\mu+\nu}\right),$$

$$W = \frac{a_R}{m\pi}(d_R\exp(-\nu\pi i) + 1) = -b_R c_R\frac{\sin(\mu\pi)}{m\pi i},$$

$$b_R = \tilde{b}_R + O(R^2) \quad \text{as} \quad R \to 0,$$
$$d_R = \tilde{d}_R + O(R^2) \quad \text{as} \quad R \to 0.$$

It is easy to see that if $\nu^2 < 0$ and we let R approach zero along the sequence $\{R^\theta{}_n;\ n=1,2,\cdots\}$, chosen so that $d_{R^\theta_n} = -(2mi\lambda)^\nu L(\theta)$, then for each x, y in $(0,\infty)$

$$G_{R^\theta_n}(x,y;\lambda) \underset{n\to\infty}{\to} G_\theta(x,y;\lambda)$$

and, also, for each θ there exists such a sequence. From simple estimates of $[G_{R^\theta_n}(x,y;\lambda) - G_\theta(x,y;\lambda)]$ in each of the regions of integration corresponding to the possible linear orderings of x, y and R^θ_n, it follows that $Q_{R^\theta_n}(\lambda)$ converges strongly to $Q_\theta(\lambda)$ and therefore from Theorem IX.2.16 of Ref. 9, $U^t_{R^\theta_n}(j)$ converges, in the strong operator topology, to $U^t_\theta(j)$ for each t in $(-\infty,\infty)$. In particular, for $\nu^2 < 0$ and fixed $l \neq 0$, $U^t_R(j)$ does not converge as R approaches zero, except along special sequences, in contrast with the imaginary mass case in Sec. 2 of Ref. 2. This makes explicit the connection between the radius of regularization in the cutoff model and the associated $U_\theta{}^t$, as discussed in Sec. IV of Ref. 1; the fact that R^θ_n is a function of j could be interpreted as a means by which to select some of the evolution operators U^t_s on $\mathcal{H} = \oplus\mathcal{H}_j$ over others. For $\nu > 0$ but not integral, the above analysis shows that $U^t_R(j)$ does converge as R approaches zero, and converges to $U^t_N(j)$. A similar analysis confirms that this latter behavior holds for all $\nu \geq 0$.

There remains the case $j=0$. When the above program is begun for $j=0$, one finds that $\tilde{H}_R$ is not essentially self-adjoint for any ν. That this problem is basically unrelated to the potential is evident from the fact that the same result would emerge for a free particle. The point is that when we have a singular potential, it is reasonable to first restrict the formal Hamiltonian H to a domain of functions with support isolated from the singularity, and then look for extensions. If the potential is not singular, this procedure can lead to unwanted solutions as it does in our problem for $j=0$. [It is important to keep in mind that $r=0$ is only a boundary

point for the radial equation (2), not the full Schrödinger equation (1); there is no reason to distinguish $r=0$ from neighboring points for the nonsingular $\tilde{V}$.] Thus the regularization method does not select out particular solutions for $j=0$ as it does for $j \geq 1$. Fortunately ν and j cannot vanish simultaneously for $m > 1/8$, so we can "justify" all the unitary restrictions of Nelson's, either by the Friedrichs extension or regularization.

We summarize our results in the following

Proposition: The nonunitary evolution operators U^t on $L_2(\mathbf{R}^3)$ for

$$\frac{\partial \psi}{\partial t} = i\left(\frac{1}{2m}\Delta + \frac{1}{r^2}\right)\psi$$

defined by Nelson in Ref. 2, i.e., those for $m > 1/8$, are (time independent) averages of unitary evolution operators $U_s{}^t$ obtained by the traditional approach discussed by Case in Ref. 1; in other terms,

$$U^t\psi = \int U_s{}^t\psi \, d\mu(s) \quad \text{for all } \psi \text{ in } L_2(\mathbf{R}^3), \quad t \geq 0,$$

for some (time independent) probability measure μ on $[0, 2\pi)^N$.

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Time-dependent dynamical symmetries, associated constants of motion, and symmetry deformations of the Hamiltonian in classical particle systems

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A study is made of time-dependent dynamical symmetry mappings of Hamilton's equations for classical particle systems. The conditions that an infinitesimal mapping $(\delta x^A, \delta t) \equiv (\xi^A(x,t)\delta a, \xi^0(x,t)\delta a)$, $A = 1, \ldots, 2n$, be a symmetry mapping are expressed in terms of a "symmetry vector" $Z^A(x,t) \equiv \xi^A - \xi^0 \eta^{AB} \partial_B H(x,t)$ (where η^{AB} defines the symplectic matrix of phase space). These conditions imply that ξ^0 is arbitrary. It is shown that the symmetry deformation of a constant of motion $M(x,t)$ will also be a ("derived") constant of motion (time-dependent related integral theorem). It follows for the case $H = H(x)$ that every time-dependent symmetry deformation of $H(x)$ is a constant of motion, and it is shown conversely that every constant of motion $M(x,t)$ can be expressed as a symmetry deformation of the Hamiltonian, that is, there exists a symmetry vector $Z^A(x,t)$ such that $M = Z^A \partial_A H$. It is found that if $Z^A (\neq 0)$ is a symmetry vector, then $M(x,t)Z^A$ will be a (scaled) symmetry vector if and only if M is a constant of motion. The existence of groups of symmetry vectors is considered, and it is shown that a complete set of r symmetry vectors Z^A_α, $\alpha = 1, \ldots, r$, determines an r-parameter continuous group of symmetries. A special class of symmetry vectors $Z^A_{(P)}(x,t) \equiv \eta^{AB}(\partial_B M - N\partial_B H)$, ("extended Poisson vectors"), where $M(x,t)$, $N(x,t)$ are constants of motion is defined and conditions that such vectors determine a symmetry group are obtained. Poisson vectors are also used to show that the related integral theorem mentioned above may be considered as a generalization of Poisson's theorem on constants of motion. Dependency relations between derived constants of motion with respect to vectors of a symmetry group are obtained.

1. INTRODUCTION

In this paper we consider time dependent dynamical symmetries and associated time dependent constants of the motion for classical particle systems described by Hamilton's equations. This work is a continuation and generalization of recently published papers[1,2] in which we limited our considerations essentially to the time independent case.[3]

We define $2n$ phase space coordinates x^A in terms of the generalized coordinates q^i of the associated configuration space and their conjugate momenta p_i such that[4]

$$(x^1, \ldots, x^n; x^{n+1}, \ldots, x^{2n}) \equiv (q^1, \ldots, q^n; p_1, \ldots, p_n). \tag{1.1}$$

In general, we shall assume the Hamiltonian H to be time dependent $[H(x,t)]$ and take Hamilton's equations in form[5]

$$\dot{x}^A = \eta^{AB} H_{,B}, \tag{1.2}$$

where η^{AB} is defined by the symplectic matrix[6]

$$[\eta^{AB}] \equiv \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix} \quad (\eta^{AB} = -\eta^{BA}). \tag{1.3}$$

The covariant form η_{AB} is defined by

$$\eta_{AB}\eta^{BC} = \delta^C_A, \quad (\eta_{AB} = -\eta_{BA}). \tag{1.4}$$

A function $M(x,t)$ will be a constant of motion of the dynamical path defined by (1.2) if

$$dM/dt = \eta^{AB} M_{,A} H_{,B} + M_{,t} = M_{,A} H^A + M_{,t} = 0, \tag{1.5}$$

where

$$H^A \equiv \eta^{AB} H_{,B} \quad (H_{,B} = \eta_{BA} H^A). \tag{1.6}$$

A dynamical symmetry is a mapping which maps the set of integral curves of (1.2) into itself.

In this paper the conditions for dynamical symmetries will be based upon infinitesimal point mappings with associated changes in parameter t (Ref. 7)

$$\bar{x}^A = x^A + \xi^A(x,t)\delta a, \tag{1.7}$$

$$\bar{t} = t + \xi^0(x,t)\delta a. \tag{1.8}$$

This form of infinitesimal mapping is a generalization of those we previously considered (see Ref. 1, 2) where it was assumed $H = H(x)$ and

$$\xi^A = \xi^A(x), \quad d\bar{t} = dt\{1 + 2\phi[x(t)]\delta a\}.$$

We give below, a brief summary of the main results of this paper.

In Sec. 2 we obtain in two different ways the conditions (see Theorem 2.1) that the transformation (1.7), (1.8) define a dynamical symmetry mapping. It is shown that the function $\xi^0(x,t)$, which appears in (1.8), may be taken as arbitrary, and that the $\xi^A(x,t)$ of (1.7) is defined in terms of a symmetry vector $Z^A(x,t)$ [a solution of (2.13)] and ξ^0.

In Sec. 3 a time dependent related integral theorem is derived which states that the symmetry deformation of a constant of motion $M(x,t)$ will also be a ("derived") constant of motion. This includes the case in which $M(x,t) = H(x)$, and hence it follows that time dependent symmetry deformations of Hamiltonians of the form $H(x)$ are constants of motion. It is also shown that if $H = H(x,t)$ (which is hence not a constant of motion) there exist [as a result of the arbitrariness of the $\xi^0(x,t)$] suitably chosen symmetry mappings for which the deformations of $H(x,t)$ will be constants of motion.

In Sec. 4 it is proved for dynamical systems with $H = H(x)$ that *every constant of motion $M(x,t)$ can be expressed as a symmetry deformation of the Hamiltonian.*

In Sec. 5 we show that if $Z^A(x,t)$ is any symmetry vector, then the "scaled" vector $M(x,t)Z^A(x,t)$ will also be a symmetry vector where $M(x,t)$ is any constant of motion.

In Sec. 6 it is shown that if $M(x,t)$, $N(x,t)$ are arbitrary constants of motion of dynamical systems with $H=F(x)+G(t)$, then the "extended Poisson" vector $Z^A_{(P)}\equiv\eta^{AB}M_{,B}-NH^A$ and its partial time-derivatives will be symmetry vectors. It is also shown that there exist $2n$ linearly independent symmetry vectors of the "Poisson form" $Z^A_{(P)\alpha}(x,t)\equiv\eta^{AB}M_{\alpha,B}$ where $M_\alpha(x,t)$ is any set of $2n$ functionally independent constants of motion.

In Sec. 7 we consider r-parameter continuous groups determined by symmetry vectors. It is first shown that the commutator of any two symmetry vectors is also a symmetry vector. Conditions are obtained in order that a set of symmetry vectors of the Poisson form determine a symmetry group. It is also shown how extended Poisson vectors can be used to define groups of symmetry mappings (1.7), (1.8). Dependency relations between derived constants of motion obtained by the symmetry deformation of a given constant of motion with respect to vectors of a symmetry group are determined in terms of the structure constants of the group.

Specific examples illustrating in detail results of this paper will appear elsewhere.

2. DERIVATION OF DYNAMICAL SYMMETRY EQUATIONS

In this section we derive the dynamical symmetry equations of the system (1.2) based upon the mapping (1.7), (1.8). The conditions for such a symmetry can be expressed in the form

$$\delta\left(\frac{dx^A}{dt}-\eta^{AB}\frac{\partial H(x,t)}{\partial x^B}\right)\equiv\left(\frac{d\bar{x}^A}{d\bar{t}}-\eta^{AB}\frac{\partial H(\bar{x},\bar{t})}{\partial\bar{x}^B}\right)-\left(\frac{dx^A}{dt}-\eta^{AB}\frac{\partial H(x,t)}{\partial x^B}\right)=0, \tag{2.1}$$

for all $x^A(t)$ which satisfy (1.2).

From (1.8) we find to first order in δa that

$$\frac{dt}{d\bar{t}}=1-\frac{d\xi^\circ(x,t)}{dt}\delta a. \tag{2.2}$$

Consider

$$\delta(\dot{x}^A)\equiv\frac{d\bar{x}^A}{d\bar{t}}-\frac{dx^A}{dt}=\frac{d}{dt}(x^A+\xi^A\delta a)\frac{dt}{d\bar{t}}-\frac{dx^A}{dt}. \tag{2.3}$$

From (2.2) and (2.3) we obtain (to first order in δa)

$$\delta(\dot{x}^A)=[d\xi^A/dt-(d\xi^\circ/dt)\dot{x}^A]\delta a. \tag{2.4}$$

By use of (1.7), (1.8) we have for any function $F(x,t)$

$$\delta F(x,t)\equiv F(\bar{x},\bar{t})-F(x,t)=(F_{,A}\,\xi^A+F_{,t}\xi^\circ)\delta a. \tag{2.5}$$

In addition,

$$dF(x,t)/dt=F_{,A}\dot{x}^A+F_{,t}=\eta^{AB}F_{,A}H_{,B}+F_{,t}. \tag{2.6}$$

We now apply (2.5) to obtain

$$\delta(H_{,B})=(H_{,BC}\xi^C+H_{,Bt}\xi^\circ)\delta a. \tag{2.7}$$

From (2.4), (2.7), (1.3), and (2.6) we evaluate the left-hand side of (2.1) to obtain the following conditions for a dynamical symmetry:

$$\xi^A_{,B}H^B-\xi^BH^A_{,B}+\xi^A_{,t}-\xi^\circ_{,B}H^BH^A-\xi^\circ H^A_{,t}-\xi^\circ_{,t}H^A=0. \tag{2.8}$$

If we define for any vector $V^A(x,t)$ the operator

$$S(V^A)\equiv V^A_{,B}H^B-V^BH^A_{,B}+V^A_{,t}, \tag{2.9}$$

then (2.8) can be written in the form

$$S(\xi^A)-S(\xi^\circ H^A)=0. \tag{2.10}$$

From the linearity of the operator S we may write (2.10) in the form

$$S(\xi^A-\xi^\circ H^A)=0. \tag{2.11}$$

Hence if we define

$$Z^A\equiv\xi^A-\xi^\circ H^A, \tag{2.12}$$

the symmetry equation (2.8) can be written in the form

$$S(Z^A)=Z^A_{,B}H^B-Z^BH^A_{,B}+Z^A_{,t}=0. \tag{2.13}$$

This indicates that to obtain a solution (ξ^A,ξ°) to the symmetry equation (2.8) it is sufficient to solve (2.13) for $Z^A(x,t)$ and then determine ξ^A from (2.12) in which ξ° may be chosen arbitrarily.

We refer to the vector ξ^A as a "symmetry mapping vector" and to Z^A as a "symmetry vector."

Theorem 2.1: For a dynamical system (1.2) where $H=H(x,t)$ every symmetry mapping (1.7), (1.8) is determined by $\xi^A(x,t)$, $\xi^\circ(x,t)$ where ξ° is chosen arbitrarily and ξ^A is defined by (2.12) in which $Z^A(x,t)$ is a solution of (2.13).

If in (2.12) the particular choice $\xi^\circ=0$ is made, we see that any solution Z^A of (2.13) will itself be a symmetry mapping vector.

We give next an alternative derivation of (2.8) based upon a generalization of a method used by Komar[8] which applies to our present case where $H=H(x,t)$ and $\xi^\circ=\xi^\circ(x,t)\neq0$ [Komar considered the case $H=H(x)$, and $\xi^\circ=0$].

Starting at any point P we move to a point Q along the trajectory passing through P as determined by (1.2). Then a point R is determined by means of the point mapping (1.7) as applied to the point Q. We now interchange the order of these two operations by starting at P and use (1.7) to obtain the point S. We then require that the point R lies on the trajectory passing through the point S.

Since P and Q are on the same dynamical path, to reach the point R through Q as described above, we may write

$$x^A(R)=x^A(Q)+\xi^A(Q)\delta a=x^A(P)+\dot{x}^A(P)\delta t+\xi^A(Q)\delta a, \tag{2.14}$$

where $\delta t\equiv t(Q)-t(P)$. For the same reason we may evaluate $\xi^A(Q)$ by

$$\xi^A(Q)=\xi^A(P)+\left[\frac{d\xi^A}{dt}\right]_P\delta t=\xi^A(P)+[\xi^A_{,B}\,\dot{x}^B+\xi^A_{,t}]_P\,\delta t. \tag{2.15}$$

From (2.15), (2.14), and (1.2) we have

$$x^A(R) = x^A(P) + \xi^A(P)\delta a + [H^A + (\xi^A_{,B}H^B + \xi^A_{,t})\delta a]_P\,\delta t. \tag{2.16}$$

By means of the second route we have

$$x^A(R) = x^A(S) + \bar{\dot{x}}^A(S)\delta\bar{t} = x^A(P) + \xi^A(P)\delta a + \bar{\dot{x}}^A(S)\delta\bar{t},$$

$$\bar{\dot{x}}^A \equiv d\bar{x}^A/d\bar{t}, \tag{2.17}$$

where $\delta\bar{t} \equiv \bar{t}(R) - \bar{t}(S)$. We may write

$$\bar{\dot{x}}^A(S) = H^A(S) = H^A(P) + [H^A_{,B}\xi^B + H^A_{,t}\xi^\circ]_P\,\delta a. \tag{2.18}$$

From (1.8) we obtain

$$\delta\bar{t} = \left[1 + \frac{d\xi^\circ}{dt}\,\delta a\right]_P \delta t = [1 + (\xi^\circ_{,C}H^C + \xi^\circ_{,t})\delta a]_P\,\delta t. \tag{2.19}$$

By use of (2.19), (2.18) in (2.17) we obtain

$$X^A(R) = X^A(P) + \xi^A(P)\delta a + [H^A + (H^A_{,B}\xi^B + H^A_{,t}\xi^\circ + H^A H^C\xi^\circ_{,C} + H^A\xi^\circ_{,t})\delta a]_P\,\delta t. \tag{2.20}$$

Equating the right-hand sides of (2.16) and (2.20) we again obtain the symmetry condition (2.8).

In order to obtain the time independent symmetry equation discussed in Ref. 1, 2 we take $H = H(x)$, $\xi^A = \xi^A(x)$, $\xi^\circ = \xi^\circ(x)$ in (2.8) and define

$$2\phi(x) \equiv \xi^\circ_{,A}H^A. \tag{2.21}$$

Then (2.8) reduces to

$$\xi^A_{,B}H^B - \xi^B H^A_{,B} - 2\phi H^A = 0, \tag{2.22}$$

which is recognized as the above-mentioned time independent symmetry equation. Thus to obtain solutions to (2.22) it is sufficient to solve (2.13) for Z^A assuming $H = H(x)$, $Z^A = Z^A(x)$ and then define ξ^A and ϕ by (2.12) and (2.21), respectively, where we consider ξ° as an arbitrary function $\xi^\circ(x)$.

3. TIME DEPENDENT RELATED INTEGRAL THEOREM

In this section we examine several means of determining time dependent constants of motion of a dynamical system. It was shown in Ref. 1 and indirectly in Ref. 2 (expressed in terms of a related integral theorem) that if $M(x)$ is a time independent constant of motion of a dynamical system with $H = H(x)$, then so also is $\delta M/\delta a \equiv M_{,A}\xi^A$ where $\xi^A(x)$ is a symmetry mapping vector given by (2.22). We now extend this result to time dependent constants of motion $M(x, t)$ for systems in which $H = H(x, t)$ and symmetry mappings are based upon (1.7), (1.8).

To obtain this extension, first observe that we may express $\delta M(x, t)$ by means of (2.5) as

$$\delta M \equiv (M_{,A}\xi^A + M_{,t}\xi^\circ)\delta a. \tag{3.1}$$

We define a deformation operator Δ by

$$\Delta \equiv (\delta a)Z^A\frac{\partial}{\partial x^A}, \tag{3.2}$$

and note by means of (2.12) and (1.5) that for any constant of motion $M(x, t)$

$$\delta M(x, t) = \Delta M(x, t) = M_{,A}Z^A\delta a. \tag{3.3}$$

If $M(x, t)$ is a constant of the motion [see (1.5)], then a simple calculation shows that for any Z^A which satisfies (2.13)

$$\frac{d}{dt}\left(\frac{\delta M}{\delta a}\right) \equiv S(Z^A)M_{,A} + (M_{,B}H^B + M_{,t})_{,A}Z^A = 0, \tag{3.4}$$

which implies that $\delta M/\delta a$ is a constant of the motion.

We summarize the above remarks as

Theorem 3.1 (Time Dependent Related Integral Theorem): If $M(x, t)$ is a constant of the motion of the dynamical system (1.2) with $H = H(x, t)$, then $\delta M/\delta a = M_{,A}\xi^A + M_{,t}\xi^\circ = \Delta M/\delta a = M_{,A}Z^A$ is also a constant of the motion, where Z^A is a symmetry vector as described in Theorem 2.1.

As an important illustration of this theorem we mention the case where $H = H(x)$ for which it is well known H is a constant of motion. Then Theorem 3.1 states that

$$\delta H(x)/\delta a = H_{,A}Z^A \tag{3.5}$$

is also a constant of the motion.

We now assume the general case $H = H(x, t)$ and show by a suitable choice of $\xi^\circ(x, t)$ there exist symmetry mappings (1.7), (1.8) for which

$$\frac{\delta H(x, t)}{\delta a} \equiv H_{,A}\xi^A + H_{,t}\xi^\circ = H_{,A}Z^A + H_{,t}\xi^\circ \tag{3.6}$$

will be a constant of the motion. The condition that $\delta H/\delta a$ be a constant of motion is

$$(\delta H)_{,A}H^A + (\delta H)_{,t} = 0. \tag{3.7}$$

We evaluate the left-hand side of (3.7) by means of (3.6) and combine the result with the equation $H_{,A}S(Z^A) = 0$ [refer to (2.13)] to obtain the condition on $\xi^\circ(x, t)$

$$\xi^\circ_{,A}H^A H_{,t} + \xi^\circ_{,t}H_{,t} + \xi^\circ(H_{,At}H^A + H_{,tt}) + H_{,At}Z^A = 0 \tag{3.8}$$

in order that $\delta H(x, t)/\delta a$ be a constant of motion.

We state this in the form of a theorem.

Theorem 3.2: Corresponding to any solution (Z^A, ξ°) of (2.13) and (3.8), $\delta H/\delta a$ as defined in (3.6) will be a constant of motion of the dynamical system (1.2) with $H = H(x, t)$. The associated symmetry mapping (1.7), (1.8) is then determined by ξ^A, ξ° where ξ^A is given by (2.12).

4. REPRESENTATION OF EVERY CONSTANT OF MOTION AS A SYMMETRY-INDUCED DEFORMATION OF THE HAMILTONIAN

In Sec. 3 it was shown by means of Theorem 3.1 that if $H = H(x)$ (and hence H is a constant of motion) then the symmetry-induced deformation of the Hamiltonian $\delta H/\delta a = \Delta H/\delta a = H_{,A}Z^A(x, t)$ is also a constant of the motion. We shall now show for such dynamical systems [i.e., those with $H = H(x)$] that corresponding to every constant of motion $M(x, t)$ there exists at least one symmetry vector $Z^A_{(M)}(x, t)$ such that

$$M(x, t) = \Delta H(x)/\delta a = H(x)_{,A}Z^A{}_{(M)}(x, t). \tag{4.1}$$

This will be done by use of a suitably chosen canonical transformation.

For any Hamiltonian $H(x)\equiv H(q,p)$ [see (1.1)] there exists a canonical coordinate transformation[9]

$$\tilde{x}^A=\tilde{x}^A(x)\Leftrightarrow \tilde{q}^i=\tilde{q}^i(q,p),\quad \tilde{p}_i=\tilde{p}_i(q,p),\quad i=1,\ldots,n, \tag{4.2}$$

such that in $(\tilde{x})$ coordinates

$$H(q,p)=\tilde{H}(\tilde{q},\tilde{p})\equiv\tilde{p}_1. \tag{4.3}$$

It follows from (4.3) and Hamilton's equations in the $(\tilde{x})$ system that

$$\tilde{x}^1-t,\ \tilde{x}^2,\ldots,\tilde{x}^{2n} \tag{4.4}$$

are constants of motion, which by inspection are seen to be functionally independent.

It should be recalled that the elements η^{AB} of the symplectic matrix $[\eta^{AB}]$ [see (1.3)] transform as the components of a second rank contravariant numerical tensor under canonical transformations, i.e.,[10]

$$\tilde{\eta}^{AB}=\frac{\partial\tilde{x}^A}{\partial x^C}\frac{\partial\tilde{x}^B}{\partial x^D}\eta^{CD}=\eta^{AB}. \tag{4.5}$$

Under the coordinate transformation (4.2) $H(x)$ transforms as a scalar as indicated by (4.3). It therefore follows that $H_{,A}$ and H^A transform as covariant and contravariant vectors, respectively:

$$H_{,A}=\frac{\partial\tilde{x}^B}{\partial x^A}\tilde{H}_{,B},\quad H^A=\frac{\partial x^A}{\partial\tilde{x}^B}\tilde{H}^B, \tag{4.6}$$

where

$$\tilde{H}_{,A}\equiv\partial\tilde{H}/\tilde{x}^A\ ,\quad \tilde{H}^B\equiv\eta^{BA}\tilde{H}_{,A}. \tag{4.7}$$

Since any symmetry vector $Z^A(x,t)$ transforms under (4.2) as a contravariant vector we may write[11]

$$Z^A(x,t)=\frac{\partial x^A}{\partial\tilde{x}^B}\tilde{Z}^B(\tilde{x},t), \tag{4.8}$$

and hence we note by (4.6) and (4.8) that ΔH is a scalar, i.e.,

$$\Delta H(x)/\delta a=H_{,A}(x)Z^A(x,t)=\tilde{H}_{,A}(\tilde{x})\tilde{Z}^A(\tilde{x},t)=\Delta\tilde{H}(\tilde{x})/\delta a. \tag{4.9}$$

Based upon the above-mentioned transformations a simple calculation shows that $S(Z^A)$ as defined by (2.13) transforms as a functionally form invariant vector, i.e.,

$$\tilde{S}(\tilde{Z}^A)\equiv\tilde{Z}^A_{,B}\tilde{H}^B-\tilde{Z}^B\tilde{H}^A_{,B}+\tilde{Z}^A_{,t}=(\partial\tilde{x}^A/\partial x^C)S(Z^C)=0 \tag{4.10}$$

(where the zero follows from the fact that Z^C is a symmetry vector). Hence (4.10) implies $\tilde{Z}^A$ is also a symmetry vector.

By means of (4.3) and (4.7) we find that

$$\tilde{H}^A=\delta^A_1, \tag{4.11}$$

and hence in (4.10) $\tilde{Z}^B\tilde{H}^A_{,B}=0$. This implies by (4.10) that

$$\tilde{Z}^A_{,B}\tilde{H}^B+\tilde{Z}^A_{,t}=0, \tag{4.12}$$

which shows [see (1.5)] that the individual components $\tilde{Z}^A(\tilde{x},t)$ are constants of motion.[12] By use of (4.11) we see that (4.12) reduces to

$$\frac{\partial\tilde{Z}^A}{\partial\tilde{x}^1}+\frac{\partial\tilde{Z}^A}{\partial t}=0. \tag{4.13}$$

The solution of (4.13) can be written as

$$\tilde{Z}^A=\tilde{F}^A(\tilde{x}^1-t,\ \tilde{x}^2,\ldots,\tilde{x}^{2n}), \tag{4.14}$$

where $\tilde{F}^A$ is an arbitrary function of the indicated arguments. We note that each of these arguments is itself a constant of motion [see (4.4)]. We state this (intermediate) result as

Theorem 4.1: For every dynamical system (1.2) with $H=H(x)$ there exists a canonical coordinate system $(\tilde{x})$ in which each component $\tilde{Z}^A(\tilde{x},t)$ of any symmetry vector is a constant of motion.

Remark: From (4.14) it follows that the $2n$ components $\tilde{Z}^A$ can always be selected as $2n$ functionally independent constants of motion.

Suppose now that $M(x,t)$ is an arbitrary constant of motion in the (x) coordinate system. In the $(\tilde{x})$ coordinate system $M(x,t)$ transforms to

$$M(x,t)=\tilde{M}(\tilde{x}^1-t,\ \tilde{x}^2,\ldots,\tilde{x}^{2n}). \tag{4.15}$$

We now define a symmetry vector $\tilde{Z}^A_{(M)}$ based on (4.14) and (4.15) by

$$\tilde{Z}^A_{(M)}\equiv\tilde{F}^A_{(M)}(\tilde{x}^1-t,\ \tilde{x}^2,\ldots,\tilde{x}^{2n}),\quad A\neq n+1,\quad \tilde{Z}^A_{(M)}\equiv\tilde{M}. \tag{4.16}$$

From (4.8) we determine the components $Z^A_{(M)}(x,t)$ in the (x) coordinate system by

$$Z^A_{(M)}=\frac{\partial x^A}{\partial\tilde{x}^B}\tilde{Z}^B_{(M)}. \tag{4.17}$$

Since $\tilde{S}(\tilde{Z}^A_{(M)})=0$ it follows from an equation similar to (4.10) that $S(Z^A_{(M)})=0$, and hence $Z^A_{(M)}(x,t)$ is a symmetry vector. It will now be shown that the $Z^A_{(M)}$ given by (4.17) will satisfy the desired condition (4.1).

From Theorem 3.1 referred to the $(\tilde{x})$ coordinates we obtain the constant of motion

$$\Delta\tilde{H}/\delta a=\tilde{H}_{,A}\tilde{Z}^A_{(M)}=\delta_{n+1,A}\tilde{Z}^A_{(M)}=\tilde{Z}^{n+1}_{(M)}=\tilde{M} \tag{4.18}$$

by use of (4.3) and (4.16). It follows from (4.9), (4.15), and (4.18) that (4.1) will be satisfied by the $Z^A_{(M)}$ given by (4.17). From the degree of arbitrariness of the components $\tilde{Z}^A_{(M)}$ as given by (4.16) it is evident that the vector $Z^A_{(M)}$ is not unique.

We may now state

Theorem 4.2: Every constant of the motion $M(x,t)$ of a dynamical system (1.2) with $H=H(x)$ can be expressed as a symmetry-induced deformation of the Hamiltonian H, that is, $M(x,t)$ may be expressed in the form (4.1) where $Z^A_{(M)}(x,t)$ is a symmetry vector.

5. SCALING OF SYMMETRY VECTORS

Given a symmetry vector $Z^B(x,t)$, i.e. a solution of (2.13), we determine if there exists a function $A(x,t)$ such that

$$Z^{*B}(x,t)\equiv A(x,t)Z^B \tag{5.1}$$

will also be a symmetry vector. From (2.13) we have

$$S(Z^{*B}) = S(AZ^B) = AS(Z^B) - (A_{,C}H^C + A_{,t})Z^B. \quad (5.2)$$

Hence (5.2) implies that if $S(Z^{*B})$ is to be zero when $S(Z^B) = 0$, then $A_{,C}H^C + A_{,t} = 0$ (assuming $Z_B \neq 0$). Therefore, $A(x, t)$ must be a constant of motion. Conversely, if $A(x, t)$ is a constant of motion, then it follows from (5.2) that Z^{*B} will be a symmetry vector.

Theorem 5.1: If Z^B ($\neq 0$) is a symmetry vector of the dynamical system (1.2) [that is, Z^B satisfies (2.13)], then a necessary and sufficient condition that $Z^{*B}(x, t) \equiv A(x, t)Z^B(x, t)$ be a symmetry vector is that A be a constant of motion.

We shall refer to Z^{*B} as a scaling-related symmetry vector obtained from Z^B by means of the scaling factor A.

In keeping with (2.12) we write

$$Z^{*B} = \xi^{*B} - \xi^{*\circ}H^B, \quad (5.3)$$

where

$$\xi^{*B} \equiv A\xi^B, \quad \xi^{*\circ} \equiv A\xi^\circ. \quad (5.4)$$

Theorem 5.2: If (1.7) and (1.8) define a symmetry mapping in terms of (ξ^B, ξ°) [that is, (2.8) is satisfied], then a scaling-related symmetry mapping is defined by $(\xi^{*B}, \xi^{*\circ}) \equiv (A\xi^B, A\xi^\circ)$, where $A = A(x, t)$ is an arbitrary constant of motion.

Since $A(x, t)$ is a constant of motion, then along a given dynamical path $A(x, t) = A_0 = \text{const}$ and hence along this path $(Z^{*B}, \xi^{*B}, \xi^{*\circ})$ differ from (Z^B, ξ^B, ξ°) by this constant factor A_0 as indicated by (5.1), (5.4).

We next show that if $Z^A(x, t)$ is any symmetry vector, i.e., a solution of (2.13), then $Z^A_{,A}$ will be a constant of motion.[13] To prove this we form from the symmetry equation $S(Z^A) = 0$ [see (2.13)]

$$[S(Z^A)]_{,A} = W_{,A}H^A + W_{,t} = dW/dt = 0, \quad W \equiv Z^A_{,A}. \quad (5.5)$$

By Theorem 5.1 the scaled vector $Z^{*B}(x, t) \equiv A(x, t)Z^B(x, t)$ is a symmetry vector and hence by (5.5) $Z^{*B}_{,B}$ is a constant of motion. We show below how this may be used to obtain an alternative proof of the time dependent related integral theorem (Theorem 3.1). From (5.1) we have

$$Z^{*B}_{,B} = (AZ^B)_{,B} = AZ^B_{,B} + A_{,B}Z^B. \quad (5.6)$$

Hence

$$A_{,B}Z^B = Z^{*B}_{,B} - AZ^B_{,B}. \quad (5.7)$$

Since the right-hand side of (5.7) is a constant of motion the left-hand side must also be a constant of motion. From the definition (2.5) we have

$$\delta A/\delta a = A_{,B}\xi^B + A_{,t}\xi^\circ = A_{,B}Z^B + \xi^\circ(A_{,B}H^B + H_{,t}) = A_{,B}Z^B, \quad (5.8)$$

because A is a constant of motion. We have thus proved that if $A(x, t)$ is any constant of motion, then $\delta A/\delta a$ (based upon the symmetry vector Z^A) is a constant of motion, which is the related integral theorem.

6. EXTENDED POISSON SYMMETRY VECTORS

In Ref. 1, 2 it was shown how to construct a class of symmetry mapping vectors derived from constants of motion. Such vectors, called Poisson symmetry vectors, were defined by $\xi^A_{(P)}(x) \equiv \eta^{AB}M(x)_{,B}$, where $M(x)$ is any constant of motion of a dynamical system (1.2) with $H = H(x)$. [Such vectors $\xi^A_{(P)}(x)$ will satisfy (2.22) with $\phi = 0$.] We now generalize this definition of a Poisson symmetry vector to the time dependent theory.

For this purpose define the "extended Poisson symmetry vector"

$$Z^A_{(P)}(x, t) \equiv \xi^A_{(P)}(x, t) - \xi^\circ_{(P)}(x, t)H^A = \eta^{AB}M_{,B} - NH^A, \quad (6.1)$$

where

$$\xi^A_{(P)} \equiv \eta^{AB}M_{,B}, \quad \xi^\circ_{(P)} \equiv N, \quad (6.2)$$

with $M(x, t)$, $N(x, t)$ any constants of motion.

We now prove that if

$$H(x, t) = F(x) + G(t) \quad (6.3)$$

the vector $Z^A_{(P)}$ defined by (6.1) will be a symmetry vector, i.e., it will satisfy (2.13). This implies that $(\xi^A_{(P)}, \xi^\circ_{(P)})$ of (6.2) will define a symmetry mapping (1.7), (1.8).

We have then from (6.1) and (2.13) that

$$S(Z^A_{(P)}) = S(\eta^{AB}M_{,B}) - S(NH^A). \quad (6.4)$$

By use of (6.3) and the conditions that $M(x, t)$ and $N(x, t)$ are constants of motion an easy calculation shows that each term on the right-hand side of (6.4) is zero. This completes the proof.[14]

We state this as follows.

Theorem 6.1: If $H(x, t) = F(x) + G(t)$, and $M(x, t)$, $N(x, t)$ are any constants of motion of the dynamical system (1.2), then the mapping (1.7), (1.8) defined by (6.2) will be a symmetry mapping, and in addition the extended Poisson symmetry vector $Z^A_{(P)}$ defined by (6.1), will be a symmetry vector [that is, it will satisfy (2.13)].

Corollary 6.1: If $H(x, t) = F(x) + G(t)$, and if $Z^A_{(P)}$ is an extended Poisson symmetry vector as defined in (6.1), then $Z^A_{(P),t}, Z^A_{(P),tt}, \cdots$ will also be symmetry vectors.

If in (6.1) we choose $N = 0$, then it is easily shown that the resulting Poisson vector

$$Z^A_{(P)}(x, t) = \eta^{AB}M_{,B}(x, t) \quad (6.5)$$

will be a symmetry vector for the dynamical system (1.2) with $H = H(x, t)$ (H arbitrary). If now $R(x, t)$ denotes any constant of motion of such a system, then by Theorem 3.1 with $Z^A = Z^A_{(P)}$ of (6.5) we have[15]

$$\delta R/\delta a = \eta^{AB}R_{,A}M_{,B} \equiv [R, M]. \quad (6.6)$$

We recognize that (6.6) gives an alternative proof of Poisson's theorem on constants of motion since the right side of (6.6) is the Poisson bracket of the arbitrary constants of motion $R(x, t)$, $M(x, t)$, and the left side of (6.6) is a constant of motion by Theorem 3.1. Hence, Theorem 3.1 may be viewed as a generalization of Poisson's theorem.[16]

Note if we consider the case $H = H(x)$ and choose

$R=H$ then (6.6) shows $\delta H/\delta a=-M_{,t}$.

Note also if H is of the form (6.3) and $Z^A_{(P)}$ is defined by (6.1), then the constant of motion $Z^A_{(P),A}=M_{,t}$.

We now show how the Poisson symmetry vector form (6.5) may be used to determine $r\leq 2n$ linearly independent symmetry vectors. Let $M_\alpha(x,t)$, $\alpha=1,\ldots,r$, be a set of functionally independent constants of motion of (1.2) with $H=H(x,t)$, where $H(x,t)$ is now taken to be arbitrary. We show that the Poisson symmetry vectors

$$Z^A_{(P)\alpha}(x,t)\equiv\eta^{AB}M_{\alpha,B},\quad \alpha=1,\ldots,r, \tag{6.7}$$

are linearly independent.

To prove this assume they are linearly dependent. Then there exist constants k^α not all zero such that

$$k^\alpha Z^A_\alpha=0,\quad \alpha=1,\ldots,r. \tag{6.8}$$

From (6.7), (6.8) it follows that

$$k^\alpha M_{\alpha,B}=0. \tag{6.9}$$

This implies $k^\alpha M_\alpha=\psi(t)$. Since $k^\alpha M_\alpha$ must be a constant of motion, it follows that $d\psi/dt=0$ or $\psi=\psi_0=\text{const}$. Hence $k^\alpha M_\alpha=\psi_0$ which contradicts the assumption that the M_α are functionally independent, and therefore the Z^A_α of (6.7) are linearly independent.

Theorem 6.2: A dynamical system (1.2) with $H=H(x,t)$ admits $r\leq 2n$ linearly independent symmetry vectors of the form (6.7) where the $M_\alpha(x,t)$ is a set of r functionally independent constants of motion.

7. GROUPS OF DYNAMICAL SYMMETRIES

In this section we examine group properties of symmetry vectors in phase space.

A. Commutator theorem

We show first that if $Z^A_\alpha(x,t)$, $Z^A_\beta(x,t)$ are any two symmetry vectors [i.e., solutions of (2.13)], then $Z^A_{\alpha\beta}$ defined by[17]

$$Z^A_{\alpha\beta}\equiv \mathcal{L}_\alpha Z^A_\beta=Z^A_{\beta,B}Z^B_\alpha-Z^B_\beta Z^A_{\alpha,B} \tag{7.1}$$

will also be a symmetry vector.

Since $S(Z^A_\alpha)=0$ and $S(Z^A_\beta)=0$, we may write

$$Z^B_\alpha[S(Z^A_\beta)]_{,B}-Z^B_\beta[S(Z^A_\alpha)]_{,B}=0. \tag{7.2}$$

If (7.2) is expanded and then use be made of (2.13) as applied to Z^A_α, Z^A_β we obtain the result

$$S(Z^A_{\alpha\beta})=0. \tag{7.3}$$

Hence $Z^A_{\alpha\beta}$ as defined by (7.1) will be a symmetry vector.

We state this as Theorem 7.1.

Theorem 7.1: Corresponding to any two symmetry vectors $Z^A_\alpha(x,t)$, $Z^A_\beta(x,t)$ [solutions to (2.13)] their commutator $Z^A_{\alpha\beta}$ defined by (7.1) will also be a symmetry vector.

If now (2.13) admits a complete set of s linearly independent solutions $\{Z\}\equiv\{Z^A_1,\ldots,Z^A_s\}$, then every other solution will be linearly dependent on the vectors of this set. If Z^A_α, $Z^A_\beta\subset\{Z\}$, then by Theorem 7.1 $Z^A_{\alpha\beta}$ will be a solution of (2.13) and hence we may write by (7.1)

$$Z^A_{\alpha\beta}\equiv Z^A_{\beta,B}Z^B_\alpha-Z^B_\beta Z^A_{\alpha,B}=C^\gamma_{\alpha\beta}Z^A_\gamma,\quad \alpha,\beta,\gamma=1,\ldots,s, \tag{7.4}$$

where $C^\gamma_{\alpha\beta}$ are constants. Defining a set of operators

$$X_\alpha\equiv Z^A_\alpha\partial_A\,(=\Delta_\alpha/\delta a), \tag{7.5}$$

we obtain from (7.4) and (7.5)

$$(X_\alpha,X_\beta)=C^\gamma_{\alpha\beta}X_\gamma, \tag{7.6}$$

where

$$(X_\alpha,X_\beta)\equiv X_\alpha X_\beta-X_\beta X_\alpha. \tag{7.7}$$

Equation (7.6) implies that $[X_1,\ldots,X_s]$ is a basis for an s-parameter (complete) group C_s of symmetry vectors.

Theorem 7.2: If the dynamical system (1.2) admits a complete set of s linearly independent symmetry vectors $Z^A_1,\ldots,Z^A_s$, then it admits an s-parameter group C_s generated by these vectors.

By Theorem 6.2 we have the following corollary to Theorem 7.2:

Corollary 7.2: The complete group of symmetries (if it exists) is of order $\geq 2n$.

B. Poisson algebras and groups of Poisson symmetry vectors

We consider the question as to when a set of r Poisson symmetry vectors $Z^A_{(P)}$ defined by (6.7), where $M_\alpha(x,t)$ is a set of r functionally independent constants of motion of (1.2) with $H=H(x,t)$, will define an r-parameter group of symmetries in that (7.4) or the equivalent (7.6) holds for the vectors $Z^A_{(P)\alpha}$.

Assume then the $Z^A_{(P)\alpha}$ of (6.7) define an r-parameter group of symmetries. From (7.4) it will follow by use of (6.7) that

$$([M_\beta,M_\alpha]-C^\gamma_{\alpha\beta}M_\gamma)_{,A}=0,\quad \alpha,\beta,\gamma=1,\ldots,r. \tag{7.8}$$

Hence we may write

$$[M_\beta,M_\alpha]-C^\gamma_{\alpha\beta}M_\gamma=G_{\alpha\beta}(t), \tag{7.9}$$

where $G_{\alpha\beta}(t)$ must be a constant of motion. This implies $dG_{\alpha\beta}/dt=0$ or $G_{\alpha\beta}=k_{\alpha\beta}=\text{const}$. Hence from (7.9) we obtain as necessary conditions on the M_α

$$[M_\beta,M_\alpha]-C^\gamma_{\alpha\beta}M_\gamma=k_{\alpha\beta}. \tag{7.10}$$

Conversely, if (7.10) is satisfied for a set of r functionally independent constants of motion M_α, it follows that (7.4) holds for the vectors $Z^A_{(P)\alpha}$ of (6.7).

Theorem 7.3: A necessary and sufficient condition that a set of r Poisson vectors $Z^A_{(P)\alpha}$, $\alpha=1,\ldots,r$, defined by (6.7) determine an r-parameter group of symmetries of the system (1.2) with $H=H(x,t)$ is that (7.10) be satisfied, where the $M_\alpha(x,t)$ is a set of $r\leq 2n$ functionally independent constants of motion and where $C^\gamma_{\alpha\beta}$ are the structure constants of the group and $k_{\alpha\beta}$ are constants.

If $k_{\alpha\beta}=0$ in (7.10), we say the M_α define a Poisson algebra.

We next determine a sufficient condition that the group of Poisson symmetry vectors based upon the constants

of motion M_α as described in Theorem 7.3 determines a Poisson algebra of order r.

Suppose then the constants $k_{\alpha\beta}$ of (7.10) are such that the equations

$$C^\gamma_{\alpha\beta}k_\gamma = k_{\alpha\beta} \tag{7.11}$$

have solutions for $k_\alpha = \text{const}$. Then

$$M'_\alpha \equiv M_\alpha + k_\alpha \tag{7.12}$$

will be constants of motion such that

$$[M'_\beta,\ M'_\alpha] = C^\gamma_{\alpha\beta}M'_\gamma, \quad \alpha,\beta,\gamma = 1,\ldots,r, \tag{7.13}$$

and hence the M'_α define a Poisson algebra of order r.

Theorem 7.4: If the conditions of Theorem 7.3 are satisfied, then a sufficient condition that the system (1.2) admit a Poisson algebra of order $r \leq 2n$ is that

$$\text{rank of matrix } [C^\gamma_{\alpha\beta}] = \text{rank of matrix } [C^\gamma_{\alpha\beta}, k_{\alpha\beta}], \tag{7.14}$$

(where γ = column and $\alpha\beta$ = row). The algebra is then defined by (7.13), where M'_α is given by (7.12), and the k_α are solutions of (7.11).

Remark: If the $k_{\alpha\beta} = 0$, then (7.11) is satisfied by $k_\gamma = 0$ and $M'_\alpha = M_\alpha$.

As an illustration of the above discussion, we consider the case $H = H(x)$ in the canonical coordinate system $(\tilde{x})$ of Sec. 4 [see (4.3)]. From (4.4) we define the $2n$ functionally independent constants of motion $\tilde{M}_\alpha$ by [see (4.4)]

$$\tilde{M}_1 \equiv \tilde{x}^1 - t, \quad \tilde{M}_2 \equiv \tilde{x}^2, \ldots, \tilde{M}_{2n} \equiv \tilde{x}^{2n}. \tag{7.15}$$

We calculate

$$\text{(a) } [\tilde{M}_\alpha, \tilde{M}_\beta] = \eta^{\alpha\beta}; \quad \text{(b) } \tilde{Z}^A_{(P)\alpha} = \eta^{AB}\tilde{M}_{\alpha,B} = \eta^{A\alpha},$$
$$\alpha,\beta = 1,\ldots,2n. \tag{7.16}$$

It is evident from (7.16) that these $\tilde{Z}^A_{(P)\alpha}$ define a $2n$-parameter Abelian group of symmetries ($C^\gamma_{\alpha\beta} = 0$). From (7.16a) the matrix rank condition (7.14) is not met and hence there is no Poisson algebra of order $2n$ of the type described in Theorem 7.4. However Abelian Poisson algebras of order $r \leq n$ may be easily obtained in the following manner: From the set (7.15) choose r of the $\tilde{M}$'s, say, $\tilde{M}_{\alpha_1}, \tilde{M}_{\alpha_2}, \ldots, \tilde{M}_{\alpha_r}$ so that $|\alpha_i - \alpha_j| \neq n$, $i,j = 1,\ldots,r$. It follows from (7.16a) that the Poisson brackets $[\tilde{M}_{\alpha_i}, \tilde{M}_{\alpha_j}] = 0$, and hence such a set of $\tilde{M}_{\alpha_i}$ defines an Abelian Poisson algebra of order $r \leq n$.

This example enables us to state the following theorem.

Theorem 7.5: Every dynamical system (1.2) with $H = H(x)$ always admits Abelian Poisson algebras of order $r \leq n$.

C. Dependency relations

We now assume a dynamical system (1.2) with $H = H(x,t)$ which admits an r-parameter group S_r of symmetries based upon r vectors $Z^A_\alpha(x,t)$ and hence which satisfy (2.13) and (7.4). Corresponding to any constant of motion $M(x,t)$ we have from Theorem 3.1 a "first derived" constant of motion

$$M_\alpha \equiv \Delta_\alpha M/\delta a = M_{,A}Z^A_\alpha, \quad \alpha = 1,\ldots,r. \tag{7.17}$$

From (7.5), (7.6) we have

$$M_{\alpha\beta} - M_{\beta\alpha} = C^\gamma_{\alpha\beta}M_\gamma, \quad \alpha,\beta,\gamma = 1,\ldots,r, \tag{7.18}$$

where $M_{\alpha\beta} \equiv \Delta_\alpha M/\delta a$ is a "second derived" constant of motion, and hence (7.18) exhibits a linear dependency relation between the *first* and *second* derived constants of motion based on the constant of motion $M(x,t)$. This result is recognized as an extension of a similar relation between constants of motion obtained in the time independent theory.[1]

As a second example of linear dependence we continue with the vectors Z^A_α which define the group S_r. We obtain from (7.4)

$$Z^A_{\alpha\beta,A} = C^\gamma_{\alpha\beta}Z^A_{\gamma,A}. \tag{7.19}$$

If we define

$$W_\alpha \equiv Z^A_{\alpha,A}, \quad W_{\alpha\beta} \equiv \Delta_\alpha W_\beta/\delta a = W_{\beta,B}Z^B{}_\alpha, \tag{7.20}$$

then (7.19) can be written in the form

$$W_{\beta,B}Z^B_\alpha - W_{\alpha,B}Z^B_\beta = W_{\alpha\beta} - W_{\beta\alpha} = C^\gamma_{\alpha\beta}W_\gamma. \tag{7.21}$$

Since W_α is a constant of motion [see (5.5)], it follows by Theorem 3.1 that $W_{\alpha\beta}$ is a first derived constant of motion, and hence (7.21) is a dependency relation between the W_α and their *first* derived constants of motion.

D. Symmetry groups determined by extended Poisson vectors

From Theorem 6.1 we know that the extended Poisson vectors $Z^A_{(P)\alpha}$ [based on the constants of motion $M_\alpha(x,t)$, $N_\alpha(x,t)$ for $H(x,t) = F(x) + G(t)$] given by

$$Z^A_{(P)\alpha} \equiv \eta^{AB}M_{\alpha,B} - N_\alpha H^A, \quad \alpha = 1,\ldots,r, \tag{7.22}$$

are symmetry vectors.

We now determine when such a set of $Z^A_{(P)\alpha}$ define an r-parameter group in that (7.4) will be satisfied. A necessary condition is obtained by substitution of (7.22) in (7.4) which gives

$$\eta^{AC}([M_\beta, M_\alpha]_{,C} + N_\alpha M_{\beta,Ct} - N_\beta M_{\alpha,Ct} - C^\gamma_{\alpha\beta}M_{\gamma,C})$$
$$+ H^A([M_\alpha, N_\beta] - [M_\beta, N_\alpha] + N_{\alpha,t}N_\beta - N_{\beta,t}N_\alpha + C^\gamma_{\alpha\beta}N_\gamma) = 0. \tag{7.23}$$

It can be shown that (7.23) is also a sufficient condition. Hence we state

Theorem 7.6: A necessary and sufficient condition that the extended Poisson symmetry vectors (7.22) determine an r-parameter group of symmetries is that (7.23) be satisfied.

To illustrate this theorem we consider two examples.

Example 1: Here we take $M_\alpha = M_\alpha(x) = N_\alpha(x)$ in (7.22) such that $[M_\alpha, M_\beta] = 0$ and choose $C^\gamma_{\alpha\beta} = 0$. An inspection of (7.23) under these assumptions shows it is satisfied.

As a specific example satisfying these conditions we select H to have a Liouville form

$$H(x)=\sum_{i=1}^{n}[\phi_i(p_i)+\psi_i(q^i)], \tag{7.24}$$

where ϕ_i is a function of p_i only and ψ_i is a function of q^i only. It is easily verified that

$$M_i(x)\equiv\phi_i(p_i)+\psi_i(q^i), \quad i=1,\ldots,n, \tag{7.25}$$

are n constants of motion such that $[M_i, M_j]=0$. Hence the $Z^A_{(P)\alpha}$ defined by (7.22), (7.25) define an n-parameter Abelian symmetry group.

Note that the n-dimensional simple harmonic oscillator is obtained by choosing $\phi_i\equiv(1/2)p_i^2$, $\psi_i\equiv(1/2)q^{i^2}$ and the geodesic system is obtained by choosing $\phi_i\equiv(1/2)p_i^2$, $\psi_i\equiv 0$.

Example 2: For this example we take $N_\alpha=M_{\alpha,t}(x,t)$ in (7.22). The corresponding extended Poisson vectors are given by

$$Z^A_{(P)\alpha}(x,t)=\eta^{AB}M_{\alpha,B}-M_{\alpha,t}H^A, \quad \alpha=1,\ldots,r. \tag{7.26}$$

In this case it can be shown that a necessary and sufficient condition that (7.23) be satisfied is that

$$[M_\beta, M_\alpha]_{,C}+M_{\alpha,t}M_{\beta,Ct}-M_{\beta,t}M_{\alpha,Ct}-C^\gamma_{\alpha\beta}M_{\gamma,C}=0,$$
$$\alpha,\beta,\gamma=1,\ldots,r. \tag{7.27}$$

As a specific illustration of this case we consider the n-dimensional harmonic oscillator with $H\equiv(1/2)\sum_{i=1}^{n}(p_i^2+q^{i^2})$. We choose $C^\gamma_{\alpha\beta}=0$, $\alpha,\beta,\gamma=1,\ldots,n$, and

$$M_1\equiv[\arctan(p_1/q^1)-t]^2, \quad M_a\equiv k_aM_1+(p_a^2+q^{a^2})^{1/2},$$
$$a=2,\ldots,n. \tag{7.28}$$

It is found that (7.27) is satisfied for these choices, and hence the $Z^A_{(P)\alpha}$ of (7.26) determine an n-parameter Abelian symmetry group.

E. Groups of symmetry mappings

Consider a set of r extended Poisson vectors $Z^A_{(P)\alpha}$ defined by (7.22) with $M_\alpha(x)=N_\alpha(x)$ such that

$$[M_\beta, M_\alpha]=C^\gamma_{\alpha\beta}M_\gamma, \quad \alpha,\beta,\gamma=1,\ldots,r. \tag{7.29}$$

From (6.1), (6.2) we have

$$\xi^A_{(P)\alpha}=\eta^{AB}M_{\alpha,B}, \ \xi^0_{(P)\alpha}=M_\alpha. \tag{7.30}$$

We define operators

$$U_\alpha\equiv\xi^A_{(P)\alpha}\partial_A, \quad T_\alpha\equiv\xi^0_{(P)\alpha}\partial_t. \tag{7.31}$$

A calculation shows that

$$(U_\alpha, U_\beta)=C^\gamma_{\alpha\beta}U_\gamma, \quad (U_\alpha, T_\beta)=C^\gamma_{\alpha\beta}T_\gamma, \quad (T_\alpha, T_\beta)=0. \tag{7.32}$$

Hence we consider the set of symmetry mappings (1.7), (1.8) determined by (7.30) [see Theorem 6.1],

$$\bar{x}^A=x^A+\xi^A_{(P)}\delta a, \quad \bar{t}=t+\xi^0_{(P)}\delta a, \tag{7.33}$$

where

$$\xi^A_{(P)}\equiv k^\alpha\xi^A_{(P)\alpha}, \quad \xi^0_{(P)}=h^\alpha\xi^0_{(P)\alpha}, \quad h^\alpha,\ k^\alpha \text{ arbitrary consts.}, \tag{7.34}$$

as defining a $2r$-parameter group of symmetry mappings.

We note that Example 1 following Theorem 7.6 illustrates the above concept.

[1] G.H. Katzin, Lett. Nuovo Cimento 7, 213 (1973).
[2] G.H. Katzin and J. Levine, J. Math. Phys. 15, 1460 (1974).
[3] A. Komar, Phys. Rev. D 8, 1028 (1973), has considered a special case of the time dependent theory.
[4] Capital indices will have the range $1, 2, \ldots, 2n$. Ranges on other indices will be as indicated.
[5] A comma (,) indicates partial differentation, and a dot (·) indicates total time derivative d/dt. Unless indicated otherwise Einstein summation notation is used.
[6] The symbols 0_n and I_n indicate nth order zero and identity matrices, respectively.
[7] Under general coordinate transformation $(x^A)\to(y^A)$, $\xi^A(x,t)$ transforms as a contravariant vector and $\xi^0(x,t)$ as a scalar.
[8] See Ref. 3.
[9] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, Mass., 1950).
[10] C.W. Kilmister, *Hamiltonian Dynamics* (American Elsevier, New York, 1965).
[11] Note that $Z^A_{,B}$ and $H^A_{,B}$ do not in general transform as tensors.
[12] Note that since the left side of (4.12) is nontensorial in character, the components $Z^A(x,t)$ in the (x) coordinate system will not in general be constants of motion.
[13] This generalizes a result of Komar (see Ref. 3) to include the case $H=H(x,t)$. Note also the fact that $\xi^A_{,A}-2\phi$ is a time independent constant of motion (which was derived in Ref. 2) follows immediately from

$$Z^A_{,A}=(\xi^A-\xi^0H^A)_{,A}=\xi^A_{,A}-\xi^0_{,A}H^A-\xi^0H^A_{,A}=\xi^A_{,A}-2\phi,$$

where use is made of (2.21) and the fact that $H^A_{,A}\equiv 0$.
[14] Note that if $H=H(x,t)$ and $\xi^A(x,t)\equiv\eta^{AB}G_{,B}(x,t)$, $\xi^0=0$, then $Z^A=\xi^A$ will by a symmetry vector if and only if $\eta^{AB}G_{,A}H_{,B}+G_{,t}=f(t)$ where $f(t)$ is arbitrary. Hence $G(x,t)$ need not be a constant of motion in order that $(\xi^A, 0)$ define a symmetry mapping. In this connection see J.L. Anderson, Am. J. Phys. 40, 541 (1972).
[15] $[R, M]$ is the familiar notation for the Poisson bracket of R and M.
[16] In Ref. 1 it was pointed out that a similar generalization held for the time independent case.
[17] The symbol $\pounds_\alpha$ denotes the Lie derivative with respect to the vector Z^A_α.

Observables, operators, and complex numbers in the Dirac theory

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The geometrical formulation of the Dirac theory with spacetime algebra is shown to be equivalent to the usual matrix formalism. Imaginary numbers in the Dirac theory are shown to be related to the spin tensor. The relation of observables to operators and the wavefunction is analyzed in detail and compared with some purportedly general principles of quantum mechanics. *An exact formulation of Larmor and Thomas precessions in the Dirac theory is given for the first time*. Finally, some basic relations among local observables in the nonrelativistic limit are determined.

1. INTRODUCTION

The Dirac electron theory is widely acknowledged to be the most precise available quantum theory of a single particle. Yet the principles and interpretation of quantum theory continue to be discussed at great length in the literature without taking the Dirac theory into account. Though the mathematical formalism of the Dirac theory unfortunately does not uniquely determine its interpretation, one should expect a reasonable interpretation to provide some understanding of the mathematical structure of the theory. On this score many widely proclaimed general principles of quantum theory prove to be profoundly deficient, if not substantially wrong. For example, if the uncertainty principle is basic to the interpretation of quantum mechanics, why has it never been given a clear formulation in the full Dirac theory? And if Planck's constant provides an absolute limit on the precision of measurements, why does it also determine the magnitude of the spin?

This paper aims to clarify the geometrical and physical interpretation of the Dirac theory and determine some of its implications for the interpretation of quantum theory in general. With a formalism developed in Refs. 1, 2, 3 the Dirac theory can be given a completely geometrical formulation, involving neither matrices nor complex numbers. In the process, the following significant *facts* are established concerning the interpretation of the theory: (1) The four gamma matrices play a completely geometrical role in the Dirac theory. They are matrix representations of four orthonormal vectors (*not* four matrix components of a single vector as often suggested). The algebra of gamma matrices has the same geometrical significance as tensor algebra. The gamma matrices have no function in the Dirac theory which entitles them to be regarded as operators with any special quantum-mechanical significance. (2) The unit imaginary $i' = (-1)^{1/2}$ in the customary formulation of the Dirac has a definite geometrical and physical significance. It is a superfluous adjunct of the mathematical formalism in the sense that it can be replaced by the tensor quantity it actually represents. Specifically, the quantity $\frac{1}{2}i'\hbar$, wherever it appears in equations of the Dirac theory, is a representation of the spin tensor by one of its eigenvalues. When $\frac{1}{2}i'\hbar$ has been replaced in the formalism by the spin bivector it represents, antiparticle conjugation can be identified as a *geometrical* transformation of observables of the theory. (3) The Dirac equation and the wavefunction can be eliminated from the Dirac theory, leaving a set of conservation laws and constitutive relations for observables.

The above facts and further details have already been established in Refs. 2 and 3. However, these papers are open to misunderstanding, because they do not explain in detail exactly how they are related to the conventional matrix formulation of the Dirac theory. This paper aims to supply the missing details and make it easy to translate expressions of the matrix formalism into the geometrical language and vice-versa. The first few sections are devoted to this end, with emphasis on establishing the first two facts cited above.

Section 3 derives the geometrical form of the Dirac equation, which involves no complex numbers.

Sections 4 and 5 analyze the relation of the wave function to observables in detail. In Sec. 5 some common notions about a correspondence between observables and operators are criticized in the light of the Dirac theory. Correspondences of observables with the wavefunction are held to be fundamental. It is suggested that the significance of eigenvalues in quantum theory is to be found more in their association with constant and homogeneous local observables than with operators.

Section 6 introduces the fundamental relative observables and analyzes the physical interpretation of the energy density in considerable detail. For the first time expressions for the Larmor and Thomas precession energies are derived from the Dirac theory without any approximations.

Section 7 proves that in the nonrelativistic limit the Gordon current is equal to the local momentum density but differs from the charge current by the magnetization current associated with the spin density.

2. GEOMETRIC SIGNIFICANCE OF THE DIRAC MATRICES

Recall some of the fundamental properties of the Dirac matrices (as developed, for example in Ref. 4). The *Dirac matrices* are defined as a set of irreducible matrices γ_μ which satisfy the anticommutation rules

$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2g_{\mu\nu}I, \tag{2.1a}$$

where the $g_{\mu\nu}$ ($\mu, \nu = 0, 1, 2, 3$) are components of the spacetime metric tensor and I is the unit matrix. Since it can be proved that the γ_μ must be 4×4 matrices, their

irreducibility can be expressed by the condition that the trace of (2.1a) gives

$$\tfrac{1}{4}\mathrm{Tr}\gamma_\mu\gamma_\nu = g_{\mu\nu}. \tag{2.1b}$$

Conditions (2.1) can be satisfied only by traceless matrices, that is,

$$\tfrac{1}{4}\mathrm{Tr}\gamma_\mu = 0. \tag{2.2}$$

Conditions (2.1) do not determine the Dirac matrices uniquely. However, it can be shown that any two sets of Dirac matrices $\{\gamma_\mu\}$ and $\{\gamma_\mu'\}$ are related by a similarity transformation, that is,

$$\gamma_\mu' = S\gamma_\mu S^{-1}, \tag{2.3}$$

where S is a nonsingular matrix. The γ_μ over the complex numbers generate the complete algebra of 4×4 matrices. But certain elements of the algebra are distinguished by their association (2.1) with the spacetime algebra, and this gives the entire algebra a geometric significance. The 4×4 matrix algebra with the geometric interpretation induced by the conditions (2.1) is called the *Dirac Algebra*.

Clearly, (2.1) indirectly assigns some geometric significance to the Dirac matrices themselves. But in the usual approach the full geometric significance of the γ_μ is not determined until their relation to a Dirac spinor has been specified. Equivalent results can be achieved more efficiently by a change in viewpoint. To see how, it is only necessary to realize that the key relation (2.1a) does not depend in any essential way on the assumption that the γ_μ are matrices. All that is required is that the γ_μ belong to an associative noncommutative algebra.

The appropriate change in viewpoint is achieved simply by interpreting the γ_μ as vectors of a spacetime frame instead of as matrices. By definition the scalar products $\gamma_\mu\cdot\gamma_\nu$ of these vectors are just the components $g_{\mu\nu}$ of the metric tensor. So the two equations (2.1a) and (2.1b) for matrices correspond to the single equation

$$\tfrac{1}{2}(\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu) = \gamma_\mu\cdot\gamma_\nu \equiv g_{\mu\nu} \tag{2.4}$$

for vectors. The vectors γ_μ generate an associative algebra over the reals which has been dubbed the *spacetime algebra* in Ref. 1, because it provides a direct and complete algebraic characterization of the geometric properties of Minkowski spacetime.

By providing a geometrical interpretation of the γ_μ which does not depend on the notion of spinor, geometric algebra releases the γ_μ from their confines in relativistic quantum theory and elevates them to a central position in the mathematical description of all physical systems in spacetime. The advantages of using spacetime algebra in place of the usual tensor methods have been adequately demonstrated in Refs. 1, 5, and 6, to which the reader is referred for details. Of course any equation in the spacetime algebra can be reexpressed as an equation in the Dirac algebra, but besides having a more direct geometric interpretation, the spacetime algebra is mathematically more efficient, as should already be evident from a comparison of (2.1) with (2.4). This becomes clearer as manipulations with the two algebras are compared in more detail.

Since the Dirac matrices in (2.1) can obviously be regarded as matrix representations of the vectors in (2.3), it is convenient to persist in using the same symbols γ_μ for both to facilitate comparison of the algebras and translation of equations from one system to the other. For the same reason, it is convenient to establish a correspondence between the nomenclatures of the two systems. The elements of the spacetime algebra are called *multivectors* and every such element can be expressed as a polynomial of the γ_μ over the *reals*, which has at most 16 linearly independent elements. (see Refs. 1 and 5 for more details). A multivector is said to be *even* (*odd*) if it does (does not) change sign on replacement of γ_μ by $-\gamma_\mu$ in its polynomial representation. The same terminology will be applied here to matrix representations of multivectors. Of course, the Dirac algebra admits polynomials of the γ_μ over the complex numbers, but, in contrast to other elements of the algebra, the unit imaginary of the complex field has no geometric significance except, as will be shown in the next section, in connection with spinors.

It may be worth pointing out that a $(-1)^{1/2}$ is commonly introduced as a "scalar" in the Dirac theory in two distinct ways, first as a root of negative terms in $g_{\mu\nu}$, and second as an essential element of the Dirac equation. Geometric algebra shows that $(-1)^{1/2}$ has a different geometrical significance in each case, and it provides the machinery to keep the distinction clear. Thus, Eq. (2.4) gives $\gamma_\mu^2 = g_{\mu\nu}$ where $\gamma_\mu = (g_{\mu\mu})^{1/2}$ (no sum on μ). More particularly, $\gamma_0^2 = 1$ has the timelike vector $\gamma_0 = (1)^{1/2}$ as a "root of unity", while $\gamma_1^2 = -1$ has the spacelike vector $\gamma_1 = (-1)^{1/2}$ as a "root of minus one." This shows that in the first of the above cases the "scalar $(-1)^{1/2}$" serves to distinguish between spacelike and timelike vectors, and that such a quantity is rendered superfluous by the use of spacetime algebra. It will be shown later that in the second case $(-1)^{1/2}$ represents a spacelike bivector.

In accordance with conventions adopted in Ref. 5, the scalar term in a polynomial representation of a multivector M is denoted by $M_{(0)}$ and called the *scalar* or (0-vector) *part* of M. From (2.2) it is easy to prove that in general

$$M_{(0)} = \tfrac{1}{4}\mathrm{Tr}M, \tag{2.5}$$

which shows that "scalar part" spacetime algebra corresponds to "trace" in the Dirac algebra. In particular, from (2.1b) and (2.4)

$$\gamma_\mu\cdot\gamma_\nu \equiv (\gamma_\mu\gamma_\nu)_{(0)} = \tfrac{1}{4}\mathrm{Tr}(\gamma_\mu\gamma_\nu). \tag{2.6}$$

Moreover, Eq. (2.2) becomes $(\gamma_\mu)_{(0)} = 0$ in spacetime algebra and simply says that a vector is not a scalar. The factor $\frac{1}{4}$ in (2.5) and (2.6) has no geometrical import. Its appearance is another indication that matrix algebra is not ideally suited to the geometrical role it plays in the Dirac theory.

Hermitian conjugation plays an important role in matrix theory, but it has no geometrical significance in the Dirac algebra except in connection with a specific matrix representation. In spacetime algebra a similar role is played by an operation called *reversion*. The

reverse $\tilde{M}$ of a multivector M is obtained from M by reversing the order of γ's in its polynomial representation. The relation of reversion to Hermitian conjugation will be given in the next section.

Equation (2.3) was presented as a change in representation of the Dirac matrices, but the fact is the same equation sppears in spacetime algebra where the notion of representation has no significance. The geometrical requirement of spacetime algebra that the γ_μ' in (2.3) must be vectors entails that they can be written as a linear combination $\gamma_\mu' = a_\mu{}^\nu \gamma_\nu$ of the γ_ν, so (2.3) must be invariant under reversion, from which it follows that S can be chosen so that $S^{-1} = \tilde{S}$. Thus (2.3) takes on the special form

$$\gamma_\mu' = a_\mu{}^\nu \gamma_\nu = S\gamma_\mu \tilde{S}. \tag{2.7}$$

This equation describes a Lorentz transformation of a frame of vectors γ_μ into a frame $\{\gamma_\mu'\}$. Moreover, Eq. (2.7) can be solved for S as a function the γ_μ' and the γ_μ alone, which proves the S is indeed a multivector and that every Lorentz transformation can be expressed in that form. Proper Lorentz transformations (i.e., transformations continuously connected to the identity) will be of special interest in the analysis of the Dirac theory. It can be shown that (2.7) is a proper Lorentz transformation if and only if S is an *even* multivector satisfying

$$S\tilde{S} = 1. \tag{2.8}$$

From this condition it is only an algebraic exercise to show that S can be put in the form

$$S = e^{B/2}, \tag{2.9}$$

where B is a bivector. Without elaborating on the important geometric notion of a bivector, it is sufficient for present purposes to remark that any bivector B can be written in the "polynomial form"

$$B = \tfrac{1}{2} B^{\mu\nu} \gamma_\mu \wedge \gamma_\nu, \tag{2.10a}$$

where the

$$\gamma_\mu \wedge \gamma_\nu = \tfrac{1}{2}[\gamma_\mu, \gamma_\nu] \equiv \tfrac{1}{2}(\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu) \tag{2.10b}$$

provide a complete basis for the space of bivectors, and the

$$B^{\mu\nu} = \gamma^\mu \cdot B \cdot \gamma^\nu = B(\gamma^\mu \wedge \gamma^\nu) = (B\gamma^\mu \gamma^\nu)_{(0)} = -B^{\nu\mu} \tag{2.10c}$$

are alternative expressions for the six independent scalar coefficients. For more details and proofs of the assertions in this paragraph see Ref. 1, Chap. IV and Appendix B.

3. THE DIRAC EQUATION WITHOUT COMPLEX NUMBERS

At first sight the Dirac algebra appears to be more general than spacetime algebra, because its "scalar field" consists of complex numbers rather than real numbers only. But, it will be shown that the imaginary unit i' of the Dirac algebra is superfluous in the physical theory, and its use serves only to obscure the geometrical and physical interpretation. This section shows that i' can be replaced by a spacelike bivector and finds the appropriate formulations of the wavefunction and Dirac equation in terms of the spacetime algebra. The next section shows that i' is superfluous in the expression for observables of the Dirac theory.

A Dirac spinor Ψ is a column matrix with four complex components, that is,

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \alpha_1 + i'\beta_1 \\ \alpha_2 + i'\beta_2 \\ \alpha_3 + i'\beta_3 \\ \alpha_4 + i'\beta_4 \end{pmatrix}, \tag{3.1}$$

where the α's and β's are real numbers and i' is the $(-1)^{1/2}$ of the matrix algebra. The representation (3.1) in terms of components $\psi_1, \psi_2, \psi_3, \psi_4$ presumes a specific representation of the Dirac matrices. It is convenient to work with the socalled *standard representation*:

$$\gamma_0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \gamma_k = \begin{pmatrix} 0 & -\sigma_k \\ \sigma_k & 0 \end{pmatrix}. \tag{3.2a}$$

Here I is the 2×2 unit matrix and where the σ_k are the usual 2×2 Pauli matrices, that is, are traceless Hermitian matrices satisfying

$$\sigma_1 \sigma_2 \sigma_3 = i'I. \tag{3.2b}$$

By virtue of the fact that the γ_μ are related to the spacetime metric by (2.1), Ψ and its components have a definite geometrical significance, a significance to be ascertained below by finding an expression for Ψ in terms of spacetime algebra which is independent of the matrix representation.

As explained in Refs. 1 and 5, in the spacetime algebra the quantities $\boldsymbol{\sigma}_k$ defined by $\boldsymbol{\sigma}_k = \gamma_k \gamma_0$ $(k = 1, 2, 3)$ are to be interpreted as vectors relative to the inertial system specified by the timelike vector γ_0. The $\boldsymbol{\sigma}_k$ generate an algebra over the reals which is isomorphic to the Pauli algebra. To emphasize this fact it is convenient to write

$$\boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \boldsymbol{\sigma}_3 = i \tag{3.3}$$

in analogy to (3.2b). On the other hand, $\boldsymbol{\sigma}_k = \gamma_k \gamma_0$ implies $\boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \boldsymbol{\sigma}_3 = \gamma_0 \gamma_1 \gamma_2 \gamma_3$. This fact can be expressed only in a 4×4 matrix representation of the $\boldsymbol{\sigma}_k$. The 4×4 matrix representations of the $\boldsymbol{\sigma}_k$ are commonly denoted by α_k in the literature (e.g., p. 69 of Ref. 4), but to help keep geometric significance to the fore the symbols $\boldsymbol{\sigma}_k$ are used here. From the standard representation (3.2),

$$\boldsymbol{\sigma}_k = \gamma_k \gamma_0 = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \tag{3.4a}$$

$$i = \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \boldsymbol{\sigma}_3 = \gamma_0 \gamma_1 \gamma_2 \gamma_3 = \gamma_5 = \begin{pmatrix} 0 & i'I \\ i'I & 0 \end{pmatrix}, \tag{3.4b}$$

which imply

$$i\boldsymbol{\sigma}_k = \begin{pmatrix} i'\sigma_k & 0 \\ 0 & i'\sigma_k \end{pmatrix}. \tag{3.5}$$

Now introduce a basis in spinor space

$$u_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad u_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad u_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad u_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

such that

$$\gamma_0 u_1 = u_1, \tag{3.6a}$$

$$i\sigma_3 u_1 = \gamma_2\gamma_1 u_1 = i' u_1, \tag{3.6b}$$

and

$$u_2 = -i\sigma_2 u_1, \quad u_3 = \sigma_3 u_1, \quad u_4 = \sigma_1 u_1. \tag{3.6c}$$

Supposing (3.1) refers to this representation, by using (3.6c) to eliminate u_2, u_3, u_4, and (3.6b) to eliminate the imaginary unit i', Ψ can be written

$$\begin{aligned}\Psi &= \psi_1 u_1 + \psi_2 u_2 + \psi_3 u_3 + \psi_4 u_4 \\ &= (\psi_1 - i\sigma_2\psi_2 + \sigma_3\psi_3 + \sigma_1\psi_4)u_1 \\ &= \{\alpha_1 + (\alpha_4\sigma_1 + \beta_4\sigma_2 + \alpha_3\sigma_3) + i(\beta_2\sigma_1 - \alpha_2\sigma_2 + \beta_1\sigma_3) + i\beta_3\}u_1.\end{aligned}$$

Thus any Dirac spinor Ψ can be written in for form

$$\Psi = \psi u_1, \tag{3.7}$$

where ψ can be written down directly from the column matrix form (3.1) by using

$$\begin{aligned}\psi &= \alpha_1 + (\alpha_4\sigma_1 + \beta_4\sigma_2 + \alpha_3\sigma_3) + i(\beta_2\sigma_1 - \alpha_2\sigma_2 + \beta_1\sigma_3) + i\beta_3 \\ &= \alpha_1 + \alpha_4\gamma_1\gamma_0 + \beta_4\gamma_2\gamma_0 + \alpha_3\gamma_3\gamma_0 \\ &\quad + \beta_2\gamma_3\gamma_2 + \alpha_2\gamma_3\gamma_1 + \beta_1\gamma_2\gamma_1 + \gamma_5\beta_3.\end{aligned} \tag{3.8}$$

The significance of (3.7) and (3.8) is that the unit imaginary i' has been eliminated to express Ψ uniquely as a function of an *even* multivector ψ. But ψ can be expressed as an element of the spacetime algebra at once simply by interpreting the γ's as vectors instead of matrices. As will be seen, this helps to make the geometrical significance of spinors explicit.

Dirac's equation for an electron with charge e and mass m in an external electromagnetic field can be written

$$\gamma_\mu\left(i'\hbar\partial_\mu - \frac{e}{c}A_\mu\right)\Psi = mc\Psi$$

where $\gamma_\mu = (\gamma_\mu)^{-1} = g^{\mu\nu}\gamma_\nu$. With

$$\Box = \gamma^\mu\partial_\mu, \quad \partial_\mu = \frac{\partial}{\partial x^\mu} \tag{3.9}$$

and

$$A = A_\mu\gamma^\mu = A^\mu\gamma_\mu, \tag{3.10}$$

the Dirac equation assumes the form

$$\left(i'\hbar\Box - \frac{e}{c}A\right)\Psi = mc\Psi. \tag{3.11}$$

It is crucial to note that the unit imaginary i' in the Dirac equation cannot be absorbed into the definition of the γ_μ while both ∂_μ and A_μ are kept real. Since the Dirac equation describes a physical property of the electron, the nontrivial explicit appearance of i' in the equation implies that i' has a physical significance. That significance remains to be determined.

The i' in the Dirac equation can be replaced by a multivector by using (3.7) along with (3.6b) to put (3.11) in the form

$$\left(\hbar\Box\psi\gamma_2\gamma_1 - \frac{e}{c}A\psi\right)\gamma_0 u_1 = mc\psi u_1. \tag{3.12}$$

The γ_0 was inserted in the right side of (3.12) by using (3.6a) to make the coefficients of u_1 even multivectors. Although u_1 does not have an inverse, the coefficients of u_1 in (3.12) can be equated, because, as (3.6c) shows, even multivectors operating on u_1 generate a complete basis for Dirac spinors. Therefore, (3.12) yields

$$\left(\hbar\Box\psi\gamma_2\gamma_1 - \frac{e}{c}A\psi\right)\gamma_0 = mc\psi,$$

or equivalently,

$$\hbar\Box\psi\gamma_2\gamma_1 - \frac{e}{c}A\psi = mc\psi\gamma_0. \tag{3.13}$$

Conversely, by multiplying (3.13) on the right by u_1 and using (3.6) and (3.7) the Dirac equation is recovered. So (3.13) is fully equivalent to the Dirac equation (3.11), and, by using (3.7), a solution of the one equation can be easily expressed as a solution of the other.

By interpreting the γ's as vectors instead of matrices, Eq. (3.13) becomes an equation in spacetime algebra which may fairly be called the *Dirac equation* in that language because of its equivalence to the usual matrix equation. Likewise, it is appropriate to refer to ψ as a *spinor* in the spacetime algebra. In the spacetime algebra, (3.10) simply expresses the potential A as a linear combination of basis vectors, and the socalled "Dirac operator" $\Box$ introduced by (3.9) can be directly interpreted as the derivative with respect to a spacetime point $x = x^\mu\gamma_\mu$.

The most significant feature of (3.13) is that the i' which appears in (3.11) has been replaced by the bivector $\gamma_2\gamma_1$, because bivectors have a straightforward geometrical interpretation in spacetime algebra. So translation of the Dirac theory into the language of spacetime algebra promises to reveal a hidden significance of imaginary numbers in the Dirac theory. This promise will be completely fulfilled in the next section.

The derivation of (3.13) made use of a specific matrix representation of the γ_μ. The consequence of using any other representation can be ascertained by considering an arbitrary change of basis in Dirac "spin space" which takes u_1 to

$$u_1' = S' u_1. \tag{3.14}$$

Now the transformation matrix S' in (3.14) can be taken to be an even multivector; for if S' has an odd part, because of (3.6a) that part can be made even without affecting (3.14) by multiplying it on the right by γ_0; similarily, any "complex coefficient" in a polynomial representation of S' can be replaced by an even multivector by using (3.6b). By an argument to be given later in connection with a more important issue, the fact that S' is even implies that it can be put in the form

$$S' = \exp(i\delta)S, \tag{3.15a}$$

where S satisfies (2.8), δ is a scalar, and it will be recalled, i satisfies (3.4b). The inverse of S' is

$$S'^{-1} = \exp(-i\delta)\tilde{S}. \tag{3.15b}$$

Hence (3.14) gives

$$u_1 = \exp(-i\delta)\tilde{S}u_1'. \tag{3.16}$$

Equations (3.6a, b) can be transformed into the new

representation by multiplying them by S' and using (3.15) and (3.16) together with the fact that $i=\gamma_5$ anticommutes with the γ_μ; one gets

$$\exp(2i\delta)\gamma_0'u_1'=u_1', \tag{3.17a}$$

$$\gamma_2'\gamma_1'u_1'=i'u_1', \tag{3.17b}$$

where the γ_μ' are related to the γ_μ by (2.7). With (3.16), (3.7) can be put in the form

$$\Psi=\psi'\exp(-i\delta)u_1' \tag{3.18a}$$

where

$$\psi'=\psi\tilde{S}. \tag{3.18b}$$

Substituting (3.18a) into the Dirac equation (3.11), and using (3.17a, b) to get an equation for ψ' in the same way that (3.6a, b) were used to get an equation for ψ, one notices that the factor $\exp(-i\delta)$ can be eliminated yielding the equation

$$\hbar\Box\psi'\gamma_2'\gamma_1'-\frac{e}{c}A\psi'=mc\psi'\gamma_0'. \tag{3.19}$$

This has the same form as (3.13). Indeed (3.19) can be obtained directly from (3.13) by multiplying it on the right by the constant factor $\tilde{S}$. For note that, by (2.8) and (2.7),

$$\psi\gamma_2\gamma_1\tilde{R}=\psi R\tilde{R}\gamma_2R\tilde{R}\gamma_1\tilde{R}=\psi'\gamma_2'\gamma_1',$$

which shows how the terms on the left of (3.13) and (3.19) are related.

Thus it has been proved that the form of (3.13) is uniquely determined, independently of the choice of a representation for the Dirac matrices. The specification of vectors γ_2, γ_1, and γ_0 in (3.13) is determined only to within a proper Lorentz transformation; this arbitrariness corresponds to the freedom to choose a matrix representation for the Dirac theory. The form of the usual Dirac equation (3.11) is representation independent. However, no solution to that equation can be exhibited without choosing a specific representation. The significance of such a choice is hidden in the matrix formulation of the Dirac theory. It has been uncovered above. A choice of representation amounts to a specific correspondence between 4×4 matrices and vectors. Though the choice is to some extent arbitrary, a definite choice must nevertheless be made. The explicit appearance of γ's in (3.13) and (3.19) is a consequence of such a choice. It has already been pointed out that this implies that i' must be interpreted geometrically as a spacelike bivector. A more complete interpretation will be provided in the next section.

It should be noted that in conventional treatments of the Dirac theory,[4] it is proved that the Dirac equation retains its form under Lorentz transformations. That proof is easily translated into the present language, but it would be superfluous, for having eliminated matrices and interpreted the γ_μ as vectors, we have put the Dirac equation in the form (3.13) which is manifestly independent of coordinates. It cannot be overemphasized that the vectors $\gamma_0, \gamma_1, \gamma_2$ appearing in (3.13) need not be associated with any coordinate frame; they are simply a set of arbitrarily chosen orthonormal vectors. Adoption of a coordinate frame with γ_0 as the time component is equivalent in the conventional theory to adopting a matrix representation for which γ_0 is Hermitian and the γ_k are anti-Hermitian. Adoption of the standard representation (3.2) associates by (3.6b) the i' of the matrix representation with the bivectors $\gamma_2\gamma_1$ in (3.13). Thus, the standard representation is distinguished by relating Hermitian conjugation and complex numbers of the matrix algebra to intrinsic features of the Dirac equation.

There is an alternative formulation of the Dirac equation in terms of spacetime algebra which should be mentioned. Define the quantity Φ by the equation

$$\Phi=\psi U \tag{3.20a}$$

where

$$U=\tfrac{1}{2}(1+\gamma_0)(1+\sigma_3). \tag{3.20b}$$

Multiplying (3.13) on the right by U and noting that $\gamma_2\gamma_1U=Ui\sigma_3=Ui$ and $\gamma_0U=U$, one gets

$$\hbar\Box\Phi i-\frac{e}{c}A\Phi=mc\Phi. \tag{3.21}$$

Except for the choice of units and a difference in sign which is merely a matter of convention, (3.21) is identical to Eq. (13.2) of Ref. 1. It is the first formulation of the Dirac equation in terms of spacetime algebra.

Comparison of (3.21) with the matrix Dirac equation (3.11) suggests that the pseudoscalar $i=\gamma_5$ in (3.22) is the geometrical quantity which corresponds to the imaginary i' in (3.11). But this is misleading, because certain essential geometrical features of the Dirac theory are hidden in the structure of U as defined by (3.20), much as they are hidden in the properties of the base spinor u_1 in (3.7). These features were first uncovered in Ref. 2, where it was concluded that (3.13) is a much more significant equation than (3.21). To nail down the interpretation of i' in the Dirac theory, it is necessary to examine the definitions of observables. This is undertaken in the next section.

4. OBSERVABLES AND THE WAVEFUNCTION

The geometrical significance of the wavefunction Ψ in Dirac's theory is determined by requiring that certain bilinear functions of Ψ be tensors. Interpretation of these tensors as observables determines the physical significance of Ψ.

This section explains how the socalled "bilinear covariants" of the Dirac theory can be expressed in terms of spacetime algebra. This makes it possible to provide a direct interpretation of the Dirac wavefunction, showing that the interpretation of the γ_μ as vectors is in complete accord with the Dirac theory and so justified by its simplicity. Moreover, the geometrical and physical interpretation of the unit imaginary i' in the Dirac theory is ascertained by proving that $\frac{1}{2}i'\hbar$ is a representation of the spin bivector by one of its eigenvalues.

Equation (3.8) explicitly shows that ψ is a sum of scalar, bivector, and pseudoscalar parts. Of course, every even multivector has this property. Note that $\tilde{i}=i$, that is, the unit pesudoscalar $i=\gamma_5=\gamma_0\gamma_1\gamma_2\gamma_3$ is invariant under reversion. However, every bivector

changes sign under reversion as is shown by $\gamma_\mu\gamma_\nu = -\gamma_\nu\gamma_\mu$ for $\mu \neq \nu$. Hence $\tilde{\psi}$ can be obtained from ψ simply by changing the sign of its bivector part. Since ψ is an even multivector, so, is $\psi\tilde{\psi}$. But $\psi\tilde{\psi}$ is clearly invariant under reversion, so its bivector part must vanish. Moreover, since $i^2 = -1$, $\psi\tilde{\psi}$ can be put in the "polar form"

$$\psi\tilde{\psi} = \rho \exp(i\beta) = \rho\cos\beta + i\rho\sin\beta, \tag{4.1}$$

where ρ and β are scalars. One can then define R by the equation $R = [\rho \exp(i\beta)]^{-1/2}\psi$, or just write

$$\psi = \rho^{1/2} \exp(\tfrac{1}{2}i\beta)R. \tag{4.2a}$$

Because of (3.9),

$$R\tilde{R} = 1. \tag{4.2b}$$

The expression (4.2a) is the "canonical form" for a spinor in the spacetime algebra, first found in Ref. 2. The quantities ρ, β, and R have distinctive geometrical and physical interpretations which are independent of any matrix representation. So it is best to use them instead of the α's and β's in (3.8).

It is simplest to set forth the interpretation of ψ categorically and after that explain how it is related to the usual formulation of the Dirac theory. The quantity R in (4.2) determines a proper Lorentz transformation of a frame $\{\gamma_\mu\}$ into a frame $\{e_\mu\}$ according to the equation

$$e_\mu = R\gamma_\mu\tilde{R}. \tag{4.3}$$

This equation has exactly the form of the Lorentz transformation (2.7), since comparison of (4.2b) with (2.8) shows that R has the same algebraic structure as S. However, $R = R(x)$ is a (generally differentiable) function of the spacetime point x, while S is constant. Thus, (4.3) specifies a (generally differentiable) set of four vector fields with values $e_\mu = e_\mu(x)$ at each point x determined by a proper Lorentz transformation of a fixed frame $\{\gamma_\mu\}$. This completely describes the *geometrical* significance of R. By virtue of (4.3), the spinor R may be regarded as a representation of a Lorentz transformation.

Since the pseudoscalar i anticommutes with the vector γ_μ, (4.2a) and (4.3) imply

$$\psi\gamma_\mu\tilde{\psi} = \rho e_\mu. \tag{4.4}$$

If (3.12) is regarded as a generalization of the transformation (4.3), then multiplication of the e_μ by ρ must be interpreted as a dilatation.

The geometrical interpretation of a Dirac spinor given here is more direct and detailed than the conventional one. Ordinarily, Dirac spinors are said to be representations of the Lorentz group because they *transform* in a certain way under Lorentz transformation (see Ref. 4). In contrast, we say that ψ represents a Lorentz transformation because, by Eq. (4.4), it *determines* a "rotation-dilatation" of the frame $\{\gamma_\mu\}$ into the frame $\{\rho e_\mu\}$. Actually, $\psi = \psi(x)$ determines a continuous infinity of Lorentz transformations, one at each spacetime point x. Perhaps it is worth adding for emphasis that ψ does not operate in some "abstract spin space" detached from spacetime, it transforms spacetime vectors into spacetime vectors.

The physical interpretations of ρ and R are fixed by specifying interpretations for the e_μ. The quantity

$$\rho v = \psi\gamma_0\tilde{\psi} \tag{4.5a}$$

is to be identified as the *probability current* of the Dirac theory. It follows that the timelike vector

$$v \equiv e_0 = R\gamma_0\tilde{R} \tag{4.5b}$$

can be interpreted the (local) "world velocity" of a Dirac particle, while ρ is the probability density in the local rest frame determined by v. The tensor components of the probability current relative to the frame $\{\gamma_\mu\}$ are

$$\rho v^\mu = \rho v \cdot \gamma^\mu = (\psi\gamma_0\tilde{\psi}\gamma^\mu)_{(0)}, \tag{4.5c}$$

and the local conservation of probability is expressed by

$$\Box \cdot (\rho v) = \partial_\mu(\rho v^\mu) = 0. \tag{4.6}$$

The spacelike vector

$$s = \frac{\hbar}{2}e_3 = \frac{\hbar}{2}R\gamma_3\tilde{R} \tag{4.7a}$$

can be identified as the (local) *spin vector* of the Dirac theory. The corresponding "current"

$$\frac{\hbar}{2}\psi\gamma_3\tilde{\psi} = \rho s \tag{4.7b}$$

has components

$$\rho s_\mu = \rho s \cdot \gamma_\mu = \frac{\hbar}{2}(\psi\gamma_3\tilde{\psi}\gamma_\mu)_{(0)}. \tag{4.7c}$$

Of course, s cannot be interpreted directly as the electron spin because angular momentum is a bivector. The "proper spin density" of the electron is ρS, where S is the (local) *spin bivector* given by

$$S = \frac{\hbar}{2}e_2e_1 = \frac{\hbar}{2}R\gamma_2\gamma_1\tilde{R} = \frac{\hbar}{2}Ri\sigma_3\tilde{R} = isv. \tag{4.8a}$$

These assorted equivalent expressions are easily related by using $R\tilde{R} = 1$ and the appropriate definitions. The tensor components of S are

$$S^{\alpha\beta} = (S\gamma^\beta\gamma^\alpha)_{(0)} = is\wedge v\wedge\gamma^\beta\wedge\gamma^\alpha = s_\mu v_\nu\epsilon^{\mu\nu\alpha\beta}, \tag{4.8b}$$

which we get by applying (2.12) to (4.8a) and introducing the "alternating tensor" defined by

$$\epsilon^{\mu\nu\alpha\beta} = -i\gamma^\mu\wedge\gamma^\nu\wedge\gamma^\alpha\wedge\gamma^\beta = -(\gamma_5\gamma^\mu\gamma^\nu\gamma^\alpha\gamma^\beta)_{(0)}. \tag{4.9}$$

The right side of (4.8a) or (4.8b) shows that S is the dual of the bivector $sv = s\wedge v$. Thus, given v, s, and S are equivalent descriptions of the spin in the sense that either one determines the other by (4.8).

In (4.5), (4.7), (4.8) the e_μ defined by (4.3) have been given a physical interpretation by relating them to the electron spin and velocity. It is important to realize that the index μ in (4.3) is a "free index," that is, it need not be related to any coordinate system. However, the physical interpretation requires that the γ_μ indexed in (4.3) be identical to the set $\gamma_0, \gamma_1, \gamma_2, \gamma_3 = i\gamma_0\gamma_1\gamma_2$ specified in the Dirac equation (3.13). It will be noted that the "change of representation" transforming (3.13) to (3.10) does not alter the e_μ since $\psi\gamma_\mu\tilde{\psi} = \psi'\gamma_\mu'\tilde{\psi}'$.

Something can now be said about the physical interpretation of the Dirac wavefunction in its canonical form (4.2a). The quantity ρ has been identified as the proper probability density. The unimodular spinor R determining the Lorentz transformation (4.3) can be specified by six scalar parameters. Five of those parameters determine the velocity and spin directions of the electron, which, of course, also determines the "spin plane" containing the vectors e_1 and e_2 orthogonal to v and s. The remaining parameter is the *phase* of the wavefunction. Geometrically, the phase determines the directions of e_1 and e_2 in the spin plane. Physically, the phase is related indirectly to the electron energy-momentum by derivatives of the wavefunction; this will be considered in the next section. To sum up, except for the phase and the parameter β in (4.2a), the Dirac wavefunction determines (or is determined by) the electron probability current and the spin direction.

To get an interpretation of β, additional physical assumptions are needed The bivector

$$M = \frac{e\hbar}{2mc}\psi\gamma_2\gamma_1\tilde{\psi} = \frac{e}{mc}\exp(i\beta)\rho S \tag{4.10}$$

is usually interpreted as the magnetization or magnetic moment density of the electron. The right side of (4.10) was obtained by using (4.2a) with (4.8a) and shows that the ratio of magnetic moment to spin density differs from the usual gyromagnetic ratio e/mc attributed to the electron by the factor $\exp(i\beta)$. Equation (4.10) shows that β can be interpreted geometrically as the angle of a "duality rotation" of S into M. It also lends a physical significance to β, but, as explained in Ref. 3, other features of the Dirac theory make a fully satisfactory physical interpretation difficult to come by.

Proof that the expressions (4.5), (4.7), and (4.10) are equivalent to conventional expressions for probability current, spin and magnetic moment in the Dirac theory is simply a matter of computation using the unique correspondence between ψ and the column spinor Ψ established in Sec. 3. The computations have been discussed in Appendix A of Ref. 3, so it suffices to display the results in Table I in the form of expressions for the so-called bilinear covariants using both mathematical systems. Table I uses the notation $\bar{\Psi} = \Psi^\dagger\gamma_0$ where $\Psi^\dagger$ denotes Hermitian adjoint, in addition to conventions already explained, especially in connection with (2.5) and (2.10).

The term "observable" is used here to refer to tensor quantities such as ρv_μ, $M_{\mu\nu}$, and s_μ which (in principle, at least) are amenable to experimental observation. The relations of wavefunction to observables given by (4.1), (4.5), (4.7), (4.10) are much simpler and easier to use than those in Table I. So the table is useful only for comparison with the conventional formulation.

Table I helps reveal the role of the unit imaginary i' in the matrix formulation of the Dirac theory. Observables are always reducible to real numbers. Some of the bilinear covariants in Table I are formed from anti-Hermitian products of the γ_μ, so a factor i' is needed to make the quantities real. This apparently trivial mathematical fact has a physical significance. To discover that significance, it should be noted first that i' never enters any expression for observables of the Dirac theory (such as those in Table I) except as a multiple of the wavefunction Ψ, and second, that i' enters only in the combination $i'\hbar$ with Planck's constant. Also, note that

$$S\psi = \tfrac{1}{2}\hbar\psi\gamma_2\gamma_1 \tag{4.11}$$

is easily proved from (4.2) and (4.8). Interpreting (4.11) as a matrix equation and using (3.7) and (3.6b), one shows immediately that

$$S\psi = \tfrac{1}{2}i'\hbar\Psi, \tag{4.12}$$

that is, $\frac{1}{2}i'\hbar$ is an eigenvalue of the bivector S describing the spin. Equation (4.12) can be used to eliminate the explicit appearance of $i'\hbar$ in equations of the Dirac theory. For example, if Γ is some matrix operator, since $S = \frac{1}{2}S^{\mu\nu}\gamma_\mu\gamma_\nu$, (4.12) yields

$$i'\hbar\bar{\Psi}\Gamma\Psi = \bar{\Psi}\Gamma\gamma_\mu\gamma_\nu\Psi S^{\mu\nu}, \tag{4.13}$$

showing the factor $i'\hbar$ to be equivalent to a contraction of the spin tensor $S^{\mu\nu}$ with some other tensor. As Table I illustrates, the factor $i'\hbar$ appears explicitly only in those expressions for observables involving the electron spin. Equation (4.12) shows us that the factor $\frac{1}{2}i'\hbar$ in the Dirac theory is in fact a representation of the electron spin by an eigenvalue of the spin tensor. The eigenvalue is imaginary, because the spin tensor $S^{\mu\nu}$ is skew-symmetric. The i' is a representation of the direction of the spin tensor, because the conventions of Dirac theory correspond, in a devious way, to the generator of rotations in the physical "spin plane" with the generator of rotations in the abstract complex plane. Of course, the factor $\frac{1}{2}\hbar$ is just the magnitude of the spin tensor.

The spin tensor $S^{\alpha\beta}$, which is crucial to the understanding of $i'\hbar$, is not mentioned in standard accounts of the Dirac theory, so some explanation is in order. Standard accounts (e.g., p. 59 of Ref. 7) either implicitly or explicitly introduce the spin (density) tensor

$$\begin{aligned}\rho S^{\nu\alpha\beta} &= \frac{i'\hbar}{2}\bar{\Psi}\gamma^\nu\wedge\gamma^\alpha\wedge\gamma^\beta\Psi \\ &= \frac{i'\hbar}{2}\bar{\Psi}\gamma_5\gamma_\mu\Psi\epsilon^{\mu\nu\alpha\beta} \quad \rho s_\mu\epsilon^{\mu\nu\alpha\beta}\end{aligned} \tag{4.14}$$

where use has been made of the identity

$$\gamma^\nu\wedge\gamma^\alpha\wedge\gamma^\beta = \gamma_5\gamma_\mu\epsilon^{\mu\nu\alpha\beta} \tag{4.15}$$

and the expression for s_μ in Table I. Contraction of (4.14) with v_ν and comparison with (4.8b) gives the desired relation

$$\rho S^{\alpha\beta} = \rho v_\nu S^{\nu\alpha\beta} = \rho s_\mu v_\nu\epsilon^{\mu\nu\alpha\beta}. \tag{4.16}$$

TABLE I. Bilinear covariants as observables.

$$\bar{\Psi}\Psi = (\psi\tilde{\psi})_{(0)} = \rho\cos\beta$$

$$\bar{\Psi}\gamma_\mu\bar{\Psi} = (\gamma_\mu\psi\gamma_0\tilde{\psi})_{(0)} = \gamma_\mu\cdot(\rho v) = \rho v_\mu$$

$$\frac{e}{mc}\frac{i'\hbar}{2}\bar{\psi}\tfrac{1}{2}\gamma_\mu\quad\gamma_\nu\Psi = \frac{e\hbar}{2mc}(\gamma_\mu\gamma_\nu\psi\gamma_2\gamma_1\tilde{\psi})_{(0)} = (\gamma_\mu\wedge\gamma_\nu)\cdot M = M_{\mu\nu}$$

$$\frac{i'\hbar}{2}\bar{\Psi}\gamma_\mu\gamma_5\psi = \frac{\hbar}{2}(\gamma_\mu\psi\gamma_3\tilde{\psi})_{(0)} = \gamma_\mu\cdot(\rho s) = \rho s_\mu$$

$$\bar{\Psi}\gamma_5\Psi = (i\psi\tilde{\psi})_{(0)} = -\rho\sin\beta$$

The $\rho S^{\alpha\beta}$ must be interpreted as the components of the electron spin angular momentum density in the local rest frame determined by the particle velocity v.

Having ascertained that the imaginary unit i' functions in the Dirac theory as a representation of the electron spin direction, it is evident that charge conjugation must have a geometrical interpretation as well as the usual physical one. Indeed, it has already been discovered in Sec. 5 of Ref. 8 that charge conjugation entails a rotation of the "observables" e_1, e_2, e_3 defined by (4.3) about an axis in the spin plane. Reference 9 pointed out that this transformation in "the space of observables" of the Dirac theory is isomorphic to the operation of charge conjugation in isospace, so by regarding them as one and the same, one gets a space-time interpretation of isospace relating spin to isospin and indicating a connection between the pseudoscalar and isospin properties of the pion. This speculative idea has not thus far been pushed by the author. Still, in view of the uncertainties of strong interaction theory, it seems sufficiently promising to merit mention once again.

5. OBSERVABLES AND OPERATORS

A number of statements about observables, operators, and eigenvalues are frequently put forward in one form or another as general principles of quantum theory. The difficulties these principles face when applied to the Dirac theory shows that they are not so general after all. Surely, since the Dirac theory is the most firmly established version of quantum theory, only those principles which are required by or are at least consistent with the Dirac theory can be regarded as both fundamental and general.

Consider, for example, the EHOO-principle that "the *E*igenvalues of *H*ermitian *O*perators correspond to *O*bserved values". In the relation $\rho v_k = \bar{\Psi}\gamma_k\Psi = \Psi^\dagger\gamma_0\gamma_k\Psi$ $(k=1,2,3)$ from Table I, the matrices $\gamma_0\gamma_k$ are Hermitian. Since $(\gamma_0\gamma_3)^2 = 1$, the eigenvalues of $\gamma_0\gamma_3$ are ± 1. So if Ψ is an eigenstate of $\gamma_0\gamma_3$, we have $\gamma_0\gamma_3\Psi = \pm\Psi$ or $\gamma_3\Psi = \pm\gamma_0\Psi$; whence, $\rho v_3 = \Psi\gamma_3\Psi = \pm\Psi\gamma_0\Psi = \pm\rho v_0$. But this says that the velocity of the electron equals the speed of light, which is inconsistent with the Dirac equation, not to mention experimental evidence. Notwithstanding the absurdity of the result, application of the EHOO-principle to the socalled "velocity operators" $\gamma_0\gamma_k$ has been perpetuated in accounts of the Dirac theory for forty years, along with fruitless attempts to explain away the problem. This and many other similar difficulties are easily resolved by admitting that EHOO is not a general principle of quantum mechanics and, in particular, does not apply to operators composed of the γ_μ. The role of the γ_μ in the Dirac theory is clear in the multivector formulation; the γ_μ are simply an othonormal set of vectors. In the expression $\gamma_\mu\cdot(\rho v) = \rho v_\mu$ appearing in Table I the interpretation of the γ_μ as operators is trivial and has nothing to do with quantum mechanics; the γ_μ simply pick out the μth component of the vector v by inner multiplication. Nor is the noncommutive multiplication rule for the γ_μ justified by any principle concerning the impossibility of simultaneous eigenvalues in the Dirac theory; it has straightforward geometrical significance already discussed in Sec. 2 and in Refs. 1 and 5. It should be evident that the γ_μ have the same geometrical role in all the relations of Table I.

To the extent that propositions about Hermitian operators and eigenvalues are significant in the Dirac theory, they are special properties of the "kinetic energy–momentum operators," customarily written

$$\hat{p}_\mu = i'\hbar\,\partial_\mu - \frac{e}{c}A_\mu \tag{5.1}$$

in the matrix formulation. It is often said that $\hat{p}_k$ $(k=1,2,3)$ corresponds to the kinetic momentum observable, but this is inaccurate and leaves room for misinterpretation. Rather, the operator $\hat{p}_k$ *determines a relation* between the wavefunction and the kinetic momentum observable. Those relations of the wavefunction to basic observables which are determined by $\hat{p}_\mu$ are given in Table II. The table gives both the multivector and matrix expressions for the observables. The relations in Table II, like those in Table I, can be proved by the method of Appendix A in Ref. 3. The operator $\hat{p}_\mu$ is defined implicitly for both the matrix and multivector formalisms by the expressions for the Gordon current. The expression for $\hat{p}_\mu$ used in the table differs from (5.1) in that it is "hermitized" to give real quantities for the observables.

Tables I and II give a complete set of relations of the wavefunction to the fundamental (local) observables in

TABLE II. Observalbe with the kinetic energy–momentum operator.

Gordon current	$k_\mu \equiv \bar{\Psi}\hat{p}_\mu\Psi \equiv i'\hbar\frac{1}{2}\{\bar{\Psi}\partial_\mu\Psi - (\partial_\mu\bar{\Psi})\Psi\} - \frac{e}{c}A_\mu\bar{\Psi}\Psi$ $\equiv (\tilde{\psi}\hat{p}_\mu\psi)_{(0)} \equiv \left(\bar{\psi}\left\{\hbar\partial_\mu\psi\gamma_2\gamma_1 - \frac{e}{c}A_\mu\psi\right\}\right)_{(0)}$
Energy–momentum tensor	$T^{\nu\mu} = \bar{\Psi}\gamma^\nu\hat{p}^\mu\Psi = (\gamma_0\tilde{\psi}\gamma^\nu\hat{p}^\mu\psi)_{(0)}$
Proper–Energy–momentum density	$\rho p^\mu \equiv v_\nu T^{\nu\mu} = v\cdot[(\hat{p}^\mu\psi)\gamma_0\tilde{\psi}]_{(1)}$ $= (\tilde{\psi}\,e^{-i\beta}\hat{p}^\mu\psi)_{(0)} = \rho(\tilde{R}\hat{p}^\mu R)_{(0)}$
Kinetic Energy density	$T^{oo} = \Psi^\dagger\hat{p}^o\Psi = (\psi^\dagger\hat{p}^o\psi)_{(0)}$
(Relative) kinetic momentum density $(k=1,2,3)$	$T^{ok} = \Psi^\dagger\hat{p}^k\Psi = (\psi^\dagger\hat{p}\psi)_{(0)}$
Total Angular momentum tensor	$J^{\mu\alpha\beta} = T^{\mu\alpha}x^\beta - T^{\mu\beta}x^\alpha - \rho s_\nu\epsilon^{\nu\mu\alpha\beta}$ $= \bar{\Psi}\{\gamma^\mu(\hat{p}^\alpha x^\beta - \hat{p}^\beta x^\alpha) - (i'\hbar/2)\gamma^\mu\wedge\gamma^\alpha\wedge\gamma^\beta\}\Psi$ $= (\gamma_0\tilde{\psi}\{\gamma^\mu(\hat{p}^\alpha x^\beta - \hat{p}^\beta x^\alpha)\psi$ $- (\hbar/2)\gamma^\mu\wedge\gamma^\alpha\wedge\gamma^\beta\psi\gamma_2\gamma_1\})_{(0)}$
Proper Total Angular momentum density	$v_\mu J^{\mu\alpha\beta} = \rho(p\wedge x + isv)\cdot(\gamma^\beta\wedge\gamma^\alpha)$
(Relative) Total Angular momentum density $(i,j,k)=(1,2,3)$	$J^{oij} = \Psi^\dagger\{\hat{p}^i x^j - \hat{p}^j x^i - (i'\hbar/2)\gamma^i\wedge\gamma^j\}\Psi$ $\equiv \Psi^\dagger\hat{J}_k\Psi = (\psi^\dagger\hat{J}_k\psi)_{(0)}$ $\equiv (\psi^\dagger\{(\hat{p}^i x^j - \hat{p}^j x^i)\psi - (\hbar/2)\gamma^i\wedge\gamma^j\psi\gamma_2\gamma_1\})_{(0)}$

the Dirac theory. Actually, Table II adds only one relation which is mathematically independent of the seven independent relations in Table I. It relates the energy–momentum tensor to the gradient of the phase of the wavefunction. The nature of this relation is best seen by expressing the (proper) kinetic energy–momentum in the form

$$p_\mu = (\tilde{R}\hat{p}_\mu R)_{(0)} = \hbar\,(\gamma_1\gamma_2)\cdot(\tilde{R}\partial_\mu R) - \frac{e}{c}A_\mu$$
$$= 2S\cdot(\partial_\mu R\tilde{R}) - \frac{e}{c}A_\mu. \tag{5.2}$$

The quantity $2\partial_\mu R\tilde{R} = 2(\partial_\mu R)R^{-1}$ can be regarded as the logarithmic derivative or angular velocity of the family of Lorentz transformations determined by R according to (4.3). The quantity $2S\cdot(\partial_\mu R\tilde{R})$ is the projection of this angular velocity onto the spin plane; it describes two effects: the rate at which the spin plane precesses and the rate at which the phase (angle of rotation in the spin plane) changes. Only the last effect appears in the Schrödinger theory, where the energy and momentum are completely determined by the phase. In spite of the fact that the "proper energy–momentum density" ρp_μ is a fundamental quantity in relativistic continuum mechanics, it is rarely considered in discussions of the Dirac theory. Indeed, the expression for ρp_μ in terms of the matrix wavefunction is so unwieldy that it has not been included in Table II, though it is not difficult to obtain from matrix expressions for $T^{\mu\nu}$ and v_μ in Tables I and II.

The significance of Eq. (5.2) lies in the insight it gives into the role of the operator $i'\hbar\partial_\mu$ in the Dirac theory. The $i'\hbar$ has been replaced in (5.2) by the physical and geometrical quantity it represents, the spin bivector S. Moreover, (5.2) shows that in relating the wavefunction to energy and momentum the $i'\hbar$ in the operator $i'\hbar\partial_\mu$ functions as a projection operator, eliminating from $\partial_\mu\psi$ the derivatives of ρ and β and retaining only the angular velocity of R in the spin plane. These specific facts about $i'\hbar\partial_\mu$ in the Dirac theory should be compared carefully with general propositions about Hermitian operators and observables in quantum mechanics. For the most part, such propositions have been developed to generalize properties of $i'\hbar\partial_\mu$. It may be concluded that in so far as they relate the phase of a wavefunction to the energy and momentum of a particle, the propositions are well grounded. Beyond this, their validity is problematic. Certainly none of the usual propositions recognize the essential relation of $i'\hbar$ to the spin. And, as shown earlier, they produce nonsense when applied to the Dirac matrices.

"Hermiticity" is often said to be an essential attribute of operators corresponding to observables. The validity of this view should be judged by examining the role of hermiticity in the Dirac theory. Several different but interrelated roles can in fact be distinguished. In the Dirac matrix algebra hermiticity is *given* a geometrical significance by adopting the standard representation in which the γ_k $(k = 1, 2, 3)$ representing spacelike vectors are anti-Hermitian, while γ_0 representing a timelike vector is Hermitian. Thus Hermitian conjugation serves to distinguish a specific, though arbitrarily chosen, rest frame in spacetime. It should be noted that assignment of this role to hermiticity is not entirely arbitrary; it is in large part dictated by Eq. (2.1) which relates the matrix representation to the indefinite metric of spacetime. Hermiticity also plays a role in the association if $i'\hbar$ with the spin through the requirement met in Table I that only *real* bilinear covariants are to be interpreted as observables. Neither of these roles is recognized in the usual discussions of operators in quantum mechanics. Moreover, when the matrix algebra and complex numbers are replaced by spacetime algebra, the indirect representation of geometrical and physical features by hermiticity is eliminated.

The significance of Hermitian matrices is quite different from the significance of Hermitian differential operators in the Dirac theory, though these two kinds of hermiticity are continually confounded in the literature. The distinction appears in a third role of hermiticity. A study of the relations in Table II reveals that hermiticity insures that the operator $i'\hbar\partial_\mu$ relates energy and momentum directly to the phase *and not* to the amplitude of the wavefunction. This is the role of hermiticity in the Schrödinger theory and seems to be the feature responsible for the successes of abstract operator formulations of quantum mechanics.

A misplaced emphasis on operators in quantum mechanics has continued to cover-up the meaning of hermiticity and the relation of complex numbers to spin. The relations of observables to the wavefunction expressed in Tables I and II is fundamental to the Dirac theory. They are only indirectly and imperfectly expressible as relations of observables to Hermitian operators. By using the relations in Tables I and II along with the Dirac equation, the wavefunction and the operator $i'\hbar\partial_\mu$ can be completely eliminated, resulting in a formulation of the Dirac theory as a set of conservation laws and constitutive equations for observables. This reformulation has been carried out in Ref. 3 and brings to light other features of the Dirac theory which are hidden in the conventional formulation.

Having determined that the purportedly fundamental correspondence between observables and operators is neither adequate nor necessary in the Dirac theory, the significance of eigenvalues in the theory should be examined closely. To begin with, it should be emphasized that the fundamental assumptions of the Dirac theory do not require any reference to eigenvalues, so acceptable assertions about the physical significance of eigenvalues must be derived rather than assumed. Consider the appearance of energy eigenvalues. Solution of the Dirac equation for a bound electron, together with the correspondence of energy to the wavefunction in Table II, gives a discrete spectrum of values for the energy. It is true that these numbers can be regarded as the eigenvalues of an energy operator, but this fact is not needed either to identify the numbers as observables or to explain the existence of a spectrum; the fundamental relation of the energy to the phase of the wavefunction suffices.

There is another property of energy eigenvalues which may be physically significant but goes unremarked in standard expositions of quantum mechanics, because they deal with the total energy without examining

the energy density. The global (or total) energy $\langle E \rangle = \int d^3x \rho_0 E$ of an electron in a stationary state is subject to fairly direct experimental measurement. The existence of a stationary state requires only that $\langle E \rangle$ be independent of time. However, the stationary state solutions of the Dirac equation entail the additional property $\langle E \rangle = E$, that is, the energy density has the striking property of being everywhere a constant multiple E of the probability density. It may be noted that this is what one would expect if it is surmised that the stationary solutions of the Dirac equation describe an ensemble of particle motions each with the same energy E. This suggests that the physical significance of eigenvalues in quantum theory is to be found in the fact that they correspond to *local* observables which are homogeneous in space and constant in time, rather than in their connection to Hermitian operators.

A local observable may well be homogeneous and constant without being the eigenvalue of some Hermitian operator. For example, without specifying any Hermitian operator, one might nevertheless say that an electron is in a velocity eigenstate with eigenvalue v if the local velocity $v = R\gamma_0\tilde{R}$ is homogeneous and constant. It is easy to show that only the free particle "plane wave" states are eigenstates of the velocity in this sense. They are also eigenstates of spin and momentum in the usual sense, but they are quite unphysical because they require uniform density ρ. The physical free particle solutions of the Dirac equation are wavepackets, for which it can be shown that the local velocity cannot be constant. So it may be that some physically significant local observables cannot be associated with physically significant eigenvalues.

Angular momentum operators have an important place in the systematic analysis of quantum theory. The angular momentum operators $\hat{J}_k$ in the Dirac theory are defined implicitly by the expressions for the (relative) angular momentum density in Table II [where the values of (i,j,k) are understood to be cyclic permutations of $(1,2,3)$]. The $\hat{J}_k$ are commonly defined by requiring first that they satisfy the well-known commutation relations of angular momentum operators and second that they commute with the Dirac Hamiltonian for a central field and so are conserved quantities (see, for example, Ref. 10). The $\hat{J}_k$ are then found to have the form given in Table II. Such an approach gives the impression that assumptions about "angular momentum algebra" are essential to the interpretation of Dirac theory. On the contrary, it was shown in Ref. 3 that given the Dirac equation and the relations of the wavefunction to the particle velocity in Table I and the energy–momentum tensor in Table II, expressions for the spin and the total angular momentum are unambiguously determined by introducing the conventional definition of orbital angular momentum. Then the form of $\hat{J}_k$ in Table II can be obtained simply by writing the resulting expressions in conventional operator form, and manifestly without an appeal to assumptions which could be called "quantum mechanical." Evidently, the physical significance of the $\hat{J}_k$ is derived from the relation they express between the wavefunction and the angular momentum tensor. But nothing in this relation implies that, as is usually supposed, the eigenvalues of $\hat{J}^2 \equiv \hat{J}_k\hat{J}_k$ should be interpreted as the square of the magnitude of the angular momentum. This is not to question the importance of $\hat{J}^2$ or the angular momentum algebra in calculations or the classification of states; the aim here is only to point out that some problems of interpretation exist. Further questions about the interpretation of angular momentum quantum numbers will be considered later.

Probably the most profound problem posed by the Dirac theory for conventional interpretations of quantum theory lies in the difficulty of reconciling the usual interpretations of the Heisenberg uncertainty principle with the properties of electron spin. As the nature of this problem has already been explained in Ref. 3, it will not be discussed here.

6. RELATIVE OBSERVABLES AND THE INTERPRETATION OF ENERGY

The most important observable in the Dirac theory is the total energy $\langle E \rangle$, for this quantity has been subjected to the most thorough experimental investigation, especially in the hydrogen atom, and it is primarily by inferences from the experimental results that the identification of other Dirac observables, such as velocity, spin, and momentum have been confirmed. To identify different physical effects contributing to the energy and study the relation to other observables, the energy must be decomposed into a sum of terms. The usual treatment associates observables with operators rather than directly with the wavefunction and, strangely, is unable to separate different physical contributions to the energy except as perturbations of the nonrelativistic limit. In contrast, the approach here is to eliminate the wavefunction along with the operators of the Dirac Hamiltonian to get an expression for the energy density of a Dirac electron in terms of the local observables identified in Tables I and II. The results are not complete in the sense that a fully satisfactory physical understanding has been achieved. However, the linear contribution of external fields is identified and exact expressions for the Thomas and Larmor precessions are found. Also, a number of peculiar features are discovered which are hidden by the operator formulation. Comparison with the usual results will be made in another paper.

Energy is a relative observable, that is, its significance is relative to some inertial frame. However, an atom binding an electron determines an inertial frame, and relative to that frame the electron's energy has an absolute significance. This frame should be kept in mind, though the following discussion makes no assumption about bound states, and the results hold for any inertial frame designated by a specific choice of the timelike vector γ_0.

As an aid to physical interpretation and in preparation for the "nonrelativistic limit," the observables in Tables I and II will be expressed as "relative observables" and related by formulas derived in Ref. 3. The procedure used for introducing relative variables is explained in detail in Ref. 5, so the results and nomenclature of Ref. 5 are freely employed with only the briefest comments.

The "relative" velocity v of the electron is related to the "proper" velocity v defined in (4.5) by the equation

$$v\wedge\gamma_0=\frac{v_0}{c}\mathbf{v}, \tag{6.1a}$$

where

$$v_0\equiv v\cdot\gamma_0=(1-\mathbf{v}^2/c^2)^{-1/2}. \tag{6.1b}$$

Thus

$$v\gamma_0=v_0(1+\mathbf{v}/c)=L^2, \tag{6.1c}$$

where L is the spinor in Eq. (6.15) below, which determines the "boost" of γ_0 into v. The " relative" probability density in the inertial system of γ_0 is

$$\rho_0\equiv(\rho v)\cdot\gamma_0=\rho v_0. \tag{6.2}$$

A spacetime point x can be designated by a time $t=c^{-1}x^0=c^{-1}x\cdot\gamma_0$ and a position $\mathbf{x}=x\wedge\gamma_0$, whence

$$x\gamma_0=ct+\mathbf{x}, \tag{6.3}$$

and the derivative $\square=\square_x$ can be expressed in terms of the derivatives

$$\partial_t=c^{-1}\partial_0=c^{-1}\gamma_0\cdot\square \quad\text{and}\quad \nabla=\nabla_x=\gamma_0\wedge\square \tag{6.4a}$$

by the equation

$$\gamma_0\square=c^{-1}\partial_t+\nabla. \tag{6.4b}$$

Accordingly, the equation for probability conservation

$$\partial_\mu(\rho v^\mu)=\square\cdot(\rho v)=0 \tag{6.5a}$$

can be written in the familiar relative form

$$\partial_t\rho_0+\nabla\cdot(\rho_0\mathbf{v})=0. \tag{6.5b}$$

Similarly, the proper time derivative

$$d_\tau=\frac{d}{d\tau}=v\cdot\square \tag{6.6a}$$

is related to the socalled "hydrodynamic derivative"

$$d_t\equiv\partial_t+\mathbf{v}\cdot\nabla \tag{6.6b}$$

by the equation

$$d_\tau=v\cdot\square=\frac{v_0}{c}d_t. \tag{6.6c}$$

Now consider the expression of mechanical quantities in terms of relative variables. The kinetic energy—momentum vector $p=\gamma^\mu p_\mu$, whose components are related to the wavefunction by (5.2), can be decomposed into an energy

$$\epsilon=cp\cdot\gamma_0 \tag{6.7a}$$

and a momentum

$$\mathbf{p}=p\wedge\gamma_0 \tag{6.7b}$$

by using the algebraic relation

$$p\gamma_0=\frac{\epsilon}{c}+\mathbf{p}. \tag{6.7c}$$

(Here the energy—momentum p has been expressed in "momentum units" instead of the "energy units" used in Ref. 5.) The (kinetic) momentum density in the inertial frame of γ_0 is thus

$$\rho_0\mathbf{p}=\rho v_0\mathbf{p}=\rho v\cdot\gamma_0 p\wedge\gamma_0. \tag{6.8}$$

Now from (5.3) and (6.7c)

$$px=(p\gamma_0)(\gamma_0 x)=\left(\frac{\epsilon}{c}+\mathbf{p}\right)(ct-\mathbf{x})$$

$$=\epsilon t-\mathbf{p}\cdot\mathbf{x}+ct\mathbf{p}-\frac{\epsilon}{c}\mathbf{x}-\mathbf{p}\wedge\mathbf{x}.$$

The scalar part of this equation is just the relation

$$p\cdot x=\epsilon t-\mathbf{p}\cdot\mathbf{x},$$

while the proper bivector part is

$$p\wedge x=ct\mathbf{p}-\frac{\epsilon}{c}\mathbf{x}+\mathbf{x}\wedge\mathbf{p}. \tag{6.9a}$$

From this, one immediately sees that the relative vector part of $p\wedge x$ is

$$[p\wedge x]_{(1)}=ct\mathbf{p}-\frac{\epsilon}{c}\mathbf{x}, \tag{6.9b}$$

while the relative bivector part is

$$[p\wedge x]_{(2)}=\mathbf{x}\wedge\mathbf{p}=i\mathbf{x}\times\mathbf{p}\equiv i\mathbf{L}, \tag{6.9c}$$

showing that $p\wedge x$ is an appropriate generalization of the usual orbital angular momentum vector $\mathbf{L}\equiv\mathbf{s}\times\mathbf{p}$, or better, the corresponding angular momentum bivector $\mathbf{x}\wedge\mathbf{p}$. In accordance with (6.8), the "relative orbital angular momentum density" is

$$\rho_0\mathbf{L}=\rho_0\mathbf{x}\times\mathbf{p}. \tag{6.10}$$

For the proper spin vector s, defined by (4.7),

$$s\gamma_0=s_0+\mathbf{s} \tag{6.11a}$$

where

$$\mathbf{s}=s\wedge\gamma_0 \tag{6.11b}$$

and, since $s\cdot v=v_0(s_0-\mathbf{s}\cdot\mathbf{v}/c)=0$,

$$s_0\equiv s\cdot\gamma_0=c^{-1}\mathbf{s}\cdot\mathbf{v}. \tag{6.11c}$$

Using (6.1) and (6.11) in (4.8), one has for the proper spin bivector

$$S=isv=i(s\gamma_0)(\gamma_0 v)$$

$$=i(s_0+\mathbf{s})v_0(1-\mathbf{v}/c)$$

$$=iv_0(\mathbf{s}-s_0\mathbf{v}/c-\mathbf{s}\wedge\mathbf{v}/c)$$

$$=\frac{v_0}{a}\mathbf{s}\times\mathbf{v}+iv_0(\mathbf{s}-s_0\mathbf{v}/c).$$

Hence,

$$S=\mathbf{s}_1+S_2=\mathbf{s}_1+i\mathbf{s}_2, \tag{6.12a}$$

where

$$\mathbf{s}_1\equiv[S]_{(1)}=\frac{v_0}{c}\mathbf{s}\times\mathbf{v}=\frac{v_0}{c}\mathbf{v}\cdot(i\mathbf{s}) \tag{6.12b}$$

is the relative vector part of S, and

$$S_2=i\mathbf{s}_2\equiv[S]_{(2)}=iv_0(\mathbf{s}-c^{-1}s_0\mathbf{v}) \tag{6.12c}$$

is the relative bivector part. From (6.9) and (6.12) one finds that the relative bivector part of the proper "total" angular momentum $J\equiv p\quad x+S$ at a point x is

$$i\mathbf{J}\equiv[J]_{(2)}=\mathbf{x}\wedge\mathbf{p}+S_2=i(\mathbf{x}\times\mathbf{p}+\mathbf{s}_2), \tag{6.13}$$

so

$$\rho_0\mathbf{J}=\rho_0\mathbf{x}\times\mathbf{p}+\rho_0\mathbf{s}_2 \tag{6.14}$$

is the total (relative) angular momentum density, expressed as a sum of orbital and spin parts.

The trouble with representing spin by the relative

vectors $\mathbf{s}$ or $\mathbf{s}_2$ is they do not have constant magnitude, one of the principle properties of the proper spin s and S. There is an alternative definition of "relative" spin which does not suffer this defect. In the manner explained in Ref. 5, the spinor R introduced by (4.2) can be factored in the form

$$R = LU, \tag{6.15}$$

where the spinor U determines a spatial rotation and L determines a boost of γ_0 to v. Now define a relative spin bivector Σ and vector $\boldsymbol{\sigma}$ by

$$\Sigma = \frac{\hbar}{2} Ui\boldsymbol{\sigma}_3\tilde{U} = i\boldsymbol{\sigma}. \tag{6.16}$$

Using (6.15) in (4.8) one easily shows that Σ is related to S by a boost:

$$S = L\Sigma\tilde{L}, \quad \Sigma = \tilde{L}SL, \tag{6.17a}$$

$$sv = L\boldsymbol{\sigma}\tilde{L}, \quad \boldsymbol{\sigma} = \tilde{L}svL = \tilde{L}sL\gamma_0. \tag{6.17b}$$

When expressed in terms of relative velocity, the relation of $\boldsymbol{\sigma}$ to $\mathbf{s}$ is found to be [see Eq. (4.38) of Ref. 5],

$$\mathbf{s} = \boldsymbol{\sigma} + \frac{(v_0 - 1)}{\mathbf{v}^2}\boldsymbol{\sigma}\cdot\mathbf{v}\mathbf{v} = \boldsymbol{\sigma} + \frac{v_0^2}{c^2(v_0+1)}\boldsymbol{\sigma}\cdot\mathbf{v}\mathbf{v}, \tag{6.18a}$$

$$cs_0 = \mathbf{s}\cdot\mathbf{v} = v_0\mathbf{v}\cdot\boldsymbol{\sigma}. \tag{6.18b}$$

Substitution of (6.18) into (6.12c) yields

$$\mathbf{s}_2 = v_0\left(\boldsymbol{\sigma} - \frac{v_0}{c^2(1+v_0)}\boldsymbol{\sigma}\cdot\mathbf{v}\mathbf{v}\right): \tag{6.19}$$

so (6.14) can be written

$$\rho_0\mathbf{J} = \rho_0\mathbf{x}\times\mathbf{p} + \rho_0 v_0\left(\boldsymbol{\sigma} - \frac{v_0}{c^2(1+v_0)}\boldsymbol{\sigma}\cdot\mathbf{v}\mathbf{v}\right). \tag{6.20}$$

This shows the correct way to combine σ with the orbital angular momentum to get the total relative angular momentum density. Especially in discussions of relativistic approximations, it is important to be clear about which of the several different representations of spin is employed.

From the kinetic energy–momentum vector p it is convenient to form the an energy–momentum vector P defined by

$$P = p + \frac{e}{c}A = 2\gamma^\mu S\cdot(\partial_\mu R\tilde{R}), \tag{6.21}$$

where $A = \gamma^\mu A_\mu$ is the electromagnetic vector potential and the right side of the equation has been obtained from (5.2). The quantity of chief interest in this section, the density $\rho_0 E$ of the total energy $\langle E\rangle = \int d^3x\rho_0 E$, is related to E by

$$E = c\gamma_0\cdot P = 2cS\cdot(\partial_0 R\tilde{R}) = \epsilon + V, \tag{6.22a}$$

where (6.21) has been used, ϵ is the kinetic energy defined by (6.7a), and

$$V \equiv eA\cdot\gamma_0 \tag{6.22b}$$

is the usual electric potential energy. The corresponding total local momentum is

$$\mathbf{P} = P\wedge\gamma_0 = \mathbf{p} + \frac{e}{c}\mathbf{A} \tag{6.22c}$$

where $\mathbf{A} \equiv A\wedge\gamma_0$. Combining (6.22a) and (6.22c), one has

$$P\gamma_0 = E/c + \mathbf{P}. \tag{6.22d}$$

Equation (6.22a) explicitly exhibits the dependence of the local energy E on the time derivative of the spinor R. Instead of analyzing this expression directly, it is advantageous first to study the energy in the local rest system determined by the velocity v. Since by (4.5), (4.7), and (4.8) the local velocity and spin are functions only of the spinor R, equations of motion for these "mechanical quantities" along a "streamline" in spacetime with tangent v are determined by an equation of motion for R, which can be put in the form

$$d_\tau R = \tfrac{1}{2}\Omega R \quad \text{or} \quad \Omega = 2(d_\tau R)\tilde{R}, \tag{6.23}$$

where Ω is a bivector and d_τ is the proper time derivative defined by (6.6a). Expressed in terms of the "angular velocity" Ω, the equations of motion for velocity and spin are

$$d_\tau v = \tfrac{1}{2}[\Omega, v] = \Omega\cdot v, \tag{6.24a}$$

$$d_\tau s = \tfrac{1}{2}[\Omega, s] = \Omega\cdot s, \tag{6.24b}$$

$$d_\tau S = \tfrac{1}{2}[\Omega, S]. \tag{6.24c}$$

By using (6.23) along with (6.21), one finds that the local energy in the local rest frame is given by the projection of the angular velocity onto the local spin frame, that is,

$$v\cdot p = (\Omega S)_{(0)} = \Omega\cdot S = v\cdot p + \frac{e}{c}v\cdot A. \tag{6.25}$$

The plan now is to attain a physical interpretation of the energy density by analyzing the "proper angular velocity" Ω. To accomplish this, some physical input is needed besides the relations of observables to the wavefunction, which is all that has been used so far. That input comes from the Dirac equation, which was used in Sec. 6 of Ref. 3 to get the following expression for Ω in terms of local observables:

$$\Omega = \overline{\Omega} + v\cdot\left(mcv\cos\beta + \frac{e}{c}A\right)S^{-1}, \tag{6.26}$$

where

$$\overline{\Omega} = -\Box\wedge v - iv\wedge\Box\beta = \frac{e}{mc^2}Fe^{i\beta} - \frac{e^{i\beta}}{mc}C, \tag{6.27a}$$

in which $F = \Box\wedge A$ is the external electromagnetic field and

$$C = \{\partial_\mu W^\mu + \tfrac{1}{4}[\gamma^\mu\gamma^\nu, [W_\mu, W_\nu]S^{-1}]\}, \tag{6.27b}$$

$$W_\mu = (\rho e^{i\beta})^{-1}\partial_\mu(\rho e^{i\beta}S) = \partial_\mu S + S(\partial_\mu\ln\rho + i\partial_\mu\beta). \tag{6.27c}$$

Substituting (6.26) and (6.27) in (6.25) and recalling the expression (4.10) for the magnetic moment density M, one gets the following expression for the "kinetic energy density" $\rho\epsilon_v$ in the local rest system

$$\rho\epsilon_v \equiv \rho cv\cdot p = \rho mc^2\cos\beta + M\cdot F - c^{-1}C\cdot M. \tag{6.28}$$

Lest the reader believe that physical interpretations are being arbitrarily imposed here, it should be pointed out that the identification of $\rho\epsilon_v$ as kinetic energy density is a consequence of adopting the conventional interpretation of the operator (5.1) as "kinetic energy–momentum operator" and of the "Dirac current" $\overline{\Psi}\gamma_\mu\Psi = \rho v_\mu$ as probability current. Unconventional as the present discussion may appear, it is based on conven-

tional assumptions of the Dirac theory and conventional principles of relativistic continuum mechanics. The ultimate aim is to discover the full consequences of those assumptions.

According to conventional principles of relativistic continuum mechanics, the quantity $\rho\epsilon_v/c^2$ should be interpreted as the electron mass density. If the Dirac theory in fact describes a statistical ensemble of particle motions then v must be only a local average (not an actual) particle velocity, and a deviation of the rest mass density from ρmc^2 due to statistical effects is to be expected. Be this as it may, the term $\rho mc^2\cos\beta$ has the appearance of a rest mass tensor, and one might guess that the unfamiliar factor $\cos\beta$ is needed to meet the constraint $v^2 = 1$ in a statistical average of particle velocities. The interpretation of the second term in (6.28) requires less speculation, for $M\cdot F = \frac{1}{2}F_{\mu\nu}M^{\nu\mu}$ will be recognized as the classical expression for the increase in mass due to the electromagnetic interaction of a dipole. Interpretation of the last term is difficult, but may be crucial to a complete understanding of the Dirac theory. Considering the expression (6.27b, c) for C in terms of the spin and the corresponding spin dependence of the momentum flux exhibited in Eq. (3.22) of Ref. 3, it may be guessed that this last term be interpreted as the enhancement of mass due to the local spin flux.

To relate (6.28) to the energy density $\rho_0 E$, note from (6.1) and (6.7) that

$$v\cdot p = \frac{v_0}{c}(\epsilon - \mathbf{v}\cdot\mathbf{p}): \tag{6.29}$$

hence the total energy density can be written

$$\begin{aligned}\rho_0 E &= c\rho v\cdot p + \rho_0\mathbf{v}\cdot\mathbf{p} + \rho_0 V\\ &= mc^2\rho\cos\beta + c\rho[\bar{\Omega}S]_{(0)} + \rho_0\mathbf{v}\cdot\mathbf{p} + \rho_0 V\end{aligned} \tag{6.30a}$$

or

$$\rho_0 E = mc^2\rho\cos\beta + M\cdot F - e^{-1}C\cdot M + \rho_0\mathbf{v}\cdot\mathbf{p} + \rho_0 V. \tag{6.30b}$$

Use of the expressions (6.26), (6.27) for Ω to get the energy density in the form (6.30), which is amenable to physical interpretation, is equivalent to the usual practice of expressing the energy density in terms of the Dirac Hamiltonian, and then systematically replacing the operators and the wavefunction by local observables. To get on with the interpretation of (6.30), it is worth remarking that the magnetic moment of the Dirac electron was first identified theoretically and experimentally precisely by isolating the contribution of the term $M\cdot F$ to the total energy (by a different method, of course). But there is another contribution to the energy due to the interaction of the spin with the external field arising from the Thomas precession. Ordinarily the contribution of the Thomas precession is identified only as a correction to the nonrelativistic approximation. But the formalism used here makes it possible to discuss the role of the Thomas precession exactly.

In Sec. 4 of Ref. 5 the generalized Larmor and Thomas precession of a classical rigid point particle is discussed. All the results obtained there apply immediately to the present problem if only the proper velocity of a particle there is identified with the velocity v of a streamline in the present formulation of the Dirac theory. This paragraph recalls those results which are most pertinent to the present discussion. The angular velocity Ω defined by Eq. (6.23) determines the precession of the velocity and spin through Eq. (6.24). It will be convenient to decompose Ω into relative vector and bivector parts; thus

$$\Omega = 2(d_\tau R)\tilde{R} = \boldsymbol{\alpha} + i\boldsymbol{\beta} \tag{6.31a}$$

$$\boldsymbol{\alpha} \equiv [\Omega]_{(1)} = \Omega\cdot\gamma_0\gamma_0, \tag{6.31b}$$

$$i\boldsymbol{\beta} = [\Omega]_{(2)} = \Omega\wedge\gamma_0\gamma_0. \tag{6.31c}$$

Introducing the factorization (6.15), one finds for the spinor U the equation of motion

$$d_\tau U = \frac{v_0}{c}d_t U = \tfrac{1}{2}\omega U, \tag{6.32}$$

for which the angular velocity can be expressed in the several useful forms

$$\begin{aligned}\omega &= \tilde{L}\Omega L - 2\tilde{L}d_\tau L = \omega^L + \omega^T\\ &= i\left(\boldsymbol{\beta} + \frac{v_0}{c(1+v_0)}\boldsymbol{\alpha}\times\mathbf{v}\right),\end{aligned} \tag{6.33}$$

$$\begin{aligned}\omega^L &= [\tilde{L}\Omega L]_2\\ &= i\left(\boldsymbol{\beta} - \frac{v_0^2}{c^2(1+v_0)}(\boldsymbol{\beta}\times\mathbf{v})\times\mathbf{v} + \frac{v_0}{c}\boldsymbol{\alpha}\times\mathbf{v}\right),\end{aligned} \tag{6.34}$$

$$\begin{aligned}\omega^T &= [2(d_\tau L)\tilde{L}]_2 = -[2\tilde{L}d_\tau L]_2\\ &= \frac{((d_\tau v)\wedge v\wedge\gamma_0)\gamma_0}{1+v_0} = \frac{v_0^2}{c^2(1+v_0)}i\mathbf{v}\times d_\tau\mathbf{v}\\ &= \frac{v_0^2}{c(1+v_0)}i\mathbf{v}\times\left(\boldsymbol{\alpha} + \frac{\mathbf{v}}{c}\times\boldsymbol{\beta}\right).\end{aligned} \tag{6.35}$$

These equations give the decomposition of ω into a sum two terms, the generalized Larmor precession ω^L and the Thomas precession ω^T, which is due solely to the acceleration of the particle. One can solve (6.33) for Ω in terms of ω:

$$\Omega = L(\omega + 2\tilde{L}d_\tau L)\tilde{L} = L\omega L + 2(d_\tau L)\tilde{L}, \tag{6.36}$$

which is the more useful when one has the formula

$$2(d_\tau L)\tilde{L} = \frac{(d_\tau v)\wedge(v+\gamma_0)}{1+v_0}. \tag{6.37}$$

Applying (6.32) and (6.33) to the relative spin vector $\boldsymbol{\sigma}$ defined by (6.16), one obtains the equation of motion

$$\begin{aligned}d_\tau\boldsymbol{\sigma} &= \frac{v_0}{c}d_t\boldsymbol{\sigma} = \omega\cdot\boldsymbol{\sigma} = \omega^L\cdot\boldsymbol{\sigma} + \omega^T\cdot\boldsymbol{\sigma}\\ &= \left(-\boldsymbol{\beta} + \frac{v_0}{c(1+v_0)}\mathbf{v}\times\boldsymbol{\alpha}\right)\times\boldsymbol{\sigma},\end{aligned} \tag{6.38}$$

a key formula derived by Thomas. Now it must be emphasized that to speak of the Thomas precession in the Dirac theory, it is essential to introduce the relative spin $\boldsymbol{\sigma}$ defined by (6.16); this is the spin obtained, as required by Thomas, from the proper spin S by a "deboost" into an *inertial* system, a system in which the acceleration of the particle is zero. It makes no sense to speak of the Thomas precession of the spin vectors $\mathbf{s}$ or $\mathbf{s}_2$ defined previously.

The formulation of the Thomas precession just given admits an immediate generalization, simply by replac-

ing the proper time derivatived d_τ by the derivative d_τ by the derivatives $\partial_\mu = \gamma_\mu \cdot \square$. Then (6.31a) is replaced by

$$\Omega_\mu = 2(\partial_\mu R)\tilde{R} = \alpha_\mu + i\beta_\mu, \tag{6.39}$$

from which (6.31a) can be recovered since $\Omega = v^\mu \Omega_\mu$ and $d_\tau = v^\mu \partial_\mu$. Similarly, (6.32) generalizes to

$$\partial_\mu U = \tfrac{1}{2}\omega_\mu U, \tag{6.40a}$$

where

$$\omega_\mu = \tilde{L}\omega_\mu L - 2\tilde{L}\partial_\mu L = \omega_\mu^L + \omega_\mu^T$$
$$= i\left(\beta_\mu + \frac{v_0}{c(1+v_0)}\,\alpha_\mu \times \mathbf{v}\right), \tag{6.40b}$$

$$\omega_\mu^T = [2(\partial_\mu L)\tilde{L}]_2 = -[2\tilde{L}\partial_\mu L]_2$$
$$= \frac{v_0^2}{c^2(1+v_0)}\, i\mathbf{v}\times\partial_\mu\mathbf{v} = \frac{v_0^2}{c(1+v_0)}\, i\mathbf{v}\times\left(\alpha_\mu + \frac{\mathbf{v}}{c}\times\beta_\mu\right). \tag{6.40c}$$

Also,

$$\Omega_\mu = L(\omega_\mu + 2\tilde{L}\partial_\mu L)\tilde{L} \tag{6.41}$$

and

$$\partial_\mu \sigma = \omega_\mu \cdot \sigma = \left(-\beta_\mu + \frac{v_0}{c(1+v_0)}\,\mathbf{v}\times\alpha_\mu\right)\times\sigma, \tag{6.42a}$$

or, equivalently,

$$\partial_\mu \Sigma = \partial_\mu(i\sigma) = \tfrac{1}{2}[\omega_\mu, \Sigma], \tag{6.42b}$$

and, differentiating (6.17a) and using (6.41),

$$\partial_\mu S = \tfrac{1}{2}[\Omega_\mu, S] = L(\partial_\mu \Sigma - \tfrac{1}{2}[\omega_\mu^T, \Sigma])\tilde{L}. \tag{6.42c}$$

We are now prepared to separate the energy–momentum due to variations in velocity from other contributions to the total energy–momentum. Using (6.39) in (6.21) followed by (6.17), (6.41), and (6.42), we find

$$\gamma_\mu \cdot P = P_\mu = [\Omega_\mu S]_{(0)} = [(\omega_\mu + 2\tilde{L}(\partial_\mu L))\Sigma]_{(0)}$$
$$= P'_\mu - \omega_\mu^T \cdot \Sigma, \tag{6.43}$$

where P'_μ is defined by

$$P'_\mu \equiv \hbar[\partial_\mu U i\sigma_3 \tilde{U}]_{(0)} = [\omega_\mu \Sigma]_{(0)} = \omega_\mu \cdot \Sigma. \tag{6.44}$$

From (6.43) one sees that

$$v \cdot P = v^\mu P_\mu = \Omega \cdot S = (\omega - \omega^T)\cdot\Sigma = \omega^L \cdot \Sigma \tag{6.45}$$

is just the generalized Larmor precession energy, whereas, from (6.44),

$$v \cdot P' = \omega \cdot \Sigma = \omega^L \cdot \Sigma + \omega^T \cdot \Sigma \tag{6.46}$$

includes also the Thomas precession energy. Removing the potential energy contribution from (6.44) by writing

$$p'_\mu = P'_\mu - \frac{e}{c}A_\mu = \hbar[\partial_\mu U i\sigma_3 \tilde{U}]_{(0)} - \frac{e}{c}A_\mu, \tag{6.47}$$

one finds, since $\omega^T = v^\mu \omega_\mu^T = v_0(\omega_0^T - c^{-1}\mathbf{v}_k\omega_k^T)$,

$$\mathbf{v}\cdot\mathbf{p} = \mathbf{v}\cdot\mathbf{p}' + \frac{c}{v_0}\,\omega^T\cdot\Sigma - c\omega_0^T\cdot\Sigma. \tag{6.48}$$

It is convenient to replace Ω by $\bar{\Omega}$ in the formulation of precession energy. This is perfectly permissible since, as is easily shown by substituting (6.26) into (6.24), it does not alter the precession of the velocity and the spin. The replacement does not affect the Thomas precession; it merely changes the definition of the generalized Larmor precession from (6.34) to

$$\bar{\omega}^L = [\tilde{L}\bar{\Omega}L]_2. \tag{6.49}$$

Corresponding changes in other quantities will also be indicated by overbars.

Now switching from Ω to $\bar{\Omega}$ and substituting (6.45) and (6.48) into (6.30a), the energy density is put in the form

$$\rho_0 E = mc^2\rho\cos\beta + c\rho\bar{\omega}\cdot\Sigma - c\rho_0\omega_0^T\cdot\Sigma + \rho_0\mathbf{v}\cdot\mathbf{p}' + \rho_0 V. \tag{6.50}$$

The term $c\rho\bar{\omega}\cdot\Sigma = \rho_0[(c/v_0)(\bar{\omega}^L + \omega^T)\Sigma]_{(0)}$ includes both the generalized Larmor and Thomas precession energies. It is important to note that the change in the definition of the kinetic momentum from $\mathbf{p}$ to $\mathbf{p}'$ is essential to make the Thomas term explicit. The term $c\rho_0\omega_0^T\cdot\Sigma$ vanishes for stationary states, since by (6.40c) $\omega_0^T = 0$ if $c\partial_0\mathbf{v} = \partial_t\mathbf{v} = 0$.

To study the dependence of the precession energy in (6.50) on relative observables, express F in terms of the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ relative to γ_0;

$$F = \mathbf{E} + i\mathbf{B}, \quad \text{hence} \quad iF = -\mathbf{B} + i\mathbf{E}. \tag{6.51}$$

Also write

$$C = \mathbf{C}_1 + C_2 = \mathbf{C}_1 + i\mathbf{C}_2 \tag{6.52}$$

where $\mathbf{C}_1 \equiv [C]_1$ and $C_2 = i\mathbf{C}_2 \equiv [C]_2$. The definition (6.27b) shows that C depends on $\partial_\mu S$ and S; these quantities can be expressed in terms of $\partial_\mu\Sigma$ and Σ by using (6.42a) and (6.17a), but this step will not be carried out, because it is not clear how to derive any physical insight from it. The terms which are difficult to understand will be kept lumped together. Now using (6.51) and (6.52) in (6.27b) and then in (6.33), one gets

$$c\rho\bar{\omega}\cdot\Sigma = -\frac{e}{mc}\left(\sigma\cdot\mathbf{B} + \frac{v_0}{c(1+v_0)}\,\sigma\cdot(\mathbf{E}\times\mathbf{v})\right)\rho\cos\beta$$
$$+\left(\sigma\cdot\mathbf{C}_2 - \frac{v_0}{c(1+v_0)}\,\sigma\cdot(\mathbf{C}_1\times\mathbf{v})\right)\frac{\rho\cos\beta}{m}$$
$$-\frac{e}{mc}\left(\sigma\cdot\mathbf{E} - \frac{v_0}{c(1+v_0)}\,\sigma\cdot(\mathbf{B}\times\mathbf{v})\right)\rho\sin\beta$$
$$+\left(\sigma\cdot\mathbf{C}_1 + \frac{v_0}{c(1+v_0)}\,\sigma\cdot(\mathbf{C}_2\times\mathbf{v})\right)\rho\frac{\sin\beta}{m}. \tag{6.53}$$

The terms in first line of (6.53) except for the factor $\cos\beta$ are exactly the terms derived by Thomas (see Ref. 5), who evaluated the precession energy under the assumption that $\bar{\Omega} = (e/mc^2)F$. Thomas wisely evaluated the energy only in the nonrelativistic approximation where $v_0(1+v_0)^{-1} \approx \frac{1}{2}$ (and, fortunately, $\cos\beta \approx 1$). In higher order approximations the effect of the external field through terms in the second line of (6.53) is probably important, though it is not clear how to make this explicit. It might be guessed that because of the smallness of $\sin\beta$, the unfamiliar terms in the last two rows are generally insignificant, but it will be seen that the $\sigma\cdot\mathbf{E}$ term may be of the same order of magnitude as the $\sigma\cdot(\mathbf{E}\times\mathbf{v})$ term in the first row.

For an electron in a central field,

$$e\mathbf{E} = -\nabla V = -V'\frac{\mathbf{x}}{|\mathbf{x}|} \quad \text{with } V' = \frac{dV}{d|\mathbf{x}|},$$

in which case the second term in (6.53) can be written

$$\frac{e}{m^2c^2}\frac{\rho}{(1+v_0)}\frac{V'}{|\mathbf{x}|}\boldsymbol{\sigma}\cdot\mathbf{L}^*, \tag{6.54a}$$

where

$$\mathbf{L}^* = \mathbf{x}\times(mv_0\mathbf{v})\cos\beta. \tag{6.54b}$$

The term (6.54a) has the well-known form of the spin-orbit coupling; however, $\mathbf{L}^*$ differs from the orbital angular momentum $\mathbf{L}=\mathbf{x}\times\mathbf{p}$, because the relation $\mathbf{p} = mv_0\mathbf{v}$ assumed by Thomas does not hold in the Dirac theory. To estimate the magnitude of this discrepancy the correct relation of $\mathbf{p}$ to $\mathbf{v}$ will now be found.

The correct relation of the kinetic energy–momentum p to the particle velocity v in the Dirac theory was found in Sec. 5 of Ref. 3 to be given by

$$\rho p = mc\rho v\cos\beta - \Box\circ(\rho S) + \Box\circ\rho(iS)\circ\Box\beta. \tag{6.55}$$

To express this as a relation among relative observables, multiply by γ_0 and recall (6.7) and (6.1) to get

$$\frac{\epsilon}{c} + \mathbf{p}mcv_0\left(1+\frac{v}{c}\right)\cos\beta - \rho^{-1}\Box\cdot(\rho S)\gamma_0 - (\Box\beta)\cdot(iS)\gamma_0. \tag{6.56}$$

But, by virtue of (6.4) and (6.12a),

$$\gamma_0\Box\cdot(\rho S) = [\gamma_0\Box(\rho S)]_{(0+1)} = [(\partial_0+\nabla)\rho(\mathbf{s}_1+i\mathbf{s}_2)]_{(0+1)}$$
$$= \nabla\cdot(\rho\mathbf{s}_1) + \partial_0(\rho\mathbf{s}_1) + \nabla\cdot(\rho i\mathbf{s}_2)$$

and

$$\gamma_0(\Box\beta)\cdot(iS) = [\gamma_0(\Box\beta)iS]_{(0+1)} = [(\partial_0\beta+\nabla\beta)(i\mathbf{s}_1-\mathbf{s}_2)]_{(0+1)}$$
$$= -\mathbf{s}_2\cdot\nabla\beta - \mathbf{s}_2\partial_0\beta + (\nabla\beta)\cdot(i\mathbf{s}_1).$$

Hence the scalar part of (6.56) can be written

$$\epsilon = mc^2v_0\cos\beta - c\rho^{-1}\nabla\cdot(\rho\mathbf{s}_1) + c\mathbf{s}_2\cdot\nabla\beta, \tag{6.57a}$$

while the vector part can be written

$$\mathbf{p} = m\mathbf{v}v_0\cos\beta - \rho^{-1}\nabla\times(\rho\mathbf{s}_2) + \mathbf{s}_1\times\nabla\beta + \rho^{-1}\partial_0(\rho\mathbf{s}_1) - \mathbf{s}_2\partial_0\beta. \tag{6.57b}$$

Using (6.57b) to eliminate $mvv_0\cos\beta$ in (6.54), one indeed gets the desired spin-orbit term with $\mathbf{L}$ instead of $\mathbf{L}^*$, but there are several additional terms as well. Some understanding of the additional terms can be achieved by comparing with results known in the literature, but to do so it is necessary to take the nonrelativistic limit, since it is only in connection with that approximation that the Thomas precession has been discussed previously. This will be done later.

The discussion of the Dirac energy density in this section has concentrated on a detailed interpretation of a few terms. A satisfactory interpretation of all the terms has not been found, but let us review the general approach. The effective mass density given by (6.28) differs from what appears to be a rest energy term $\rho mc^2\cos\beta$ by a term commonly called the internal energy density. Accordingly, it is natural to call the "generalized Larmor" term $c\bar{\Omega}\cdot S = c\bar{\omega}^L\cdot\Sigma$ the *internal energy* of the system. The magnitude of the internal energy depends, of course, on the interaction with external fields, which (6.30b) expresses to terms linear in the external field F by $c\rho\bar{\omega}^L\circ\Sigma = M\cdot F + e^{-1}C\cdot M$. The kinetic energy density $\rho_0\mathbf{v}\cdot\mathbf{p}$ of the system is also influenced by external fields, which was found to terms linear in the field by separating the Thomas precession energy from other contributions to the kinetic energy with $\rho_0\mathbf{v}\cdot\mathbf{p} = \rho_0\mathbf{v}\cdot\mathbf{p}' + \rho c\omega^T\cdot\Sigma - c\rho_0\omega_0^T\cdot\Sigma$. The Larmor and Thomas precessions were combined in (6.50) to get the total influence of external fields (aside from the potential energy V of course). Nevertheless, it is very important to be able to separate contributions to the mass density from contributions to the kinetic energy.

7. OBSERVABLES IN THE NONRELATIVISTIC LIMIT

The exact constitutive relations found for relative observables in the last section are rather complicated and difficult to interpret. The relations simplify greatly in the nonrelativistic limit to be determined here; still they remain nontrivial. It will be shown that the local momentum and the Gordon current are equal in that limit, but they differ from the local velocity by a "magnetization current." In a subsequent paper this result will be shown to have important implications for the interpretation of spin-orbit coupling and the Pauli and Schrödinger theories. Also, for future use, the nonrelativistic form of the spin-electric energy density is found.

The adjective "relativistic" was criticized in Ref. 5, but it will nevertheless be employed here, because it is almost universally used in connection with the topic under discussion. It may be well to recall, therefore, that sometimes the word "relativistic" means that the relative speed $|\mathbf{v}|$ is of the order of the velocity of light c; sometimes it means that accelerations are small, and sometimes it means that an expression or quantity is completely independent of the relative velocity. The term "nonrelativistic" will be used here especially to mean $|\mathbf{v}| \ll c$. Furthermore, it should be emphasized that the so-called "nonrelativistic limit" of the Dirac theory involves a number of other assumptions—reasonable assumptions about the magnitude of external fields, and about which quantities are slowly varying functions of position, in particular, about the curious quantity β.

It will not be necessary to spell out such assumptions, because they will be implicit in the approximate equations written down. From (6.16) one gets in the nonrelativistic limit

$$v_0 = (1-\mathbf{v}^2/c^2)^{-1/2} = 1 + \frac{1}{2}\frac{\mathbf{v}^2}{c^2} + \cdots \approx 1. \tag{7.1}$$

Using this in the several equations defining the relative spins one finds

$$\mathbf{s} \approx \mathbf{s}_2 \approx \boldsymbol{\sigma}, \tag{7.2a}$$

$$S \approx S_2 \approx \Sigma \approx i\mathbf{s}, \tag{7.2b}$$

$$s_0 \ll |\mathbf{s}|, \tag{7.2c}$$

$$\mathbf{s}_1^2 \ll \mathbf{s}^2 \approx |S|^2 = -S^2 = \tfrac{1}{4}\hbar^2. \tag{7.2d}$$

Also, of course,

$$\rho_0 = \rho v_0 \approx \rho,$$

and (6.20) reduces to the familiar expression

$$\rho_0 \mathbf{J} \approx \rho \mathbf{J} \approx \rho(\mathbf{x}\times\mathbf{p}+\mathbf{s}).$$

From Eq. (2.18) of Ref. 3, one gets

$$-mc\rho \sin\beta = c^{-1}\partial_t(\rho s_0) + \nabla\cdot(\rho\mathbf{s}).$$

Hence for stationary or slowly varying states one has

$$\sin\beta = \frac{-1}{mc}\frac{\nabla\cdot(\rho s)}{\rho}. \tag{7.3a}$$

To this may be added the condition

$$|\sin\beta| \approx |\beta| \leq |\mathbf{v}|/c, \tag{7.3b}$$

which seems reasonable in view of the numerical factor $|\mathbf{s}|/mc = \hbar/2mc$ on the right side of (7.3a). Better justification will be given in a subsequent paper.

Employing the above approximations, one finds that (6.57b) reduces to the important equation

$$\mathbf{p} = m\mathbf{v} - \rho^{-1}\nabla\times(\rho\mathbf{s}) = m\mathbf{v} - \rho^{-1}\nabla\cdot(\rho S). \tag{7.4}$$

Higher order terms must be carried to get the appropriate approximation to (6.57a), since the corrections to the large "rest energy" term mc^2 are of interest. Accordingly, recalling especially (6.12b), one finds

$$\begin{aligned}\epsilon - mc^2 &\approx \tfrac{1}{2}m\mathbf{v}^2 - \tfrac{1}{2}mc^2\beta^2 + \rho^{-1}\nabla\cdot(\rho\mathbf{s}\times\mathbf{v}) + c\mathbf{s}\cdot\nabla\beta \\ &= \tfrac{1}{2}m\mathbf{v}^2 + \tfrac{1}{2}mc^2\beta^2 + \rho^{-1}\nabla\cdot[\rho(c\beta\mathbf{s}) + \mathbf{v}\times\mathbf{s}] \\ &\approx \tfrac{1}{2}m\mathbf{v}^2 + \frac{1}{2m}\left(\frac{\nabla\cdot(\rho\mathbf{s})}{\rho}\right)^2 + \rho^{-1}\nabla\cdot\left(-\frac{1}{m}\mathbf{s}\nabla\cdot(\rho\mathbf{s}) + \rho\mathbf{v}\times\mathbf{s}\right).\end{aligned} \tag{7.5}$$

This is an appropriate place to discuss the physical interpretation and examine the N.R. Limit of the Gordon current k, whose components are defined in Table II. In Sec. 5 of Ref. 3 the Gordon current was found to be related to the velocity and magnetization or spin by the exact equation

$$j \equiv e\rho v = \frac{e}{mc}k + \Box\cdot M = \frac{e}{mc}k + e\Box\cdot(\rho e^{i\beta}S), \tag{7.6}$$

and to the proper energy–momentum density by

$$k = \rho p\cos\beta - \rho q\sin\beta, \tag{7.7a}$$

where

$$q = \gamma^\mu v\cdot\partial_\mu s = -\gamma^\mu s\cdot\partial_\mu v. \tag{7.7b}$$

Given the conservation law (6.5) for the Dirac current $j = e\rho v$ and the identity $\Box\cdot(\Box\cdot M) = 0$, one finds from (7.6), the conservation law

$$\Box\cdot k = \partial_\mu k^\mu = 0. \tag{7.8}$$

Accepting the conventional interpretation of j as the total charge current and identifying $\Box\cdot M$ as a magnetization current, one is lead by (7.6) to interpret $(e/mc)k$ as a convection current. In this way the Gordon current is given a physical interpretation, however, the significance of its close relation to the energy–momentum exhibited by (7.7) remains obscure, though it is clearly tied up with the significance of β. Since, as has already been mentioned, $\sin\beta$ should be regarded as a small quantity, (7.7) shows that the Gordon current is nearly proportional to the energy–momentum density. However, it is not possible in the exact Dirac theory to identify $(e/mc)\rho p$ as a charge current density, because it does not have vanishing divergence. One can express $\Box\cdot(\rho p)$ in terms of other observables by taking the divergence of (6.55), obtaining immediately

$$\Box\cdot(\rho p) = -mc\rho v\cdot(\Box\beta)\sin\beta + \{\Box\cdot(\rho i S)\}\cdot\Box\beta.$$

But, as shown in Sec. 5 of Ref. 3 the Dirac equation also implies

$$\Box\cdot(i\rho S) = mc\rho v\sin\beta + (\Box\beta)\cdot(\rho S) + \rho q.$$

Hence, one gets the exact relations

$$\Box\cdot(\rho p) = \rho q\cdot\Box\beta = \rho v\cdot\{(\Box\beta)\cdot\Box s\} = -\rho s\cdot\{(\Box\beta)\cdot\Box v\}. \tag{7.9}$$

Regarding β as small, one gets immediately from (7.7a)

$$k \approx \rho p. \tag{7.10}$$

By (6.7) and (7.5), the "time component" of the Gordon current is, in the N.R. limit,

$$\gamma_0\cdot k \approx \rho\frac{\epsilon}{c} \approx mc\rho, \tag{7.11a}$$

while the "space component" is

$$\mathbf{k} \equiv k\wedge\gamma_0 = \rho\mathbf{p}. \tag{7.11b}$$

And, if β is slowly varying, one gets from (7.9)

$$\Box\cdot(\rho p) \approx m\partial_t\rho + \nabla\cdot(\rho\mathbf{p}) = 0. \tag{7.12}$$

Substituting (7.11b) into (7.4), one gets

$$e\rho\mathbf{v} = \frac{e}{m}\mathbf{k} + \nabla\times\left(\rho\frac{e}{m}\mathbf{s}\right), \tag{7.13}$$

the N.R. expression for a charge current expressed as a conduction current plus a magnetization current.

Returning now to the expression (6.53) for the interaction energy density, we are particularly interested in the N.R. limit of the two terms explicitly involving the electric field. Let us refer to these terms collectively as the *spin-electric* energy density and denote them by $\rho_0 E_{SE}$. Recalling (7.3b), we find that (6.53) gives us

$$\rho_0 E_{SE} \approx -\frac{e}{2mc^2}\rho\mathbf{s}\cdot(\mathbf{E}\times\mathbf{v}) - \frac{e}{mc}\mathbf{s}\cdot\mathbf{E}\rho\beta. \tag{7.14}$$

Using (7.4) we can determine how the first term in (7.14) couples to the momentum instead of the velocity. Thus, using the fact that $\mathbf{s}^2 = \frac{1}{4}\hbar^2$ implies $\mathbf{s}\cdot(\partial_k\mathbf{s}) = 0$, we find that

$$\begin{aligned}m\rho\mathbf{s}\cdot(\mathbf{E}\times\mathbf{v}) - \rho\mathbf{s}\cdot(\mathbf{E}\times\mathbf{p}) &= \mathbf{s}\cdot[\mathbf{E}\times(\nabla\times\rho\mathbf{s})] \\ &= -\mathbf{s}^2\mathbf{E}\cdot\nabla\rho + \mathbf{E}\cdot\mathbf{s}\mathbf{s}\cdot\nabla\rho + \rho\mathbf{E}\cdot(\mathbf{s}\cdot\nabla\mathbf{s}).\end{aligned} \tag{7.15}$$

By virtue of (7.3a) the last term in (7.14) can be written

$$-\frac{e}{mc}\mathbf{s}\cdot\mathbf{E}\rho\beta = \frac{e}{m^2c^2}\mathbf{s}\cdot\mathbf{E}\nabla\cdot(\rho\mathbf{s}), \tag{7.16}$$

which reveals that it gives a contribution of the same order of magnitude as the next to last term in (7.14). With the help of (7.15) and (7.16) we can write (7.14) in the form

$$\rho_0 E_{SE} = -\frac{e}{2m^2c^2}\{\rho\mathbf{s}\cdot(\mathbf{E}\times\mathbf{p}) + \mathbf{s}^2(\rho\nabla\cdot\mathbf{E} - \nabla\cdot(\rho\mathbf{E}))\}$$

$$-\frac{e}{2m^2c^2}\mathbf{E}\cdot\{\mathbf{s}(\mathbf{s}\cdot\nabla\rho+2\nabla\cdot(\rho\mathbf{s}))+\mathbf{s}\cdot\nabla\mathbf{s}\}. \quad (7.17)$$

Discussion of this result will be deferred until a subsequent paper, when we will be in a position to compare it with results obtained by conventional methods.

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Consistency in the formulation of the Dirac, Pauli, and Schrödinger theories

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Properties of observables in the Pauli and Schrödinger theories and first order relativistic approximations to them are *derived* from the Dirac theory. They are found to be *inconsistent* with customary interpretations in many respects. For example, failure to identify the "Darwin term" as the s-state spin–orbit energy in conventional treatments of the hydrogen atom is traced to a failure to distinguish between charge and momentum flow in the theory. Consistency with the Dirac theory is shown to imply that the Schrödinger equation describes not a spinless particle as universally assumed, but a particle in a spin eigenstate. The bearing of spin on the interpretation of the Schrödinger theory is discussed. Conservation laws of the Dirac theory are formulated in terms of relative variables, and used to derive virial theorems and the corresponding conservation laws in the Pauli–Schrödinger theory.

1. INTRODUCTION

In quantum mechanics three different equations are widely used to describe the motion of a single electron, namely, the Schrödinger, Pauli, and Dirac equations. Each of these equations must be supplemented by physical assumptions which prescribe how to calculate observables from the electron wavefunction. The three waveequations are intimately related; the Pauli equation being an approximation to Dirac equation for small electron velocities, while the Schrödinger equation approximates the Pauli equation by neglecting magnetic interactions of the spin.

Obviously, the observables associated with the three equations should be related to one another by the same approximations. In fact, however, quite a few inconsistencies in this regard are to be found in the literature. Consider, for example the usual expressions for probability density ρ and probability current in the Schrödinger theory,

$$\rho = \Psi^\dagger \Psi, \tag{1.1a}$$

$$\rho u_k = -\frac{i\hbar}{2m}\{\Psi^\dagger \partial_k \Psi - \partial_k \Psi^\dagger \Psi\} - \frac{e}{mc} A_k \Psi^\dagger \Psi. \tag{1.1b}$$

In the Schrödinger theory, Eq. (1.1b) plays a triple role role; besides the probability current ρu_k, it determines the charge current $e\rho u_k$ associated with a charge density $e\rho$ and a kinetic momentum density $m\rho u_k$ associated with a mass density $m\rho$.

In the Pauli theory the same expressions (1.1a,b) are usually used for probability density and current, Ψ being understood as the two component Pauli wavefunction instead of the Schrödinger wavefunction (e.g., Ref. 1). In both the Schrödinger and Pauli theories the waveequation implies the conservation law

$$\partial_t \rho + \partial_k(\rho u_k) = 0. \tag{1.1c}$$

Though $e\rho$ is still interpreted as charge density, the Pauli theory differs from Schrödinger theory in that $e\rho u_k$ must be supplemented by a "spin magnetization current" $c\nabla\times\mathbf{m}$ to get the total charge current

$$\mathbf{j} = e\rho\mathbf{u} + c\nabla\times\mathbf{m}, \tag{1.2a}$$

where

$$m_k = \frac{e\hbar}{2mc}\Psi^\dagger \sigma_k \Psi \tag{1.2b}$$

and the σ_k are the usual Pauli matrices. The fact that (1.2a) is the correct expression for the charge current has been established for a long time,[2] though its importance seems to be frequently unappreciated.

Following history, textbooks show how to get from the Schrödinger theory to the Pauli theory by heuristic arguments (e.g., Ref. 1). Reversing the procedure, the Schrödinger theory can be derived rigorously (rather than heuristicly) from the Pauli theory, with some consequences that seem to have been completely overlooked. When the magnetic field is small or zero, the Pauli wave equation is identical to the Schrödinger equation and posesses solutions of the form

$$\Psi = \begin{pmatrix}\phi\\0\end{pmatrix}. \tag{1.3}$$

So from (1.1a) we have $\rho = \Psi^\dagger\Psi = \phi^\dagger\phi$ and from (1.1b) we get an expression for ρu_k with ϕ replacing Ψ. Since ϕ is a complex function satisfying the Schrödinger equation, and since its relation to the probability density and current has been derived, it would seem that we have arrived at the Schrödinger theory.

But here's the rub! we must take account of fact that Eq. (1.3) means that the electron is in an eigenstate of the spin. So what we have proved is that the *Schrödinger theory is identical to the Pauli theory when the electron is in an eigenstate of the spin.* Of course, this is at variance with the usual view that the Schrödinger theory describes a particle without spin, but it is a rigorous consequence of requiring that the theory be derivable from the Pauli theory. The difference is important! Though Eq. (1.3) yields some of the usual features of the Schrödinger theory, it also implies nonvanishing values for (1.2b), specifically, if σ_3 is diagonal as usual, then

$$m_3 = \frac{e\hbar}{2mc}\phi^\dagger\phi = \frac{e\hbar}{2mc}\rho, \quad m_1 = m_2 = 0. \tag{1.4}$$

Equation (1.4) leads to nonvanishing values for the magnetization current $\nabla\times\mathbf{m}$. Hence, the expression for the charge current $\mathbf{j}$ given by (1.2a) does not reduce to $e\rho\mathbf{u}$ when the passage to the Schrödinger theory is made. That is, the usual expression for charge current in the

Schrödinger theory obtained by multiplying (1.1b) by the charge e is *inconsistent* with the assumption that the Schrödinger theory is derivable from the Pauli theory. To put it bluntly, everyone to date has been using the wrong expression for charge current density in the Schrödinger theory. Of course there is no way that this error could be revealed directly by experiment, because the only direct experimental means of testing for the existence of a magnetization current is by introducing a magnetic field. But in that case everyone knows enough to discard the Schrödinger theory and use the Pauli or Dirac theories. However, the existence of a magnetization current has important bearing on the interpretation of the Schrödinger theory even in the absence of a magnetic field. For instance, it implies that there is a nonvanishing charge current in the s-states of hydrogen, eliminating one of the reputedly fundamental differences between the Schrödinger and Bohr theories. It also leads to the conclusion that the appearance of complex numbers in the Schrödinger theory is inseparably related to the existence of the spin, the factor $i\hbar$ being significant in the theory only because $\frac{1}{2}i\hbar$ is an eigenvalue of the matrix representing the spin. This is difficult to reconcile with conventional interpretations of the uncertainty principle.

Though it is supported experimentally, the expression (1.2a) for the charge current was originally introduced into the Pauli theory as an *ad hoc* assumption. So it is important to know that it can be justified on deeper theoretical grounds. The charge current in the Dirac theory is given by the wellknown expression

$$j^\mu = e\bar{\Psi}\gamma_\mu\Psi, \tag{1.5}$$

where Ψ is now the four component Dirac wavefunction. The Dirac equation implies the conservation law

$$\partial_\mu j^\mu = 0 \tag{1.6}$$

as well as the decomposition

$$j^\mu = \frac{e}{mc}k^\mu + \partial_\nu M^{\mu\nu}, \tag{1.7a}$$

where

$$k^\mu = \frac{i\hbar}{2}\{\bar{\Psi}\partial^\mu\Psi - (\partial^\mu\bar{\Psi})\Psi\} - \frac{e}{c}A^\mu\bar{\Psi}\Psi \tag{1.7b}$$

is the so-called Gordon current,[3] and

$$M^{\mu\nu} = \frac{ie\hbar}{2mc}\Psi\tfrac{1}{2}[\gamma^\nu, \gamma^\mu]\Psi \tag{1.7c}$$

is interpreted as the magnetic moment density due to the electron spin. In the nonrelativistic limit, the time and space components of (1.7b) reduce, respectively, to (1.1a) and (1.1b), while the nonvanishing components of (1.7c) are given in (1.2b), so the space components of (1.7a) reduce exactly to Eq. (1.2a). Thus, the expression (1.2a) for the charge current in the Pauli theory is fully justified by the requirement of consistency with the Dirac theory. It is important to realize that the particular combination of currents in (1.7a) is a consequence of the Dirac equation, whereas the limiting result (1.2a) is not a consequence of the Pauli equation.

The interpretation of the Dirac current (1.5) as a charge current is well established experimentally. But the Dirac current is also interpreted as a probability current by dropping the charge e. Here we run into another inconsistency with the Schrödinger theory, for the Schrödinger current (1.1b), which is supposed to be a probability current, corresponds to the Gordon current (1.7b) and not, as we have seen, to the Dirac current. One way to resolve this difficulty might be to identify the Gordon current as the probability current in the Dirac theory. The required conservation law

$$\partial_\mu k^\mu = 0 \tag{1.8}$$

is indeed satisfied, but then new problems of normalization and interpretation arise in the Dirac theory. The only alternative is to conclude that (1.2a) rather than (1.1b) determines the correct probability current as well as the charge current. This does not mean that the Schrödinger current should be dispensed with. Indeed, by comparison with the Dirac theory, it can be shown to be proportional to the momentum density, and (1.2a) suggests it can be interpreted as a convective charge current.

The main objective of this paper is to establish a consistent identification of observables in the Dirac, Pauli, and Schrödinger theories. This will be accomplished by beginning with the formulation of the Dirac theory in terms of local observables as given in Refs. 4 and 5, and obtaining the corresponding formulations of the Pauli and Schrödinger theories as limiting cases. The unusual formulation of quantum theory employed here is fully equivalent mathematically to the conventional one. However, it brings to light certain problems in physical interpretation which, as already argued in Ref. 4, may require for their resolution some modification of current theory. No such modification of quantum theory will be attempted here. But we cannot resist expressing the opinion that the Dirac theory is best interpreted as describing statistical ensemble of particle motions and pointing out from time to time how this may help the understanding of mathematical relations in the theory. Though some of the unusual physical interpretations we suggest are open to dispute and hopefully at some time to experimental test, the mathematical steps alone show what is required to establish consistency among the Dirac, Pauli, and Schrödinger theories.

A formulation of the Dirac theory in terms of local observables like the one given in Ref. 4 is sometimes called a "hydrodynamic formulation" of quantum theory. Hydrodynamics provides a ready-made terminology for the description of continuous distributions and flows of mechanical quantities such as energy, momentum, angular momentum, and charge; as such it is useful in quantum theory, but it should be understood that the use of hydrodynamic terminology does not imply that any classical model or interpretation has been presumed. A hydrodynamic formulation of Schrödinger theory was first given by Madelung[7]; it has been discussed since by numerous authors, recently, for example, by Wilhelm.[8] Complete hydrodynamic formulations of the Pauli and Dirac theories were first given by Takabayasi,[9] though other authors, notably Costa de Beauregard,[10] achieved partial results earlier. These formulations of the Schrödinger, Pauli, and Dirac theories, though fully consistent with more conventional formulations of quan-

tum theory, are inconsistent with one another in their identifications of observables. In Ref. 6 it was shown that if the Schrödinger theory is regarded as an approximation to the Pauli theory, then it necessarily contains spin (albeit in a degenerate form). Here we show how the identification of observables in Ref. 5 must be adjusted to be consistent with the more fundamental formulation of the Dirac theory in Refs. 4 and 5.

Section 2 obtains the Pauli theory as the nonrelativistic approximation to the Dirac theory and discusses relativistic corrections. The usual physical interpretation of these results is held to be incorrect because of insufficient attention to the identification of observables, especially failure to bring the nonrelativistic limit of the Dirac (charge) current into the discussion and distinguish it from the momentum density. The Darwin term in the energy is proved to be a spin–orbit energy for s-states in exact accordance with the original argument of Thomas.

Section 3 summarizes the definitions and interrelations of observables in the Pauli–Schrödinger theory which are *required* for the sake of consistency with the Dirac theory. Some implications of the consistency requirement for the Schrödinger hydrogen atom are pointed pointed out to show that the conventional interpretation of the Schrödinger theory must be drastically revised, but no attempt is made to carry any such revision to completion.

Section 4 expresses the hydrodynamic equations of the Dirac theory in terms of relative observables, uses them to derive a virial theorem, and obtains their nonrelativistic limit.

The nomenclature and results of Refs. 4, 5, and 11 are used throughout this paper. The reader is advised to become familiar especially with Ref. 5 before attempting to follow the arguments here in any detail.

2. NONRELATIVISTIC APPROXIMATIONS TO THE DIRAC THEORY

In the literature two methods have been widely used to generate nonrelativistic approximations to the Dirac theory, namely, separation of the Dirac wavefunction into large and small components,[12,13,14] and the F–W transformation.[15] To facilitate comparison with our approach, we translate the first of these methods into multivector language. Then we criticize the physical interpretation usually accorded to the method and give reasons for interpreting it differently. Our arguments also have bearing on the F-W transformation and suggest rather different mathematical methods for generating relativistic corrections, but we do not pursue either of these points in any detail. Our objective is only to show in multivector language how the Pauli equation and relativistic corrections to it can be obtained from the Dirac equation and provided with a consistent physical interpretation.

The definition of electron energy in the Dirac theory differs from the definition in the nonrelativistic theories by including the rest energy. We can remove the rest energy while retaining the definition of the energy in terms of the wavefunction by changing the wave equation with the transformation

$$\psi \to \psi \exp\{-i\sigma_3 mc^2 t/\hbar\}, \tag{2.1}$$

whereupon the Dirac equation (3.11) of Ref. 5 becomes

$$\hbar\Box\psi i\sigma_3 + mc\gamma_0\psi = mc\psi\gamma_0 + \frac{e}{c}A\psi. \tag{2.2}$$

To express (2.2) in terms of relative variables we multiply it by $c\gamma_0$ and, recalling the definitions (6.4) and (6.22) of Ref. 5, obtain

$$\hbar(\partial_t + c\nabla)\psi i\sigma_3 = mc^2(\psi^* - \psi) + (V - e\mathbf{A})\psi, \tag{2.3}$$

where

$$\psi^* \equiv \gamma_0\psi\gamma_0. \tag{2.4}$$

The wavefunction ψ can be expressed as the sum of an even part ψ_e and an odd part ψ_o, that is,

$$\psi = \psi_e + \psi_o, \tag{2.5a}$$

where distinction between "even" and "odd" is best made by the equation

$$\psi^* = \psi_e - \psi_o. \tag{2.5b}$$

As is easily shown by the method of Appendix A in Ref. 4, this separation of ψ into even and odd multivector parts is exactly equivalent to the usual separation of the wavefunction into large and small components in the matrix version of the Dirac theory, but we shall see only later what this separation means physically. After substituting (2.5) into (2.3) and separately equating even and odd parts we obtain the coupled equations:

$$\hbar\partial_t\psi_e i\sigma_3 = -c\left\{\hbar\nabla\psi_o i\sigma_3 + \frac{e}{c}\mathbf{A}\psi_o\right\} + V\psi_e, \tag{2.6a}$$

$$\hbar\partial_t\psi_o i\sigma_3 - V\psi_o + 2mc^2\psi_o = -c\left\{\hbar\nabla\psi_e i\sigma_3 + \frac{e}{c}\mathbf{A}\psi_e\right\}. \tag{2.6b}$$

Equations (2.6) can be solved to lowest order by neglecting the first two terms in the left of (2.6b) in relation to the third, yielding

$$\psi_o = -\frac{1}{2mc}\left\{\hbar\nabla\psi_e i\sigma_3 + \frac{e}{c}\mathbf{A}\psi_e\right\}. \tag{2.7a}$$

If we use this to eliminate ψ_0 from (2.6a), then after expanding, simplifying and using the identity

$$\mathbf{A}\psi_e + \nabla(\mathbf{A}\psi_e) = (\nabla\mathbf{A}\cdot\nabla)\psi_e = (i\mathbf{B} + 2\mathbf{A}\cdot\nabla)\psi_e,$$

we arrive at the Pauli equation

$$\hbar\partial_t\psi_e i\sigma_3 = \frac{1}{2m}\left\{-\hbar^2\nabla^2 + \frac{e^2}{c^2}\mathbf{A}^2\right\}\psi_e + \frac{e\hbar}{2mc}\{i\mathbf{B} + 2\mathbf{A}\cdot\nabla\}\psi_e i\sigma_3 + V\psi_e \tag{2.7b}$$

For readers who are still not completely at home with the multivector algebra used here, we prove that (2.7) is equivalent to the usual matrix form of the Pauli equation. This is most easily done by replacing each vector σ_k in (2.7) by a corresponding Pauli matrix σ_k according to the rules

$$\sigma_1 \to \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_2 \to \sigma_2 = \begin{pmatrix} 0 & -i' \\ i' & 0 \end{pmatrix}, \tag{2.8}$$

$$\boldsymbol{\sigma}_3 \to \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The i' here is a mathematical square root of -1 with no geometrical interpretation; however, i' multiplied by the unit matrix is a matrix representation of the pseudoscalar i, a fundamental geometrical entity. This follows from (2.8), thusly:

$$i = \boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3 \to \sigma_1\sigma_2\sigma_3 = i'\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

By (2.8) ψ_e corresponds to a matrix ψ_e' which becomes a column matrix Ψ_e by operating on an eigenmatrix u_1 of σ_3; so we make the correspondence

$$\psi_e \to \psi_e', \quad \Psi_e = \psi_e' u_1 \quad \text{where } u_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{2.9a}$$

From (2.8) we also have

$$\mathbf{B} = \boldsymbol{\sigma}_i B^i \to \sigma_i B^i \equiv \sigma \cdot \mathbf{B}. \tag{2.9b}$$

Hence regarding (2.7) as a matrix equation and multiplying it on the right by u_1, we get, by (2.8) and (2.9), the Pauli equation in its usual matrix form:

$$i'\hbar\partial_t\Psi_e = \frac{1}{2m}\left\{-\hbar^2\nabla^2 + \frac{e^2}{c^2}\mathbf{A}^2\right\}\Psi_e + \frac{e\hbar}{2mc}\{-\sigma\cdot\mathbf{B} + 2i'\mathbf{A}\cdot\nabla\}\Psi_e + V\Psi_e. \tag{2.10}$$

Now we return to the multivector formalism and the coupled equations (2.6a,b).

To obtain higher order approximations to (2.6a,b) in a systematic way and to discuss the usual physical interpretation of the results, it is convenient to introduce operators $\hat{K}$, $\hat{\mathbf{p}}$, and $\hat{p}_k$ defined by

$$\hat{K}\psi \equiv \hbar\partial_t\psi i\boldsymbol{\sigma}_3 - V\psi, \tag{2.11}$$

$$\hat{\mathbf{p}}\psi \equiv -\hbar\nabla\psi i\boldsymbol{\sigma}_3 - \frac{e}{c}\mathbf{A}\psi = \boldsymbol{\sigma}_k p_k\psi, \tag{2.12a}$$

$$\hat{\mathbf{p}}_k\psi \equiv -\hbar\partial_k\psi i\boldsymbol{\sigma}_3 - \frac{e}{c}\mathbf{A}_k\psi \equiv \boldsymbol{\sigma}_k\cdot\hat{p}\psi. \tag{2.12b}$$

The Pauli equation (2.7b) can then be written

$$\hat{K}\psi_e = \frac{1}{2m}\hat{\mathbf{p}}^2\psi_e = \frac{1}{2m}\hat{p}^2\psi_e - \frac{e\hbar}{2mc}\mathbf{B}\psi_e\boldsymbol{\sigma}_3, \tag{2.13}$$

where we have used the obvious operator notation

$$\hat{p}^2 \equiv \hat{\mathbf{p}}\cdot\hat{\mathbf{p}} = \hat{p}_k\hat{p}_k. \tag{2.14}$$

Equations (2.6a,b) can be put in the form

$$\hat{K}\psi_e = c\hat{\mathbf{p}}\psi_0, \tag{2.15a}$$

$$(1 + \hat{K}/2mc^2)\psi_0 = (1/2mc)\hat{\mathbf{p}}\psi_e. \tag{2.15b}$$

Assuming $|\hat{K}\psi| \ll 2mc^2|\psi|$, (2.15b) can be solved for ψ_0 in the form

$$\psi_0 = \frac{1}{2mc}(1 + \hat{K}/2mc^2)^{-1}\hat{\mathbf{p}}\psi_e \approx \frac{1}{2mc}(1 - \hat{K}/2mc^2)\hat{\mathbf{p}}\psi_e. \tag{2.16}$$

Substituting this into (2.15a) and using the identity

$$(\hat{K}\hat{\mathbf{p}} - \hat{\mathbf{p}}\hat{K})\psi = \hbar\left(-\frac{e}{c}\partial_t\mathbf{A} - \nabla V\right)\psi i\boldsymbol{\sigma}_3 = e\hbar\mathbf{E}\psi i\boldsymbol{\sigma}_3,$$

we get

$$\hat{K}\psi_e = \frac{1}{2m}\hat{\mathbf{p}}^2\psi_e - \frac{1}{4m^2c^2}(\hat{\mathbf{p}}^2\hat{K}\psi_e + e\hbar\hat{\mathbf{p}}(\mathbf{E}\psi_e)i\boldsymbol{\sigma}_3). \tag{2.17}$$

Using (2.13) in the first and second terms on the right-hand side of this equation and the identity

$$e\hbar\hat{\mathbf{p}}(\mathbf{E}\psi)i\boldsymbol{\sigma}_3 = e\hbar^2(\nabla\mathbf{E})\psi + e\hbar(\mathbf{E}\cdot\hat{\mathbf{p}} - i\mathbf{E}\times\hat{\mathbf{p}})\psi i\boldsymbol{\sigma}_3$$

in the third term, we arrive finally at the first order correction to the Pauli equation:

$$\hat{K}\psi_e = \frac{1}{2m}\hat{p}^2\psi_e - \frac{e\hbar}{2mc}\mathbf{B}\psi_e\boldsymbol{\sigma}_3 - \frac{1}{8m^3c^2}\hat{\mathbf{p}}^2\psi_e - \frac{e\hbar^2}{4m^2c^2}(\nabla\cdot\mathbf{E} + i\nabla\times\mathbf{E})\psi_e - \frac{e\hbar}{4m^2c^2}\mathbf{E}\cdot\hat{\mathbf{p}}\psi_e i\boldsymbol{\sigma}_3 - \frac{e\hbar}{4m^2c^2}\mathbf{E}\times\hat{\mathbf{p}}\psi_e\boldsymbol{\sigma}_3. \tag{2.18}$$

With (2.8) and (2.9) it is easy to show that (2.18) is equivalent to the usual matrix equation obtained in Refs. 12–14 as the first order relativistic correction to the Pauli equation. The usual physical interpretation of (2.18) proceeds by identifying $\hat{p}_k$ as a "kinetic momentum operator" and, neglecting the difference between $\hat{p}^2$ and $\hat{\mathbf{p}}^2$ given by (2.13), interpreting the first and third terms of (2.18) as the first two terms in the expansion of a relativistic "kinetic energy operator"

$$(\hat{p}^2 + m^2c^4)^{1/2} - mc^2 = \frac{\hat{p}^2}{2m} - \frac{\hat{p}^4}{8m^3c^2} + \cdots. \tag{2.19}$$

The second and last terms of (2.15) are interpreted as spin precession energies, with the latter (spin–orbit) term being reduced in magnitude by a factor of $\frac{1}{2}$ attributed to the Thomas precession. The $\nabla\times\mathbf{E}$ term is usually neglected; in any case it does not contribute to the energy directly. With neglect of the vector potential, the $\mathbf{E}\cdot\hat{\mathbf{p}}$ term in (2.18) can be shown to contribute to the energy the negative of half the amount of the $\nabla\cdot\mathbf{E}$ term. So, for the purpose of calculating the energy, these two terms in (2.18) can be replaced by a single term $(-e\hbar^2/8m^2c^2)(\nabla\cdot\mathbf{E})\psi_e$, the so-called "Darwin term," which is usually regarded as a quantum-mechanical effect without classical interpretation. The contributions of the last four terms in (2.18) to the energy levels of hydrogen can be evaluated by perturbation theory from the hydrogen solutions to the Schrödinger equation; it has been found[16] that, as one might expect, they combine to give the α^4 term in the expansion of the Sommerfeld fine structure formula.

To sum up, the usual interpretation regards (2.18) as an approximate separation of the Dirac energy into kinetic and interaction energies. Simple and natural as this interpretation appears from the operator formulation of (2.18), it is inconsistent with the identification of kinetic energy and momentum already made in the exact Dirac theory. Nothing in the Dirac theory justifies the interpretation of (2.19) as a "kinetic energy operator." Indeed, if the operator $\hat{p}_k$ is to be interpreted as the "kinetic momentum operator," then on the basis of "relativistic invariance" alone, the operator $\hat{K}$ defined by (2.11) must be regarded as the "kinetic energy operator," which is certainly inconsistent with the interpretation of (2.18) reviewed above.

Nevertheless, in the "Schrödinger approximation" to be discussed later, $\hat{K}\psi_e = (2m)^{-1}\hat{p}^2\psi_e$, showing at least that the usual interpretation of $(2m)^{-1}\hat{p}^2$ as an *approximate* kinetic energy operator is consistent with the Dirac theory.

Section 6 of Ref. 5 gave an exact derivation of the Larmor precession energy and found that it arises from the electron mass density. Of course, in a statistical theory it is possible to identify in the mass density contributions from the kinetic and interaction energies of the statistical ensemble, but this is not allowed in the conventional Dirac theory, where the best that can be done is to determine how the mass is affected by external fields. New interpretations cannot emerge from approximations to an exact theory.

It was also shown that the Thomas precession energy came from the kinetic momentum, and to identify it the kinetic momentum was separated into two parts in Eq. (6.48) of Ref. 5. Heretofore, no one has paid attention to the fact that a similar separation was made implicitly in the derivation of (2.18). So much emphasis is laid on the correspondence between operators and observables that it is sometimes overlooked that an operator must act on a wavefunction to produce an observable quantity. This simple fact obviously implies that a change in the wavefunction while an operator is kept fixed will generally change the correspondence with observables. Exactly this kind of change was made in arriving at (2.18). The operator $\hat{p}_k$ introduced in (2.12) can indeed (with due attention to its relation of the energy–momentum tensor) be regarded as a momentum operator when it acts on the Dirac wavefunction ψ. It follows that the operator equation $\hat{p}_k\psi = \hat{p}_k\psi_e + \hat{p}_k\psi_0$ corresponds to a separation of the momentum into two parts. But only $\hat{p}_k\psi_e$ is associated with momentum in (2.12) and (2.18), though $\hat{p}_k\psi_0$ is negligible only in the zeroth order (Pauli) approximation; this amounts to a change in the interpretation of the theory by identifying a different quantity as momentum. As a result, the Larmor and Thomas precession energies appear (magically) as interaction terms. Of course, as long as only the total energy is being measured experimentally it does not matter what part of it is called kinetic; only the coupling with external fields is important. However, the spin and momentum are related to one another by the angular momentum conservation law, and the interpretation of one cannot be changed without affecting the other. When this is taken into account, arbitrariness in the interpretation of various contributions to the energy is eliminated.

Before (2.18) can be correctly interpreted, the relation of ψ_e to the Dirac observables must be determined. The physical meaning of the decomposition $\psi = \psi_e + \psi_0$ is revealed by the decomposition

$$\psi = \rho^{1/2}\exp(i\beta/2)LU \tag{2.20}$$

obtained from Eqs. (4.2) and (6.15) of Ref. 5. The spinor L can be expressed in terms of the relative velocity $\mathbf{v}$ by taking the square root of (6.1c) in Ref. 5 to obtain (e.g., Eq. (18.14) of Ref. 17)

$$L = \frac{v_0^{1/2}}{\sqrt{2}}\left(\frac{1}{\alpha} + \frac{\alpha v}{c}\right)$$

$$\text{where } \alpha \equiv \frac{v_0^{1/2}}{(v_0+1)^{1/2}} \text{ and } v_0 = (1-\mathbf{v}^2/c^2)^{1/2}. \tag{2.21}$$

Hence (2.20) can be written

$$\psi = \frac{\exp(i\beta/2)}{\sqrt{2}}\left(\frac{1}{2} + \frac{\alpha\mathbf{v}}{c}\right)\rho_0^{1/2}U, \tag{2.22}$$

where of course $\rho_0 = \rho v_0$. The separation of (2.22) into even and odd parts is easily accomplished by noting that $\mathbf{v}$ and i are odd (i.e., $\gamma_0\mathbf{v}\gamma_0 = -\mathbf{v}$ and $\gamma_0 i\gamma_0 = -i$), while U is even (i.e., $\gamma_0 U\gamma_0 = U$); hence

$$\psi_e = \frac{1}{\sqrt{2}}\left(\frac{\cos\frac{1}{2}\beta}{\alpha} + i\frac{\mathbf{v}\alpha}{c}\sin\tfrac{1}{2}\beta\right)\rho_0^{1/2}U, \tag{2.23a}$$

$$\psi_0 = \frac{1}{\sqrt{2}}\left(\frac{i\sin\frac{1}{2}\beta}{\alpha} + \frac{\mathbf{v}\alpha}{c}\cos\tfrac{1}{2}\beta\right)\rho_0^{1/2}U. \tag{2.23b}$$

For $|\mathbf{v}/c \ll 1$, $\alpha \approx (2)^{-1/2}$, in which case it is clear from (2.23) that $|\psi_0| \ll |\psi_e|$ only if β is simultaneously small (modulo π of course). Thus β small is a prerequisite for the Pauli equation to obtain as the N.R. limit of the Dirac equation. We do not attempt to explain this fact here, we merely record it as another clue to the physical interpretation of the mysterious parameter β, and we note that (2.23) shows exactly how the separation of ψ into even and odd parts depends on $\mathbf{v}/c$, a fact which we now exploit.

Expanding (2.23a,b) in β and $|\mathbf{v}|/c$ and keeping terms to first order only in both quantities, we get

$$\psi_e \approx \rho^{1/2}U \approx \rho_0^{1/2}U \equiv \chi, \tag{2.24a}$$

$$\psi_0 \approx \tfrac{1}{2}(i\beta + \mathbf{v}/c)\chi. \tag{2.24b}$$

Substitutting these in (2.7a) and multiplying on the right by $2\tilde{\chi}$, we obtain

$$\left(i\beta + \frac{\mathbf{v}}{c}\right)\rho = -\frac{1}{mc}\left\{\hbar\nabla\chi i\sigma_3 + \frac{3}{c}\mathbf{A}\chi\right\}\tilde{\chi} = \frac{1}{mc}(\hat{\mathbf{p}}\chi)\tilde{\chi}. \tag{2.25a}$$

Separating this into relative vector and pseudovector parts, we get

$$\mathbf{v} = -\frac{\hbar}{m\rho}[\nabla\chi i\sigma_3\tilde{\chi}]_{(1)} - \frac{e}{c}\mathbf{A} \tag{2.25b}$$

and

$$\beta = -\frac{\hbar}{mc\rho}[\nabla\chi\sigma_3\tilde{\chi}]_{(0)} = -\frac{1}{mc}\frac{\hbar}{2}\nabla\cdot(\chi\sigma_3\tilde{\chi})$$

$$= -\frac{1}{mc\rho}\nabla\cdot(\rho\mathbf{s}), \tag{2.25c}$$

where we have used (6.16) and (7.3a) of Ref. 5 to identify the relation of the spin to the Pauli wavefunction χ as

$$\rho\mathbf{s} = \frac{\hbar}{2}\rho U\sigma_3\tilde{U} = \frac{\hbar}{2}\chi\sigma_3\tilde{\chi}. \tag{2.26}$$

The result (2.25c) is just an approximate derivation of (7.3a) in Ref. 5, which has already been shown to hold under more general assumptions. Equation (2.25b) is the correct expression for the electron velocity in terms of the Pauli wavefunction. This reveals the physical significance of Eq. (2.7a) in the Pauli theory.

We are now in a position to examine the physical significance of the spin-electric coupling terms in (2.18) by expressing them in terms of local observables. The

last three terms in (2.18) are equivalent to the single term in (2.17)

$$-\frac{e\hbar}{4m^2c^2}\hat{\mathbf{p}}(\mathbf{E}\psi_e)i\sigma_3=-\frac{e\hbar^2}{4m^2c^2}\nabla(\mathbf{E}\psi_e)$$

$$=-\frac{e\hbar^2}{4m^2c^2}[(\nabla\mathbf{E})\psi_e+2\mathbf{E}\cdot\nabla\psi_e-\mathbf{E}\nabla\psi_e], \tag{2.27}$$

which we have reexpressed by using (2.12a) and neglecting the vector potential $\mathbf{A}$. In the present approximation, we can replace ψ_e in (2.27) by the Pauli wavefunction $\chi=\rho^{1/2}U$, whereupon, after multiplication on the right by $\tilde{\chi}$, (2.27) becomes

$$-\frac{e\hbar}{4m^2c^2}(\hat{\mathbf{p}}\mathbf{E}\chi)i\sigma_3\tilde{\chi}=-\frac{e\hbar^2}{4m^2c^2}(\rho\nabla\mathbf{E}+\mathbf{E}\cdot\nabla\rho+2(\mathbf{E}\cdot\nabla U)\tilde{U})$$

$$+\frac{e}{2mc}\mathbf{E}\left(\frac{\hbar^2}{2mc}(\nabla\chi)\tilde{\chi}\right). \tag{2.28}$$

But if (2.25a) is multiplied by $i\mathbf{s}$ and (2.26) is used, one finds, neglecting $\mathbf{A}$,

$$\frac{\hbar^2}{2mc}(\nabla\chi)\tilde{\chi}=\left(i\frac{\mathbf{v}}{c}-\beta\right)\rho\mathbf{s}. \tag{2.29}$$

Noting that $\mathbf{s}^2=\frac{1}{4}\hbar^2$, that $(\mathbf{E}\cdot\nabla U)\tilde{U}$ is a bivector, and that $i\mathbf{E}\mathbf{v}\mathbf{s}=\mathbf{E}\cdot\mathbf{v}i\mathbf{s}-(\mathbf{E}\times\mathbf{v})\mathbf{s}$, we obtain, on substituting (2.29) and (2.28) and taking the scalar part,

$$-\frac{e\hbar}{4m^2c^2}[(\hat{\mathbf{p}}\mathbf{E}\chi)i\sigma_3\tilde{\chi}]_{(0)}=-\frac{e\mathbf{s}^2}{m^2c^2}\nabla\cdot(\rho\mathbf{E})$$

$$-\frac{e}{2mc^2}\rho\mathbf{s}\cdot(\mathbf{E}\times\mathbf{v})-\frac{e}{2mc}\mathbf{s}\cdot\mathbf{E}\rho\beta. \tag{2.30}$$

Of course, the perfect divergence $\nabla\cdot(\rho\mathbf{E})$ in (2.30) has a vanishing contribution to the total energy so, with $\sin\beta=\beta$, (2.30) is seen to differ from the expression (7.14) of Ref. 5 for the spin-electric energy density essentially by a factor $\frac{1}{2}$ in the last term. We shall not look into the reason for this discrepancy, because it does not affect matters of interpretation which concern us now.

The importance of the last term in (2.30) depends on the magnitude of β relative to $|\mathbf{v}|/c$, and that can be determined only by computation from the solution to the wave equation. The hydrogen atom solutions to the Pauli equation gives $\mathbf{s}$ constant, in which case (2.25c) gives $\beta=-(mc)^{-1}\mathbf{s}\cdot\nabla\ln\rho$; so if ρ is a sufficiently slowly varying function of position, we have $\beta\ll|\mathbf{v}|/c$, and (2.30) is equivalent to (7.14) and (7.17) in Ref. 5, giving us in this approximation

$$\rho E_{SE}=-\frac{e}{2mc^2}\rho\mathbf{s}\cdot(\mathbf{E}\times\mathbf{v})$$

$$=-\frac{e}{2m^2c^2}\{\rho\mathbf{s}\cdot(\mathbf{E}\times\mathbf{p})+\mathbf{s}^2(\rho\nabla\cdot\mathbf{E}-\nabla\cdot(\rho\mathbf{E})\}. \tag{2.31}$$

This shows that the hydrogen spin-electric energy given by (2.18) is identical to the one arrived at by Thomas from purely classical considerations (see Ref. 1). This fact is disguised in (2.18) by the use of operators and the failure to distinguish between velocity and momentum.

The mysterious Darwin term is completely explained by (2.31). Since $\nabla\cdot\mathbf{E}$ is proportional to a delta function vanishing everywhere except at the origin and ρ is non-vanishing at the origin only for s-states, the Darwin term contributes only to s-states. But $\mathbf{p}=0$ for s-states, so (2.31) shows that the Darwin term gives the entire spin–orbit coupling for s-states. Even though the momentum density $\rho\mathbf{p}$ vanishes for s-states, spin–orbit coupling is possible because the charge current $e\rho\mathbf{v}=em^{-1}\nabla\times\rho\mathbf{s}$ is finite. The numerical coefficient of the Darwin term is notable; as (2.31) shows a factor $\hbar^2/8$ arises from the "Thomas factor" $\frac{1}{2}$ and the spin $\mathbf{s}^2=\frac{1}{4}\hbar^2$.

For other than s-states the distinction between velocity and momentum is not so important, being responsible only for a term $-\frac{1}{2}em^{-2}c^{-2}\mathbf{E}\cdot\mathbf{s}\mathbf{s}\cdot\nabla\rho$ which was neglected in relating (7.17) of Ref. 5 to (2.31) here. This is to say that the magnetization current makes an important contribution to the energy only for s-states, where it is the entire current.

The identification of Thomas precession in the Dirac theory is justified in current textbooks solely by noting the factor $\frac{1}{2}$ in the spin orbit term of (2.18) which remains after associating a factor $\frac{1}{2}\hbar$ with the spin. The identification of the "Thomas factor" is correct, as we have shown by the same general argument as Thomas, based primarily on the fact that the proper spin S is always orthogonal to the proper particle velocity v. But it's appearance in (2.18) is rather fortuitous, because the separation of the Dirac momentum into $\hat{p}_k\psi_e+p_k\psi_0$ which makes the Thomas precession explicit in (2.18) is equivalent to the exact separation made in (6.48) of Ref. 5 only to first order. It must be remembered that, as cautioned in Ref. 5, it is possible to talk of the Thomas precession only when $\Sigma=Ui\sigma_3\tilde{U}$ is taken to be the spin.

3. OBSERVABLES IN THE PAULI–SCHRÖDINGER THEORY

In the introduction we pointed out that the interpretation of the Schrödinger theory as a theory of an electron without spin is inconsistent with the view that it is an approximation to the Dirac theory. *Consistency requires that the Schrödinger theory be regarded as describing an electron in an eigenstate of spin.* Here the term "eigenstate" can be taken in the usual sense. But we think that the sense suggested in Sec. 5 of Ref. 5 is more revealing. Accordingly, *we say that an electron is in an eigenstate of the spin if and only if the local spin vector* $\mathbf{s}=U\sigma_3\tilde{U}$ is uniform, i.e., constant in time and homogeneous in space.

To emphasize the fact that the Schrödinger theory is identical to the Pauli theory for an electron in an eigenstate of spin, we speak of the "Pauli–Schrödinger (P–S) theory." The P–S theory has already been discussed in Ref. 6, and everything mentioned there is consistent with the Dirac theory. But the derivation of the P–S theory from the Dirac theory which has been carried out in the preceeding sections reveals some important features of the P–S theory which were not mentioned in Ref. 6. This has particularly significant consequences for the interpretation of the Schrödinger theory.

Let us summarize the *assumptions* of the P–S theory

which we have *derived* from the Dirac theory in Sec. 2. The P–S wavefunction χ can be written in the form

$$\chi = \rho^{\frac{1}{2}} U, \tag{3.1a}$$

where

$$UU^\dagger = 1, \tag{3.1b}$$

$$U^\dagger \equiv \gamma_0 \tilde{U} \gamma_0 = \tilde{U} \tag{3.1c}$$

and

$$\rho = \chi^\dagger \chi = \chi \chi^\dagger \tag{3.2a}$$

is a scalar to be interpreted as the probability density. The wavefunction χ is determined by assuming that it is a solution of the Pauli equation (2.7b) or (2.13). As emphasized in Ref. 6, the Pauli equation reduces to the Schrödinger equation when the magnetic field is sufficiently small. Besides the probability density (3.2a), the fundamental observables of the P–S theory are the energy density ρE, the momentum density $\rho \mathbf{p}$, the spin density $\rho \mathbf{s}$, and the charge current $\mathbf{j} = e\rho \mathbf{v}$; they are expressible in terms of the wavefunction by the equations

$$\rho E = \hbar(\partial_t \chi i\sigma_3 \chi^\dagger)_{(0)} = \rho\hbar(\partial_t U i\sigma_3 U^\dagger)_{(0)}, \tag{3.2b}$$

$$\rho \mathbf{s} = \frac{\hbar}{2} \chi \boldsymbol{\sigma}_3 \chi^\dagger = \frac{\hbar}{2} \rho U \boldsymbol{\sigma}_3 U^\dagger, \tag{3.2c}$$

$$(\hat{p}_k \chi)\chi^\dagger \equiv -\left\{\hbar\partial_k \chi i\boldsymbol{\sigma}_3 + \frac{e}{c} A_k \chi\right\}\chi^\dagger = \rho p_k - i\partial_k(\rho \mathbf{s}), \tag{3.2d}$$

$$m^{-1}(\hat{\mathbf{p}}\chi)\chi^\dagger \equiv -m^{-1}\left\{\hbar\nabla\chi i\boldsymbol{\sigma}_3 + \frac{e}{c}\mathbf{A}\chi\right\}\chi^\dagger = \rho(\mathbf{v} + ic\beta). \tag{3.2e}$$

This completes the list of assumptions derived for the P–S theory.

For purposes of comparison, we use (2.8) and (2.9) to express the observables (3.2) in the usual matrix notation. Writing $\Psi = \chi u_1$, as in (2.9a), for the matrix wavefunction, introducing $\hat{p}_k \Psi \equiv -(i'\hbar\partial_k + (e/c)A_k)\Psi$, and using Re to denote "real part," we get

$$\rho = \chi^\dagger \chi = (\chi^\dagger \chi)_{(0)} = \Psi^\dagger \Psi, \tag{3.3a}$$

$$\rho E = \hbar(\chi^\dagger \partial_t \chi i\boldsymbol{\sigma}_3)_{(0)} = \mathrm{Re}\{i'\hbar\Psi^\dagger \partial_t \Psi\}, \tag{3.3b}$$

$$\rho s_k = \rho \mathbf{s}\cdot\boldsymbol{\sigma}_k = \frac{\hbar}{2}(\boldsymbol{\sigma}_k \chi \boldsymbol{\sigma}_3 \chi^\dagger)_{(0)} = \frac{\hbar}{2}\Psi^\dagger \boldsymbol{\sigma}_k \Psi, \tag{3.3c}$$

$$\rho p_k = \rho(U^\dagger \hat{p}_k U)_{(0)} = (\chi^\dagger \hat{p}_k \chi)_{(0)} = \mathrm{Re}\{\Psi^\dagger \hat{p}_k \Psi\}, \tag{3.3d}$$

$$\rho v_k = \rho \mathbf{v}\cdot\boldsymbol{\sigma}_k = m^{-1}(\chi^\dagger \boldsymbol{\sigma}_k \hat{\mathbf{p}}\chi)_{(0)}$$
$$= m^{-1}\,\mathrm{Re}\{\Psi^\dagger \boldsymbol{\sigma}_k \boldsymbol{\sigma}_j \hat{p}_j \Psi\}. \tag{3.3e}$$

Equations (3.3) can be used instead of (3.2) to relate observables to the wavefunction, but (3.2) is easier to work with. For example, using $m^{-1}\hat{\mathbf{p}} = m^{-1}\boldsymbol{\sigma}_k \hat{p}_k$, we get immediately from (3.2d) and (3.2e)

$$\rho \mathbf{p} - i\nabla(\rho \mathbf{s}) = m\rho(\mathbf{v} + ic\beta). \tag{3.4a}$$

Since $\nabla(\rho \mathbf{s}) = \nabla\cdot(\rho \mathbf{s}) + i\nabla\times(\rho \mathbf{s})$, the vector part of (3.4a) is

$$m\rho\mathbf{v} = \rho\mathbf{p} + \nabla\times(\rho \mathbf{s}), \tag{3.4b}$$

while the pseudovector part gives

$$mc\rho\beta = -\nabla\cdot(\rho \mathbf{s}). \tag{3.4c}$$

In Sec. 7 of Ref. 5 the fundamental relation (3.4b) was derived from a "constitutive equation" determined by the Dirac equation. In Sec. 2 we saw that a decoupling of (3.4b) from the waveequation was brought about by the separation of the Dirac wavefunction into large and small components. So (3.4b) must be introduced into the P–S theory as an assumption independent of the P–S waveequation. It has already been pointed out in Sec. 7 of Ref. 5 that (3.4b) expresses the separation of the total charge current $j = e\rho\mathbf{v}$ into a convection current $em^{-1}\rho\mathbf{p}$ and a magnetization current $\nabla\times(em^{-1}\rho \mathbf{s})$ written as Eq. (1.2) in the introduction. The physical significance of (3.4c) is not as obvious as that of (3.4b). Indeed, since the function β is given in terms of ρ and $\mathbf{s}$ by (3.4c), it need not be introduced into the theory at all. However, we have already observed the peculiar role of β in the Dirac theory, so it should be interesting to see how it enters the P–S theory.

From the set of basic observables (3.2) other observables can be constructed. Chief among these are the "orbital angular momentum density"

$$\rho\mathbf{L} \equiv \mathbf{x}\times(\rho\mathbf{p}) = \rho\mathbf{x}\times\mathbf{p} \tag{3.5}$$

and the "total angular momentum density"

$$\rho J \equiv \rho(\mathbf{L} + \mathbf{s}). \tag{3.6}$$

Since, according to (3.4b), $\mathbf{p} \neq m\mathbf{v}$, the moment of charge differs from the moment of momentum. To express this difference we introduce the orbital momentum density

$$\rho\mathbf{L}^* \equiv \mathbf{x}\times(\rho m\mathbf{v}) = m\rho\mathbf{x}\times\mathbf{v}. \tag{3.7}$$

By virtue of (3.4b), the relation between the two orbital moment densities can be put in the form

$$\rho\mathbf{L}^* = \rho\mathbf{L} + 2\rho\mathbf{s} + \partial_k\{\rho\mathbf{x}\times(\boldsymbol{\sigma}_k\times\mathbf{s})\}. \tag{3.8}$$

Other important observables appear when we use the Pauli equation to derive equations of motion for the local observables. With $\mathbf{p}$ and $\mathbf{v}$ related to the wave equation by (3.2d,e), it is easy to show that the Pauli equation implies the conservation laws

$$\partial_t\rho + \nabla\cdot(m^{-1}\rho\mathbf{p}) = 0, \tag{3.9}$$

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{v}) = 0. \tag{3.10}$$

Indeed, either of these equations follows from the other by virtue of (3.4b). Equation (3.9) implies the existence of momentum streamlines. We can always write the equation for momentum conservation on such a streamline in the general form

$$\rho D_t\mathbf{p} \equiv \rho(\partial_t + (\mathbf{p}/m)\cdot\nabla)\mathbf{p} = \rho\mathbf{f}' - \partial_k\mathbf{N}'_k. \tag{3.11a}$$

This introduces the *force density* $\rho\mathbf{f}'$ and the stress $\mathbf{N}'_k$ on a volume element moving with the streamline as local observables. In Ref. 6, the Pauli equation was shown to lead to the specific expressions

$$\mathbf{f}' = e\{\mathbf{E} + (\mathbf{p}/mc)\times\mathbf{B}\} + (e/mc)\boldsymbol{\sigma}_k\mathbf{s}\cdot\partial_k\mathbf{B}, \tag{3.11b}$$

$$\mathbf{N}'_k = -M^{-1}\rho\boldsymbol{\sigma}_j\mathbf{s}\cdot(\partial_j\partial_k\mathbf{s} + \mathbf{s}\partial_j\partial_k\ln\rho) \tag{3.11c}$$

for $\mathbf{f}'$ and $\mathbf{N}'_k$ in terms of the basic local observables of (3.2).

On the other hand, Eq. (3.10) rather than (3.9) rather than (3.9) is the charge conservation equation, and momentum conservation along a *charge* (or *velocity*)

streamline has the general form

$$\rho d_t \mathbf{p} \equiv \rho(\partial_t + \mathbf{v}\cdot\nabla)\mathbf{p} = \rho\mathbf{f} - \partial_k \mathbf{N}_k. \tag{3.12a}$$

By the method of Ref. 6 it can be shown that the Pauli equation leads to the expressions

$$\mathbf{f} = e\{\mathbf{E} + (\mathbf{v}/c)\times\mathbf{B}\}, \tag{3.12b}$$

$$\mathbf{N}_k = \rho c\sigma_k \cdot \mathbf{s}\nabla\beta + \sigma_j \mathbf{s}\cdot(\sigma_k \times \partial_j \mathbf{v}). \tag{3.12c}$$

We will not carry out the derivation here, because in Sec. 4 the same results will be obtained from the hydrodynamic formulation of the Dirac theory. The corresponding conservation laws for angular momentum will also be obtained. Our object here is only to compare the conservation laws (3.11) and (3.12) on the momentum and charge streamlines.

The structure of the stress terms (3.11c) and (3.12b) appears to be difficult to understand. But (3.12b) shows that the force on a charge streamline is exactly the classical "Lorentz force"; this by itself is nearly sufficient to show that the electromagnetic interaction in quantum theory is the same as in classical theory. On the other hand, (3.11b) shows that the force on a momentum streamline consists of a "Lorentz force" supplemented by a "Stern–Gerlach force." In the light of (3.12b), we conclude that the "Stern–Gerlach force" arises from the circulation of charge relative to the momentum streamlines. The same general conclusion was reached in Ref. 4 by an examination of the hydrodynamic formulation Dirac theory. But it should be recalled that the analysis there is complicated by the fact that there are no momentum streamlines in the exact Dirac theory, though there are streamlines generated by the Gordon current.

We have summarized how observables are brought into the P–S theory. A basic set such as (3.2) must be defined in terms of the wavefunction, while the remaining observables arise when the wave equation is used to construct the conservation laws. In this connection it is well to recall that, as shown in Ref. 6, even the spin does not have to be introduced by definition in the Dirac theory, because it is determined by the conservation laws. The conservation laws are equations of motion for the observables, and as we have seen with (3.11) and (3.12) they have properties which can be interpreted physically. In this way the physical consequences of the wave equation are revealed.

So far we have discussed only local observables in the P–S theory. The "average" (or "global") observables obtained by averaging local observables over spaces are easier to study experimentally, so we now ascertain some of their properties.

The average momentum has the classical relation to the average velocity

$$\langle\mathbf{p}\rangle \equiv \int d^3x\rho\mathbf{p} = m\langle\mathbf{v}\rangle. \tag{3.13}$$

This follows from (3.4b) since the contribution of the "spin current" vanishes by Gauss's theorem. However, by integrating (3.8) we find that the angular momentum differs from the average moment of charge according to the formula

$$\langle\mathbf{L}^*\rangle = \langle\mathbf{L}\rangle + 2\langle\mathbf{s}\rangle. \tag{3.14}$$

Multiplying the Pauli equation (2.13) by $\psi_e^\dagger = \chi^\dagger$, taking the scalar part and integrating, we get the expression for the average kinetic energy

$$\langle K\rangle = \left\langle\frac{\hat{p}2}{2m}\right\rangle - \frac{e}{mc}\langle\mathbf{B}\cdot\mathbf{s}\rangle = \langle E\rangle - \langle V\rangle, \tag{3.15}$$

where, in particular,

$$\langle\hat{p}^2\rangle = \int d^3x(\chi^\dagger\hat{p}^2\chi)_{(0)}, \tag{3.16}$$

$$\langle\mathbf{B}\cdot\mathbf{s}\rangle = \int d^3x\rho\mathbf{B}\cdot\mathbf{s}. \tag{3.17}$$

The "operator expectation" (3.16) can be reexpressed in terms of the velocity, with the striking result

$$\langle\hat{K}\rangle = \langle\tfrac{1}{2}m\mathbf{v}^2\rangle + \langle\tfrac{1}{2}mc^2\beta^2\rangle. \tag{3.18}$$

In Sec. 4 this result will be obtained from an exact relation holding in the Dirac theory.

According to (2.15) the operator $(2m)^{-1}\hat{p}^2$ can be interpreted as the *kinetic energy* operator only if $\langle\mathbf{B}\cdot\mathbf{s}\rangle = 0$, that is, in the Schrödinger approximation to the Pauli theory. The expression $\langle\hat{p}^2\rangle$ is unsatisfactory from our point of view, because it has not been expressed in terms of the basic local observables in (2.2). We can easily reexpress it in terms of the momentum (2.3d) by using Eq. (4.11) of Ref. 6, which shows us that

$$(\chi^\dagger\hat{p}^2\chi)_0 = \rho\{\mathbf{p}^2 - \mathbf{s}^2[2\nabla^2\ln\rho + (\nabla\ln\rho)^2] - \mathbf{s}\cdot(\nabla^2\mathbf{s})\}. \tag{3.19}$$

Hence

$$\langle\hat{p}^2\rangle = \langle\mathbf{p}^2\rangle - \langle\mathbf{s}^2[2\nabla^2\ln\rho + (\nabla\ln\rho)^2] - \mathbf{s}(\nabla^2\mathbf{s})\rangle. \tag{3.20}$$

Equation (3.20) shows, at least, that $\langle p^2/2m\rangle$ does not give the entire contribution to the kinetic energy, so, on the basis of general principles of continuum mechanics, one is tempted to interpret the spin and density terms in (3.20) as a kind of heat energy associated with the local angular momentum flux, but it is difficult to account for the specific form of the terms on the basis of this idea.

Obviously, the kinetic energy is much more simply expressed in terms of the velocity by (3.18) than in terms of the momentum. Notice that, in contrast to (3.15), (3.18) displays no explicit interaction with the magnetic field. This is entirely in accordance with the idea that the spin arises from a circulation of charge. But the problem remains to understand the β^2 term in (3.18). We shall comment on this later.

A virial theorem for the P–S theory is easily derived with the help of (3.12) [but not by using (3.11)!]. Since, in Sec. 4 we will obtain a more general theorem from the Dirac theory by a similar method, we do not give the derivation. Looking ahead, we merely note that from Eqs. (4.20)-(4.23) we get, recalling that the rest energy is omitted from the Pauli theory, the general virial theorem for stationary states

$$\langle E\rangle = -\langle\tfrac{1}{2}m\mathbf{v}^2\rangle - \langle\tfrac{1}{2}mc^2\beta^2\rangle + \langle V\rangle - e\langle\mathbf{x}\cdot(\mathbf{E} + c^{-1}\mathbf{v}\times\mathbf{B})\rangle, \tag{3.21}$$

which for a Coulomb field alone reduces to

$$\langle E\rangle = -\langle\tfrac{1}{2}m\mathbf{v}^2\rangle - \tfrac{1}{2}mc^2\langle\beta^2\rangle. \tag{3.22}$$

Equating this to $\langle E\rangle + \langle K\rangle + \langle V\rangle$ and using (3.18), we get the alternative form of the virial theorem

$$m\langle \mathbf{v}^2\rangle + mc^2\langle \beta^2\rangle + \langle V\rangle = 0. \tag{3.23}$$

Let us consider some implications of the above relations among observables for the interpretation of the Schrödinger solution of the hydrogen atom. As has been explained, we get the Schrödinger theory *with spin* by taking $\mathbf{s}$ constant. This determines a preferred direction in the theory, so it is convenient to write

$$\mathbf{s} = \tfrac{1}{2}\hbar\sigma_3. \tag{3.24}$$

Obviously,

$$\langle \mathbf{s}\rangle = \mathbf{s} = \tfrac{1}{2}\hbar\sigma_3 \tag{3.25}$$

for any solution of the Schrödinger equation. From the Schrödinger wavefunctions for the hydrogen atom we get

$$\langle \mathbf{L}\rangle = m\hbar\sigma_3 = 2m\mathbf{s}, \tag{3.26}$$

where m is the magnetic quantum number. This is identical to the usual result

$$\langle \hat{L}_3\rangle = m\hbar, \quad \langle \hat{L}_1\rangle = 0 = \langle \hat{L}_2\rangle,$$

where the $\hat{L}_k$ are the usual angular momentum operators, that is,

$$\langle \hat{L}_k\rangle = \sigma_k \cdot \langle \mathbf{L}\rangle = \langle \sigma_k \cdot \mathbf{L}\rangle.$$

The total angular momentum is clearly

$$\langle \mathbf{J}\rangle = (m + \tfrac{1}{2})\hbar\sigma_3 = (2m+1)\mathbf{s}. \tag{3.27}$$

The spin is coupled to other observables by Eq. (3.46), which, in the Schrödinger theory can be written

$$m\rho v = \rho\mathbf{p} - \mathbf{s}\times\nabla\rho. \tag{3.28}$$

For s-states the Schrödinger wavefunctions imply $\mathbf{p} = 0$, but (3.28) shows that $\mathbf{v} \neq 0$. In fact, since ρ is spherically symmetric $\nabla\rho$ is directed radially, so (3.28) implies that the charge streamlines circulate about the "spin axis." Thus, the *charge distribution of an s-state is not static* as it is usually supposed to be when $(e/m)\mathbf{p}$ is wrongly assumed to describe the charge flow. It must be emphasized that this conclusion is solely a consequence of requiring that the Schrödinger theory be a consistent approximation to the Dirac theory. Of course, we have already seen that the charge current in the s-state gives the "Darwin spin-orbit energy" when the first order relativistic correction is included.

The correspondence between Schrödinger and Bohr theories of hydrogen is significantly improved by corresponding $\mathbf{v}$ rather than $\mathbf{p}/m$ with the velocity of the electron in the Bohr theory. All observables can be expressed in terms of $\mathbf{v}$ rather than $\mathbf{p}$ by using (3.28). The angular momentum to compare with the Bohr theory is therefore $\mathbf{L}^*$ defined by (3.7) rather than $\mathbf{L}$. Indeed, substitution of (3.25), (3.26) into (3.14) yields

$$\langle L^*\rangle = (m+1)\hbar\sigma_3 \ . \tag{3.29}$$

As in the Bohr theory, (3.29) associates a finite angular momentum with the s-states. Since spin is separately conserved it appears that we can just omit it from the angular momentum balance. But a deeper analysis may show that the half-integral values of the "azimutal quantum number" in the Schrödinger theory are related to the spin.

It is tempting to suppose that the Schrödinger theory describes in some sense a statistical ensemble of Bohr-like orbits. The expression (3.18) for the kinetic energy seems to be very close to what one might expect in such a case. Consider the strange quantity β which appears there. From (3.4c) we have

$$\beta = \frac{-1}{mc}\nabla\cdot(\rho\mathbf{s}) = -\frac{\hbar}{2mc}\sigma_3\cdot\nabla\ln\rho, \tag{3.30}$$

so in the Schrödinger theory (3.12) can be written

$$\langle \tilde{K}\rangle = \tfrac{1}{2}m\langle \mathbf{v}^2\rangle + \frac{\mathbf{s}^2}{2m}\left\langle\left(\frac{\partial\ln\rho}{\partial z}\right)^2\right\rangle. \tag{3.31}$$

Thus the contribution of β to the energy is determined by by the derivative of the density along the "axis of quantization." But the Bohr orbits are confined to a plane, while the Schrödinger $\mathbf{v}$-orbits are distributed throughout space, though they too circulate about a preferred axis. Perhaps the last term in (3.31) is only needed to compensate for this difference; or perhaps it represents the entire contribution of the spin to the energy. Perhaps the biggest difference between the Bohr and Schrödinger theories is that the latter contains spin. No doubt the last word on the subject has not been spoken.

4. HYDRODYNAMIC EQUATIONS FOR RELATIVE OBSERVABLES

In Sec. 6 of Ref. 5 the fundamental *relative* local observables, velocity, spin, energy, and momentum were introduced and the basic constitutive relations among them were ascertained and discussed. This section derives the *relative* equations of motion for these quantities. The resulting equations are exact but probably too complicated to be of practical interest. We use them only to derive a virial theorem and to find the corresponding hydrodynamic equations of the Pauli–Schrödinger theory in the nonrelativistic limit. However, it may be possible to use these equations to compute relativistic dynamical corrections to the Pauli theory, a problem which is difficult to handle with a wave equation.

Le us recall the dynamical conservation laws of the Dirac theory. According to Eqs. (2.26) and (3.22) of Ref. 4, the energy–momentum conservation law can be written

$$\rho d_\pi p = \frac{e}{c}\rho F\cdot v - \partial_\mu N^\mu, \tag{4.1a}$$

where

$$N(\gamma^\mu) = N^\mu = \gamma^\nu\rho(v\wedge\gamma^\mu)\cdot W = -\rho s^\mu\Box\beta + \gamma^\nu\rho[v\gamma^\mu\partial_\nu S]_{(0)}. \tag{4.1b}$$

Note that $N(v) = v_\mu N^\mu = 0$, so $N(n)$ can be identified as the proper stress tensor, describing the flux of momentum through a hypersurface with normal n into a particle streamline. Equation (4.1a) says that the Lorentz force is the only body force on the electron; the "Stern–Gerlach" force does not appear explicitly in (4.1a) because it is not a body force, rather it has been shown in 4 to arise from the term $\partial_\mu N^\mu$, so it expresses the influence of the external field on the local momentum flux.

According to Eqs. (2.34) and (2.33) of Ref. 4, angular

momentum conservation in the Dirac theory can be expressed by the equation

$$\rho d_\tau S = -\partial_\mu M^\mu + \rho v \wedge p + \gamma_\mu \wedge N^\mu \tag{4.2a}$$

where

$$M(\gamma^\mu) \equiv M^\mu = \rho S \cdot \gamma^\mu v = \rho \tfrac{1}{2}[S, \gamma^\mu \wedge v]. \tag{4.2b}$$

The last two terms of (4.2a) describe the coupling of the spin to the energy–momentum density a flux via the skew-symmetric part of the energy–momentum tensor. Also $M(v) = 0$, so the tensor $M(n)$ gives the flux of angular momentum in the direction n onto a streamline. Thus (4.2a) says that the spin is subject to no body torques; the "Larmor term" does not appear explicitly in (4.2a), because, as shown in Ref. 4, it describes the influence of the external field on the local angular momentum flux.

The main task of this section is to reexpress the conservation laws (4.1) and (4.2) in relative form. This work completes the job of expressing the Dirac theory in terms of relative variables which was begun in Sec. 6 of Ref. 5, so familiarily with the characterization of relative variables developed there is presumed.

Consider first the conservation Eq. (4.1a) for energy energy–momentum. Using (6.6) and (6.7) of Ref. 5, we write

$$\rho d_\tau p \gamma_0 = c^{-1} \rho_0 d_t \left(\frac{\epsilon}{c} + \mathbf{p} \right). \tag{4.3}$$

Also it is easy to show that [Eq. (2.15) of Ref. 11]

$$F \cdot v \gamma_0 = v_0 [c^{-1} \mathbf{E} \cdot \mathbf{v} + \mathbf{E} + c^{-1} \mathbf{v} \times \mathbf{B}]. \tag{4.4}$$

Hence after multiplication by γ_0, Eq. (4.1a) can be separated into the two equations

$$\rho_0 d_t \epsilon = \rho_0 e \mathbf{E} \cdot \mathbf{v} - \partial_\mu N_0^\mu, \tag{4.5a}$$

$$\rho_0 d_t \mathbf{p} = \rho_0 e (\mathbf{E} + c^{-1} \mathbf{v} \times \mathbf{B}) - \partial_\mu \mathbf{N}^\mu, \tag{4.5b}$$

where we have introduced the notation

$$N_0^\mu \equiv c^2 N^\mu \cdot \gamma_0, \quad \mathbf{N}^\mu \equiv c N^\mu \wedge \gamma_0.$$

To get the flux terms expressed in terms of relative local observables, we use (4.26).

Introducing the frame of relative vectors

$$\sigma_k \equiv \gamma_k \gamma_0 = -\gamma_0 \gamma_k = \gamma_0 \gamma^k \quad (k = 1, 2, 3),$$

and recalling (6.4b) of Ref. 5, we have

$$c^{-1} N_0^\mu = -\rho s^\mu \partial_t \beta + \rho [v \gamma^\mu \partial_t S]_{(0)}, \tag{4.6a}$$

$$c^{-1} \mathbf{N}^\mu = \rho s^\mu \nabla \beta - \sigma_j \rho [v \gamma^\mu \partial_j S]_{(0)}, \tag{4.6b}$$

and, recalling (6.1) and (6.12a) of Ref. 5, we have

$$[v \gamma^0 \partial_\nu S]_{(0)} = \frac{v_0}{c} [\mathbf{v} \partial_\nu (\mathbf{s}_1 + S_2)]_{(0)} = \frac{v_0}{c} \mathbf{v} \cdot \partial_\nu \mathbf{s}_1$$

$$\begin{aligned} [v \gamma^k \partial_\nu S]_{(0)} &= [v \gamma_0 \gamma_0 \gamma^k \partial_\nu S]_{(0)} \\ &= v_0 [(1 + \mathbf{v}/c) \sigma_k \partial_\nu (\mathbf{s}_1 + S_2)]_{(0)} \\ &= v_0 \{ \partial_\nu (\sigma_k \circ \mathbf{s}_1) + c^{-1} (\mathbf{v} \wedge \sigma_k) \cdot \partial_\nu S_2 \}. \end{aligned}$$

Hence,

$$N_0^0 = -c \rho s_0 \partial_t \beta + \rho_0 \mathbf{v} \cdot \partial_t \mathbf{s}_1, \tag{4.7a}$$

$$N_0^k \equiv N_{0k} = -c \rho s^k \partial_t \beta + \rho_0 \{ c \partial_t \mathbf{s}_1 \cdot \sigma_k + (\mathbf{v} \wedge \sigma_k) \cdot \partial_t S_2 \}, \tag{4.7b}$$

$$\mathbf{N}^0 = c \rho s_0 \nabla \beta - \rho_0 \sigma_j \mathbf{v} \cdot \partial_j \mathbf{s}_1 \tag{4.7c}$$

$$\mathbf{N}^k \equiv \mathbf{N}_k = c \rho s^k \nabla \beta - \rho_0 \{ c \nabla \mathbf{s}_1 \cdot \sigma_k + \sigma_j (\mathbf{v} \wedge \sigma_k) \cdot \partial_j S_2 \}. \tag{4.7d}$$

It will be noted that these flux terms are expressed in terms of several quantities which are not independent of one another. By (6.12), (6.18), (6.19) of Ref. 5 and (2.18) of Ref. 4, s_0, s, s_1, S_2, and β can all be expressed in terms of σ and $\mathbf{v}$. In terms of σ, the flux terms (4.7) appear very much more complicated, but simplify considerably if one retains only first order relativistic corrections. Equations (4.5) for energy and momentum coupled to the equation of motion (6.38) of Ref. 5 for σ are appropriate equations to study if one is interested in the dynamical role of the Thomas precession. Instead, however, we here obtain equations of motion for $\mathbf{s}_1$ and S_2, because they have the general form of conservation laws. To keep the general features of the equations apparent, we do not express s^μ and β in terms of s_1 and S_2, as would be necessary if we were looking for solutions. Therefore, we regard (4.7) as a satisfactory expression of the flux in terms of local observables. So substituting (4.7) into (4.5), we get

$$\begin{aligned} \rho_0 d_t \epsilon = \rho_0 e \mathbf{E} \cdot \mathbf{v} &+ \partial_t \{ \rho s_0 \partial_t \beta - c^{-1} \rho_0 \mathbf{v} \cdot \partial_t \mathbf{s}_1 \} \\ &- \partial_k \{ -c \rho s^k \partial_t \beta + c \rho_0 \partial_t \mathbf{s} \cdot \sigma_k + \rho_0 (\mathbf{v} \wedge \sigma_k) \cdot \partial_t S_2 \} \end{aligned} \tag{4.8a}$$

$$\begin{aligned} \rho_0 d_t \mathbf{p} = \rho_0 e (\mathbf{E} + c^{-1} \mathbf{v} \times \mathbf{B}) &+ \partial_t \{ -\rho s_0 \nabla \beta + c^{-1} \sigma_j \mathbf{v} \cdot \partial_j \mathbf{s}_1 \} \\ &+ \partial_k \{ c \rho s^k \nabla \beta + c \rho_0 \nabla s_1 \circ \sigma_k + \rho_0 \sigma_j (\mathbf{v} \wedge \sigma_k) \cdot \partial_j S_2 \}. \end{aligned} \tag{4.8b}$$

We now get equations of motion for s_1 and S_2 by taking the relative vector and bivector parts of (4.2a) to get

$$\rho d_\tau \mathbf{s}_1 = -\partial_\mu [M^\mu]_1 + \rho [v \wedge p]_1 + [\gamma_\mu \wedge N^\mu]_1, \tag{4.9a}$$

$$\rho d_\tau S_2 = -\partial_\mu [M^\mu]_2 + \rho [v \wedge p]_2 + [\gamma_\mu \wedge N^\mu]_2. \tag{4.9b}$$

Now to express the right side of (4.9) in relative observables. In the process we keep in mind the facts that $\sigma_k \cdot \mathbf{s} = s^k$ while $\sigma_k \circ \nabla = \partial_k$, as follows from the definitions of $\mathbf{s}$ and ∇ in (6.11) and (6.4) of Ref. 5.

$$\begin{aligned} c \gamma_\mu \wedge N^\mu = c [\gamma_\mu N^\mu]_2 &= [\gamma_\mu \gamma_0 (c^{-1} N_0^\mu - \mathbf{N}^\mu)]_2 \\ &= -\mathbf{N}^0 + c^{-1} \sigma_k N_0^k - \sigma_k \wedge \mathbf{N}^k. \end{aligned}$$

So from (4.7),

$$\begin{aligned} [\gamma_\mu \wedge N^\mu]_1 &= -c^{-1} \mathbf{N}^0 + c^{-2} \sigma_k N_0^k \\ &= -\rho s_0 \nabla \beta + c^{-1} \rho_0 \sigma_j \mathbf{v} \cdot \partial_j \mathbf{s}_1 \\ &\quad - c^{-1} \rho \mathbf{s} \partial_t \beta + c^{-1} \rho_0 \{ \partial_t \mathbf{s}_1 - c^{-1} \mathbf{v} \cdot \partial_t S_2 \}, \end{aligned} \tag{4.10a}$$

$$\begin{aligned} [\gamma_\mu \wedge N^\mu]_2 &= -c^{-1} \sigma_k \wedge \mathbf{N}^k = -c^{-1} \sigma_k \wedge \mathbf{N}_k \\ &= -\rho \mathbf{s} \wedge \nabla \beta - \rho_0 \nabla \wedge \mathbf{s}_1 + c^{-1} \rho_0 \sigma_j \wedge (\mathbf{v} \circ \partial_j S_2). \end{aligned} \tag{4.10b}$$

Also

$$\begin{aligned} v \wedge p &= [v_0 (1 + \mathbf{v}/c)(\epsilon/c - \mathbf{p})]_{(1)+(2)} \\ &= v_0 \left(\frac{\epsilon}{c^2} \mathbf{v} - \mathbf{p} \right) - \frac{v_0}{c} \mathbf{v} \wedge \mathbf{p}. \end{aligned} \tag{4.11}$$

From (4.2b) we get

$$\begin{aligned} M^0 = \rho \tfrac{1}{2} [\mathbf{s}_1 + S_2, \gamma^0 \wedge v] &= \rho v_0 \{ \tfrac{1}{2} [\mathbf{v}, \mathbf{s}_1] + \tfrac{1}{2} [\mathbf{v}, S_2] \} \\ &= \rho_0 \{ \mathbf{v} \wedge \mathbf{s}_1 = \mathbf{v} \cdot S_2 \}, \end{aligned} \tag{4.12a}$$

and, since

$$\gamma^k \wedge v = [\gamma^k \gamma_0 \gamma_0 v]_2 = -[\sigma_k v_0 (1 - \mathbf{v}/c)]_2$$

$$= -v_0\{\sigma_k - c^{-1}\sigma_k \wedge \mathbf{v}\},$$

we also get from (4.2b),

$$M^k = -\rho_0 \tfrac{1}{2}[\mathbf{s}_1 + S_2, \sigma_k - c^{-1} i\sigma_k \times \mathbf{v}]$$
$$= \rho_0\{\sigma_k \wedge \mathbf{s}_1 + \sigma_k \cdot S_2 - c^{-1}\mathbf{s}_1 \times (\sigma_k \times \mathbf{v}) - c^{-1}\tfrac{1}{2}[\sigma_k \wedge \mathbf{v}, S_2]\}. \tag{4.12b}$$

Hence,

$$c\partial_\mu [M^\mu]_1 = \partial_t(\rho_0 \mathbf{v} \cdot S_2) + c\nabla \cdot (\rho_0 S_2) - \partial_k(\rho_0 \mathbf{s}_1 \times (\sigma_k \times \mathbf{v})),$$
$$c\partial_\mu [M^\mu]_2 = \partial_t(\rho_0 \mathbf{v} \wedge \mathbf{s}_1) + c\nabla \wedge (\rho_0 \mathbf{s}_1) - \partial_k(\rho_0 \tfrac{1}{2}[\sigma_k \wedge \mathbf{v}, S_2]).$$

So, at last Eqs. (4.9a,b) can be written

$$\rho_0 d_t \mathbf{s}_1 = -\partial_t(\rho_0 \mathbf{v} \cdot S_2) - c\nabla \cdot (\rho_0 S_2) + \partial_k(\rho_0 \mathbf{s}_1 \times (\sigma k \times \mathbf{v}))$$
$$+ \rho_0(c^{-1}\epsilon \mathbf{v} - c\mathbf{p}) - c\rho s_0 \nabla\beta + \rho_0 \sigma_j \mathbf{v} \cdot \partial_j \mathbf{s}_1$$
$$- \rho \mathbf{s}\partial_t\beta + \rho_0 \partial_t \mathbf{s}_1 - c^{-1}\rho_0 \mathbf{v} \cdot (\partial_t S_2), \tag{4.13a}$$

$$\rho_0 d_t S_2 = -\partial_t(\rho_0 \mathbf{v} \wedge \mathbf{s}_1) - c\nabla \wedge (\rho_0 \mathbf{s}_1) + \partial_k(\rho_0 \tfrac{1}{2}[\sigma_k \wedge \mathbf{v}, S_2])$$
$$- \rho_0 \mathbf{v} \wedge \mathbf{p} - c\rho \mathbf{s} \wedge \nabla\beta - c\rho_0 \nabla \wedge \mathbf{s}_1$$
$$+ \rho_0 \sigma_j \wedge (\mathbf{v} \cdot \partial_j S_2). \tag{4.13b}$$

With Eqs. (4.8a,b) and (4.13a,b) we have completed the formulation of the Dirac hydrodynamic equations in terms of relative observables. No one can fail to notice how much more complicated these equations are than their proper counterparts (4.1a,b) and (4.2a,b). So, for most purposes it is clearly best to deal with the proper equations.

The relative hydrodynamic equations become much simpler in the N.R. limit. To attain this limit, as we saw in Sec. 7 of Ref. 5, we need only express all spins in terms of S or $\mathbf{s}$ with the identifications

$$S_2 = S = i\mathbf{s}, \quad c\mathbf{s}_1 = \mathbf{v} \cdot S, \quad cs_0 = \mathbf{s} \cdot \mathbf{v},$$

take $\rho_0 = \rho$, and regarding $c|\boldsymbol{\beta}| \approx |\mathbf{v}|$, neglect all terms of relative order c^{-1} or less. Then from (4.8b) we easily get the momentum conservation equation

$$\rho d_t \mathbf{p} = \rho e(\mathbf{E} + c^{-1}\mathbf{v} \times B) - \partial_k \mathbf{N}_k, \tag{4.14a}$$

where the momentum flux $\mathbf{N}_k$ is the limit of (4.7d)

$$\mathbf{N}_k = \rho c s^k \nabla\beta + \sigma_j \rho S \cdot (\partial_j \mathbf{v} \wedge \sigma_k), \tag{4.14b}$$

and from (4.9b) we get the angular momentum conservation equation in terms of the spin

$$\rho d_t S = \rho \mathbf{p} \wedge \mathbf{v} - \sigma_k \wedge \mathbf{N}_k - \partial_k M_k, \tag{4.15a}$$

where the spin flux M_k is given by

$$M_k \equiv \rho \tfrac{1}{2}[S, \sigma_k \wedge \mathbf{v}] - \rho \sigma_k \wedge (S \cdot \mathbf{v}). \tag{4.15b}$$

In addition, from (4.8a) we get the energy conservation equation

$$\rho d_t \epsilon_p = e\rho \mathbf{E} \cdot \mathbf{v} + \partial_k\{c\rho s^k \partial_t\beta - S \cdot (\partial_t \mathbf{v} \wedge \sigma_k)\}. \tag{4.16}$$

As already mentioned in the last section, these are the hydrodynamic equations of the Pauli theory.

As an application of the relative hydrodynamic equations we derive a virial theorem for the Dirac theory, though actually it is hardly more difficult to derive the theorem directly from the proper hydrodynamic equations. Differentiating $\mathbf{x} \cdot \mathbf{p}$ and using (4.5b), we get

$$d_t(\mathbf{x} \cdot \mathbf{p}) = \mathbf{v} \cdot \mathbf{p} + \mathbf{x} \cdot [e(\mathbf{E} + c^{-1}\mathbf{v} \times \mathbf{B}) - \rho_0^{-1}\partial_\mu \mathbf{N}^\mu].$$

But, by (4.7d)

$$-\mathbf{x} \cdot (\partial_\mu \mathbf{N}^\mu) = -\partial_\mu(\mathbf{x} \cdot N^\mu) + \sigma_k \cdot \mathbf{N}^k$$
$$= -\partial_\mu(\mathbf{x} \cdot N^\mu) + c\rho \mathbf{s} \cdot \nabla\beta - \rho v_0(c\nabla \cdot \mathbf{s}_1 + \mathbf{v} \cdot (\nabla \cdot S_2)).$$

So

$$\rho_0 d_t(\mathbf{x} \cdot \mathbf{p}) = \rho_0 \mathbf{v} \cdot \mathbf{p} + e\rho_0 \mathbf{x} \cdot (\mathbf{E} + c^{-1}\mathbf{v} \times \mathbf{B}) - \partial_\mu(\mathbf{x} \cdot \mathbf{N}^\mu)$$
$$+ \rho_0\left(\frac{c}{v_0}\mathbf{s} \cdot \nabla\beta - c\nabla \cdot \mathbf{s}_1 - \mathbf{v} \cdot (\nabla \cdot S_2)\right),$$

and since

$$\int d^3x \rho_0 d_t(\mathbf{x} \cdot \mathbf{p}) = \partial_t \int d^3x \rho_0 \mathbf{x} \cdot \mathbf{p} = \partial_t \langle \mathbf{x} \cdot \mathbf{p} \rangle,$$

we have

$$\partial_t \langle \mathbf{x} \cdot \mathbf{p} \rangle = \langle \mathbf{v} \cdot \mathbf{p} \rangle + e\langle \mathbf{x} \cdot (\mathbf{E} + c^{-1}\mathbf{v} \times \mathbf{B}) \rangle - \partial_t \left\langle\!\!\left\langle \frac{\mathbf{x} \cdot \mathbf{N}^0}{c\rho_0} \right\rangle\!\!\right\rangle$$
$$+ \left\langle\!\!\left\langle \left(\frac{c}{v_0}\mathbf{s} \cdot \nabla\beta - c\nabla \cdot \mathbf{s}_1 - \mathbf{v} \cdot S_2\right) \right\rangle\!\!\right\rangle. \tag{4.17}$$

Hence, for stationary states we have

$$\langle \mathbf{v} \cdot \mathbf{p} \rangle + e\langle \mathbf{x} \cdot (\mathbf{E} + c^{-1}\mathbf{v} \times \mathbf{B}) \rangle = -\left\langle\!\!\left\langle \left(\frac{c}{v_0}\mathbf{s} \cdot \nabla\beta - c\nabla \cdot \mathbf{s}_1 - \mathbf{v} \cdot (\nabla \cdot S_2)\right) \right\rangle\!\!\right\rangle. \tag{4.18}$$

This can be related to the energy by taking the expectation value of (6.30) in Ref. 5 to get

$$\langle E \rangle = \left\langle c\frac{\bar{\Omega} \cdot S}{v_0} \right\rangle + mc^2 \left\langle \frac{\cos\beta}{v_0} \right\rangle + \langle \mathbf{v} \cdot \mathbf{p} \rangle + \langle V \rangle. \tag{4.19}$$

Now we recall from (6.27a) in Ref. 5 that $\bar{\Omega} = -\Box \wedge v + v \cdot (i\Box\beta)$. To express $\bar{\Omega} \cdot S$ in terms of relative variables, note that the divergence of $v \cdot S = 0$ gives

$$(\Box \wedge v) \cdot S = (v \wedge \Box) \cdot S = (v\Box S)_{(0)}.$$

Hence

$$-(\Box \wedge v) \cdot S = -v_0[(1 + \mathbf{v}/c)(\partial_0 + \nabla)(\mathbf{s}_1 + S_2)]_{(0)}$$
$$= -\frac{v_0}{c}[\mathbf{v} \cdot \partial_0 \mathbf{s}_1 + c\nabla \cdot \mathbf{s}_1 + \mathbf{v} \cdot (\nabla \cdot S_2)].$$

Also,

$$S \cdot (v \cdot (i\Box\beta)) = [Svi\Box\beta]_{(0)} = s \cdot \Box\beta = s_0\partial_0 + \mathbf{s} \cdot \nabla\beta.$$

Hence, we have the general formula,

$$c\rho\bar{\Omega} \cdot S = \rho_0\left\{\frac{cs_0}{v_0}\partial_0\beta - \mathbf{v} \cdot \partial_0 \mathbf{s}_1 + \frac{c}{v_0}\mathbf{s} \cdot \nabla\beta - c\nabla \mathbf{s}_1 - \mathbf{v} \cdot (\nabla \cdot S_2)\right\}. \tag{4.20}$$

Taking the expectation value of (4.20) and comparing with (4.18), we find *for stationary states*

$$\left\langle c\frac{\bar{\Omega} \cdot S}{v_0} \right\rangle = \left\langle\!\!\left\langle \left(\frac{c}{v_0}\mathbf{s} \cdot \nabla\beta - c\nabla \cdot \mathbf{s}_1 - \mathbf{v} \cdot (\nabla \cdot S_2)\right) \right\rangle\!\!\right\rangle$$
$$= -\langle \mathbf{v} \cdot \mathbf{p} \rangle - e\langle \mathbf{x} \cdot (\mathbf{E} + c^{-1}\mathbf{v} \times \mathbf{B}) \rangle = \left\langle c\frac{\bar{\omega}^L \cdot \Sigma}{v_0} \right\rangle. \tag{4.21}$$

Recall that the last term in (4.21) is equal to the first by (6.17) and (6.49) of Ref. 5; the factor c/v_0 would be missing, as (6.38) of Ref. 4 shows, if $\bar{\omega}^L$ were defined as the angular velocity corresponding to the total time derivative instead of the proper time derivative. Thus, (4.21) is exactly a virial theorem for the generalized

Larmor precession energy, or as it was called in Sec. 6 of Ref. 4, the *internal energy*.

Substituting (4.21) in (4.19), we obtain the result that for any stationary state in the Dirac theory

$$\langle E\rangle = mc^2\left\langle\frac{\cos\beta}{v_0}\right\rangle + \langle V\rangle - e\langle \mathbf{x}\cdot(\mathbf{E} + c^{-1}\mathbf{v}\times\mathbf{B})\rangle. \tag{4.22}$$

A Coulomb field has the special property that

$$e\mathbf{x}\cdot\mathbf{E} = -\mathbf{x}\cdot\nabla V = V. \tag{4.23}$$

Hence for a Coulomb field alone, (4.22) reduces to the simple form

$$\langle E\rangle = mc^2\left\langle\frac{\cos\beta}{v_0}\right\rangle = mc^2\int d^3x\rho\cos\beta. \tag{4.24}$$

This ought to tell us something important about the interpretation of β, but we do not know what. At least we can use it as additional support for our contention that β must, on the average, be a small quantity. Thus, if $\langle E\rangle$ does not deviate much from mc^2, then, since $v_0 \geq 1$ everywhere, (4.29) implies that $\langle\cos\beta\rangle \approx 1$. This being true, we can expand v_0 and $\cos\beta$ in (4.24) to get the approximate expression

$$\langle E\rangle - mc^2 \approx -\langle\tfrac{1}{2}mv^2\rangle - \tfrac{1}{2}mc^2\langle\beta^2\rangle. \tag{4.25}$$

This, as should be expected, is just the virial theorem one obtains by using the Pauli theory. It should be compared with

$$\langle E\rangle - mc^2 \approx \langle\tfrac{1}{2}m\sigma^2\rangle + \langle\tfrac{1}{2}mc^2\beta^2\rangle + \langle V\rangle, \tag{4.26}$$

which is obtained immediately by integrating (7.5) of Ref. 5.

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On Chapman–Kolmogorov equations for neutron population in a multiplying assembly*

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We prove that the Chapman–Kolmogorov system for neutron population in a multiplying assembly admits a unique positive and norm invariant solution belonging to the Banach space of summable sequences. We then show that the standard kinetic equation can be deduced in a rigorous way from such a system of a countably infinite number of partial differential equations. Finally, we indicate how the Chapman–Kolmogorov initial-value problem can be approximated by a problem in a finite-dimensional space.

1. INTRODUCTION

Chapman—Kolmogorov equations for neutron population in a multiplying assembly at zero power have been extensively investigated in the literature (Refs. 1 to 12).

In this paper, we shall examine such a system by using the theory of semigroups of linear bounded transformations (Refs. 12, 14, 15). We shall first prove existence and uniqueness of a solution in a suitable Banach space and, successively, we shall derive some properties of physical interest in a rigorous way.

Following Ref. 12, the Chapman—Kolmogorov system under consideration has the form

$$\frac{\partial}{\partial t}P(n,t) = -pnP(n,t) + p\sum_{s=0}^{n} b(s)(n+1-s)P(n+1-s,t) + q[P(n-1,t) - P(n,t)], \quad t>0,\ n=0,1,2,\cdots, \tag{1}$$

where we let $P(-1,t)\equiv 0$ and where

$P(n,t)$ = the probability that n neutrons are in the multiplying assembly at the instant t;

$p = 1/l$, where l is the average lifetime;

$b(s)$, $s=0,1,2,\cdots$ = the probability that s neutrons are emitted if one neutron is absorbed;

$\sum_{s=0}^{\infty} b(s) = 1, \quad 0 \le b(s) \le 1;$

q = the probability per unit time interval that a nonfission source emits a neutron.

System (1) must be supplemented with an initial condition of the form

$$P(n,0) = P_0(n), \quad n=0,1,2,\cdots, \tag{2}$$

where

$$\sum_{n=0}^{\infty} P_0(n) = 1, \quad 0 \le P_0(n) \le 1. \tag{3}$$

Conditions (3) have an obvious physical meaning.

2. DEFINITIONS AND PRELIMINARY REMARKS

Due to (3), we now introduce the Banach space $X = l^1$ of all numerical vectors $f = \{f(n), n=0,1,2,\cdots\}$ with a countably infinite number of real components $f(n)$, such that (Ref. 13, p. 127)

$$\|f\| = \sum_{n=0}^{\infty} |f(n)| < \infty.$$

Further, let us define the following operators:

$$[Af]_n = -pnf(n) + p\sum_{s=0}^{n} b(s)(n+1-s)f(n+1-s), \quad n=0,1,2,\cdots, \tag{4}$$

$$[Sf]_n = qf(n-1), \quad n=1,2,3,\cdots, \quad [Sf]_0 = 0, \tag{5}$$

$$[Hf]_n = pnf(n), \quad n=0,1,2,\cdots, \tag{6}$$

$$[Kf]_n = p\sum_{s=0}^{n} b(s)(n+1-s)f(n+1-s), \quad n=0,1,2,\cdots, \tag{7}$$

where $[Af]_n$ indicates the $(n+1)$th component of the vector Af and where the domains of A, S, H, and K are given as

$$D(A) = \{f : f\in X,\ \sum_{n=0}^{\infty} |[Af]_n| < \infty\} \tag{8}$$

$$D(S) = X, \tag{9}$$

$$D(H) = D(K) = D = \{f : f\in X,\ \sum_{n=0}^{\infty} n|f(n)| < \infty\}. \tag{10}$$

We note that $D = D(H)$ is the "largest" subset of X on which H can be defined, whereas the largest subset on which K can be defined contains D [see (11)]. However, we take $D(K) = D$ by definition since we are interested in the operator $(-H+K)$ for which $D(-H+K) = D(H)\cap D(K)$.

Given any $f\in D$, we have

$$\sum_{n=0}^{N}\sum_{s=0}^{n} b(s)(n+1-s)|f(n+1-s)| = \sum_{s=0}^{N}\sum_{n=s}^{N} b(s)(n+1-s)|f(n+1-s)| \le \sum_{s=0}^{N} b(s)\sum_{m=1}^{\infty} m|f(m)| \le \sum_{m=1}^{\infty} m|f(m)| < \infty \tag{11}$$

since $\sum_{s=0}^{\infty} b(s) = 1$. Hence, $f\in D(A)$ and, consequently, $D\subset D(A)$ and $-H+K\subset A$. We also observe that definition (10) is justified by the fact that the mean number of neutrons $\langle n\rangle = \sum_{n=0}^{\infty} nf(n)$ is finite provided that $f\in D_+ = D\cap X_+$, where

$$X_+ = \{f : f\in X,\ f(n)\ge 0,\ n=0,1,2,\cdots\}$$

is the (closed) positive cone of X (Ref. 16).

Moreover, let D_0 be the linear manifold spanned by the canonical base of X. D_0 is the family of all vectors of X with a finite number of nonzero components, it is dense in X and it is contained in D. By definition, A_0 is the restriction of A with domain $D(A_0) = D_0$.

Following Ref. 15, we finally put

$$G_r = -H + rK, \quad D(G_r) = D \tag{12}$$

where r is a real parameter, such that $0 \leq r < 1$.

3. PROPERTIES OF H AND OF K

We have:

Lemma 1: For every $\alpha > 0$, $(\alpha I + H)^{-1} \in \beta(X)$ (Ref. 13, p. 149), $(\alpha I + H)^{-1}[X_+] \subset X_+$, $\|(\alpha I + H)^{-1}\| \leq 1/\alpha$; $H \in \mathcal{C}(X)$ (Ref. 13, p. 164), $H[X_+] \subset X_+$, $D(H) = D \supset D_0$ is dense in X; H is the closure of H_0, where H_0 is the restriction of H to D_0.

Lemma 1 follows directly from the definition (6) of H and from the explicit expression of $(\alpha I + H)^{-1}$

$$[(\alpha I + H)^{-1} f]_n = (\alpha + pn)^{-1} f(n), \tag{13}$$

where $n = 0, 1, 2, \cdots$ and $\alpha > 0$ (see also Ref. 15, p. 6).

Lemma 2: $K[D_+] \subset X_+$; $\|Kf\| \leq \|Hf\|$, $f \in D$; $\|Kf\| = \|Hf\|$, $f \in D_+$.

Lemma 2 follows from the definition (7) of K and from inequality (11).

Starting from Lemma 1 and from Lemma 2 and following Ref. 15, we obtain (see also the remark at the end of p. 3 of Ref. 15)

Lemma 3: $G_r \in \mathcal{G}(1, 0)$ (Ref. 13, Chap. 9), $0 \leq r < 1$; the semigroup $Z_r(t) = \exp(tG_r)$ is such that: (i) $Z_r(t)[X_+] \subset X_+$ for any $t \geq 0$; (ii) $[Z_r(t)f]_n \leq [Z_{r'}(t)f]_n$, $n = 0, 1, 2, \cdots$, $f \in X_+$ and $r \leq r'$.

If we now put

$$Z(t)f = \lim_{r \to 1^-} Z_r(t)f, \quad t \geq 0, \ f \in X \tag{14}$$

we have:

Theorem 1: (a) $Z(t)$ is a semigroup such that $\|Z(t)\| \leq 1$, $Z(t)[X_+] \subset X_+$; (b) the limit (14) holds uniformly in each finite interval of t, i.e., $\|Z(t)f - Z_r(t)f\| < \epsilon$, $t \in [0, \bar{t}]$; provided that $1 - \delta < r < 1$ where $\delta = \delta(\epsilon, f)$ does not depend on $t \in [0, \bar{t}]$; (c) if G is the generator of $Z(t)$, then $A_0 \subset -H + K \subset G \subset A$; (d) if there is a semigroup $\{Z'(t), 0 \leq t\}$ such that $Z'(t)[X_+] \subset X_+$ and its generator G' is an extension of A_0, then $[Z'(t)f]_n \geq [Z(t)f]_n$, $f \in X_+$, $n = 0, 1, 2, \cdots$.

Theorem 1 follows from Lemma 3 (Ref. 15, pp. 7 to 10).

Remark: The preceding lemmas and Theorem 1 summarize some basic results obtained by Kato in Ref. 15.

4. THE INITIAL-VALUE PROBLEM

Due to the results of Theorem 1, the initial-value problem

$$\begin{aligned} &\frac{du}{dt} = Gu(t) - qIu(t) + Su(t), \quad t > 0, \\ &\lim_{t \to 0+} u(t) = u_0 \in D(G) \end{aligned} \tag{15}$$

admits a unique solution of the form

$$u(t) = \exp[t(G - qI + S)]u_0, \quad u_0 \in D(G), \ t \geq 0, \tag{16}$$

where

$$\exp[t(G - qI + S)][X_+] \subset X_+ \text{ and } \|\exp[t(G - qI + S)]\| \leq 1, \quad t \geq 0.$$

In fact, we have (Ref. 13 p. 495)

$$\exp[t(G + S)]f = \sum_{j=0}^{\infty} T^{(j)}(t)f, \quad t \geq 0, \tag{17}$$

where

$$\begin{aligned} &T^{(0)}(t)f = \exp(tG)f = Z(t)f, \\ &T^{(j+1)}(t)f = \int_0^t Z(t - s)ST^{(j)}(s)f\,ds, \quad j = 0, 1, 2, \cdots, \end{aligned} \tag{18}$$

and where, according to (5), $\|Sf\| = q\|f\|$, $f \in X$, $S[X_+] \subset X_+$. It follows from relations (18)

$$T^{(j)}(t)[X_+] \subset X_+, \quad \|T^{(j)}(t)f\| \leq [(qt)^j / j!]\|f\| \tag{19}$$

where we used (a) of Theorem 1. We conclude that $\exp[t(G + S)][X_+] \subset X_+$ and that $\|\exp[t(G + S)]\| \leq \exp(qt)$, at any $t \geq 0$. Since I is the identity operator, qI commutes with $(G + S)$. Consequently, (Ref. 13, p. 495)

$$\exp[t(G + S - qI)] = \exp(-qt)\exp[t(G + S)], \quad t \geq 0. \tag{20}$$

Hence, $\exp[t(G + S - qI)][X_+] \subset X_+$ and $\|\exp[t(G + S - qI)]\| \leq 1$ at any $t \geq 0$ as announced.

We conclude that, given any $u_0 \in D(G) \cap X_+$, the solution of system (15) is such that $u(t) \in D(G) \cap X_+$ at any $t \geq 0$ and $\|u(t)\| \leq \|u_0\|$.

Remark 1: In particular, let us assume that $u_0 = \{P_0(0), P_0(1), P_0(2), \cdots\} \in D_+ = D(H) \cap X_+ = D(-H + K) \cap X_+$ and that $\|u_0\| = \sum_{n=0}^{\infty} P_0(n) = 1$. Relations (3) are then satisfied and $\langle n \rangle(0) = \sum_{n=1}^{\infty} nP_0(n) < \infty$, where

$$\langle n \rangle(t) = \sum_{n=1}^{\infty} nP(n, t), \quad t \geq 0, \tag{21}$$

is the first moment of the neutron population.

It also follows that $u(t) = \{u(0; t), u(1; t), u(2; t), \cdots\} \in D(G) \cap X_+ \subset D(A) \cap X_+$ at any $t \geq 0$, since $G \subset A$ due to (c) of Theorem 1. In other words, $Gu(t) = Au(t)$ at any $t \geq 0$ and system (15) becomes just the "physical" system (1) + (2). Thus, system (1) + (2) admits a positive solution $u(t) \in X$, such that $\|u(t)\| = \sum_{n=0}^{\infty} u(n; t) \leq 1$ at any $t \geq 0$. Obviously, the preceding results remain valid if $u_0 \in D_0 \cap X_+$ and $\|u_0\| = 1$.

5. PRESERVATION OF THE NORM OF $u(t)$

In order to prove that

$$\|\exp[t(G + S - qI)]f\| = \|f\|, \quad f \in X_+, \ t \geq 0, \tag{22}$$

we introduce the space X^* of all bounded linear forms on X (Ref. 13 p. 134):

$$X^* = \{f^* : f^* = \{f^*(n), n = 0, 1, 2, \cdots\}, \|f^*\| < \infty\},$$

$$\|f^*\| = \{\sup |f^*(n)|, \ n = 0, 1, 2, \cdots\}.$$

Given a vector $f \in D_0 = D(A_0)$, we have

$$\begin{aligned} (f^*, A_0 f) &= p \sum_{n=0}^{\infty} f^*(n) \left(-nf(n) + \sum_{s=0}^{n} b(s)(n + 1 - s)f(n + 1 - s) \right) \\ &= p \sum_{m=0}^{\bar{n}} [-mf^*(m)]f(m) + \sum_{n=0}^{\bar{n}-1} f^*(n) \\ &\quad \left(\sum_{m=1}^{n+1} b(n + 1 - m)mf(m) \right) \\ &\quad + \sum_{n=\bar{n}}^{\infty} f^*(n) \sum_{m=1}^{\bar{n}} b(n + 1 - m)mf(m) \quad , \end{aligned}$$

where, since $f\in D_0$, $\bar{n}=\bar{n}(f)$ is such that $f(n)=0$, $n=\bar{n}+1,\bar{n}+2,\cdots$. It follows easily from the preceding equality

$$(f^*,A_0f)=(g^*,f),\quad f\in D_0, \tag{23}$$

where

$$g^*(m)=-pmf^*(m)+pm\sum_{s=0}^{\infty}b(s)f^*(m+s-1). \tag{24}$$

Since $g^*\in X^*$ provided that $\{\sup|g^*(m)|, m=0,1,2,\cdots\}<\infty$, we conclude that (Ref. 13, p. 167)

$$[A_0^*f^*]_m=g^*(m),\quad D(A_0)=\{f^*: f^*\in X^*, g^*\in X^*\}. \tag{25}$$

Let us now investigate whether or not the equation

$$(\alpha I-A_0^*)f^*=0 \tag{26}$$

has a nontrivial solution $f^*\in D(A_0^*)$, where α is a suitable positive number. We obtain from (26) and from (24)

$$\begin{aligned}&\alpha f^*(0)=0,\\ &(\alpha+pm)f^*(m)=pm\sum_{s=0}^{\infty}b(s)f^*(m+s-1),\\ &m=1,2,3,\cdots,\end{aligned} \tag{27}$$

where $\|f^*\|=\{\sup|f^*(m)|,\ m=1,2,3,\cdots\}<\infty$.

It follows from system (27) that

$$f^*(1)=(l\alpha+1)^{-1}\sum_{s=1}^{\infty}b(s)f^*(s) \tag{28}$$

$$\varphi^*(m)=(l\alpha+m)^{-1}\sum_{s=0}^{\infty}b(s)(m+s-1)\varphi^*(m+s-1),\quad m=2,3,\cdots, \tag{29}$$

where $\varphi^*(m)=f^*(m)/m$, $m=2,3,\cdots$. Hence, if system (27) has a nontrivial solution $f^*\in X^*$, then system (29) has a solution such that $|\varphi^*(m)|\to 0$ as $m\to+\infty$. Then there exists an integer $\bar{m}$, such that $\mu=\{\sup|\varphi^*(m)|, m=2,3,\cdots\}=|\varphi^*(\bar{m})|$. Consequently, we have from (29)

$$\begin{aligned}|\varphi^*(m)|&\le\mu(l\alpha+m)^{-1}\sum_{s=0}^{\infty}b(s)(m+s-1)\\ &=\mu(l\alpha+m)^{-1}(m+\bar{\nu}-1),\end{aligned} \tag{30}$$

where $\bar{\nu}=\sum_{s=0}^{\infty}sb(s)$ is the mean number of neutrons emitted if one neutron is absorbed and where we took into account the relation $\sum_{s=0}^{\infty}b(s)=1$. It follows from (30) that

$$\mu\le\mu[(\bar{m}+\bar{\nu}-1)/(\bar{m}+l\alpha)],$$

which leads to $\mu=0$, provided that $\alpha>\alpha_0=(\bar{\nu}-1)/l$. Hence, if $\alpha>\alpha_0$, $\varphi^*(m)=0$ and $f^*(m)=0$, $m=2,3,\cdots$, and $f^*(1)=0$ due to (28). We conclude that Eq. (26) admits only the trivial solution provided that $\alpha>\alpha_0$. Condition (ii) of Theorem 3 of Ref. 15 is then verified and, as a consequence, we have

$$\|\exp(tG)f\|=\|f\|,\quad t\ge 0,\ f\in X_+. \tag{31}$$

Moreover, $\exp(tG)$ is the only semigroup whose generator is an extension of A_0. It also follows from relations (18) that

$$\|T^{(j)}(t)f\|=[(qt)^j/j!]\|f\|,\quad t\ge 0,\ f\in X_+$$

and, consequently,

$$\|\exp[t(G+S)]f\|=\exp(qt)\|f\|,\quad t\ge 0,\ f\in X_+, \tag{32}$$

$$\|\exp[t(G+S-qI)]f\|=\|f\|,\quad t\ge 0,\ f\in X_+. \tag{33}$$

Relation (33) implies that

$$\|u(t)\|=\sum_{n=0}^{\infty}u(n;t)=\|u_0\|,\quad u_0\in D(G)\cap X_+,\ t\ge 0. \tag{34}$$

Remark 2: Let u_0 be as in Remark 1. Then, (34) implies that $u(t)=\exp[t(G+S-qI)]u_0$ is the physical solution of system (1)+(2). In other words, $u(t)=\{u(0;t), u(1,t),\cdots\}=\{P(0,t),P(1,t),\cdots\}\in X_+$ and $\|u(t)\|=\sum_{n=0}^{\infty}P(n,t)\equiv 1$, in agreement with the physical meaning of the $P(n,t)$'s.

6. FINITE-DIMENSIONAL APPROXIMATION OF (15)

We shall now indicate how the initial-value problem (15) can be approximated by a suitable problem in a finite-dimensional space $X^{(\lambda)}$. Let us in fact define $X^{(\lambda)}$ as the set of all $(\lambda+1)$-tuples of real numbers $f^{(\lambda)}=\{f^{(\lambda)}(n), n=0,1,\cdots\lambda\}$ with norm

$$\|f^{(\lambda)}\|_\lambda=\sum_{n=0}^{\lambda}|f^{(\lambda)}(n)|.$$

Moreover, let us introduce the operator $Q^{(\lambda)}\in\beta(X,X^{(\lambda)})$ as follows:

$$Q^{(\lambda)}f=g^{(\lambda)},\quad g^{(\lambda)}=\{f(n), n=0,1,\cdots,\lambda\},\quad D(Q^{(\lambda)})=X, \tag{35}$$

where it is easy to prove that

$$\|Q^{(\lambda)}\|\le 1,\quad \lim_{\lambda\to\infty}\|Q^{(\lambda)}f\|_\lambda=\|f\|,\quad f\in X. \tag{36}$$

Hence, the sequnce $\{X^{(1)},X^{(2)},\cdots,X^{(\lambda)},\cdots\}$ is a sequence of Banach spaces approximating X (Refs. 17, 18, and 19, p. 202).

Finally, let us define the following operations from $X^{(\lambda)}$ into $X^{(\lambda)}$:

$$\begin{aligned}&[S^{(\lambda)}f^{(\lambda)}]_n=qf^{(\lambda)}(n-1),\quad n=1,2,\cdots,\lambda,\\ &[S^{(\lambda)}f^{(\lambda)}]_0=0,\quad D(S^{(\lambda)})=X^{(\lambda)},\\ &[G_r^{(\lambda)}f^{(\lambda)}]_n=-pnf^{(\lambda)}(n)+rp\sum_{s=0}^{n}b(s)(n+s-1)\\ &\qquad f^{(\lambda)}(n+s-1),\quad n=0,1,\cdots\lambda-1,\\ &[G_r^{(\lambda)}f^{(\lambda)}]_\lambda=-p\lambda f^{(\lambda)}(\lambda)+rp\sum_{s=1}^{\lambda}b(s)(\lambda+s-1)\\ &\qquad f^{(\lambda)}(\lambda+s-1),\end{aligned} \tag{37, 38}$$

where $D(G_r^{(\lambda)})=Q^{(\lambda)}[D]$ (see Sec. 2) and where r is a fixed value of the real parameter, such that $0\le r<1$ [see (12) of Sec. 2].

We have from (37) and from (38)

$$\|Q^{(\lambda)}Sf-S^{(\lambda)}Q^{(\lambda)}f\|_\lambda=0,\quad \lambda=1,2,\cdots,\ f\in X,$$

$$\|Q^{(\lambda)}G_rf-G_r^{(\lambda)}Q^{(\lambda)}f\|_\lambda=[b(0)/l](\lambda+1)|f(\lambda+1)|,\quad f\in D,$$

and also

$$\lim_{\lambda\to\infty}\|Q^{(\lambda)}Sf-S^{(\lambda)}Q^{(\lambda)}f\|_\lambda=0,\quad f\in X, \tag{39}$$

$$\lim_{\lambda\to\infty}\|Q^{(\lambda)}G_r f - G_r^{(\lambda)}Q^{(\lambda)}f\|_\lambda = 0, \quad f\in D, \tag{40}$$

since $\lim[(\lambda+1)|f(\lambda+1)|]=0$ as $\lambda\to\infty$ provided that $f\in D(G_r)=D$ (see Sec. 2).

Finally, it is not difficult to prove that $G_r^{(\lambda)}$ is a generator of class $\mathcal{G}(1,0)$ in $X^{(\lambda)}$ just as $G_r\in\mathcal{G}(1,0)$ in X. As a conclusion, we have (Refs. 17, 18, and Ref. 19, p. 205)

$$\lim_{\lambda\to\infty}\|Q^{(\lambda)}\exp[t(G_r+S-qI)]f-\exp[t(G_r^{(\lambda)}+S^{(\lambda)} - qI^{(\lambda)})]Q^{(\lambda)}f\|_\lambda = 0 \tag{41}$$

uniformly with respect to t in any finite interval $[0,\bar{t}]$, where $I^{(\lambda)}$ is the identity operator in $X^{(\lambda)}$.

Due to (b) of Theorem 1, if we choose r close enough to 1, we obtain from (41)

$$\|Q^{(\lambda)}[\exp t(G+S-qI)]f-\exp[t(G_r^{(\lambda)}+S^{(\lambda)} - qI^{(\lambda)})]Q^{(\lambda)}f\|_\lambda < \epsilon, \tag{42}$$

uniformly in any finite interval of t, provided that λ is large enough.

Let us now consider the following initial-value problem in $X^{(\lambda)}$:

$$\frac{d}{dt}u^{(\lambda)}(t) = [G_r^{(\lambda)}+S^{(\lambda)}-qI^{(\lambda)}]u^{(\lambda)}(t), \quad t>0,$$
$$\lim_{t\to 0^+}\|u^{(\lambda)}(t)-u_0^{(\lambda)}\|_\lambda = 0, \quad u_0^{(\lambda)}\in D(G_r^{(\lambda)}); \tag{43}$$

then, if we choose $u_0^{(\lambda)}=Q^{(\lambda)}u_0$, the solution $u(t)$ of problem (15) is such that

$$\|Q^{(\lambda)}u(t)-u^{(\lambda)}(t)\| < \epsilon, \tag{44}$$

uniformly with respect to $t\in[0,\bar{t}]$, provided that λ is large enough.

Relation (44) has an obvious interpretation. The first $(\lambda+1)$ components of the vector $u(t)\in X$ can be approximated by the corresponding components of $u^{(\lambda)}\in X^{(\lambda)}$ with an error not larger than an arbitrarily small $\epsilon>0$.

We dwell on the fact that (43) is an initial-value problem in a finite-dimensional space. As a consequence, it is not difficult to obtain a numerical solution of system (43).

7. THE KINETIC EQUATION

We are finally going to show how an equation for the first moment of the neutron population $\langle n\rangle(t)$ can be deduced from (1) in a rigorous way.

If we multiply both sides of (1) by n, we obtain

$$\frac{\partial P_1(n,t)}{\partial t} = -pnP_1(n,t)+pn\sum_{s=0}^{n}b(s)P_1(n+1-s,t) + q[P_1(n-1,t)-P_1(n,t)]+qP(n-1,t), \quad n=1,2,\cdots, \tag{45}$$

where $P_1(n,t)=nP(n,t)$, $n=1,2,\cdots$, and where we let $P_1(0,t)=0$. System (35) must be supplemented with an initial condition of the form

$$P_1(n,0)=P_{10}(n)=nP_0(n), \quad n=1,2,\cdots, \tag{46}$$

where $0\le P_{10}(n)\le n$ [see (2) and (3)].

The definition (21) of $\langle n\rangle(t)$ leads us to introduce the Banach space X_1 of all vectors $f_1=\{f_1(n), n=1,2,\cdots\}$ with norm

$$\|f_1\|_1=\sum_{n=1}^{\infty}|f_1(n)|<\infty.$$

Remark 3: X_1 may be identified, if necessary, with the closed subspace of X composed of all vectors of X, such that $f(0)=0$.

We also define the following operators:

$$[H_1f_1]_n = p(n-1)f_1(n), \quad n=1,2,\cdots, \tag{47}$$

$$[K_1f_1]_n = p\sum_{s=0}^{n}b(s)(n-s)f_1(n+1-s), \quad n=1,2,\cdots, \tag{48}$$

$$[B_1f_1]_n = p\sum_{s=1}^{n}sb(s)f_1(n+1-s), \quad n=1,2,\cdots, \tag{49}$$

$$[S_1f_1]_n = qf_1(n-1), \quad n=2,3,\cdots, \quad [S_1f_1]_1=0, \tag{50}$$

where $[H_1f_1]_n$ indicates the nth component of the vector $H_1f_1\in X_1$ and where

$$D(H_1)=D(K_1)=D_1=\{f_1: f_1\in X_1, \ \sum_{n=1}^{\infty}n|f_1(n)|<\infty\},$$
$$D(B_1)=D(S_1)=X_1. \tag{51}$$

Remark 4: H_1 and K_1 operate on each $f_1\in D_1\subset X_1$ just as H and K do on each $f\in D\subset X$. In other words, H_1 and K_1 are respectively H and K evaluated by an "X_1-observer." This can be verified by comparing $[H_1f_1]_n$ and $[K_1f_1]_n$ with $[Hf]_{n-1}$ and with $[Kf]_{n-1}$.

As far as B_1 is concerned, we have

$$\|B_1f_1\|_1 \le p\sum_{n=1}^{\infty}\sum_{s=1}^{n}sb(s)|f(n+1-s)| = p\sum_{s=1}^{\infty}sb(s)\sum_{n=s}^{\infty}|f(n+1-s)| = (\bar{\nu}/l)\|f_1\|_1, \tag{52}$$

$$B_1[X_{1+}]\subset X_{1+}, \quad \|B_1f_1\|_1=(\bar{\nu}/l)\|f_1\|_1, \quad f_1\in X_{1+}, \tag{53}$$

where $X_{1+}=\{f_1: f_1\in X_1; f_1(n)\ge 0, \ n=1,2,\cdots\}$ and where $\bar{\nu}=\sum_{s=1}^{\infty}sb(s)$ (see Sec. 5).

Finally, we obtain from (50)

$$S_1[X_{1+}]\subset X_{1+}, \quad \|S_1f_1\|_1=q\|f_1\|_1. \tag{54}$$

By using definitions (47)–(50), the abstract version of system (45) + (46) becomes

$$\frac{d}{dt}u_1 = (-H_1+K_1+S_1-qI_1)u_1(t)+(B_1-pI_1)u_1(t)+qI_1v(t), \quad t>0,$$
$$\lim_{t\to 0^+}\|u_1(t)-u_{10}\|=0, \tag{55}$$

where $u_{10}=\{P_{10}(1),P_{10}(2),\cdots\}$ and where $v(t)=\{u(0;t), u(1;t),\cdots\}$ is just the $u(t)$ of the preceding sections considered as an element of X_1.

Since H_1 and K_1 are just the operators H and K considered in X_1 (see Remark 4), a semigroup $\{\exp(tG_1), t\ge 0\}$ exists, such that

$$\exp(tG_1)[X_{1+}]\subset X_{1+}, \quad \|\exp(tG_1)f_1\|_1=\|f_1\|_1, \quad f_1\in X_{1+}, \tag{56}$$

where G_1 is a closed operator and where

$$(-H_1+K_1)\subset G_1\subset A_1. \tag{57}$$

Here, A_1 is defined as follows:

$$[A_1f_1]_n=-p(n-1)f_1(n)+p\sum_{s=0}^{n}(n-s)f_1(n+1-s)=g_1(n),$$
$$n=1,2,\cdots, \tag{58}$$
$$D(A_1)=\{f_1: f_1\in X_1,\quad g_1\in X_1\}\supset D_1,$$

and it is the version of A in X_1 [see (4) and Remark 4].

Starting from (56) and by a procedure similar to that of Sec. 5, we obtain successively for any $f_1\in X_{1+}$

$$\|\exp[t(G_1+S_1-qI_1)]f_1\|_1=\|f_1\|_1, \tag{59}$$

$$\|\exp[t(G_1+S_1-qI_1+B_1)]f_1\|_1=\exp[(\bar\nu/l)t]\,\|f_1\|_1, \tag{60}$$

$$\|\exp(t\chi_1)f_1\|_1=\exp\left(\frac{\bar\nu-1}{l}t\right)\|f_1\|_1, \tag{61}$$

where all the preceding semigroups transform X_{1+} into itself and where

$$\chi_1=G_1+S_1-qI_1+B_1-pI_1,\quad D(\chi_1)=D(G_1). \tag{62}$$

Let us now consider the following initial-value problem:

$$\frac{du_1}{dt}=\chi_1u_1(t)+qI_1v(t),\quad t>0,$$
$$\lim_{t\to0^+}u_1(t)=u_{10}\in D(\chi_1)\cap X_{1+}, \tag{63}$$

where $v(t)\in X_{1+}$ for any $t\geq0$ and $\|v(t)\|_1=1$ (see Remark 2). We have from (63) (Ref. 13, p. 486)

$$u_1(t)=\exp(t\chi_1)u_{10}+q\int_0^t\exp[(t-s)\chi_1]v(s)\,ds, \tag{64}$$

and also

$$\|u_1(t)\|_1=\exp\left(\frac{\bar\nu-1}{l}\right)\|u_{10}\|_1+q\int_0^t\exp\left(\frac{\bar\nu-1}{l}(t-s)\right)ds, \tag{65}$$

since we are dealing with elements of X_{1+}.

Equation (64) is equivalent to the following system:

$$\frac{d}{dt}\|u_1(t)\|_1=\frac{\bar\nu-1}{l}\|u_1(t)\|_1+q,\quad t>0,$$
$$\lim_{t\to0^+}\|u_1(t)\|_1=\|u_{10}\|_1. \tag{66}$$

The first of (66) has the form of the standard kinetic equation of a multiplying medium with a source q.

8. CONCLUDING REMARKS

Let $u_0=\{P_0(0),P_1(0),\cdots\}\in D_0\cap X_+\subset D\cap X_+$ with $\|u_0\|=1$ (see Remarks 1 and 2). Then, $u_{10}=\{P_0(1),2P_0(2),3P_0(3),\cdots\}\in D_1\cap X_{1+}\subset D(\chi_1)\cap X_{1+}$ and the physical conditions (3) and (46) are satisfied since $P_0(n)\equiv0$ provided n is large enough (which is indeed physically correct). It follows that $u(t)=\{u(0;t),u(1;t),\cdots\}$ given by (16) is a positive solution of (1) + (2) such that $\|u(t)\|=\sum_{n=0}u(n;t)\equiv1$ (see Remark 2). Moreover, due to (57), $u_1(t)=\{u_1(1;t),u_1(2;t),\cdots\}$ given by (64) is a positive solution of system (45) + (46). Hence, $u_1(t)=\{u(1;t),2u(2;t),3u(3;t),\cdots\}$ and, consequently, $\|u_1(t)\|_1=\sum_{n=1}nu(n;t)=\langle n\rangle(t)$. In other words, if we put $w(t)=\{w(n,t)=u_1(n,t)/n-u(n,t),\ n=1,2,\cdots\}$, we have that $w(t)=0$ at any $t\geq0$. This result follows from some properties of $u_r=u_r(t)$, where $u_r(t)$ is the solution of system (15) with G_r instead of G. (A further paper will be devoted to the study of this and of other properties of the "approximate" solution u_r.)

Remark 5: The procedures of Sec. 7 can be used in order to find an equation for the second moment $\langle n^2\rangle(t)$. To this aim, we multiply both sides of (45) by n and we put $P_2(n,t)=nP_1(n,t)$, $n=1,2,\cdots$. Since $P_2(1,t)=P_1(1,t)$ is already known, we introduce the Banach space X_2 of all vectors $f_2=\{f_2(n),n=2,3,\cdots\}$ with norm $\|f_2\|_2=\sum_{n=2}|f_2(n)|$ to study the evolution of $u_2(t)=\{P_2(2,t),P_2(3,t),\cdots\}$. We also define the operators H_2 amd K_2 (the versions of H and K in X_2, see Remark 4) and we then proceed as in Sec. 7.

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Wave propagation in media undergoing uniform linear acceleration

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Wave propagation in a homogenous material undergoing uniform linear acceleration is considered. The covariant constitutive equations for a holohedral, nondispersive, dielectric material derived by Lianis are applied. Expressions are found for initially plane waves propagating in the direction of accelerated motion for the case where the material functions are constant. Expressions are also found for the radiation reflected and refracted at the surface of a half-space undergoing uniform linear acceleration. A detailed energy balance across this interface is also presented.

1. INTRODUCTION

The problem of wave propagation in a uniformly linear accelerated medium has been considered by Mo.[1] He applied a theory of local electrodynamics in noninertial frames based on the principle of equivalence. The constitutive theory used by Mo, as applied to media undergoing rigid rotation, has been questioned by Post and Bahulikar.[2] Recently Lianis[3] developed an invariant constitutive theory for the interaction of matter with electromagnetic fields based on the theory of general relativity. This theory has been applied to problems involving uniform rigid rotation by Lianis[3] and by Lianis and Whicker[4] in order to study the Sagnac effect.

Previous work involving the reflection and refraction of electromagnetic waves on interfaces moving at constant velocity has been done by such authors as Yeh,[5] Pyati,[6] and Daly and Gruenberg.[7] Yeh calculates reflection and transmission coefficients using the classical expression $\frac{1}{2}$ Re $(\mathbf{E}\times\mathbf{H}^*)$ for the time averaged Poynting vector. Berger[8] discussed the validity of using this time averaged Poynting vector. Daly and Gruenberg pointed out that a detailed consideration of the energy balance across the moving interface must take into account such effects as radiation pressure.

In this paper we consider the problem of wave propagation in a material undergoing uniformly linear acceleration. We apply the constitutive equations for a holohedral, nondispersive, dielectric material derived in covariant form in Ref. 3. These equations, under certain assumptions about the material functions, reduce to those used by Mo for this problem. In Sec. 2 we formulate the problem and summarize the relevant sections of Ref. 3. In Sec. 3 we consider the problem of electromagnetic radiation propagating along the direction of the accelerated motion as viewed by an inertial observer. Expressions are found for the electromagnetic fields for the case where the material functions are constant. In Sec. 4 we consider the radiation reflected and refracted at the surface of a material halfspace undergoing uniform linear acceleration. Expressions for the reflected and transmitted waves as a function of the time of incidence τ are found for two cases. In Sec. 5 expressions for the instantaneous reflection and transmission coefficients at time τ are found. A detailed energy balance across the moving interface is also considered. The results of this study are summarized in Sec. 6. In Appendix B we compare the results of the approach presented here to those obtained in Ref. 1.

2. LINEAR UNIFORM ACCELERATION

Let $\{x^\mu\}=\{x,y,z,ct\}$ denote the coordinates of an event in an inertial Minkowski reference frame and let $\{x'^\mu\}=\{x',y',z',ct'\}$ denote the coordinates of an event in a medium comoving reference frame. Here $\{x^m\}=\{x,y,z\}$ and $\{x'^m\}=\{x',y',z'\}$ are spatial Cartesian coordinates. The temporal coordinate is $x^4=ct$ in the inertial reference rame and $x'^4=ct'$ in the medium comoving frame. (Greek indices in this paper take the values 1, 2, 3, or 4 with the value 4 corresponding to the temporal coordinate. Italic indices take the value 1, 2, or 3 and correspond to spatial coordinates. The customary convention of summation over repeated indices is also used.) Here t denotes the time in the inertial frame, t' the time in the medium comoving frame, and c is the speed of light in vacuum. For a medium moving with uniform linear acceleration the inertial and comoving coordinates are related by the transformations (Rindler, Ref. 9)

$$\begin{aligned} x^1 &= x'^1 + \frac{c}{a}\cosh\frac{a}{c}x'^4 - 1\ , \\ x^2 &= x'^2, \\ x^3 &= x'^3, \\ x^4 &= c/a\sinh a/cx'^4, \end{aligned} \tag{2.1}$$

where the origins have been adjusted so that at $x^4=0=x'^4$ their relative velocity is zero. The inverse relations are given by

$$\begin{aligned} x'^1 &= x^1 - \frac{c}{a}\{\sqrt{1+(a/cx^4)^2}-1\}, \\ x'^2 &= x^2, \\ x'^3 &= x^3, \\ x'^4 &= \frac{c}{a}\ln\left\{\frac{a}{c}x^4+\sqrt{1+(a/cx^4)^2}\right\}, \end{aligned} \tag{2.2}$$

The covariant and contravariant metrics defined by the quadratic form

$$dS^2 = -G_{\alpha\beta}dx^\alpha dx^\beta, \tag{2.3}$$

where dS is the differential of proper time are, in the Cartesian coordinate system x^μ,

$$\|G_{\alpha\beta}\|=\mathrm{diag}\{1,1,1,-1\}, \tag{2.4}$$

$$\|G^{\alpha\beta}\| = \mathrm{diag}\{1, 1, 1, -1\}.$$

We will denote quantities expressed in the comoving coordinate system as primed quantities.

The metric $g'_{\alpha\beta}$ in the comoving coordinate system $\{x'^{\mu}\}$ is found using the equation

$$\|g'_{\alpha\beta}\| = \left\| \frac{\partial x^{\mu}}{\partial x'^{\alpha}} \frac{\partial x^{\nu}}{\partial x'^{\beta}} G_{\mu\nu} \right\|. \tag{2.5}$$

The result is

$$\|g'_{\alpha\beta}\| = \begin{Vmatrix} 1 & 0 & 0 & \sinh\frac{a}{c}x'^4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh\frac{a}{c}x'^4 & 0 & 0 & -1 \end{Vmatrix}. \tag{2.6}$$

Note also that

$$\sqrt{-g} = \cosh\frac{a}{c}x'^4 \tag{2.7}$$

where $g' = \det g'_{\alpha\beta}$.

The contravariant metric in the comoving system $\{x'^{\mu}\}$ may be found by inverting (2.6).

Now consider a point of fixed spatial position in the comoving frame $x'^1 = \text{const}$, $x'^2 = \text{const}$, $x'^3 = \text{const}$. For this situation using (2.1) we find that

$$\begin{aligned} dx^1 &= \sinh\frac{a}{c}x'^4\, dx'^4, \\ dx^2 &= 0, \\ dx^3 &= 0, \\ dx^4 &= \cosh\frac{a}{c}x'^4\, dx'^4 \end{aligned} \tag{2.8}$$

and thus from (2.3)

$$dS = dx'^4. \tag{2.9}$$

Using the relations

$$u^{\alpha} = \frac{dx^{\alpha}}{dS}, \quad u_{\alpha} = G_{\alpha\beta}u^{\beta}, \tag{2.10}$$

we find that the covariant and contravariant components in the inertial frame of the 4-velocity of a particle fixed in the comoving frame are given by

$$\begin{aligned} \{u^{\alpha}\} &= \left\{\sinh\frac{a}{c}x'^4, 0, 0, \cosh\frac{a}{c}x'^4\right\} \\ &= \left\{\frac{a}{c}x^4, 0, 0, \left[1 + \left(\frac{a}{c}x^4\right)^2\right]^{1/2}\right\}, \\ \{u_{\alpha}\} &= \left\{\sinh\frac{a}{c}x'^4, 0, 0, -\cosh\frac{a}{c}x'^4\right\} \\ &= \left\{\frac{a}{c}x^4, 0, 0, -\left[1 + \left(\frac{a}{c}x^4\right)^2\right]^{1/2}\right\}. \end{aligned} \tag{2.11}$$

Using the tensor transformations

$$u'^{\alpha} = \frac{\partial x'^{\alpha}}{\partial x^{\beta}}u^{\beta}, \quad u'_{\beta} = \frac{\partial x^{\beta}}{\partial x'^{\alpha}}u_{\beta}, \tag{2.12}$$

the 4-velocity of the same particle in the comoving frame is found to be

$$\begin{aligned} \{u'^{\alpha}\} &= \{0, 0, 0, 1\}, \\ \{u'_{\alpha}\} &= \left\{\sinh\frac{a}{c}x'^4, 0, 0, -1\right\}. \end{aligned} \tag{2.13}$$

To be consistent with Ref. 3 we assume that the motion starts from a reference state at $x^4 = 0$. The medium, referred to an inertial frame, is undeformed, unpolarized, and unmagnetized in this reference state. Let us call

$$X^K = (X, Y, Z)$$

the Cartesian coordinates of a material particle in the reference state. Then the motion $x^{\alpha} = x^{\alpha}(X^K, x^4)$ is given by

$$\begin{aligned} x^1 &= X + \frac{c}{a}\left\{\left[1 + \left(\frac{a}{c}x^4\right)^2\right]^{1/2} - 1\right\}, \\ x^2 &= Y, \\ x^3 &= Z, \\ x^4 &= ct. \end{aligned} \tag{2.14}$$

The deformation gradient of the uniformly linear accelerated medium referred to the inertial frame $x^{\alpha}_{,K}$, the projector tensor $S^{\alpha}{}_{\rho}$, the relativistic deformation gradient $\phi^{\alpha}{}_{K}$, and the relativistic left Green–Cauchy tensor are defined by the expressions

$$\|x^{\alpha}{}_{,K}\| = \left\| \frac{\partial x^{\alpha}(X^K, x^4)}{\partial X^K} \right\|, \tag{2.15}$$

$$S^{\alpha}{}_{\rho} = \delta^{\alpha}{}_{\rho} + u^{\alpha}u_{\rho}, \tag{2.16}$$

$$\phi^{\alpha}{}_{K} = S^{\alpha}{}_{\rho}x^{\rho}{}_{,K}, \tag{2.17}$$

$$b^{\alpha\beta} = G^{KL}\phi^{\alpha}{}_{K}\phi^{\beta}{}_{L}, \tag{2.18}$$

where the metric of the coordinate system in the reference state is

$$\|G^{KL}\| = \mathrm{diag}(1, 1, 1).$$

The integral powers of **b** are defined in the way that integral powers of tensors are normally defined. The zeroth power of **b**, however, is defined to be equal to the projector tensor **s**.

Now let $\mathbf{E} = \{E_i\}$, $\mathbf{B} = \{B^i\}$, $\mathbf{D} = \{D^i\}$, and $\mathbf{H} = \{H_i\}$ be the spatial components in some coordinate system θ^{μ} of the electric field, the magnetic induction, the dielectric displacement, and the magnetic intensity, respectively. The corresponding relativistic vectors with tensoral properties in space–time are

$$\mathcal{E}_{\alpha} = \phi_{\alpha\beta}u^{\beta}, \quad \mathcal{B}^{\alpha} = \tfrac{1}{2}e^{\alpha\beta\gamma\delta}\phi_{\beta\gamma}u_{\delta}, \tag{2.19}$$

where the components of the skew-symmetric electromagnetic flux tensor $\phi_{\alpha\beta}$ are given by

$$\phi_{ij} = \sqrt{g^*}\, e^{\alpha\beta\gamma\delta}B^k, \quad \phi_{i4} = -\phi_{4i} = E_i \tag{2.20}$$

and

$$g^* = \det g_{km}.$$

also

$$\mathcal{H}_{\alpha} = \tfrac{1}{2}e_{\alpha\beta\gamma\delta}\eta^{\beta\gamma}u^{\delta}, \quad \mathcal{D}^{\alpha} = \eta^{\alpha\beta}u_{\beta} \tag{2.21}$$

where $\eta^{\alpha\beta}$ is the skew-symmetric electromagnetic potential tensor given by

$$\eta^{ij} = e^{ijk}H_k, \quad \eta^{4i} = -\eta^{i4} = \sqrt{g^*}D^i. \tag{2.22}$$

Here $e^{\alpha\beta\gamma\delta}$ and $e_{\alpha\beta\gamma\delta}$ are the four-dimensional permutation symbols with $e_{1234}=1$ and $e^{1234}=-1$ while e_{ijk} and e^{ijk} are the three-dimensional permutation symbols with $e_{123}=e^{123}=1$.

Maxwell's equations are expressed in terms of the spatial vectors **E**, **B**, **D**, and **H**. In the absence of free charges and currents they are given in all reference frames by (we use here the Lorentz—Heaviside electromagnetic units)

$$\operatorname{curl}\mathbf{E} + \frac{\partial \mathbf{B}}{\partial \theta^4} = 0, \tag{2.23a}$$

$$\operatorname{div}\mathbf{B} = 0, \tag{2.23b}$$

$$\operatorname{curl}\mathbf{H} - \frac{\partial \mathbf{D}}{\partial \theta^4} = 0, \tag{2.23c}$$

$$\operatorname{div}\mathbf{D} = 0. \tag{2.23d}$$

In this paper we consider holohedral, nondispersive, dielectric materials. Lianis (Ref. 3) has derived constitutive equations in covariant form for such materials. These equations for linear dielectries are

$$\mathcal{D}^\rho = \sqrt{-g}\sum_{m=0}^{2}(\mathbf{b}^m)^{\rho\theta}\alpha_{(m)}\mathcal{E}_\theta, \tag{2.24}$$

$$\mathcal{H}_\rho = \sum_{m=0}^{2}(\mathbf{b}^m)_{\rho\theta}\delta_{(m)}\frac{B^\theta}{\sqrt{-g}}, \tag{2.25}$$

where $\alpha_{(m)}$ and $\delta_{(m)}$ are functions of the invariants I_1, I_2, and I_3 of the deformation. These invariants are defined by (The symbol Tr**A** denotes the trace of tensor **A**. If **A** is a 4-tensor in space—time then

$$\mathrm{Tr}\mathbf{A} = A^\mu{}_\mu = g^{\mu\nu}A_{\nu\mu}$$

where $g^{\mu\nu}$ is the metric of the coordinate system θ^μ.)

$$I_1 = J_1, \quad I_2 = \tfrac{1}{2}(J_1^2 - J_2), \quad I_3 = \tfrac{1}{6}(J_2^2 - 3J_1J_2 + 2J_3), \tag{2.26}$$

where

$$J_1 = Trb, \quad J_2 = \mathrm{Tr}b^2, \quad J_3 = \mathrm{Tr}b^3. \tag{2.27}$$

We also need an expression for the relativistic energy—momentum tensor of the electromagnetic field. We will use the expression derived by DeGroot and Suttorp, Ref. 10, from a microscopic model of interaction of the electromagnetic field with matter. This expression is

$$\begin{aligned} S^{\alpha\beta} &= -\phi^\alpha{}_\nu\eta^{\nu\beta} + \tfrac{1}{4}\eta^{\mu\nu}\phi_{\nu\mu}g^{\alpha\beta} \\ &= (\mathcal{E}_\rho\mathcal{D}^\rho + \mathcal{H}_\rho\mathcal{B}^\rho)(u^\alpha u^\beta + \tfrac{1}{2}g^{\alpha\beta}) \\ &\quad + e^{\beta\nu\delta\lambda}\mathcal{E}_\nu\mathcal{H}_\delta u_\lambda u^\alpha + e^{\alpha\nu\delta\lambda}\mathcal{D}_\nu\mathcal{B}_\delta u_\lambda u^\beta \\ &\quad - (\mathcal{E}^\alpha\mathcal{D}^\beta + \mathcal{H}^\alpha\mathcal{B}^\beta). \end{aligned} \tag{2.28}$$

3. WAVE PROPAGATION VIEWED BY INERTIAL OBSERVER

Let us consider the problem where we have a monochromatic plane wave propagating in the positive x^1 direction in an infinite slab of material characterized by the constitutive equations (2.24) and (2.25). At time $x^4 = 0$ the material starts moving according to equations (2.1) and (2.2). We seek expressions for the **B** and **E** observed by an inertial observer.

For a homogeneous medium in which the wave is propagating in the x^1-direction the vectors **B**, **E**, **D**, and **H** are functions of x^1 and x^4 only. Clearly then from Maxwell's equations B^1 and D^1 must be space—time constants. A spatially uniform static field may be superimposed on any solution of Maxwell's equations and the result is a solution. Therefore, without loss of generality we may take $B^1 = 0$, $D^1 = 0$.

For this problem the expressions relating the relativistic electromagnetic fields and their corresponding spatial vector components are found by substituting the velocities (2.12) into (2.19) and (2.21) are making use of the expressions (2.20) and (2.22). The required expressions for the relativistic left Green—Cauchy tensor and its powers are found by using Eqs. (2.14)—(2.18). Substituting these results into the constitutive equations (2.24) and (2.25), we find that the nonzero components of **D** and **H** are related to the nonzero components of **B** and **E** by the expressions (when the index m in $\alpha_{(m)}$ or $\delta_{(m)}$ takes a specific numerical value, we drop the parentheses for convenience)

$$\begin{aligned} D^2 &= \left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right](\alpha_0+\alpha_1+\alpha_2) - \left(\frac{a}{c}x^4\right)^2(\delta_0+\delta_1+\delta_2)\right\}E_2 \\ &\quad + \left(\frac{a}{c}x^4\right)\left[1+\left(\frac{a}{c}x^4\right)^2\right]^{1/2}[(\delta_0+\delta_1+\delta_2) - (\alpha_0+\alpha_1+\alpha_2)]B^3, \end{aligned} \tag{3.1}$$

$$\begin{aligned} D^3 &= \left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right](\alpha_0+\alpha_1+\alpha_2) - \left(\frac{a}{c}x^4\right)^2(\delta_0+\delta_1+\delta_2)\right\}E_3 \\ &\quad - \left(\frac{a}{c}x^4\right)\left[1+\left(\frac{a}{c}x^4\right)^2\right]^{1/2}[(\delta_0+\delta_1+\delta_2) - (\alpha_0+\alpha_1+\alpha_2)]B^2, \end{aligned} \tag{3.2}$$

$$\begin{aligned} H_2 &= \left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right](\delta_0+\delta_1+\delta_2) - \left(\frac{a}{c}x^4\right)^2(\alpha_0+\alpha_1+\alpha_2)\right\}B^2 \\ &\quad + \left(\frac{a}{c}x^4\right)\left[1+\left(\frac{a}{c}x^4\right)^2\right]^{1/2}[(\delta_0+\delta_1+\delta_2) - (\alpha_0+\alpha_1+\alpha_2)]E_3, \end{aligned} \tag{3.3}$$

$$\begin{aligned} H_3 &= \left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right](\delta_0+\delta_1+\delta_2) - \left(\frac{a}{c}x^4\right)^2(\alpha_0+\alpha_1+\alpha_2)\right\}B^3 \\ &\quad - \left(\frac{a}{c}x^4\right)\left[1+\left(\frac{a}{c}x^4\right)^2\right]^{1/2}[(\delta_0+\delta_1+\delta_2) - (\alpha_0+\alpha_1+\alpha_2)]E_2. \end{aligned} \tag{3.4}$$

Substituting (3.1)—(3.4) into (2.23c), operating on the resulting expression with $\partial/\partial x^1$, and then using (2.23a) to eliminate **E**, we find that the components B^2 and B^3 must satisfy an equation of the form

$$a_{11}\frac{\partial^2 B}{\partial x^1\partial x^1} + 2a_{12}\frac{\partial^2 B}{\partial x^1\partial x^4} + a_{22}\frac{\partial^2 B}{\partial x^4\partial x^4} + b_1\frac{\partial B}{\partial x^1} + b_2\frac{\partial B}{\partial x^4} = 0, \tag{3.5}$$

where B is used to denote either B^1 or B^2 and the coefficients are given in the Appendix. The characteristic

equation of (3.5) yields

$$\frac{dx^4}{dx^1}=\frac{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)\pm\sqrt{gh}}{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}, \tag{3.6}$$

where we have defined

$$g=\alpha_0+\alpha_1+\alpha_2, \quad h=\delta_0+\delta_1+\delta_2. \tag{3.7}$$

Obviously (3.5) is hyperbolic and may be transformed to its canonical form by the transformations

$$\alpha=x^1-\int_0^{x^4}\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}(g-h)+\sqrt{gh}}dx^4, \tag{3.8}$$

$$\beta=x^1-\int_0^{x^4}\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}(g-h)-\sqrt{gh}}dx^4. \tag{3.9}$$

The transformed equation is given by

$$2\bar{a}_{12}\frac{\partial^2 B}{\partial\alpha\,\partial\beta}+\bar{b}_1\frac{\partial B}{\partial\alpha}+\bar{b}_2\frac{\partial B}{\partial\beta}=0, \tag{3.10}$$

where the coefficients are given in Appendix A.

Let us now consider (3.10) for the special case where α_0, α_1, α_2, δ_0, δ_1, and δ_2 are constants. For this case g and h are constants and thus $\bar{b}_1=\bar{b}_2=0$. Equation (3.10) reduces to

$$\frac{\partial^2 B}{\partial\alpha\,\partial\beta}=0 \tag{3.11}$$

and thus we may write

$$B=f_1(\alpha)+f_2(\beta),$$

where f_1 and f_2 are arbitrary functions of their variables and α and β are defined by (3.8) and (3.9). First consider the case where

$$B^3=f_1(\alpha)+f_2(\beta). \tag{3.12}$$

Using (3.12) in (2.33a) we can show that

$$E_2=k_1(x^4)f_1(\alpha)+k_2(x^4)f_2(\beta)-q(x^4) \tag{3.13}$$

where $q(x^4)$ is an arbitrary function of x^4. Similarly, for

$$B^2=\bar{f}_1(\alpha)+\bar{f}_2(\beta), \tag{3.14}$$

then

$$E_3=-k_1(x^4)\bar{f}_1(\alpha)-k_2(x^4)\bar{f}_2(\beta)+\bar{q}(x^4), \tag{3.15}$$

where we used the notation

$$k_1(x^4)=\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)+\sqrt{g}\,h},$$

$$k_2(x^4)=\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)-\sqrt{gh}}. \tag{3.16}$$

For the problem under consideration we may orient the x^2 and x^3 axes so that the initial conditions are given by

$$B^2(x^1,0)=B_0\exp(ikx^1), \quad E_3(x^1,0)=-E_0\exp(ikx^1), \tag{3.17}$$

where

$$k=\frac{\omega}{c}\sqrt{g/h}, \quad B_0=\sqrt{g/h}\,E_0 \tag{3.18}$$

and all other components are zero. With the definition of α and β given by (3.8) and (3.9) the functions of α are associated with a wave traveling in the negative x^1 direction and the functions of β are associated with a wave traveling in the positive x^1 direction. Applying the initial conditions, we find

$$B^2(x^1,x^4)=B_0\exp[ik(x^1-\textstyle\int_0^{x^4}k_2(\gamma)\,d\gamma)], \tag{3.19}$$

$$E_3(x,x)=-B_0\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)-\sqrt{gh}}$$

$$\times\exp[ik(x^1-\textstyle\int_0^{x^4}k_2(\gamma)\,d\gamma)]+\bar{q}(x^4) \tag{3.20}$$

with the initial condition $\bar{q}(0)=0$. Using the constitutive equations (3.19) and (3.20) in (2.23c), we solve for $\bar{q}(x^4)$.

After applying the initial condition on $\bar{q}(x^4)$, we find

$$E_3(x^1,x^4)=-B_0\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}(g-h)-\sqrt{gh}}$$

$$\times\exp[ik(x^1-\textstyle\int_0^{x^4}k_2(\gamma)\,d\gamma)]. \tag{3.21}$$

Similarly, if we consider the case of a wave propagating in the negative x^1 direction, the initial conditions are

$$B^2(x^1,0)=B_0\exp(-ikx^1), \quad E_3(x^1,0)=E_0\exp(-ikx^1) \tag{3.22}$$

with all other components zero. Applying these conditions, we find

$$B^2(x^1,x^4)=B_0\exp[-ik(x^1-\textstyle\int_0^{x^4}k_1(\gamma)\,d\gamma)], \tag{3.23}$$

$$E_3(x^1,x^4)=-B_0\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}(g-h)+\sqrt{gh}}$$

$$\times\exp[-ik(x^1-\textstyle\int_0^{x^4}k_1(\gamma)\,d\gamma)]. \tag{3.24}$$

4. UNIFORMLY ACCELERATED HALF SPACE

We now consider the case where the half space $x^1>0$ is occupied by a material while the half space $x^1<0$ contains only free space. At time $x^4=0$ the material half space begins to move in the positive x^1 direction with a motion described by (2.1) or (2.2). At some later time $x^4=\tau$, the surface $x'^1=0$ occupies the position $x^1=d$. We will consider the interaction of a monochromatic plane wave propagating in the positive x^1 direction with this surface for two types of material. First, we will consider the case where the material is a perfect conductor. Secondly, we will consider the case where the material obeys the constitutive equations (2.24) and (2.25) with the material functions $\alpha_{(m)}$ and $\delta_{(m)}$ being constants.

The conditions across a moving boundary $\Sigma(\theta^\mu)=0$ are given by (Ref. 11)

$$\exp^{\alpha\beta\gamma\delta}[\phi_{\gamma\delta}]\,\Sigma_{,\beta}=0, \tag{4.1}$$

$$[\eta^{\alpha\beta}]\Sigma_{,\beta}=\omega^\alpha|\nabla\Sigma|, \tag{4.2}$$

where ω^α is the surface charge-current and $|\nabla\Sigma| = \sqrt{g^{ij}\Sigma_{,i}\Sigma_{,j}}$. We have used the notation [ ] to represent the jump of a quantity across the surface $\Sigma(\theta^\mu)=0$, that is $[A]=A^+ - A^-$ where $A^+=\lim_{\Sigma\to 0}A_+$ and $A^-=\lim_{\Sigma\to 0}A_-$. In our problem

$$\Sigma = x^1 - \frac{c}{a}\left\{\left[1+\left(\frac{a}{c}\,x^4\right)^2\right]^{1/2}-1\right\}=0. \tag{4.3}$$

Case 1. Perfect conductor

Without loss of generality the x^2, x^3 axes may be chosen so that the incident wave is represented by the expressions

$$E_1^{(i)}=0,\quad E_2^{(i)}=0,\quad E_3^{(i)}=E_0\exp\left(i\frac{\omega}{c}(x^1-x^4)\right) \tag{4.4}$$

$$B^1{}_{(i)}=0,\quad B^2{}_{(i)}=-E_0\exp\left(i\frac{\omega}{c}(x^1-x^4)\right),\quad B^3{}_{(i)}=0. \tag{4.5}$$

The reflected radiation may then be described by the expressions

$$E_1^{(r)}=0,\quad E_2^{(r)}=0,\quad E_3^{(r)}=E_r\exp\left[i\left(k_r x^1-\frac{\omega^r}{c}x^4\right)\right], \tag{4.6}$$

$$B^1{}_{(r)}=0,\quad B^2{}_{(r)}=-\frac{k_r}{(\omega^r/c)}E_r\exp\left[i\left(k_r x^1-\frac{\omega^r}{c}x^4\right)\right],$$

$$B^3{}_{(r)}=0, \tag{4.7}$$

where Maxwell's equations have been used to find (4.7) from (4.6) (In this section and the next section the subscripts or superscripts r and t are used to denote quantities associated with the reflected and transmitted waves respectively. They do not take the values 1, 2, or 3.)

We also use the fact that the wave 4-vector in free space $k_\alpha=(k_m,\ \omega/c)$ has zero magnitude, i.e.,

$$k_\alpha k^\alpha = 0.$$

From this condition for the reflected wave we obtain

$$(k_r)^2=(\omega^r/c)^2. \tag{4.8}$$

Now we consider the interaction of the wave with the boundary at $x^1=d$ and $x^4=\tau$. From (4.3) d and τ are related by

$$d=\frac{c}{a}\{\sqrt{1+[(a/c)\tau]^2}-1\}. \tag{4.9}$$

Using the expressions (4.4)–(4.7) for the incident and reflected waves, making use of the fact that there are no fields in a perfect conductor, and using (4.3) and the constitutive equations, we find that in order to satisfy (4.1) for a general d and τ related by (4.9) we must require that

$$\frac{\omega}{c}(d-\tau)=k_r d-\frac{\omega^r}{c}\tau, \tag{4.10}$$

$$\left(1-\frac{(a/c)\tau}{\sqrt{1+[(a/c)\tau]^2}}\right)E_0+\left(1-\frac{k_r}{(\omega^r/c)}\frac{(a/c)\tau}{\sqrt{1+[(a/c)\tau]^2}}\right)E_r=0. \tag{4.11}$$

The positive root of (4.8) yields $\omega^r=\omega$. Using the negative root in (4.10) and (4.11) yields

$$\frac{\omega^r}{c}=-k_r=\left(\frac{\tau-d}{\tau+d}\right)\frac{\omega}{c}$$

$$=\frac{(a/c)\tau-\{\sqrt{1+[(a/c)\tau]^2}-1\}}{(a/c)\tau+\{\sqrt{1+[(a/c)\tau]^2}-1\}}\frac{\omega}{c}, \tag{4.12}$$

$$E_r=-\left(\frac{1-[(a/c)\tau]/\{\sqrt{1+[(a/c)\tau]^2}\}}{1+[(a/c)\tau]/\{\sqrt{1+[(a/c)\tau]^2}\}}\right)E_0. \tag{4.13}$$

Thus the nonzero components of the reflected radiation are given by

$$E_3^{(r)}=E_r\exp\left[i\left(\frac{d-\tau}{d+\tau}\right)\frac{\omega}{c}(x^1+x^4)\right],$$

$$B_2^{(r)}=+E_r\exp\left[i\left(\frac{d-\tau}{d+\tau}\right)\frac{\omega}{c}(x^1+x^4)\right] \tag{4.14}$$

where E_r is given by (4.13).

Using (4.13), (4.14) and the free space relations $\mathbf{D}=\mathbf{E}$, $\mathbf{B}=\mathbf{H}$ (in Lorentz–Heaviside units) in (4.2) yields the expression

$$\omega^3(d,\tau)=-2E_0\left(1-\frac{(a/c)\tau}{\sqrt{1+[(a/c)\tau]^2}}\right)\cos\frac{\omega}{c}(d-\tau). \tag{4.15}$$

Similarly, the other components of the surface charge-current are found to be zero.

Case 2. A class of linear dielectrics

For $x^1>0$ the constitutive equations (2.24) and (2.25) lead to the results expressed in Eqs. (3.1)–(3.4). We again choose the x^2 and x^3 axes so that the incident and reflected fields in free space are given by (4.4)–(4.7). The transmitted waves will be functions of the form (3.14) and (3.15). They will be functions that take the form of plane waves at the time and position of interaction ($x^1=d$, $x^4=\tau$) with the interface. Specifically,

$$B^2(d,\tau)=-B_t\exp\left(i\frac{\omega^t}{c}\sqrt{g/h}\,(d-\tau)\right),$$

$$E_3(d,\tau)=+\sqrt{h/g}\,B_t\exp\left(i\frac{\omega^t}{c}(\sqrt{g/h}\,d-\tau)\right). \tag{4.16}$$

Now our solutions will be of the form of (3.14) and (3.15). We are seeking solutions which represent waves travelling in the positive x^1 direction. That is our solutions should be of the form

$$B^2(x^1,x^4)=\bar{f}_2(\beta),\quad E_3(x^1,x^4)=-k_2(x^4)\bar{f}_2(\beta)+\bar{q}(x^4). \tag{4.17}$$

Imposing the conditions (4.16) on (4.17) and using Maxwell's equations, we find that the transmitted fields are given by

$$B^2(x^1,x^4)=-B_t\exp\left\{i\frac{\omega^t}{c}\left[\sqrt{g/h}\,(x^1-\int_\tau^{x^4}k_2(\gamma)\,d\gamma)-\tau\right]\right\} \tag{4.18}$$

$$E_3(x^1,x^4)=k_2(x^4)B_t\exp\left\{i\frac{\omega^t}{c}\left[\sqrt{g/h}\,(x^1-\int_\tau^{x^4}k_2(\gamma)\,d\gamma)-\tau\right]\right\}$$

$$+\frac{(\{1+[(a/c)\tau]^2\}g-[(a/c)\tau]^2h)}{(\{1+[(a/c)x^4]^2\}g-[(a/c)x^4]^2h)}$$

$$\times[\sqrt{h/g}-k_2(\tau)]B_t\exp[i\frac{\omega^t}{c}(\sqrt{g/h}\,d-\tau)] \tag{4.19}$$

where the function $k_2(x^4)$ is given by (3.16).

For convenience we introduce the notation

$$l(\tau)=\frac{(a/c)\tau}{\sqrt{1+[(a/c)\tau]^2}}. \tag{4.20}$$

In order to satisfy (4.1) for general values of τ (or d), we must require

$$\frac{\omega}{c}(d-\tau)=k_r d-\frac{\omega^r}{c}\tau=\frac{\omega^t}{c}[\sqrt{g/h}\,d-\tau], \tag{4.21}$$

$$(1-l(\tau))E_0+\left(1-\frac{k_r}{(\omega^r/c)}l(\tau)\right)E_r=[\sqrt{h/g}-l(\tau)]B_t. \tag{4.22}$$

Again using (4.8) we find for ω^r and k_r Eq. (4.19). Also from (4.21) we find

$$\frac{\omega^t}{c}=\left(\frac{d-\tau}{\sqrt{g/h}\,d-\tau}\right)\frac{\omega}{c}. \tag{4.23}$$

Using the constitutive equations (3.2) and (3.3), the condition that $\omega^\alpha=0$, and the expressions for the incident, transmitted, and reflected waves in (4.2) at $x^1=d$ and $x^4=\tau$, and using (4.12) in the resulting equation and in (4.22), we find

$$\begin{aligned}&[\sqrt{h/g}-l]B_t=E_r(1+l)+E_0(1-l),\\ &-h[1-l\sqrt{h/g}]B_t=E_r(1+l)-E_0(1-l).\end{aligned} \tag{4.24}$$

Solving this set of equations for B_t and E_r in terms of E_0 yields the expressions

$$B_t=\frac{2(1-l)}{\sqrt{h/g}-l+h[1-\sqrt{h/g}\,l]}E_0, \tag{4.25}$$

$$E_r=\frac{1-l\sqrt{h/g}-l-h[1-\sqrt{h/g}\,l]}{1+l\sqrt{h/g}-l+h[1-\sqrt{h/g}\,l]}E_0, \tag{4.26}$$

where the function l is evaluated at $x^4=\tau$. For Case 2, therefore, the reflected wave is given by (4.14) where E_r is given by (4.26). The transmitted wave is given by (4.28) and (4.19) where ω^t is given by (4.23) and B_t by (4.25).

5. ENERGY CONSIDERATIONS AT THE MOVING INTERFACE

In the problems discussed in Sec. 4 the portion of the wave transmitted and of that reflected is a function of the time τ at which the wave front interacts with the interface. The frequency of the reflected and transmitted waves is also a function of τ.

In this section we calculate expressions for the instantaneous reflection coefficients R and transmission coefficients T at time τ by using the instantaneous Poynting vector at time τ in the expressions

$$R=(-\mathbf{n})\cdot\mathbf{S}_{(r)}/\mathbf{n}\cdot\mathbf{S}_{(i)},\quad T=\mathbf{n}\cdot\mathbf{S}_{(t)}/\mathbf{n}\cdot\mathbf{S}_{(i)}. \tag{5.1}$$

Here $\mathbf{n}$ is a unit vector normal to the interface pointing into the medium into which the transmitted wave propagates. The vectors $\mathbf{S}_{(r)}$, $\mathbf{S}_{(i)}$, and $\mathbf{S}_{(t)}$ are the Poynting vectors of the reflected, incident, and transmitted waves, respectively. The three components of the Poynting vector are given by S^{4m} where $S^{\alpha\beta}$ is defined by (2.28). Using the expressions (2.11) for the velocity, (2.4) for the metric, and the appropriate relativistic fields in (2.28), we find that for the problems of Sec. 5

$$\begin{aligned}\mathbf{S}_{(i)}&=(-E_3^{(i)}H_2^{(i)},0,0),\\ \mathbf{S}_{(r)}&=(-E_3^{(r)}H_2^{(r)},0,0),\\ \mathbf{S}_{(t)}&=(-E_3^{(t)}H_2^{(t)},0,0),\end{aligned} \tag{5.2}$$

where E_3 and H^2 are the real part of the appropriate expressions found in Sec. 4.

In this section we also apply the energy–momentum continuity conditions as derived by Grot and Eringen[12] across the boundary $\Sigma(\theta^\mu)=0$. For the problems of Sec. 4 this continuity condition reduces to

$$[-\tau^{\mu\beta}+S^{\mu\beta}]\Sigma_{,\beta}=0, \tag{5.3}$$

where $S^{\mu\beta}$ is given by (2.28) and $\tau^{\mu\beta}$ is the mechanical 4-stress. The tensor $\tau^{\mu\beta}$ is a spacelike tensor, i.e.,

$$u_\mu\tau^{\mu\beta}=0,\quad \tau^{\mu\beta}u_\beta=0. \tag{5.4}$$

For the problems of Sec. 4, Eq. (5.3) is identically satisfied except for $\mu=1$ and $\mu=4$. Substituting the velocities (2.11), Eqs. (4.3) and (5.4) into (5.3), we obtain the expressions

$$[S^{11}]-l(\tau)[S^{14}]=\tau^{11}\{1-l(\tau)^2\}, \tag{5.5}$$

$$[S^{41}]-l(\tau)[S^{44}]=l(\tau)\tau^{11}\{1-l^2(\tau)\}, \tag{5.6}$$

where $l(\tau)$ is defined by (4.20), and τ^{11} is the normal component of stress in the moving medium at the interface.

Case 1.

For this problem the instantaneous Poynting vector of the incident and reflected waves at time τ is given by

$$\begin{aligned}S^{41}{}_{(i)}&=E_0{}^2\cos^2\frac{\omega}{c}(d-\tau),\\ S^{41}{}_{(r)}&=-E_r{}^2\cos^2\frac{\omega}{c}(d-\tau),\end{aligned} \tag{5.7}$$

where E_r is given by (4.13). Thus the instantaneous reflection coefficient is given by

$$R=\{[1-l(\tau)]/[1+l(\tau)]\}^2. \tag{5.8}$$

Using the fact that $\mathbf{D}=\mathbf{E}$ and $\mathbf{B}=\mathbf{H}$ in free space and expression (4.13) for E_r in (5.7), we can show that

$$E_0^2\frac{2\cos^2(\omega/c)(d-\tau)}{\{1-l(\tau)\}^2}=-\tau^{11}. \tag{5.9}$$

We observe that (5.6) is identically satisfied due to (5.9).

Case 2

For this case upon using the constitutive equation (3.3), the instantaneous transmitted Poynting vector in the x^1 direction becomes

$$\begin{aligned}S^{41}{}_{(t)}=&\left\{\left[1+\left(\frac{a}{c}\tau\right)^2\right]h-\left(\frac{a}{c}\tau\right)^2 g\right\}\sqrt{h/g}\,B_t^2\cos^2\frac{\omega}{c}(d-\tau)\\ &+\frac{a}{c}\tau\sqrt{1+[(a/c)\tau]^2}\,(g-h)\frac{h}{g}B_t{}^2\cos^2\frac{\omega}{c}(d-\tau)\end{aligned} \tag{5.10}$$

where B_t is given by (4.25).

The instantaneous Poynting vectors for the incident and reflected waves are given by (5.7) where E_r is given by (4.26). Thus from (5.1) we find

$$R=\left(\frac{1-l(\tau)}{1+l(\tau)}\,\frac{\sqrt{h/g}-l(\tau)-h[1-\sqrt{h/g}\,l(\tau)]}{\sqrt{h/g}-l(\tau)+h[1-\sqrt{h/g}\,l(\tau)]}\right)^2, \tag{5.11}$$

$$T=\left(\left\{\left[1+\left(\frac{a}{c}\tau\right)^2 h-\left(\frac{a}{c}\tau\right)^2 g\right\}\sqrt{h/g}+\frac{a}{c}\tau\sqrt{1+[(a/c)\tau]^2}\,(g-h)\frac{h}{g}\right)\times\left(\frac{2(1-l(\tau))}{\sqrt{h/g}-l(\tau)+h(1-\sqrt{h/g}\,l(\tau))}\right)^2. \tag{5.12}$$

For this case we find that (5.5) yields the results

$$\tau^{11}=\left(\frac{E_0^2\cos^2(\omega/c)(d-\tau)}{(1+l(\tau))^2[\sqrt{h/g}-l(\tau)+h(1-\sqrt{h/g}\,l(\tau))]^2}\right)\times\left(4h+2l(\tau)^2 g-2\frac{h}{g}-4l(\tau)g\sqrt{h/g}-4l(\tau)h\sqrt{h/g}+4l(\tau)\sqrt{h/g}+2l(\tau)^2\frac{h^2}{g}-2h^2-2l(\tau)^2+4l(\tau)h^2\sqrt{h/g}-2l(\tau)^2\frac{h^3}{g}\right). \tag{5.13}$$

In a similar fashion to Case 1 we find that (5.6) reduces to an identity upon using (5.13). Specifically,

$$l(\tau)\tau^{11}(1-l^2(\tau))=l(\tau)\tau^{11}(1-l^2(\tau)). \tag{5.14}$$

It should be emphasized that the energy–momentum continuity condition (5.3) can only be used to show that $R+T=1$ for the case of a stationary interface. For a moving interface the interaction between the mechanical stress and electromagnetic energy–momentum tensor must be considred.

6. DISCUSSION

In this paper we have found expressions for waves propagating in the direction of the motion in media undergoing uniform linear acceleration. It was possible to find the expressions without resorting to the use of iteration methods. It is interesting to note that the expression found in Appendix B for **E** is equivalent to that found by Mo[1] using an iteration method. The expression for **B**, however, differs from that found by Mo. It is also interesting to note that the expressions for **E** and **B** have the same form for materials where $\alpha_{(m)}$ and $\delta_{(m)}$ are constants as they do for materials for which $\mathbf{D}=\epsilon_r E$ and $\mathbf{B}=\chi_r \mathbf{H}$.

The general solution found consists of a function associated with a wave propagating in the positive x^1 direction with phase velocity v^1 and one associated with a wave propagating in the negative x^1 direction with phase velocity v^2. From the viewpoint of an inertial observer

$$v^1=\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{[(a/c)x^4]\sqrt{1+[(a/c)x^4]^2}\,(g-h)-\sqrt{gh}},$$

$$v^2=\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}(g-h)+\sqrt{gh}}.$$

It should also be emphasized that the continuity conditions across a moving interface discussed in Sec. 5 involve both the electromagnetic energy–momentum tensor and the mechanical 4-stress. It is not true that the sum of the reflection coefficient R and the transmission coefficient T is equal to one for moving interfaces. For such moving interfaces the energy flow carried by the incident wave is in general not carried away by the reflected and transmitted waves. Such effects as radiation pressure must be considered for an accurate energy balance.

APPENDIX A

The coefficients of Eq. (3.5) are found to be

$$a_{11}=\left(\frac{a}{c}x^4\right)^2 g-\left[1+\left(\frac{a}{c}x^4\right)^2\right]h, \tag{A1}$$

$$a_{12}=\frac{a}{c}x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h), \tag{A2}$$

$$a_{22}=+\left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right]g-\left(\frac{a}{c}x^4\right)^2 h\right\}, \tag{A3}$$

$$b_1=\frac{\partial}{\partial x^4}\left(\frac{a}{c}x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)\right), \tag{A4}$$

$$b_2=+\frac{\partial}{\partial x^4}\left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right]g-\left(\frac{a}{c}x^4\right)^2 h\right\}. \tag{A5}$$

The coefficients of Eq. (3.10) are found to be

$$\bar{a}_{12}=\frac{2gh([(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h)}{(g-h)^2[(a/c)x^4]^2\{1-[(a/c)x^4]^2\}-gh}, \tag{A6}$$

$$\bar{b}_1=\left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right]g-\left(\frac{a}{c}x^4\right)^2 h\right\}\times\frac{-([(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h)}{\{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)+\sqrt{gh}\}^2}\times\left[\frac{a}{c}x^4\sqrt{1+[(a/c)x^4]^2}\left(\frac{\partial g}{\partial x^4}-\frac{\partial h}{\partial x^4}\right)+\frac{1}{2\sqrt{gh}}\left(h\frac{\partial g}{\partial x^4}+g\frac{\partial h}{\partial x^4}\right)\right]+\frac{[(a/c)x^4]^2(\partial g/\partial x^4)-\{1+[(a/c)x^4]^2\}(\partial h/\partial x^4)}{\{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)+\sqrt{gh}\}}\Bigg\}+\frac{a}{c}x^4\sqrt{1+[(a/c)x^4]^2}\left(\frac{\partial g}{\partial x^4}-\frac{\partial h}{\partial x^4}\right)+\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)+\sqrt{gh}}\times\left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right]\frac{\partial g}{\partial x^4}-\left(\frac{a}{c}x^4\right)^2\frac{\partial h}{\partial x^4}\right\}, \tag{A7}$$

$$\bar{b}_2=\left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right]g-\left(\frac{a}{c}x^4\right)^2 h\right\}\times\frac{-([(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h)}{\{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)-\sqrt{gh}\}^2}\times\left[\frac{a}{c}x^4\sqrt{1+[(a/c)x^4]^2}\left(\frac{\partial g}{\partial x^4}-\frac{\partial h}{\partial x^4}\right)-\frac{1}{2\sqrt{gh}}\left(h\frac{\partial g}{\partial x^4}+g\frac{\partial h}{\partial x^4}\right)\right]+\frac{[(a/c)x^4]^2(\partial g/\partial x^4)-\{1+[(a/c)x^4]^2\}(\partial h/\partial x^4)}{\{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}\,(g-h)-\sqrt{gh}\}}$$

$$+\frac{a}{c}x^4\sqrt{1+[(a/c)x^4]^2}\left(\frac{\partial g}{\partial x^4}-\frac{\partial h}{\partial x^4}\right)$$
$$+\frac{[(a/c)x^4]^2 g-\{1+[(a/c)x^4]^2\}h}{(a/c)x^4\sqrt{1+[(a/c)x^4]^2}(g-h)-\sqrt{gh}}$$
$$\times\left\{\left[1+\left(\frac{a}{c}x^4\right)^2\right]\frac{\partial g}{\partial x^4}-\left(\frac{a}{c}x^4\right)^2\frac{\partial h}{\partial x^4}\right\} \tag{A8}$$

APPENDIX B

In Ref. 1, Mo considered the problem of Sec. 3 from the viewpoint of a comoving observer. He applied a constitutive theory and a theory of local electrodynamics in noninertial frames to find expressions for the **B** and **E** observed by this medium-comoving observer. In order to compare the results of Sec. 3 to those obtained in Ref. 1, it is necessary to obtain expressions for the **B** and **E** observed by a comoving observer. Such expressions may be readily obtained by a straightforward, although tedious, tensor transformation of the results of Sec. 3 to the comoving frame. Unfortunately the results of such a transformation cannot be readily compared to the results of Mo. For example, the exponential naturally comes out in the terms of an integral of the function $k_2(x^4)$ defined by Eq. (3.16). In order to compare the real parts of the two wave forms found, the integration must be carried out for all appropriate regions of g and h and the results used to compare the real parts of the transformed expression to the results of Mo. This procedure is conceptually simple, but it is not a trivial manipulation.

To avoid these difficulties, we may simply repeat the procedure of Sec. 3 for the case of a comoving observer. Expression (2.13) is used for the velocities and the needed relativistic left Green–Cauchy tensor (and its powers) is readily obtained from those previously found for the inertial observer by a tensor transformation. Again the x'^2 and x'^3 axes are oriented so that the initial conditions are given by

$$B^2(x'^1,0)=B_0\exp(ikx'^1),\quad E_3(x'^1,0)=-E_0\exp(ikx'^1) \tag{B1}$$

with all other components zero. Equation (3.18) is again satisfied.

The expressions for B^2 and E_3 which result from this procedure are

$$B^2(x'^1,x'^4)=B_0\exp[ik(x'^1-\textstyle\int_0^{x'^4}k_1(\gamma)\,d\gamma)], \tag{B2}$$

$$E_3(x'^1,x'^4)=\frac{-\sqrt{g/h}\,E_0}{\sinh(a/c)x'^4+\sqrt{g/h}\cosh a/c\,x'^4}$$
$$\times\exp[ik(x'^1-\textstyle\int_0^{x'^4}k_1(\gamma)\,d\gamma)], \tag{B3}$$

where

$$k_1(x^4)=\{\sinh\frac{a}{c}x'^4+\sqrt{g/h}\cosh\frac{a}{c}x'^4\}^{-1}. \tag{B4}$$

The constitutive equations (2.24) and (2.25) reduce to $\mathbf{D}=\epsilon_r\mathbf{E}$ and $\mathbf{H}=\chi_r\mathbf{B}$ for $\alpha_0=\epsilon_r$, $\alpha_1=\alpha_2=0$, $\delta_1=\delta_2=0$, and $\delta_0=\chi_r$. For this case $g=\epsilon_r$ and $h=\chi_r$ and thus (B3) becomes

$$E_3(x'^1,x'^4)=\frac{-\sqrt{\epsilon_r/\chi_r}\,E_0}{\sinh(a/c)x'^4+\sqrt{\epsilon_r/\chi_r}\cosh(a/c)x'^4}$$
$$\times\exp[ik(x'^1-\textstyle\int_0^{x'^4}k_1(\gamma)\,d\gamma)]. \tag{B5}$$

By using (5.29) of Ref. 1 in (5.24) of Ref. 1, we find that Eq. (B5) is equivalent to (5.24) of Ref. 1.

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Nonlinear differential-difference equations

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A method is presented which enables one to obtain and solve certain classes of nonlinear differential–difference equations. The introduction of a new discrete eigenvalue problem allows the exact solution of the self-dual network equations to be found by inverse scattering. The eigenvalue problem has as its singular limit the continuous eigenvalue equations of Zakharov and Shabat. Some interesting differences arise both in the scattering analysis and in the time dependence from previous work.

1. INTRODUCTION

It is well known that a number of physically interesting problems can be modeled by nonlinear differential–difference equations. In this paper we will be primarily concerned with outlining a procedure that allows us to find and solve certain important classes of these problems. The method of solution requires knowledge of inverse scattering. This work is similar, in spirit, to the work of Flaschka[1,2] on the solution of the Toda lattice,[3,4] and of Case and Kac,[5] and Case[6] on the inverse scattering of a discretized Schrödinger equation.

In particular, we show the following:

(i) An analysis of a new discrete eigenvalue problem leads to the solution of the nonlinear self-dual network

$$\frac{1}{1+V_n^2}\frac{\partial V_n}{\partial t} = I_n - I_{n+1}, \tag{1.1}$$

$$\frac{1}{1+I_n^2}\frac{\partial I_n}{\partial t} = V_{n-1} - V_n, \tag{1.2}$$

proposed by Hirota.[7] This eigenvalue problem has as its singular continuous limit, the Zakharov–Shabat system.[8] The relationship is clear viewed from discrete to continuous, but not visa versa.

(ii) An algebraic procedure is outlined which allows one to systematically obtain evolution equations such as (1.1), (1.2) and indeed more general ones. The algebraic complexity of the problem requires such systematic procedures as discussed in Ref. 9. In addition, we show how such a procedure is applicable to the discretized Schrödinger equation.

(iii) The inverse scattering analysis is presented for the eigenvalue problem associated with (1.1), (1.2). There are some interesting differences between this and the analysis for the discretized Schrödinger equation. We also note that the time dependence of the scattering data must be considered quite carefully (see also Ref. 10).

The inverse scattering transform was first discovered by Gardner, Green, Kruskal, and Miura,[11] and a detailed examination of all the ideas, many of which are relevant to this work, is presented by Ablowitz, Kaup, Newell, and Segur.[12]

2. TIME DEPENDENCE AND EVOLUTION EQUATIONS

Consider the discretized eigenvalue problem

$$v_{1_{n+1}} = z v_{1_n} + Q_n(t) v_{2_n} + S_n(t) v_{2_{n+1}},$$

$$v_{2_{n+1}} = \frac{1}{z} v_{2_n} + R_n(t) v_{1_n} + T_n(t) v_{1_{n+1}}, \tag{2.1}$$

with the potentials Q_n, R_n, S_n, T_n, and the eigenvalue z on the interval $|n| < \infty$. In addition, let the time dependence of the eigenfunction

$$\mathbf{v}_n(t) = \begin{pmatrix} v_{1n} \\ v_{2n} \end{pmatrix}$$

obey the differential equation

$$\frac{\partial v_{1n}}{\partial t} = A_n(z,t) v_{1_n} + B_n(z,t) v_{2_n},$$

$$\frac{\partial v_{2n}}{\partial t} = C_n(z,t) v_{1_n} + D_n(z,t) v_{2_n}. \tag{2.2}$$

Solutions v_{1_n}, v_{2_n} with the eigenvalue z invariant exist when the following equations are satisfied:

$$(z + R_n S_n)\Delta A_n + (z T_n + R_n) B_{n+1} - (Q_n + S_n/z) C_n = \frac{1}{\Lambda_n}(\Lambda_n (z + R_n S_n)_t - \Lambda_{nt}(z + R_n S_n)),$$

$$(Q_n + S_n/z) A_{n+1} + (T_n Q_n + 1/z) B_{n+1} - (z + R_n S_n) B_n - (Q_n + S_n/z) D_n = \frac{1}{\Lambda_n}(\Lambda_n (Q_n + S_n/z)_t - \Lambda_{nt}(Q_n + S_n/z)),$$

$$(z + R_n S_n) C_{n+1} - (T_n Q_n + 1/z) C_n + (z T_n + R_n) D_{n+1} - (z T_n + R_n) A_n = \frac{1}{\Lambda_n}(\Lambda_n (z T_n + R_n)_t - \Lambda_{nt}(z T_n + R_n)),$$

$$(Q_n + S_n/z) C_{n+1} + (T_n Q_n + 1/z)\Delta D_n - (z T_n + R_n) B_n = \frac{1}{\Lambda_n}(\Lambda_n (T_n Q_n + 1/z)_t - \Lambda_{nt}(T_n Q_n + 1/z)), \tag{2.3}$$

where $\Lambda_n \equiv 1 - S_n T_n$, $(\cdots)_t \equiv \partial/\partial t(\cdots)$, and $\Delta(\cdots)_n = (\cdots)_{n+1} - (\cdots)_n$. (2.3) is most easily arrived at by putting (2.1) in the form

$$v_{1_{n+1}} = \frac{z + R_n S_n}{\Lambda_n} v_{1_n} + \frac{(Q_n + S_n/z)}{\Lambda_n} v_{2_n},$$

$$v_{2_{n+1}} = \frac{z T_n + R_n}{\Lambda_n} v_{1_n} + \frac{T_n Q_n + 1/z}{\Lambda_n} v_{2_n}, \tag{2.4}$$

and using (2.2) to force the consistency

$$\frac{\partial}{\partial t} v_{i_{n+1}} = \left(\frac{\partial v_i}{\partial t}\right)_{n+1}, \qquad i = 1, 2.$$

Equations (2.3) are then obtained by equating coefficients of v_{i_n} $(i = 1, 2)$ in the resulting system. We prefer the form (2.1) so as to more easily see the continuum analogy.

The purely algebraic procedure needed to deduce the differential—difference equations proceeds as follows. Expand A_n, B_n, C_n, D_n as

$$A_n = A_n^{(0)}(t) + A_n^{(1)}(t)z, \quad C_n = C_n^{(0)}(t) + C_n^{(1)}(t)z$$
$$B_n = B_n^{(0)}(t) + B_n^{(-1)}(t)/z, \quad D_n = D_n^{(0)}(t) + D_n^{(-1)}(t)/z. \tag{2.5}$$

The structure of (2.5) is suggested by a careful examination of Eqs. (2.3), the time dependence of the special soliton solutions, and the meaning of the linearized "dispersion" relation. With the assumed form (2.5), Eqs. (2.3) yield a sequence of equations corresponding to the powers z^2, z, z^0, z^{-1}, z^{-2} all of which must be independently satisfied. We found it most direct to solve the equations corresponding to the highest and lowest powers of z first. The results of these computations yield $A_n, \ldots, D_n$, as well as the required evolution equations. It may be verified that

$$\begin{aligned} A_n &= A_-^{(1)} z - T_{n-1} Q_n A_-^{(1)} - \sum_{-\infty}^{n-1} \frac{\Lambda_{Kt}}{\Lambda_K} + A_-^{(0)}, \\ B_n &= Q_n A_-^{(1)} + S_{n-1} D_-^{(-1)}/z, \\ C_n &= T_{n-1} A_-^{(1)} z + R_n D_-^{(-1)}, \\ D_n &= -R_n S_{n-1} D_-^{(-1)} - \sum_{-\infty}^{n-1} \frac{\Lambda_{Kt}}{\Lambda_K} + D_-^{(0)} + D_-^{(-1)}/z, \end{aligned} \tag{2.6}$$

along with the evolution equations

$$\begin{aligned} R_{nt} &= (1 - R_n Q_n)(T_n D_-^{(-1)} - T_{n-1} A_-^{(1)}), \\ S_{nt} &= (1 - S_n T_n)(Q_{n+1} A_-^{(1)} - Q_n D_-^{(-1)}), \\ Q_{nt} &= (1 - R_n Q_n)(S_n A_-^{(1)} - S_{n-1} D_-^{(-1)}), \\ T_{nt} &= (1 - S_n T_n)(R_{n+1} D_-^{(-1)} - R_n A_-^{(1)}), \end{aligned} \tag{2.7}$$

where $A_-^{(1)}$, $A_-^{(0)}$, $D_-^{(-1)}$, $D_-^{(0)}$ are all constants obtained as $n \to -\infty$ (and for convenience we choose $A_-^{(0)} = D_-^{(0)}$). Special cases are now apparent. Letting $R_n = \mp Q_n = I_n$, $S_n = \mp T_n = V_n$, and $D_-^{(-1)} = A_-^{(1)} = 1$, we find

$$\begin{aligned} I_{n_t} &= (1 \pm I_n^2)(\pm V_{n-1} \mp V_n), \\ V_{n_t} &= (1 \pm V_n^2)(\pm I_n \mp I_{n+1}) \end{aligned} \tag{2.8}$$

which is the self-dual network (1.1), (1.2) for the first choice of sign. Similarly, if we let $R_n = \mp Q_n^*$, $S_n = \mp T_n^*$, with $D_-^{(-1)} = -A^{(1)} = i$, we find

$$\begin{aligned} R_{n_t} &= i(1 \pm R_n R_n^*)(\mp S_n^* \mp S_{n-1}^*), \\ S_{n_t} &= i(1 \pm S_n S_n^*)(\pm R_{n+1}^* \pm R_n^*) \end{aligned} \tag{2.8'}$$

a discretized "second order in time nonlinear Schrödinger equation."

Alternatively, if $R_n = 0$, $T_n = 1$, $Q_n = \beta_n$, $S_n = 1 - \alpha_n$, we have

$$\begin{aligned} \alpha_{nt} &= \alpha_n(\beta_n - \beta_{n+1}), \\ \beta_{nt} &= \alpha_{n-1} - \alpha_n, \end{aligned} \tag{2.9}$$

whereupon letting $\alpha_n = \exp(\tilde{Q}_n - \tilde{Q}_{n+1})$, we see that $\beta_n = \tilde{Q}_{nt}$; hence

$$\tilde{Q}_{ntt} = \exp[-(\tilde{Q}_n - \tilde{Q}_{n-1})] - \exp[-(\tilde{Q}_{n+1} - \tilde{Q}_n)] \tag{2.10}$$

and the Toda lattice equation is deduced. We also note that other evolution equations can be deduced by expanding $A_n, \ldots, D_n$ in a more general expansion in z, rather than (2.5).

Finally, we point out that if $R_n = T_n = 0$ then the evolution equation linearizes to the discretized wave equation.

It should be noted that the Toda lattice equations can be deduced from the discretized Schrödinger equation (proposed by Flaschka[1,2]) in an algebraic manner as well. In that case the eigenvalue problem is given by

$$a_n v_{n+1} + a_{n-1} v_{n-1} + b_n v_n = \lambda v_n \tag{2.11}$$

where λ is the eigenvalue (we take $a_n \to 1$, $b_n \to 0$ as $|n| \to \infty$). Suitable time dependence, analogous to (2.2) may be written as

$$v_{nt} = A_n(t, \lambda) v_{n+1} + B_n(t, \lambda) v_n. \tag{2.12}$$

Differentiation of (2.11) with respect to time and using (2.11), (2.12) yields two equations (coefficients of v_{n+1}, and v_n).

$$\begin{aligned} &A_n(b_n - \lambda) + \frac{a_n}{a_{n+1}}(\lambda - b_{n+1})A_{n+1} + a_n(B_{n+1} - B_{n-1}) \\ &\quad = a_{n-1_t} a_n / a_{n-1} - a_{n_t}, \\ &-a_n^2 \frac{A_{n+1}}{a_{n+1}} + B_n(b_n - \lambda) + (\lambda - b_n)B_{n-1} + a_{n-1}A_{n-1} \\ &\quad = \frac{a_{n-1\,t}}{a_{n-1}}(b_n - \lambda) - b_{n_t}. \end{aligned} \tag{2.13}$$

Expanding A_n, B_n as

$$\begin{aligned} A_n &= A_n^{(0)}(t) + A_n^{(1)}(t)\lambda + A_n^{(2)}(t)\lambda^2, \\ B_n &= B_n^{(0)}(t) + B_n^{(1)}(t)\lambda + B_n^{(2)}(t)\lambda^2 \end{aligned} \tag{2.14}$$

and requiring the coefficients of $\lambda^3, \ldots, \lambda^0$ to vanish independently yields A_n, B_n and the evolution equations. We find

$$\begin{aligned} A_n &= 2a_n A_-^{(2)}\lambda^2 + (2a_n A_-^{(1)} + 2a_n b_n A_-^{(2)})\lambda \\ &\quad + 2a_n A_-^{(0)} + 2A_-^{(2)} a_n(a_n^2 + a_{n-1}^2 - 2 + b_n^2) + 2A_-^{(1)} a_n b_n, \\ B_n &= B_-^{(2)}\lambda^2 + (B_-^{(1)} - 2(a_n^2 - 1)A_-^{(2)})\lambda \\ &\quad + B_-^{(0)} + 2A_-^{(1)}(1 - a_n^2) - 2A_-^{(2)} a_n^2 b_n \\ &\quad + \sum_{-\infty}^{n} \left(\frac{a_{K-1_t}}{a_{K-1}} + 2A_-^{(2)}(b_K a_{K-1}^2 - b_{K+1} a_K^2) \right), \end{aligned} \tag{2.15}$$

as well as the evolution equations

$$\begin{aligned} a_{n_t} &= A_-^{(0)} a_n(b_{n+1} - b_n) + A_-^{(1)} a_n(a_{n+1}^2 - a_{n-1}^2 + b_{n+1}^2 - b_n^2) \\ &\quad + A_-^{(2)}(a_n(2(b_{n+1}a_{n+1}^2 - b_n a_{n-1}^2) + b_{n+2}a_{n+1}^2 - b_{n-1}a_{n-1}^2 \\ &\quad + b_{n+1}^3 - b_n^3 + a_n^2(b_{n+1} - b_n) + 2(b_n - b_{n+1})), \\ b_{n_t} &= A_-^{(0)} 2(a_n^2 - a_{n-1}^2) + 2A_-^{(1)}(a_n^2(b_{n+1} + b_n) \\ &\quad - a_{n-1}^2(b_n + b_{n-1})) + 2A_-^{(2)}(a_n^2(a_{n+1}^2 + a_n^2 - 2 + b_{n+1}^2) \\ &\quad - a_{n-1}^2(a_{n-1}^2 + a_{n-2}^2 - 2 + b_{n-1}^2) + b_n^2(a_n^2 - a_{n-1}^2) \\ &\quad + b_n(a_n^2 b_{n+1} - a_{n-1}^2 b_{n-1})); \end{aligned} \tag{2.16}$$

for example, if we set $A_-^{(1)} = A_-^{(2)} = 0$, $A_-^{(0)} = \frac{1}{2}$, we have

$$\begin{aligned} a_{nt} &= a_n(b_{n+1} - b_n)/2, \\ b_{nt} &= (a_n^2 - a_{n-1}^2), \end{aligned} \tag{2.17}$$

which reduces to the Toda lattice (2.10) if we let

$$a_n = \exp[-(\tilde{Q}_{n+1} - \tilde{Q}_n)/2], \quad b_n = -\tilde{Q}_{nt}.$$

It should be stressed that the above ideas can be extended to find more general nonlinear differential—

difference equations whose associated eigenvalue problems are either (2.1) or (2.11).

3. DIRECT AND INVERSE SCATTERING

In this section we first sketch the important aspects of the direct and inverse scattering technique for (2.1) assuming Q_n, R_n, S_n, T_n all vanish sufficiently rapidly as $|n| \to \infty$. The analysis results in a system of coupled summation equations, which play the role of the integral equations derived by Zakharov–Shabat.[8]

We begin by defining particular solutions of the eigenvalue problem (2.1). Let

$$\phi_n \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} z^n, \qquad \bar{\phi}_n \sim \begin{pmatrix} 0 \\ -1 \end{pmatrix} z^{-n}, \quad \text{as } n \to -\infty, \tag{3.1}$$

and

$$\psi_n \sim \begin{pmatrix} 0 \\ 1 \end{pmatrix} z^{-n}, \qquad \bar{\psi}_n \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} z^{n}, \quad \text{as } n \to +\infty. \tag{3.2}$$

It may be shown that for appropriately decaying potentials, $z^{-n}\phi$, $z^n\psi$ are analytic for $|z| > 1$, and $z^n\bar{\phi}$, $z^{-n}\bar{\psi}$ are analytic for $|z| < 1$. The asymptotic forms (3.1), (3.2) are expecially convenient, and are suggested by the fact that if

$$v = \begin{pmatrix} v_{1_n} \\ v_{2_n} \end{pmatrix}$$

is a solution of (2.1) at z then

$$\bar{v} = \begin{pmatrix} v^*_{2_n} \\ \mp v^*_{1_n} \end{pmatrix}$$

is a solution at $z = 1/z^*$ when $Q_n = \mp R^*_n$, $T_n = \mp S^*_n$. The important Wronskian relation obeys the equation

$$W_{n+1} = \frac{1 - R_n Q_n}{1 - S_n T_n} W_n, \tag{3.3}$$

where $W_n(w, v) \equiv (w_{1_n} v_{2_n} - w_{2_n} v_{1_n})$. Thus on the unit circle

$$W_n(\bar{\psi}, \psi) = \prod_n^{\infty} \frac{(1 - S_i T_i)}{(1 - R_i Q_i)}, \tag{3.4}$$

$$W_n(\bar{\phi}, \phi) = \prod_{-\infty}^{n-1} \frac{1 - R_i Q_i}{1 - S_i T_i}. \tag{3.5}$$

In the important case where $T_i = -S^*_i$, $Q_i = -R^*_i$, (3.4) and (3.5) are positive definite, hence the functions $\{\psi, \bar{\psi}\}$, $\{\phi, \bar{\phi}\}$ are, respectively, linearly independent. In all other cases we assume the amplitudes of the functions keep (3.4), (3.5) of one sign; hence we write on the unit circle

$$\bar{\phi}_n = -\bar{a}(z, t)\psi_n + \bar{b}(z, t)\bar{\psi}_n, \tag{3.6}$$

$$\phi_n(z) = a(z, t)\bar{\psi}_n + b(z, t)\psi_n. \tag{3.7}$$

We remark that $a, b, \bar{a}, \bar{b}$ depend parametrically on time through the potentials. The explicit dependence on time is found in Sec. 4. Note also that (3.4)–(3.7) imply that on the unit circle

$$a\bar{a} + b\bar{b} = \prod_{i=-\infty}^{\infty} \frac{1 - R_i Q_i}{1 - S_i T_i}, \tag{3.8}$$

and in the special case where $Q_i = -R^*_i$, $T_i = -S^*_i$ we have

$$|a|^2 + |b|^2 = \prod_{i=-\infty}^{\infty} \frac{1 + |R_i|^2}{1 + |S_i|^2}, \tag{3.9}$$

since $\bar{a} = a^*$, $\bar{b} = b^*$ for this choice of potentials.

The inverse scattering proceeds as follows. Form the combinations

$$\bar{\phi}_n/\bar{a} = -\psi_n + (\bar{b}/\bar{a})\bar{\psi}_n, \tag{3.10}$$

and

$$\phi_n/a = \bar{\psi}_n + (b/a)\psi_n. \tag{3.11}$$

Multiply (3.10) by $z^n/(z - \bar{\zeta})$, and (3.11) by $z^{-n}/(z - \zeta)$ and integrate about the unit circle. Assuming $\bar{a}(z)$ and $a(z)$ have a finite number of simple zeros inside and outside the unit circle, respectively [i.e., $|\bar{z}_k| < 1$, $\bar{a}(\bar{z}_k) = 0$, and $|z_k| > 1$, $a(z_k) = 0$], and at these zeros

$$\bar{\phi}(\bar{z}_k) = \bar{d}_k \bar{\psi}(\bar{z}_k) \equiv \bar{d}_k \bar{\psi}_k = \bar{\phi}_k, \tag{3.12}$$

$$\phi(z_k) = d_k \psi(z_k) \equiv d_k \psi_k = \phi_k, \tag{3.13}$$

we find by contour integration

$$\sum_{k=1}^{N} \frac{\bar{z}_k^n}{(\bar{z}_k - \bar{\zeta})} \bar{C}_k \bar{\psi}_{n,k} + \frac{\bar{\zeta}^n}{\bar{a}(\bar{\zeta})} \bar{\phi}_n(\bar{\zeta}) \Theta(1 - |\bar{\zeta}|) + I_{\infty,n}$$
$$= \bar{\zeta}^n \psi_n(\bar{\zeta}) \Theta(|\bar{\zeta}| - 1) + \frac{1}{2\pi i} \oint \frac{\bar{\Phi}_n}{z - \bar{\zeta}} dz, \tag{3.14}$$

$$-\sum_{k=1}^{N} \frac{z_k^{-n}}{z_k - \zeta} C_k \psi_{n,k} - \frac{\zeta^{-n}}{a(\zeta)} \phi_n(\zeta) \Theta(|\zeta| - 1) + J_{\infty,n}$$
$$= \zeta^{-n} \bar{\psi}(\zeta) \Theta(1 - |\zeta|) + \frac{1}{2\pi i} \oint \frac{\Phi_n}{z - \zeta} dz, \tag{3.15}$$

where we have defined

$$C_k = \frac{d_k}{a'_k}, \qquad \bar{C}_k = \frac{\bar{d}_k}{\bar{a}'_k}, \tag{3.16}$$

$$I_{\infty,n} = \lim_{|z| \to \infty} z^n \psi_n(z), \tag{3.17}$$

$$J_{\infty,n} = \lim_{|z| \to \infty} \frac{z^{-n}}{a} \phi_n(z), \tag{3.18}$$

$$\bar{\Phi}_n = z^n \frac{\bar{b}}{\bar{a}} \bar{\psi}_n, \qquad \Phi_n = z^{-n} \frac{b}{a} \psi_n, \tag{3.19}$$

and $\Theta(z)$ is the usual Heaviside function. Note that the contributions $I_{\infty,n}$, $J_{\infty,n}$ are due to the nonvanishing loop integrals at infinity. In (3.14) we take $\bar{\zeta}$ just outside the unit circle [e.g., $\bar{\zeta} = (1 + \epsilon)e^{i\theta}$], and in (3.15) ζ just inside the unit circle [e.g., $\zeta = (1 - \epsilon)e^{i\theta}$]. Substituting for ψ_n and $\bar{\psi}_n$ the representations

$$\psi_n = \sum_{n'=n}^{\infty} \begin{pmatrix} K_1(n, n') \\ K_2(n, n') \end{pmatrix} z^{-n'}, \tag{3.20}$$

$$\bar{\psi}_n = \sum_{n'=n}^{\infty} \begin{pmatrix} \bar{K}_1(n, n') \\ \bar{K}_2(n, n') \end{pmatrix} z^{n'}, \tag{3.21}$$

multiplying (3.14) by $(2\pi i)^{-1} z^{m-n-1}$, (3.15) by $(2\pi i)^{-1} z^{-m+n-1}$, integrating about the unit circle, and then taking the limit $\bar{\zeta}$, ζ approaching the unit circle ($\epsilon \to 0$), we find after some manipulation

$$K(n, m) - I_{\infty,n}\delta(m, n) - \sum_{n'=n}^{\infty} \bar{K}(n, n') F(m + n')(1 - \delta(m, n)) = 0 \tag{3.22}$$

and

$$\bar{K}(n, m) - J_{\infty,n}\delta(m, n) + \sum_{n'=n}^{\infty} K(n, n') F(m + n') = 0, \tag{3.23}$$

where

$$\bar{F}(m+n)=\frac{1}{2\pi i}\oint\frac{\bar{b}}{\bar{a}}z^{m+n-1}dz-\sum_{K=1}^{N}\bar{C}_k\bar{z}_k^{m+n-1},\tag{3.24}$$

$$F(m+n)=\frac{1}{2\pi i}\oint\frac{b}{a}z^{-m-n-1}dz+\sum_{K=1}^{N}C_kz_k^{-m-n-1},\tag{3.25}$$

and $\delta(m,n)$ is the Kronecker delta function. The limiting forms $I_{\infty,n}$, $J_{\infty,n}$ are found directly from the eigenvalue problem (2.1) as $|z|\to\infty$. In particular, we find

$$I_{\infty,n}=\begin{pmatrix}0\\1\end{pmatrix}\prod_{i=n}^{\infty}\left(\frac{1}{(1-R_iQ_i)}\right)\tag{3.26}$$

and

$$J_{\infty,n}=\begin{pmatrix}1\\T_{n-1}\end{pmatrix}\prod_{i=n}^{\infty}(1-S_iT_i).\tag{3.27}$$

In practice it is more convenient to write (3.22), (3.23) as forced summation equations. Before doing this, we first show how the potentials relate to the kernels $K(n,m)$, $\bar{K}(n,m)$, and why in fact these kernels are independent of z. Using (3.20) and substituting into (2.1), we find

$$K_1(n,n)=0,\tag{3.28}$$

$$K_2(n,n)=\prod_{i=n}^{\infty}\left(\frac{1}{1-R_iQ_i}\right),\tag{3.29}$$

$$Q_n=-K_1(n,n+1)/K_2(n,n),\tag{3.30}$$

$$K_n(n+1,n')-K_1(n,n'+1)-Q_nK_2(n,n')-S_nK_2(n+1,n')=0,\quad n'\geq n+1,\tag{3.31}$$

$$K_2(n+1,n')-K_2(n,n'-1)-R_nK_1(n,n')-T_nK_1(n+1,n')=0,\quad n'\geq n+1.\tag{3.32}$$

Similarly, using (3.21) and substituting into (2.1) yields

$$\bar{K}_1(n,n)=\prod_{i=n}^{\infty}\left(\frac{1}{1-R_iQ_i}\right),\tag{3.33}$$

$$\bar{K}_2(n,n)=0,\tag{3.34}$$

$$R_n=-\frac{\bar{K}_2(n,n+1)}{\bar{K}_1(n,n)},\tag{3.35}$$

$$\bar{K}_1(n+1,n')-\bar{K}_1(n,n'-1)-Q_n\bar{K}_2(n,n')-S_n\bar{K}_2(n+1,n')=0,\quad n'\geq n+1,\tag{3.36}$$

$$\bar{K}_2(n+1,n')-\bar{K}_2(n,n'+1)-R_n\bar{K}_1(n,n')-T_n\bar{K}_1(n+1,n')=0,\quad n'\geq n+1.\tag{3.37}$$

Thus given the $K(n,m)$, $\bar{K}(n,m)$ we may find Q_n, R_n from (3.30), (3.35) and S_n, T_n from (3.31), (3.37) for $n'=n+1$ typically. Similarly, the above relations insure the kernels are independent of the eigenvalue z.

The solution process is best effected by obtaining forced summation equations. Letting for $m>n$

$$K(n,m)=\prod_{i=n}^{\infty}\left(\frac{1}{1-R_iQ_i}\right)\kappa(n,m),\tag{3.38}$$

$$\bar{K}(n,m)=\prod_{i=n}^{\infty}\left(\frac{1}{1-R_iQ_i}\right)\bar{\kappa}(n,m),\tag{3.39}$$

we have from (3.12),

$$\kappa(n,m)-\begin{pmatrix}1\\0\end{pmatrix}\bar{F}(m+n)-\sum_{n'=n+1}^{\infty}\bar{\kappa}(n,n')\bar{F}(m+n')=0,\tag{3.40}$$

and from (3.23)

$$\bar{\kappa}(n,m)+\begin{pmatrix}0\\1\end{pmatrix}F(m+n)+\sum_{n'=n+1}^{\infty}\kappa(n,n')F(m+n')=0,\tag{3.41}$$

which are analogous to the continuous integral equations of Zakharov–Shabat.[8] The potentials are obtained from the relations

$$Q_n=-\kappa_1(n,n+1),\tag{3.42}$$

$$R_n=-\bar{\kappa}_2(n,n+1),\tag{3.43}$$

$$S_n=-\left(\frac{1}{1-R_nQ_n}\right)(\kappa_1(n,n+2)+Q_n\kappa_2(n,n+1)),\tag{3.44}$$

$$T_n=-\left(\frac{1}{1-R_nQ_n}\right)(\bar{\kappa}_2(n,n+2)+R_n\bar{\kappa}_1(n,n+1)),\tag{3.45}$$

without need to determine $K(n,n)$ directly, unlike the case in Refs. 5, 6. We note in passing that the problem when $R_n\equiv 0$, $T_n\equiv 1$ [(see Eq. (2.10)] is best inverted by procedures analogous to the discretized Schrödinger equation, but the results are similar to the above in that the potentials depend simply on the kernel.

In the special case where

$$Q_n=\mp R_n^*,\quad T_n=\mp S_n^*,$$

$$\bar{\kappa}(n,m)\equiv\begin{pmatrix}\bar{\kappa}_1(n,m)\\\bar{\kappa}_2(n,m)\end{pmatrix}=\begin{pmatrix}\kappa_2^*(n,m)\\\mp\kappa_1^*(n,m)\end{pmatrix}\tag{3.46}$$

and

$$\bar{F}(m+n)=\pm F^*(m+n).\tag{3.47}$$

In these cases only one of the Eqs. (3.40), (3.41) need be used. For example,

$$\kappa_1(n,m)\mp F^*(m+n)\mp\sum_{n'=n+1}^{\infty}\kappa_2^*(n,n')F^*(m+n')=0,\tag{3.48}$$

$$\kappa_2(n,m)+\sum_{n'=n+1}^{\infty}\kappa_1^*(n,n')F^*(m+n')=0,\tag{3.49}$$

where

$$R_n=\pm\kappa_1^*(n,n+1),\tag{3.50}$$

$$S_n=-\frac{1}{(1\pm|R_n|^2)}\left[\kappa_1(n,n+2)\mp R_n^*\kappa_2(n,n+1)\right].\tag{3.51}$$

In solving for the kernels it is often easier to use the form

$$\kappa_1(n,m)\mp F^*(m+n)\pm\sum_{n'=n+1}^{\infty}\sum_{n''=n+1}^{\infty}\kappa_1(n,n'')F^*(m+n')F(n'+n'')=0\tag{3.52}$$

and then find κ_2 from (3.49).

4. TIME DEPENDENCE AND SOLITON SOLUTIONS

The scattering results of Sec. 3 can now be used in conjunction with the time dependent equations (2.2) to solve the class of nonlinear differential–difference equations contained in (2.3) when the potentials R_n, Q_n, S_n, T_n vanish sufficiently rapidly as $|n|\to\infty$. Certain aspects of the time dependence are quite different than previous problems. In the case at hand A_n, B_n, C_n, D_n are given by (2.6) and the evolution equations are (2.7).

In obtaining the required time dependence of the scattering data one need only the asymptotic form of the

time dependent equations (2.2) (a remarkable fact due to inverse scattering!). As $n \to -\infty$, (2.2) takes the form

$$\frac{\partial v_{1n}}{\partial t} = (A_-^{(1)} z + A_-^{(0)}) v_{1_n},$$
$$\frac{\partial v_{2n}}{\partial t} = (D_-^{(-1)}/z + D_-^{(0)}) v_{2_n}; \tag{4.1}$$

as $n \to +\infty$, we have

$$\frac{\partial v_{1n}}{\partial t} = \left(A_-^{(1)} z + A_-^{(0)} - \sum_{k=-\infty}^{\infty} \frac{\partial}{\partial t} \log \Lambda_k\right) v_{1_n},$$
$$\frac{\partial v_{2n}}{\partial t} = \left(A_-^{(0)} + D_-^{(1)}/z - \sum_{k=-\infty}^{\infty} \frac{\partial}{\partial t} \log \Lambda_k\right) v_{2_n}, \tag{4.2}$$

where again $\Lambda_k \equiv 1 - S_k T_k$ and $\Lambda_{k,0} = \Lambda_k$ $(t=0)$. There are various ways to proceed, but since the off diagonal terms in (2.2) vanish asymptotically the time dependent eigenfunctions are chosen to satisfy

$$\phi_n^{(t)} = \phi_n \exp[(A_-^{(1)} z + A_-^{(0)})t],$$
$$\bar{\phi}_n^{(t)} = \bar{\phi}_n \exp\left(\frac{D_-^{(-1)}}{z} + A_-^{(0)}\ t\right),$$
$$\psi_n^{(t)} = \left[\psi_n \exp\left(\frac{D_-^{(-1)}}{z} + A_-^{(0)}\right)t\right] \prod_{-\infty}^{\infty} \frac{\Lambda_k}{\Lambda_{k,0}},$$
$$\bar{\psi}_n^{(t)} = \{\bar{\psi}_n \exp[(A_-^{(1)} z + A_-^{(0)})t]\} \prod_{-\infty}^{\infty} \frac{\Lambda_k}{\Lambda_{k,0}}, \tag{4.3}$$

where $\phi_n^{(t)}$, $\bar{\phi}_n^{(t)}$, $\psi_n^{(t)}$, $\bar{\psi}_n^{(t)}$ all satisfy Eqs. (2.1), (2.2), and ϕ_n, $\bar{\phi}_n$, ψ_n, $\bar{\psi}_n$ have the time independent boundary conditions (3.1), (3.2) (necessary for the direct use of the scattering results of Sec. 3). ϕ_n, $\bar{\phi}_n$, ψ_n, $\bar{\psi}_n$ satisfy (2.1) and a set of equations similar to (2.2) obtained by use of (4.3).

Since the Wronskians (3.4), (3.5) are assumed to be of one sign [in the important case when $S_n = -T_n^*$, $Q_n = -R_n^*$ (3.4), (3.5) are positive definite], we may write

$$\phi_n^{(t)} = a_0 \bar{\psi}_n^{(t)} + b_0 \psi_n^{(t)},$$
$$\bar{\phi}_n^{(t)} = -\bar{a}_0 \psi_n^{(t)} + \bar{b}_0 \bar{\psi}_n^{(t)}, \tag{4.4}$$

where a_0, b_0, $\bar{a}_0$, $\bar{b}_0$ are time independent. Using (4.3), (4.4) a, b, $\bar{a}$, $\bar{b}$ can be shown to satisfy the relations

$$a = \frac{a_0}{\prod_{k=-\infty}^{\infty} \Lambda_k/\Lambda_{k,0}},$$
$$b = \frac{b_0 \exp[(D_-^{(-1)}/z - A_-^{(1)} z)t]}{\prod_{k=-\infty}^{\infty} \Lambda_k/\Lambda_{k,0}},$$
$$\bar{a} = \frac{\bar{a}_0}{\prod_{k=-\infty}^{\infty} \Lambda_k/\Lambda_{k,0}}, \tag{4.5}$$
$$\bar{b} = \frac{\bar{b}_0 \exp[(A_-^{(1)} z - D_-^{(-1)}/z)t]}{\prod_{k=-\infty}^{\infty} \Lambda_k/\Lambda_{k,0}},$$

where a_0, $\bar{a}_0$, b_0, $\bar{b}_0$ are obtained from initial conditions. The difference between this problem and previous problems is that the scattering data a, $\bar{a}$, b, $\bar{b}$ *individually* depend on the potential through Λ_k. Since we wish to find the potentials by inversion this could be a serious difficulty. The resolution of the problem hinges on the fact that we need the time dependence of b/a, $\bar{b}/\bar{a}$, C_k, and $\bar{C}_k$ which satisfy

$$\frac{b}{a} = \frac{b_0}{a_0} \exp[(D_-^{(-1)}/z - A_-^{(1)} z)t],$$
$$\frac{\bar{b}}{\bar{a}} = \frac{\bar{b}_0}{\bar{a}_0} \exp[(A_-^{(1)} z - D_-^{(-1)}/z)t],$$
$$C_k = C_{k,0} \exp[(D_-^{(-1)}/z_k - A_-^{(1)} z_k)t], \tag{4.6}$$
$$\bar{C}_k = \bar{C}_{k,0} \exp[(A_-^{(1)} \bar{z}_k - D_-^{(-1)}/\bar{z}_k)t].$$

Now $F(m+n)$ and $\bar{F}(m+n)$ defined by (3.24), (3.25) depend only on initial data, and the inversion can be simply effected. Note that when $R_n = \mp Q_n^* = I_n$, $S_n = \mp T_n^* = V_n$, and $D_-^{(-1)} = A_-^{(1)} = 1$ the formulas (3.48)–(3.52) with the $F(m+n)$, $\bar{F}(m+n)$ defined using (4.6) lead to the solution of (2.8) and therefore the self-dual network equations (1.1), (1.2).

We remark in passing that the relationship (3.8) written in the form

$$a\bar{a} + b\bar{b} = \prod_{k=-\infty}^{\infty} \frac{1 - R_k Q_k}{\Lambda_k} \tag{4.7}$$

is intimately connected with a conservation law of (2.7). Using the set of Eqs. (4.5), we have

$$a_0 \bar{a}_0 + b_0 \bar{b}_0 = \prod_{k=-\infty}^{\infty} (1 - R_k Q_k)(1 - S_k T_k) / [1 - S_k(t=0) T_k(t=0)]^2. \tag{4.8}$$

The right-hand side must be independent of time. Formulating the expression $Q_n R_{nt} + Q_{nt} R_n + S_n T_{nt} + S_{nt} T_n$ from (2.7) and summing, we find

$$\frac{\partial}{\partial t} \sum_{k=-\infty}^{\infty} \log(1 - R_k Q_k)(1 - S_k T_k) = 0. \tag{4.9}$$

Thus,

$$\prod_{k=-\infty}^{\infty} (1 - R_k Q_k)(1 - S_k T_k) = \text{const}, \tag{4.10}$$

as it must.

In a future paper we will discuss in detail the various aspects of the solution. Here we shall only present the single soliton results. The results are in agreement with those found by Hirota.[7] Assuming $Q_n = -R_n = -I_n$ and $T_n = -S_n = -V_n$, and $A_-^{(1)} = D_-^{(-1)} = 1$, Eqs. (3.48), (3.49) can be used with the appropriate sign. If $b = \bar{b} = 0$, and only one bound state exist, then

$$\bar{F}(m+n) = -\bar{C}_1 \bar{z}_1^{m+n-1}$$

and (4.11)

$$F(m+n) = -\bar{C}_1^* \bar{z}_1^{*m+n-1}.$$

Using (3.52), $\kappa_1(n,m)$ satisfies,

$$\kappa_1(n,m) + \bar{C}_1 \bar{z}_1^{m+n-1} + \sum_{n'=n-1}^{\infty} \sum_{n''=n+1}^{\infty} \kappa_1(n,n'') \bar{C}_1 \bar{C}_1^* \bar{z}^{m+n'-1} \bar{z}_1^{*n'+n''-1} = 0. \tag{4.12}$$

Defining

$$\tilde{\kappa}_1(n) = \sum_{m=n+1}^{\infty} \bar{z}_1^{*m} \kappa_1(n,m), \tag{4.13}$$

we find

$$\tilde{\kappa}_1(n) = -\frac{\bar{C}_1(1 - \bar{z}_1 \bar{z}_1^*) \bar{z}_1^{n-1} (\bar{z}_1 \bar{z}_1^*)^{n+1}}{(1 - \bar{z}_1 \bar{z}_1^*)^2 + \bar{C}_1 \bar{C}_1^* (\bar{z}_1 \bar{z}_1^*)^{2n+1}}, \tag{4.13}$$

whereupon $\kappa_1(n,m)$, $\kappa_2(n,m)$ are found to satisfy

$$\kappa_1(n,m) = -\frac{\bar{C}_1 \bar{z}_1^{m+n-1}}{1+[\bar{C}_1\bar{C}_1^*/(1-\bar{z}_1\bar{z}_1^*)^2](\bar{z}_1\bar{z}_1^*)^{2n+1}} \tag{4.14}$$

and

$$\kappa_2(n,m) = \frac{-\bar{C}_1\bar{C}_1^*(\bar{z}_1\bar{z}_1^*)^n \bar{z}_1^{*n}\bar{z}_1^m}{\{1+[\bar{C}_1\bar{C}_1^*/(1-\bar{z}_1\bar{z}_1^*)^2](\bar{z}_1\bar{z}_1^*)^{2n+1}\}(1-\bar{z}_1\bar{z}_1^*)}. \tag{4.15}$$

Thus using (3.50) and (3.51) we may find the soliton solutions. When $\bar{z}_1 = \pm e^{-w}$, $w > 0$ and real,

$$R_n = -\operatorname{sgn}\bar{C}_{1,0}\sinh w \operatorname{sech}(2wn \pm 2(\sinh w)t + \phi_0), \tag{4.16}$$

$$S_n = \pm \operatorname{sgn}\bar{C}_{1,0}\sinh w \operatorname{sech}(2wn \pm 2(\sinh w)t + \phi_0 + w), \tag{4.17}$$

where

$$\phi_0 = -\log(|\bar{C}_{1,0}|/2\sinh w). \tag{4.18}$$

Note that the solitons can move left or right, and can be positive or negative in amplitude. In the more general case, complex solitons, as well as paired soliton bound states [a soliton "pair" each with the same velocity (see also Ref. 8)], exist.

5. CONCLUDING REMARKS

In this article we have presented a method by which the solution of the self-dual network (1.1), (1.2) and other closely related problems (2.7) can be solved. These equations are actually only one consistency condition relating to (2.3); other differential–difference equations can be deduced in the same manner as outlined in Sec. 2. There are a number of interesting questions remaining, such as multisoliton solutions, bound state (paired soliton) solutions, the continuous spectrum, "exploding" solitons, the analogy to similarity solutions, numerical investigation and the continuous limit. We will report on progress in future papers. With regard to the continuum note that the limit is actually somewhat singular.

One possible passage to the continuum is to let

$$\begin{aligned} z &= 1 - i\zeta h, \\ Q_n &= h\tilde{\omega}_n, \\ R_n &= h\rho_n, \\ S_n &= h\sigma_n, \\ T_n &= h\tau_n. \end{aligned} \tag{5.1}$$

Substituting (5.1) into (2.1) and taking the limit $h \to 0$, we have the continuum equations

$$\begin{aligned} v_{1x} + i\zeta v_1 &= \bar{q}v_2, \\ v_{2x} - i\zeta v_2 &= \bar{r}v_1, \end{aligned} \tag{5.2}$$

where $\bar{q} = \tilde{\omega} + \sigma$, $\bar{r} = \rho + \tau$. This eigenvalue problem,[9] a somewhat more general case of Ref. 8 contains only two potentials $(\bar{q}, \bar{r})$. The discrete problem must contain four potentials (Q_n, R_n, S_n, T_n) in order to obtain interesting, second order in time evolution equations. This situation is not obvious when one tries to discretize (5.2) naively.

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Ergodicity of observable and ergodic hypothesis in Markovian kinetics

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The time average of any observable, which evolves following an irreducible Markov process with countable states each of which is a persistent state, equals the ensemble average of the same quantity if and only if the corresponding master equation does not exhibit the accumulation of its eigenvalues around the infinitesimal neighborhood of the point with the value zero and if the steady distribution as the eigenfunction with the eigenvalue zero is uniform. The nonuniform steady distribution invalidates the ergodicity of observable. The principle of *a priori* equal weight is identical to the ergodicity of observable.

1. INTRODUCTION

The individual and the mean ergodic theorems of Birkhoff and von Neumann show that the metric-transitive dynamical system, which is no longer separable as being subject to Liouville's theorem, is ergodic.[1] The ergodic theorem provides a useful clue to statistical mechanics of a completely isolated system. Nevertheless, it must be noted that linear and nonlinear statistical mechanics off equilibrium is outside the realm of the theorem. Markovian kinetics has been supposed to be a model kinetics of linear and nonlinear systems off equilibrium. So long as one concerns onself with the probability measure in phase space without paying attention to a time series of observables which really occur in a single system, the ergodic theorem can be extended to the case of the Markov process only in the sense that the conserved quantity is the probability measure instead of the volume measure of phase space in the former dynamical system.

The ergodicity of the probability measure results if the Markov process is irreducible. However, one should realize that the ergodicity of the probability measure does not necessarily result in the ergodicity of physical observables. The probability measure and the associated ensemble theory are always a mathematical trick to deal with the probabilistic kinetics of observables which evolve in a single system instead of in an ensemble of the similar systems. The probabilistic kinetics of the Markov process predicts the probability that a particular event would be expected at a later time only with the use of the definite knowledge of the event appearing at a previous time.

If experimental observation takes place at each fixed time interval, the observer necessarily identifies a series of definite events and the entropy of information on the side of the observer always decreases as time goes on. This is a real situation of experimental measurement. Above all, one notes that the raw data themselves have nothing to do with the probability measure in phase space. Only after a certain sampling out of the collected events has been done, one might expect to understand the sampled events in terms of the probability measure of the ensemble theory.

In the present paper, we investigate the extent to which the ensemble point of view of the Markov process holds its plausibility specifically in comparison to experiment. The principal subject to be examined is whether or not the time average of an observable is identical to the ensemble average of the same quantity. If the ergodicity of physical observables is not maintained, one cannot rely on the ensemble theory for purpose of interpreting the collection of events measured in a single system over a long time. All one has to do is to follow the time evolution of observables by the help of the probabilistic kinetics of a single system.

In order to complete our program, we present in Sec. 2 an explicit form of the time average of any observable which follows the master equation of an irreducible Markov process. The role of the observer is stressed specificially with respect to the entropy of information. The argument on the ensemble average is given in Sec. 3. Since the time average of observables has been evaluated independently of the ensemble average, the comparison of both the averages provides a reference by which one can test whether the ergodicity of the observable is maintained. A principal result is that the ergodicity of the observable does not hold if the steady distribution is not uniform. A detailed account is presented in Sec. 4.

2. TIME AVERAGE

We restrict ourselves to the discussion of an irreducible Markov process with countable states

$$\{i\}, \quad i=1,\ 2,\ \ldots,N, \tag{2.1}$$

in which the total number N of the states does not necessarily remain finite. The Markov process is supposed to follow the master equation

$$\frac{\partial}{\partial t}P(i,t\,|\,k,t_0)=\sum_{j\neq i}W(i\leftarrow j)P(j,t\,|\,k,t_0) - \sum_{j\neq i}W(j\leftarrow i)P(i,t\,|\,k,t_0), \tag{2.2}$$

where $P(i,t\,|\,k,t_0)$ is the transition probability that the state i occurs at time t under the initial condition that the state at an earlier time $t_0(<t)$ is k, and $W(i\leftarrow j)$ is the transition probability rate from the state j to i. First of all, we suppose that the transition probability satisfies the translational invariance

$$P(i,t+t'\,|\,k,t_0+t')=P(i,t\,|\,k,t_0), \quad i,k=1,\ 2,\ \ldots,N \quad \text{with an arbitrary } t', \tag{2.3}$$

because of the definition of the Markov process.

Suppose an observer performs measurement at each time interval of $\tau(>0)$ in order to identify the states which appear at every interval of τ. Since the states follow the Markovian kinetics obeying the master equation (2.2), the observer, who has already known that the state, say, k was measured at time $t=t'$, can find the probability that the state i would be expected at the next measurement at $t=t'+\tau$ with the use of the knowledge of the measurement done at $t=t'$. The probability of expecting the state i at $t=t'+\tau$ turns out to be

$$P_c(i, t'+\tau \mid k, t') = P(i, t'+\tau \mid k, t'). \tag{2.4}$$

On the other hand, if the observer does not have any information about the events which occurred before $t=t'$ and if he is asked to predict the probability that the state k at $t=t'$ would be followed by the state i at $t=t'+\tau$, the result he obtains by the help of the Markovian kinetics (2.2) will be expressed as

$$P_c^{(a)}(i, t'+\tau \mid k, t') = \alpha_k P_c(i, t'+\tau \mid k, t') \tag{2.5}$$

with

$$\sum_{k=1}^{N} \alpha_k = 1 \quad \text{and} \quad \alpha_k > 0 \tag{2.6}$$

in terms of the *a priori* probability α_k of expecting the state k at an arbitrary time without any knowledge of the past history preceding the expectation. Once it is agreed that an objective explanation as a kind of rigorous epistemology could be established, the *a priori* probability $\{\alpha_k\}$ $(k=1, 2, \ldots, N)$ must remain the same to any one of observers who are not informed of any past history. If it were not the same to a certain observer, who is of course not informed of any past events, and if he is asked to present the logic leading to the difference, the observer would have to explain the origin of the discrepancy in terms of *a priori* preconception which can never be tested physically.

One readily notes the conservation of the *a priori* probabilities of expectation as follows:

$$\sum_{i,k=1}^{N} P_c^{(a)}(i, t'+\tau \mid k, t') = \sum_{k=1}^{N} \alpha_k = 1. \tag{2.7}$$

The first step comes from the irreducibility of the Markov process

$$\sum_{i=1}^{N} P(i, t'+\tau \mid k, t') = 1 \quad \text{for an arbitrary } k, \tag{2.8}$$

and the second step from (2.6).

In general, it is beyond the control of any theoretical analysis to fix the *a priori* probability, since one can never determine the initial state with a necessary and sufficient reasoning. One realizes, for example, that the very initial condition of a dynamical system is simply given through a certain untouched agent and never be deduced by following a sufficient reasoning. However, if only Markov process is concerned, we can prove the following theorem:

Theorem: Suppose the irreducible Markov process with N states $\{i\}$ $(i=1, 2, \ldots, N)$ which follows the master equation (2.2). Then, an observer, who is not informed of any past history of events, expects an arbitrary Markovian state k at an arbitrary time with the *a priori* probability

$$\alpha_k = 1/N \quad \text{for } k=1, 2, \ldots, N. \tag{2.9}$$

Proof: Suppose four different observers A, B, C, and D, all of whom are not informed of any past history of events before they are asked to perform measurement. Furthermore, it is assumed that the *a priori* probability $\{\alpha_k\}$ $(k=1, 2, \ldots, N)$ is common to all the observers. This will be verified at the final stage of this proof. Next, suppose that observer A asks observer B to predict the probability that the state k at time $t=t'$ is followed by the state j' at $t=t'+\tau$. The probability of expectation predicted by observer B is

$$P_c^{(a)}(j', t'+\tau \mid k, t') = \alpha_k P_c(j', t'+\tau \mid k, t') \tag{2.10}$$

with the aid of (2.5). Similarly, let observer A ask observer C to predict the probability that the state j'' at $t=t'+\tau$ is followed by the state i at $t=t'+2\tau$. The result of the probability is

$$P_c^{(a)}(i, t'+2\tau \mid j'', t'+\tau) = \alpha_{j''} P_c(i, t'+2\tau \mid j'', t'+\tau). \tag{2.11}$$

Consequently, if observer A predicts the probability that the state k at $t=t'$ is followed by the state i at $t=t'+2\tau$ only with the use of the information which both observers B and C prepare by following the Markovian kinetics (2.2), the result will be

$$\begin{aligned} \tilde{P}_c^{(a)}(i, t'+2\tau \mid k, t') &= \sum_{j'=1}^{N} P_c^{(a)}(i, t'+2\tau \mid j', t'+\tau) \\ &\quad \times P_c^{(a)}(j', t'+\tau \mid k, t') \\ &= \sum_{j'=1}^{N} \alpha_k \alpha_{j'} P_c(i, t'+2\tau \mid j', t'+\tau) \\ &\quad \times P_c(j', t'+\tau \mid k, t'). \end{aligned} \tag{2.12}$$

The entropy density of information which observer A assigns to the probabilistic event is

$$\tilde{I}_A(i, t'+2\tau \mid k, t') = -\log_2 \tilde{P}_c^{(a)}(i, t'+2\tau \mid k, t'). \tag{2.13}$$

If observer A really measures the state k at $t=t'$ and the state i at $t=t'+2\tau$, he will loose the entropy of information by the amount of $\tilde{I}_A(i, t'+2\tau \mid k, t')$. Here, it must be borne in mind that observer A performs measurement even at $t=t'+\tau$ in addition to at $t=t'$ and at $t=t'+2\tau$ since he divides the event continuing from $t=t'$ to $t=t'+2\tau$ into two parts at $t=t'+\tau$.

Similarly, observer D is supposed to predict the probability that the state k at $t=t'$ is followed by the state i at $t=t'+2\tau$ with the aid of the Markovian kinetics (2.2). The result is

$$P_c^{(a)}(i, t'+2\tau \mid k, t') = \alpha_k P_c(i, t'+2\tau \mid k, t'). \tag{2.14}$$

The entropy density of information which observer D assigns to the probabilistic event is

$$I_D(i, t'+2\tau \mid k, t') = -\log_2 P_c^{(a)}(i, t'+2\tau \mid k, t'). \tag{2.15}$$

If observer D really measures the state k at $t=t'$ and the state i at $t=t'+2\tau$, he will loose the entropy of information by the amount of $I_D(i, t'+2\tau \mid k, t')$. The difference in the decrease of the entropy of information between observers A and D is just the amount of

$$I_0 = -\sum_{i=1}^{N} \alpha_i \log_2 \alpha_i, \tag{2.16}$$

since observer A is more informed than observer D in that observer A can identify which state out of the total N states really appears at $t=t'+\tau$ although observer D cannot. Here, it is noted that observer A expects the state i at an arbitrary time with the *a priori* probability α_i. As a result, we obtain the expression

$$\tilde{I}_A(i, t'+2\tau \mid k, t') - I_D(i, t'+2\tau \mid k, t') = I_0. \tag{2.17}$$

This gives

$$\sum_{j'=1}^{N} \alpha_k \alpha_{j'} P_c(i, t'+2\tau \mid j', t'+\tau) P_c(j', t'+\tau \mid k, t') = 2^{-I_0} \alpha_k P_c(i, t'+2\tau \mid k, t'). \tag{2.18}$$

Because of the transitivity of the Markov process

$$P_c(i, t'+2\tau \mid k, t') = \sum_{j'=1}^{N} P_c(i, t'+2\tau \mid j', t'+\tau) P_c(j', t'+\tau \mid k, t'), \tag{2.19}$$

expression (2.18) reduces to

$$\sum_{j'=1}^{N} \alpha_k (\alpha_{j'} - 2^{-I_0}) P_c(i, t'+2\tau \mid j', t'+\tau) P_c(j', t'+\tau \mid k, t') = 0. \tag{2.20}$$

Since the states i and k and the time τ are arbitrary, the result is

$$\alpha_1 = \alpha_2 \cdots = \alpha_N = 2^{-I_0} \tag{2.21a}$$

or, equivalently,

$$\alpha_{j'} = 1/N \quad \text{for } j' = 1, 2, \ldots, N \tag{2.21b}$$

because of the conservation of the total *a priori* probabilities. It must, however, be remembered that the result (2.21) has been obtained only under the ansatz that the *a priori* probability $\{\alpha_k\}$ $(k=1, 2, \cdots, N)$ is common to all the concerned observers.

In order to prove the objectivity of the result (2.21), let us consider the situation that observer A measures the two events. One is that the state k at $t=t_1$ is followed by the state i at $t=t_1+2\tau$. And the other is that the state k at $t=t_2(>t_1)$ is followed by the state i at $t=t_2+2\tau$. If observer A divides the first event into two parts at $t=t_1+\tau$, he can also play both the roles of observers B and C of the previous case. Furthermore, the second event permits observer A to assimilate himself to observer D of the previous case. Since the *a priori* probability $\{\alpha_k\}$ $(k=1, 2, \ldots, N)$ remains invariant as far as a single observer is concerned, one can follow the same argument as before only with the substitution of observer A for each of observers B, C, and D. Hence, the result (2.21) is obtained again. The necessary and sufficient condition for this statement is that the time difference (t_2-t_1) remains finite, otherwise observer A would miss the second event. As a matter of fact, the finiteness of the time difference, which is equivalent to the recurrence time, is guaranteed since an irreducible Markov process with countable states has only the set of persistent states.[2] The *a priori* probability $\{\alpha_k\}$ characteristic of a group of several observers, all of whom are supposed to establish the same *a priori* probability, have been shown identical to the proability characteristic of a single subjective observer. This confirms the objectivity of the *a priori* probability, verifying that it never occurs that any one of observers opposes the universality of the result presented in (2.21). QED

With the aid of the present theorem, the *a priori* probability of expectation that the state k at $t=t'$ is followed by the state i at $t=t'+\tau$ reduces to

$$P_c^{(a)}(i, t'+\tau \mid k, t') = \frac{1}{N} P_c(i, t'+\tau \mid k, t'). \tag{2.22}$$

One can calculate the time average of any observable in terms of the *a priori* probability of expectation. For example, let us consider a physical observable $X(t)$ satisfying

$$X(t) = X_i \tag{2.23}$$

if the state at time t is i with $i=1, 2, \ldots, N$.

The time average of the moment

$$\overline{X(t'+\tau)X(t')} \equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T X(t'+\tau)X(t')\, dt' \tag{2.24}$$

turns out to be

$$\overline{X(t'+\tau)X(t')} = \sum_{i,k=1}^{N} X_i X_k P_c^{(a)}(i, t'+\tau \mid k, t') \tag{2.25}$$

because of both the definition of the *a priori* probability of expectation and the translational invariance presented in (2.3).[3]

3. ENSEMBLE AVERAGE

The master equation (2.2) is rewritten to a reduced form

$$\frac{\partial}{\partial t} P = M \cdot P, \tag{3.1}$$

where the vector P and the tensor M have the components as

$$P^i \equiv P(i, t \mid k, t_0), \quad i=1, 2, \ldots, N, \tag{3.2}$$

and

$$M_j^i \equiv \begin{cases} -\sum_{l\neq i} W(l \leftarrow i) & \text{for } i=j \\ W(i \leftarrow j) & \text{for } i\neq j. \end{cases} \tag{3.3}$$

The eigenvalue problem of the operator M is formulated in such a way

$$M \cdot P_m = \lambda_m P_m, \quad m = 0, 1, 2, \ldots, N', \tag{3.4}$$

where λ_m is an eigenvalue with the eigenvector P_m. The inequality

$$N'+1 \leq N \tag{3.5}$$

is always satisfied since the rank of the operator M does not exceed N. The eigenvalue λ_0 is chosen to be identically zero. The corresponding eigenvector P_0 gives the steady distribution of the present Markov process. If pure imaginary eigenvalues are absent and if the eigenvalue $\lambda_0=0$ is not an accumulation point of other eigenvalues, the eigenvector P_0 leads to

$$P(i) \equiv P_0^i \tag{3.6}$$

$$= \lim_{(t-t_0)\to\infty} P(i, t \mid k, t_0) \quad \text{for any } i \text{ and } k. \tag{3.7}$$

We shall first consider the case that the operator M does not have pure imaginary eigenvalues and that $\lambda_0 = 0$ is not an accumulation point of eigenvalues λ_n with $n \geq 1$. If one prepares an ensemble of systems each of which follows the master equation (3.1) and if the ensemble is sufficiently aged, then the probability of expecting that a representative system out of the ensemble finds itself in the state i at an arbitrary time is

$$P(i) \tag{3.8}$$

of (3.7). This is rather the definition of the aged ensemble, whose existence is supported by the assumption that $\lambda_0 = 0$ is not an accumulation point. Similarly, the probability of expecting that a representative system finds itself in the state k at $t = t'$ and successively in the state i at $t = t' + \tau$ is

$$P_c^{(e)}(i, t' + \tau \,|\, k, t') = P(k) P_c(i, t' + \tau \,|\, k, t'). \tag{3.9}$$

One can evaluate the ensemble average of any observable in terms of the two-time probability distribution function (3.9).

If the operator M has pure imaginary eigenvalues, the transition probability $P(i, t \,|\, k, t_0)$ will oscillate in the limit $(t - t_0) \to \infty$. This behavior is specific to a single system. On the other hand, the probability distribution function in the ensemble would not exhibit such an oscillatory behavior because of the ensemble dephasing.[4] This is because the phase relation between systems constituting the ensemble is arbitrary. As a result, the probability of expecting that a representative system finds itself in the state i at an arbitrary time is again the eigenfunction $P(i)$ of (3.6) which does not, however, satisfy (3.7). The two-time probability distribution function also reduces to (3.9).

One notes that a possibility of the eigenvalue accumulation to $\lambda_0 = 0$ could not totally be disregarded if the limit $N \to \infty$ is taken. If such an accumulation really occurs, one cannot argue that the steady distribution (3.6) may be the probability distribution in the aged ensemble.

4. ERGODICITY AND ERGODIC HYPOTHESIS

The ansatz that the time average of any observable should be equal to the ensemble average of the same quantity is stated as

$$P_c^{(a)}(i, t' + \tau \,|\, k, t') = P_c^{(e)}(i, t' + \tau \,|\, k, t') \tag{4.1}$$

for arbitrary i, k, t' and $\tau (> 0)$ with the aids of (2.22) and (3.9). The result is

$$P(k) = 1/N \quad \text{for } k = 1, 2, \ldots, N. \tag{4.2}$$

The present expression tells that the ergodicity of observable is maintained if and only if the eigenvalue $\lambda_0 = 0$ is not an accumulation point and if the steady distribution as the eigenfunction with the eigenvalue $\lambda_0 = 0$ is uniform. The ergodicity is necessarily invalidated if the steady distribution is not uniform. As a matter of fact, the principle of *a priori* equal weight,[1] when it is applied to an irreducible Markov process, is identical to the assertion for the ergodicity of observable. The principle of *a priori* equal weight and the ergodicity of observable are just a tautology with each other.

5. CONCLUDING REMARKS

Even if a statistical mechanical system with a large number of degrees of freedom follows an irreducible Markov process, the condition of the irreducibility may sometimes be too strict specifically from a physical point of view. If the irreducible Markov process with N degrees of freedom is physically reducible in the sense that it may constitute an ensemble of N' of weakly coupled subsystems each of which follows an irreducible Markov process with n degrees of freedom satisfying the constraint $N = N'n$, one may hope to regard the large irreducible system approximately as the ensemble of the small subsystems each of which is irreducible. From a mathematical point of view, however, any irreducible Markov process is no longer reducible because of its very definition. Hence it must be stressed that the reducibility quoted here is stated only as a physical approximation. If the number N' of the subsystems is much greater than unity, the probability function fixed by the Markovian kinetics of a single subsystem would be interpreted as the ensemble probability function of N' subsystems. The value of a physical observable per each subsystem at any moment is thus determined by its ensemble average over the subsystems. One should note that such an observable must be additive in the sense that the observable of the original large system is approximated by the summation of the observables allotted to each subsystem. The ergodicity of the additive observable is maintained if the ensemble average over the subsystems is independent of time, since the time average is just the time average of the quantity which has been subject to the ensemble average. As a result, even if the steady distribution of a subsystem is not uniform, the ergodicity of an additive observable would be kept. This statement could be only approximately valid to additive observables which would admit the introduction of the physical reducibility into the Markov process which is originally irreducible.

Once an irreducible Markovian kinetics is established of a single system, it will be straightforward to examine whether or not the resulting probabilistic kinetics maintains the ergodicity of observable. If the steady distribution is not uniform, the ergodicity does not hold. This observation causes a serious reconsideration of the concept of potential which has been introduced into the Markovian kinetics by several authors. The kinetics in terms of the potential which is related to the probability function of a given Markov process cannot cope with once and for all events which evolve in the single system. This is because the potential kinetics considers the kinetic behavior of only an ensemble of many similar systems and not of an irreducible single system.

If one comes to stress the probabilistic kinetics of an irreducible single system instead of the ensemble kinetics of stochastic process, the role of the observer who always decreases the entropy of information at each measurement must fully be scrutinized.

[1] D. ter Haar, *Elements of Statistical Mechanics* (Holt, Rinehart and Winston, New York, 1961) Appendix I, and references cited therein.

[2]It should be realized that any observer is never unlimited with respect to his ability of measurement. If the recurrence time is greater than the upper bound of the time interval which the observer can measure, the reasoning presented in this proof will fail. One compromise, however, would be as follows: If observer A is succeeded by observer $A^{(2)}$ as the second generation of the former observer A and if observer $A^{(2)}$ is further succeeded by the third generation $A^{(3)}$ and so on, the present proof will work only under the ansatz that all of observer A and his later generations $A^{(2)}$, $A^{(3)}$, $\cdots$ have the common *a priori* probability $\{\alpha_k\}$ $(k=1, 2, \ldots, N)$. Nevertheless, the present ansatz would by no means be self-evident.

[3]Since only the events each of which continues over the interval τ are concerned when the autocorrelation function (2.24) is evaluated, one can prepare a set of two-time events continuing over only the interval τ by dividing the event lasting from $t=0$ to $t=\infty$. If an observer, who is not informed of any past history of events, tries to find the time average of the moment (2.24), the expected value will be the average of the moment over the two-time events belonging to the set. Since the two-time event that the state k at $t=t'$ is followed by the state i at $t=t'+\tau$ is expected with the probability $\alpha_k P_c(i, t'+\tau \mid k, t')$ and since the probability of expectation is independent of the initial time t' because of (2.3), expression (2.25) follows. Here, the right hand side of (2.24) is supposed to converge. If one concerns oneself with the time average of the observable $X(t)$, the interval at which each measurement of $X(t)$ is done must be known. If the interval is τ, one can also prepare the set of the two-time events continuing over τ by dividing the event lasting from $t=0$ to $t=\infty$. If the state k at $t=t'$ is followed by the state i at $t=t'+\tau$, the mean value of $X(t)$ is $(X_i+X_k)/2$. Hence, an observer, who is not informed of any past history of events, can find the time average $\overline{X(t)}$ in terms of the *a priori* probability of expectation. The result is $\overline{X(t)}=\sum_{i,k}[(X_i+X_k)/2]\alpha_k P_c(i, t'+\tau \mid k, t')$. It is, however, not surprising that the average is dependent upon the interval τ. This is because the state at $t=t'+\tau$ is always affected by the state at $t=t'$, depending upon how the initial information would die away in the course of the stochastic evolution over the interval τ.

[4]K. Tomita, T. Ohta, and H. Tomita, Prog. Theor. Phys. 52, No. 6 (1974) (to be published).

On first order smoothing theory*

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This paper is concerned with the validity of an approximation known variously as first order smoothing theory (FOST), first order cumulant discard, quasilinear theory, and the adiabatic approximation. This approximation has been widely used in turbulent dynamo theory, which provides a number of the examples considered below. On the basis of such examples, Lerche and Parker have recently contended that first order smoothing is under no circumstances trustworthy; i.e., even when the method might have been expected to yield solutions in agreement with those of the exact theory, it does not necessarily do so. We show that the discrepancies between the exact and approximate theories that they claim to have uncovered are, in fact, nonexistent. It is established, however, from one of their examples that FOST may be legitimately criticized on a completely different ground connected with the high velocity tail of the probability distribution.

I. INTRODUCTION

Lerche and Parker[1] and Lerche[2,3,4] have recently cast doubt on the validity of a closure approximation often used in statistical physics and frequently called "first order smoothing theory" (FOST). The present authors[5,6,7] and indeed many others (see, for example, Ref. 8) have made extensive use of the method in turbulent dynamo theory, that is, the theory of electromagnetic induction in fluid conductors in turbulent motion. If the claims of Lerche and Parker prove well-founded, turbulent dynamo theory will, as they state, suffer a serious setback. It is an object of this paper to allay this fear by raising a number of difficulties inherent in their analyses.

We will first use the dynamo application to illustrate FOST, and to discuss when FOST may be expected to yield a good approximation to the exact results. Starting from the equation

$$\frac{\partial \mathbf{B}}{\partial t} = \mathrm{curl}(\mathbf{u}' \times \mathbf{B}) + \eta \nabla^2 \mathbf{B}, \tag{1}$$

which governs the induction of magnetic field $\mathbf{B}$ by a given motion $\mathbf{u}'$, which we will suppose is turbulent and of zero mean, one writes $\mathbf{B} = \langle \mathbf{B} \rangle + \mathbf{B}'$, where $\langle \mathbf{B} \rangle$ is the ensemble mean of $\mathbf{B}$, and obtains by averaging (1)

$$\frac{\partial \langle \mathbf{B} \rangle}{\partial t} = \mathrm{curl}\, \langle \mathbf{u}' \times \mathbf{B}' \rangle + \eta \nabla^2 \langle \mathbf{B} \rangle, \tag{2}$$

$$\frac{\partial \mathbf{B}'}{\partial t} = \mathrm{curl}[\mathbf{u}' \times \langle \mathbf{B} \rangle + \{\mathbf{u}' \times \mathbf{B}' - \langle \mathbf{u}' \times \mathbf{B}' \rangle\}] + \eta \nabla^2 \mathbf{B}'. \tag{3}$$

FOST rests on the idea that, provided the root mean square velocity $U = \sqrt{\langle \mathbf{u}'^2 \rangle}$ is "sufficiently small," the terms in curly brackets in (3) may be neglected, leading to

$$\frac{\partial \mathbf{B}'}{\partial t} - \eta \nabla^2 \mathbf{B}' = \mathrm{curl}\, (\mathbf{u}' \times \langle \mathbf{B} \rangle). \tag{4}$$

This equation, together with (2) and the relevant boundary, initial, and continuity conditions, give a closed mathematical system, from which $\langle \mathbf{B} \rangle$ and $\mathbf{B}'$ may be determined. The consequent simplifications introduced by FOST are clearly enormous.

Lerche and Parker[1] state that "the general validity of first order smoothing has not been established," but they do not give references in which claims for its general validity have been made. It has certainly been argued often that circumstances exist (see below) in which FOST will provide the first approximation, in a well-defined sense, to the correct results. But Lerche and Parker[1] state that, "There do exist particular investigations (e.g., ... this paper) which demonstrate its invalidity under conditions where it might have been believed, *a priori*, to be valid.... After completing a calculation in the first order smoothing approximation, one does not know whether the answer is close to the truth." It is this severe, possibly lethal, criticism of FOST that we wish to contest in this paper.

In the context of the turbulent dynamo, a comparison of the magnitude of the terms in (3) strongly suggests[8] that (4) will be a valid approximation provided

$$\textit{either } U' \ll L'/T' \tag{5}$$

$$\textit{or } U'^{\frac{1}{2}} \ll \eta/L', \tag{6}$$

where U' is a characteristic velocity, and L' and T' are typical length and time scales of $\mathbf{B}'$. Since the right-hand side of (4) is the source to which $\mathbf{B}'$ owes its existence in FOST, it appears that we may write

$$U' \approx U, \tag{7a}$$

$$L' \approx \lambda, \tag{7b}$$

$$T' \approx \tau, \tag{7c}$$

where λ and τ are the correlation length and time of the turbulence. If (7a)—(7c) hold, we may write (5) and (6) as

$$\textit{either } U \ll \lambda/\tau \tag{5'}$$

$$\textit{or } U \ll \eta/\lambda. \tag{6'}$$

Inequalities (5') and (6') should be applied with some caution. We may note two cases in which failure of one of (7a)—(7c) renders (5') and (6') misleading, even though (5) and (6) are faithful guides. First, consider the "sudden" approximation in which (5') holds. It may be shown[9] that, if $U\lambda/\eta$ is sufficiently large, i.e., if (6) or (6') is sufficiently violated, $|\mathbf{B}'|$ becomes large compared with $|\langle \mathbf{B} \rangle|$, according to (4). Far from being negligible, the term $\mathbf{u}' \times \mathbf{B}' - \langle \mathbf{u}' \times \mathbf{B}' \rangle$ in (3) ultimately dominates the term $\mathbf{u}' \times \langle \mathbf{B} \rangle$ retained in (4)! The turbulence has the effect of "breaking up the scales"[10] of the magnetic field as it evolves in a highly conducting fluid.

Eventually L' becomes small compared with λ, and (5) is violated even though (5′) is not. Since neither (5) nor (6) are valid when this stage has been reached, there is no reason to accept FOST, and the paradox is resolved. One might argue the point differently by urging that, starting from any initial state, (5) will fail in a time of at most $0(\lambda/U') \approx 0(\lambda/U)$. We are left with one case, the low conductivity limit (6) or (6′), for which the ultimate breakdown of FOST is not inevitable. As in any kinematic dynamo problem, the choice of $\mathbf{u}'$ is open, but dynamical considerations lead one to believe that U should be chosen to be of the same order as λ/τ and ν/λ, where ν is the kinematic viscosity. It is, in fact, for this reason[11] that FOST is impotent in the dynamical theory of the inducing turbulence. Nevertheless, it seems clear that, if the magnetic Prandtl number ν/η is sufficiently small, so that (6′) holds even though $U = O(\nu/\lambda)$, the magnetic fields induced by the turbulence can be studied validly by FOST.

A second difficulty arises from the failure of (5) and (6) in the high velocity tail of the probability distribution of $\mathbf{u}'$. No matter how well (5′) and (6′) are satisfied, (5) and (6) must both be violated for sufficiently large U'. This appears to provide genuine grounds for the criticism of FOST and indeed of other approximation methods. One might intuitively expect that, provided the relevant parts of the tail are sufficiently improbable, global properties of the solution, such as the growth rate of the magnetic field, will not be greatly in error. This is confirmed in an example given in Sec. III below.

The objections of Lerche and Parker[1] were of quite a different sort. They arose from a study of two examples both of which were governed by the equation

$$\frac{\partial^2 B}{\partial t^2} = (1 + \epsilon v)\, \partial B/\partial x, \tag{8}$$

where ϵ is a constant, t is a scaled time, x is a scaled distance, and v is normally distributed with zero mean and unit variance. In their first example, v depends on t alone; in their second, it depends on x alone. In the first case, they obtained conflict between the exact solution of (8) and FOST, even at $O(\epsilon^2)$ as $\epsilon \to 0$, the case in which we would have expected agreement between the two approaches. This apparent inconsistency led them to their criticisms of FOST which we have quoted above. We show in Sec. II that the inconsistency they claim exists is an illusion, and that FOST must always agree with the equations obtained by truncating the exact theory at order ϵ^2.

In their second model, for which $v = v(x)$, Lerche and Parker[1] obtained agreement between FOST and the truncated exact theory, to $O(\epsilon^2)$. It appears to us, however, that this example gives rise to serious difficulties of interpretation. These are dealt with at length in Sec. II. Suffice it to say here that their exact theory seeks to apply the Markovian concept of the "gradual unfolding of a transition probability" with increasing time (e.g., Chandrasekhar[12]) to the gradual unfolding of a transition probability with increasing coordinate distance x. This analogy would lead to the replacement of a Focker–Planck equation

$$\frac{\partial P}{\partial t} = \mathcal{L}(v)P, \tag{9}$$

where

$$\mathcal{L}(v)P = \frac{\partial^2 P}{\partial v^2} + \frac{\partial (vP)}{\partial v}, \tag{10}$$

and its fundamental Rayleigh–Greens function solution

$$G(v,\ t;\ v_0) = [2\pi(1 - \exp(-2t))]^{-1/2} \times \exp[-\tfrac{1}{2}(v - v_0 \exp(-t))^2/(1 - \exp(-2t))], \tag{11}$$

by

$$\frac{\partial P}{\partial x} = \mathcal{L}(v)P, \tag{12}$$

and

$$G(v, x;\ v_0) = [2\pi(1 - \exp(-2x))]^{-1/2} \times \exp[-\tfrac{1}{2}(v - v_0 \exp(-x))^2/(1 - \exp(-2x))]. \tag{13}$$

The physical interpretation of (11) is well known: Given that $v = v_0$ at $t = 0$, $G(v, t; v_0)dv$ is the probability that the velocity v will lie between v and $v + dv$ at a *subsequent* time $t > 0$. The restriction to positive t incorporates a physical idea sometimes called "the statistical arrow of time." The notion is reflected mathematically in the parabolic character of (9), which has significance only for initial-value problems. The physical meaning of a statistical arrow in space is not obvious, and it does not appear to be possible to adapt the usual derivations of Eq. (9), given for example in Ref. 12 or by Uhlenbeck and Ornstein[13], to obtain (12).

We argue in Sec. II that (12) may have meaning for initial-value problems in space, e.g., for situations in which a solution is sought in $x > 0$ from specified conditions on $x = 0$, but that it leads to serious difficulties if applied to boundary value problems, including particularly the search for normal modes proportional to $\exp(ikx)$ in $-\infty < x < \infty$. The dangers are clearly illustrated by the following two examples. Lerche[14] has used the method to develop from (1) a theory of induction by a static one-dimensional turbulent motion, that is a motion that is independent of time and depends on one space coordinate, x, alone over which it varies randomly. He concluded that field amplification could occur, even for incompressible flows. The relevant motion is a special case of the planar analog of toroidal flow in spherical geometry. It is well known that toroidal flows are incapable of dynamo action and the proof[15] of this fact can readily be adapted to exclude the analogous planar motions also. One concludes that Lerche's claim that these flows can regenerate field is untenable. Second, Lerche[16] has considered the diffusion of heat in

a moving conductor containing no internal sources of heat, and governed by

$$\frac{\partial T}{\partial t} + \mathbf{u}' \cdot \nabla T = \eta \nabla^2 T. \tag{14}$$

He used the analogy described above to examine the case of static one-dimensional motions by exact methods. He concluded that the temperature of the fluid could rise spontaneously through its motion, in violation of the second law. (See also Refs. 17 and 18.)

Lerche[2,3,4] has criticized FOST for reasons that arise from his application of Kraichnan's direct interaction approximation (DIA)[11,19] to induction (1) by turbulently moving conductors. When one wishes to release turbulent dynamo theory from the straightjacket imposed by (5) and (6), DIA offers a number of attractions. As Kraichnan[19] has emphasized, DIA provides an exact description of a possible dynamical system: It therefore evades physical absurdities, such as negative energy spectra, or the violation of Bochner's theorem[20] and its generalizations. Also, although solutions are more difficult to obtain than after FOST closure, DIA is not intractable. It is perhaps worth bearing in mind, however, that (as its name implies) DIA does not provide an exact description of the actual physical system, and so does not yield precise results. Therefore any criticism of FOST based on DIA is itself questionable.

The first use to which Kraichnan[21] put his DIA was to magnetohydrodynamic turbulence and, as a by-product, his analysis contains the dispersion relationship implied by DIA for kinematic dynamo action by a statistically steady isotropic turbulence without helicity, that is turbulence possessing mirror-symmetric statistical properties. Kraichnan supposed, however, that $\langle \mathbf{B} \rangle = 0$. The corresponding theory for nonzero $\langle \mathbf{B} \rangle$ was first developed by Lerche,[2] who also examined[3,4] the case of pseudo-isotropic turbulence, which (though statistically isotropic) lacks mirror-symmetry.

Lerche[2] observed that, when (5) or (6) hold (equivalent to inequality (27) of Ref. 2), the dispersion relationship obtained from DIA reduces to that given by FOST. He urged however that the implied iteration procedure for small U is not uniformly convergent throughout wavevector space, and that FOST therefore does not provide a reliable approximation to DIA for small U. His case rests on an implied hope that certain conditions, proved by Hammerstein[22] to be sufficient for the existence of solutions to integral equations of the type raised by DIA, are also necessary. Even if this could be established, the discrepancies between FOST and DIA which would then arise at large times (or small frequencies) could equally well be attributed to a failure of DIA, for it is known[11] that DIA does not necessarily give reliable results for large times (or small frequencies). We continue to regard Lerche's demonstration[2] of the equivalence of FOST and DIA under conditions (5) or (6) as a valuable proof of the consistency of the two approximations, rather than grounds for criticising either.

When the helicity is zero, Lerche's dispersion relationship [Eq. (25) in Ref. 2] based on the induction equation (1) coincides, under DIA, with that obtained[23] from the heat conduction equation (14). Since it is clear on physical grounds that the latter can only admit solutions that decay with time, we may conclude[24] that mirror-symmetric turbulent motions cannot regenerate mean magnetic fields by dynamo action, at least as far as DIA is a reliable guide.

Lerche[3] attempted to solve the DIA dispersion relationship for nonmirror symmetric flows in the particular case of static turbulence, in which the energy spectrum $E(k, \omega)$ has the form $\xi(k)\delta(\omega)$. His solution led him to believe that field amplification could not occur in any circumstances, a conclusion that is in direct conflict with FOST, which predicts that in general dynamo amplification of fields of all sufficiently long wavelengths would occur. Lerche concluded that the results of FOST were not trustworthy. This conclusion is difficult to accept in view of the close parallel that exists between induction by homogeneous turbulence and induction by spatially periodic flows. The mathematics of the latter are amenable to precise treatment, and powerful theorems have been proved by Childress[25] and Roberts,[26] including for example the result[26] that nearly all (in a well-defined mathematical sense) spatially-periodic flows will regenerate field for nearly all electrical conductivities.

It is also disturbing that the method used by Lerche to solve his dispersion relationship cast up modes that grow even for zero motion. The implication appears to be either that the dispersion relationship provided by DIA is physically untenable, or that the method used to solve it is mathematically untenable, and it seems to us[27] that the latter explanation is the correct one.

The remainder of this paper presents arguments in support of some of the statements above. We summarize these here by reiterating our faith in FOST in an admittedly limited set of circumstances, but one that is larger than the "short-sudden" approximation.[1]

II. EXACTLY SOLUBLE PROBLEMS

The exactly soluble problems discussed by Lerche and Parker[1] and by Lerche[14,16] can all be written in the form

$$\frac{dy_i}{dt} = A_{ij}(\epsilon v) y_j, \quad (i, j = 1, 2, \ldots, N) \tag{15}$$

where ϵ is a small parameter, v is Gaussianly distributed over t with unit variance and zero mean and the summation convention is used. It is postulated that the probability density $P(y_i, v, t)$ at $\{y_i\}$, v and t is governed by

$$\frac{\partial P}{\partial t} = \mathcal{L}(v) P - \frac{\partial}{\partial y_i}\left(\frac{dy_i}{dt} P\right). \tag{16}$$

This postulate can be supported by physical arguments in the case in which t is time,[12,13] but the equation is also used when t is a space coordinate x. Attention is focused on the means

$$\langle y_i \rangle \equiv \int P y_i \, d^N y, \tag{17}$$

which according to (15) and (16) obey

$$\frac{\partial \langle y_i \rangle}{\partial t} = \mathcal{L}(v) \langle y_i \rangle + A_{ij}(\epsilon v) \langle y_j \rangle, \tag{18}$$

an equation which may be solved uniquely from specified

initial conditions and the requirement that $\langle y_i \rangle$ is exponentially small as $v \to \pm\infty$ (see Sec. III).

Lerche and Parker[1], and Lerche,[14,16] used an expansion method to solve (18), writing $\langle y_i \rangle$ as a linear combination of the eigenfunctions $\phi_n(v)$ of the equation $\mathcal{L}(v)\phi_n = -n\phi_n$, the coefficients $y_i^{(n)}(t)$ being functions of t. We will work instead with the moments

$$Y_i^{(n)}(t) = \int_{-\infty}^{\infty} \langle y_i \rangle v^n dv \tag{19}$$

of $\langle y_i \rangle$, which are linear combinations of the $y_i^{(n)}$.

Suppose, for simplicity, that A_{ij} may be written as a sum (finite or infinite):

$$A_{ij}(\epsilon v) = A_{ij}^{(0)} + \epsilon v A_{ij}^{(1)} + \epsilon^2 v^2 A_{ij}^{(2)} + \cdots. \tag{20}$$

Multiply (18) by v^n and integrate over all v, making use of the result

$$\int_{-\infty}^{\infty} v^n \mathcal{L}(v) \langle y_i \rangle dv = n(n-1) Y_i^{(n-2)} - n Y_i^{(n)}. \tag{21}$$

Obtain in this way the hierarchy of moment equations

$$0 = \frac{dY_i^{(0)}}{dt} - \sum_{s=0}^{\infty} \epsilon^s A_{ij}^{(s)} Y_j^{(s)}, \tag{22}$$

$$-Y_i^{(1)} = \frac{dY_i^{(1)}}{dt} - \sum_{s=0}^{\infty} \epsilon^s A_{ij}^{(s)} Y_j^{(s+1)}, \tag{23}$$

$$2Y_i^{(0)} - 2Y_i^{(2)} = \frac{dY_i^{(2)}}{dt} - \sum_{s=0}^{\infty} \epsilon^s A_{ij}^{(s)} Y_j^{(s+2)}, \tag{24}$$

. . .

The solution to order ϵ^2 obtained by Lerche and Parker and Lerche [see Eqs. (19) and (31) of Ref. 1, and Eq. (41) of ref. 16], ultimately depends on neglecting the right-hand side of (24) (note $dY_i^{(2)}/dt = A_{ij}^{(0)} Y_j^{(2)}$, to lowest order), which yields

$$Y_i^{(2)} = Y_i^{(0)}. \tag{25}$$

This is the particular case $t_0 = t$ of the more general approximation

$$\langle v(t_0) v(t) y_i(t) \rangle = \langle v(t_0) v(t) \rangle Y_i^{(0)}(t), \tag{26}$$

to which we return below. We note that (26) is not required for closure: (22), (23), and (25) give

$$\frac{dY_i^{(0)}}{dt} = (A_{ij}^{(0)} + \epsilon^2 A_{ij}^{(2)}) Y_j^{(0)} + \epsilon A_{ij}^{(1)} Y_j^{(1)}, \tag{27}$$

$$\frac{dY_i^{(1)}}{dt} + Y_i^{(1)} = A_{ij}^{(0)} Y_j^{(1)} + \epsilon A_{ij}^{(1)} Y_j^{(0)}. \tag{28}$$

We will refer to this as the "approximate form of the exactly soluble problem."

The necessity of regarding (18) as an initial value problem with $\langle y_i \rangle$ prescribed at $t = 0$ becomes apparent if we recast that differential equation into an equivalent integral form

$$\langle y_i \rangle(v, t) = \int_0^t \int_{-\infty}^{\infty} G(v, t-t'; v') A_{ij}(\epsilon v') \langle y_j \rangle (v', t') dv' \, dt + \int_{-\infty}^{\infty} G(v, t; v') \langle y_i \rangle (v', 0) \, dv', \tag{29}$$

where G is the Greens function (11). It is then clear that the solution $\langle y_i \rangle(v, t)$ at time t depends on $\langle y_i \rangle (v, t')$ for earlier times $t' < t$ only. From (11) we obtain the velocity correlation for $t > t'$

$$\langle v(t) v(t') \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (2\pi)^{-1/2} v' \exp(-\tfrac{1}{2} v'^2) v G(v, t-t'; v') \, dv dv' = \exp[-|t-t'|]. \tag{30}$$

Let us now apply FOST. This requires (26) to hold. It is sensible to ask whether (26) will lead to (27) and (28) if (15) is regarded as an initial value problem, with correlation function (30).

The mean value of (15) clearly gives (27) to order ϵ^2. To rederive (28), we multiply (15) by $v(t_0)$, average over v, and neglect terms of order ϵ^2, to obtain

$$\frac{d}{dt} \langle v(t_0) y_i(t) \rangle = A_{ij}^{(0)} \langle v(t_0) y_j(t) \rangle + \epsilon A_{ij}^{(1)} \exp(-|t-t_0|) Y_j^{(0)}(t). \tag{31}$$

Alternatively, we may write (31) as

$$\left(1 + \frac{d}{dt}\right) [\exp(-(t-t_0)) \langle v(t_0) y_i(t) \rangle] - A_{ij}^{(0)} [\exp(-(t-t_0)) \langle v(t_0) y_j(t) \rangle] = \epsilon A_{ij}^{(1)} Y_j^{(0)}(t), \quad (t \geq t_0). \tag{32}$$

Comparing (28) and (32) we see that the solution $\langle v(t_0) y_i(t_0) \rangle$ of (32) when solved subject to the initial condition

$$\langle v(t_0) y_i(0) \rangle = 0, \quad (t_0 > 0) \tag{33}$$

is identical to the solution of (28) subject to the initial condition

$$Y_i^{(1)}(0) = 0. \tag{34}$$

In short, to order ϵ^2, there is no conflict between FOST and the approximate form of the exactly soluble problem.

Suppose that, in place of this initial value problem (called "Case A" below), we wish to consider a boundary value problem (called "Case B" below). In what follows we will often replace t by a space coordinate x, as this was used by Lerche[16] in the example we will take as our principal illustration. This is a heat conduction problem governed by (14), with u' having a single component in the y direction that depends on x alone. After transformations, we can write this in the form (15) with $N = 2$ and

$$A_{ij}^{(0)} = \begin{pmatrix} 0 & 1 \\ \lambda^2 & 0 \end{pmatrix}, \quad A_{ij}^{(1)} = \begin{pmatrix} 0 & 0 \\ i & 0 \end{pmatrix}, \quad A_{ij}^{(n)} = 0, \quad (n \geq 2), \tag{35}$$

where $\Re(\lambda) > 0$. In case (A), the correlation function satisfies the condition (33) but for x rather than t; in case (B), we require instead that

$$\langle v(x_0) y_i(x) \rangle \to 0, \quad \text{as } x - x_0 \to \pm\infty. \tag{36}$$

In case (B) the correlation (30), with x replacing t, must hold for $x - x'$ both positive and negative. Solving (15) and (35) directly, multiplying by $v(x_0)$, and averaging

(using this correlation function and FOST), we obtain

$$\langle v(x_0)y_1(x)\rangle = i\epsilon(2\lambda)^{-1} \int_{-\infty}^{\infty} \exp[-|x'-x_0| - \lambda|x'-x|]\, Y_1(x')\,dx'. \quad (37)$$

On setting $x = x_0$, we find $Y_1^{(1)}$. It is bounded at $x = \pm\infty$ and satisfies

$$\frac{d^2Y_1^{(1)}}{dx^2} - (1+\lambda)^2\, Y_1^{(1)} = i\epsilon(1+\lambda^{-1})Y_1^{(0)}. \quad (38)$$

This should be contrasted with the result (28) of the initial value problem (A) which, with x replacing t, gives

$$\left(\frac{d}{dx}+1\right)^2 Y_1^{(1)} - \lambda^2 Y_1^{(1)} = i\epsilon Y_1^{(0)}. \quad (39)$$

For both A and B, (27) gives

$$\frac{d^2Y_1^{(0)}}{dx^2} - \lambda^2 Y_1^{(0)} = i\epsilon Y_1^{(1)}. \quad (40)$$

It should be clear from a comparison of (38) and (39) that care must be taken to distinguish initial value problems of type (A) from boundary value problems of type (B). Moreover, although both types of situation are apparently amenable to FOST, the exactly soluble problem, starting from (18), presupposes that an initial value situation (A) is under study.

We are now in a position to understand some of the difficulties encountered by Lerche[14,16] and Lerche and Parker[1]. If we seek solutions of (39) and (40) that are proportional to $\exp(ikx)$ where k and λ are $O(\epsilon)$ we obtain the dispersion relationship

$$k^2 + \lambda^2 = \epsilon^2, \quad (41)$$

[cf. Ref. 16, Eq. (41)], which if interpreted as an eigenvalue problem for λ rather than k leads to difficulties when $\epsilon \leq k$. But (39) is valid for initial value problems (A) and not for boundary problems (B) in which $Y_1^{(0)}$ is proportional to $\exp(ikx)$ for all x. The correct equations are therefore (38) and (40), which yield

$$k^2 + \lambda^2 = -\epsilon^2, \quad (42)$$

as though the diffusivity λ were increased to $\sqrt{(\lambda^2+\epsilon^2)}$.

The first of the two examples given by Lerche and Parker[1] is based on (8) and is timelike. It may be written in the form (15) with $N=2$ and

$$A_{ij}^{(0)} = \begin{pmatrix} 0 & 1 \\ i\alpha & 0 \end{pmatrix}, \quad A_{ij}^{(1)} = \begin{pmatrix} 0 & 0 \\ i\alpha & 0 \end{pmatrix}, \quad A_{ij}^{(n)} = 0, \quad (n \geq 2). \quad (43)$$

Equations analogous to (39) and (40) yield the correct dispersion relationship for the initial value problem (A), viz.,

$$[\alpha + i(i\nu)^2][\alpha + i(1+i\nu)^2] = \alpha^2\epsilon^2, \quad (44)$$

for solutions proportional to $\exp(i\nu t + i\alpha x)$; see Ref. 1, Eq. (19). The apparent discrepancy between (44) and an earlier result,[28] which they derived using FOST, may be attributed to the fact that the earlier result was relevant to a boundary value problem B. We may confirm this from equations analogous to (38) and (40), which yield the dispersion relationship

$$[\alpha + i(i\nu)^2]\left[i\sqrt{(i\alpha)}/\{1+\sqrt{(i\alpha)}\}\right]\left[(i\nu)^2 - \{1+\sqrt{(i\nu)}\}^2\right] = \alpha^2\epsilon^2. \quad (45)$$

This agrees completely with their FOST (Ref. 28, Eq. (12) in the limit $L \to \infty$). Alternatively, we may observe that their time integrations in Ref. 28 are performed by Fourier transformations, but that their contours of integration in the corresponding ω''-plane are not one-sided, i.e., they do not pass below all singularities. Their solution[28] has, therefore, no bearing on the initial value problem A, and cannot be expected to reproduce (44). It happens, however, to give the correct result (45) for the boundary value problem B.

The second model based on (8) considered by Lerche and Parker[1] is spacelike. Since $N=1$, it cannot be used to formulate a boundary-value problem. There is no possibility therefore of confusing situations of types A and B. Not unexpectedly, the results of FOST agree with those derived from the approximate form of the exactly soluble problem.

We have shown in this section that, when due distinction is made between initial-value and boundary-value problems, the results obtained from FOST coincide with the solutions of a truncated set of equations obtained from the exact theory at the appropriate approximation level, here order ϵ^2. This should serve to dispel from the reader's mind doubts of the kind raised by Lerche and Parker[1]. There is, however, a completely separate cause for concern, namely, whether the solution obtained from FOST or from the truncated set of equations will differ in a significant way from the full solution of the exact equations, appropriately approximated for small ϵ. Although we have described FOST and the truncated equations as being valid to order ϵ^2, it would be more correct to say that they give solutions valid to order $(\epsilon v)^2$. The solutions they predict are not expected to be correct for $V \equiv \epsilon v = O(1)$. It is possible to derive a new expansion for $V = O(1)$ and to obtain solutions for $v = O(1)$ which, while they do *not* vanish as $|v| \to \infty$, match with these new solutions in V. It is not obvious that the resulting dispersion relationship will agree with FOST or the truncated equations. The matter is taken further in the next section where it is established unequivocally that the use of FOST or the truncated form of the exact equations for all v introduces numerically small, but nonzero, errors.

III. THE HIGH VELOCITY TAIL

We aim to illustrate how the high velocity tail of the probability distribution can cause the results of FOST, or equivalently of the truncated form of the exact theory, to differ from those from the exact theory even at order ϵ^2. We continue to use the heat conduction problem considered by Lerche[16] as our example, and examine solutions independent of x (i.e., $k=0$). We ignore the question of physical interpretation; as a mathematical problem the situation is well posed. We have seen that, in the initial-value context, FOST and a truncated version of the exact theory (which we called "the approxi-

mate exact theory") agree in predicting that the eigenvalue $(\lambda/\epsilon)^2$ is unity; see (41) with $k=0$. We prove below, however, that its correct value, to four figures, is 0.9162.

As before, the problem may be cast in the form of (15) and (35). If we set

$$T=\langle y_1\rangle, \quad \Psi=\langle y_2\rangle, \quad \lambda^2=\delta\epsilon^2, \tag{46}$$

and seek a solution independent of x, we obtain

$$\mathcal{L}(v)T=-\Psi, \quad \mathcal{L}(v)\Psi=-(\delta\epsilon^2+i\epsilon v)T, \tag{47}$$

where $\mathcal{L}(v)$ is given by (10). This poses an eigenvalue problem for δ when we add the demands

$$T, \Psi \to 0, \quad v\to\pm\infty. \tag{48}$$

We determine the smallest eigenvalue δ in the limit $\epsilon\to 0$. Only part of the inner solution [that is, the solution valid for $v=O(1)$] may be obtained by the expansion proposed by Lerche[16] as a sum of eigenfunctions $\phi_n(v)$ of $\mathcal{L}\phi_n=-n\phi_n$. The remainder of the inner solution contains terms (e.g., T_2 below) which cause the expansion to be nonuniform in the limit $|v|\to\infty$. An outer solution, valid when $v=O(\epsilon^{-1})$, must be constructed, and must be matched to the inner solution. This matching is possible only for one value of δ.

The inner solutions are expansions of T and Ψ about $\epsilon=0$ in series whose coefficients are functions of v. We write

$$\begin{aligned} T&=T_0+\epsilon T_1+\epsilon^2(T_2+T_{21}\log\epsilon)+\cdots,\\ \Psi&=\epsilon\Psi_1+\epsilon^2(\Psi_2+\Psi_{21}\log\epsilon)+\cdots, \end{aligned} \tag{49}$$

where it is easily shown that

$$\begin{aligned} &T_0=(2\pi)^{-1/2}\exp(-v^2/2), \quad T_1=\Psi_1=ivT_0,\\ &\Psi_{21}=-\mu_r T_0, \quad T_{21}=(2\pi)^{1/2}\mu_r G+i\mu_i F,\\ &\Psi_2=\tfrac{1}{2}v^2T_0-(\delta-1)G+i\beta F,\\ &T_2=-\tfrac{1}{4}v^2T_0-\tfrac{1}{2}G+\exp(-v^2/2)\int_0^v\exp(x^2/2)\\ &\qquad\int_0^x[(\delta-1)G(y)-i\beta F(y)]\,dy\,dx, \end{aligned} \tag{50}$$

and

$$\begin{aligned} F(v)&=\tfrac{1}{2}\exp(-v^2/2)\int_0^v\exp(x^2/2)\,dx,\\ G(v)&=\exp(-v^2/2)\int_0^v\exp(x^2/2)\int_0^x T_0(y)\,dy\,dx. \end{aligned} \tag{51}$$

Here β, μ_r, and μ_i are real constants whose values can be determined, together with δ, by matching with the outer solution; we shall denote $\mu_r+i\mu_i$ by μ.

The outer solution may be obtained by writing $V=\epsilon v$ in (47) and developing expansions of T and Ψ about $\epsilon=0$ in series whose coefficients are functions of V. The leading term for T is found to be, for $V>0$,

$$T=\mu\epsilon^2 v^{-1}K_0(2\exp(\pi i/4)\sqrt{(\epsilon v)}), \tag{52}$$

where $K_\nu(z)$ is the modified Bessel function, of the second kind, of order ν and argument z. The solution for $V<0$ is $T_0^*(|v|)$, where $T_0(v)$ is given by (52) and the asterisk denotes the complex conjugate. The choice of μ for multiplication constant in (52) implies that some matching has already been performed.

From (52) we have, for $\epsilon v\to 0+$,

$$T=-\tfrac{1}{2}\mu[\log\epsilon+\log v+\tfrac{1}{2}i\pi+2\gamma], \tag{53}$$

where $\gamma\doteq 0.5772$ is Euler's constant. It may be shown from (51) that, for $v\to\infty$,

$$\begin{aligned} \int_0^v F(y)\,dy&=\tfrac{1}{2}[\log v+\tfrac{1}{2}(\log 2+\gamma)]+O(1/v),\\ \int_0^v G(y)\,dy&=\tfrac{1}{2}[\log v-\tfrac{1}{2}(\log 2-\gamma)]+O(1/v), \end{aligned} \tag{54}$$

results that are useful in matching (49) to (52). It is now found that this matching requires that

$$\begin{aligned} &\mu=(1-\delta)+i\beta,\\ &2\mu(\tfrac{1}{2}\pi i+2\gamma)=1-(1-\delta)(\log 2-\gamma)+i\beta(\log 2+\gamma), \end{aligned} \tag{55}$$

whence the required eigenvalue is

$$\delta=1-(3\gamma-\log 2)/[9\gamma^2+\pi^2-(\log 2)^2]\doteq 0.91617. \tag{56}$$

It may be particularly noted that the individual terms of Lerche's expansion in terms of $\phi_n(v)$ are proportional to $\exp(-\frac{1}{2}v^2)$ for $v\to\pm\infty$. Equation (52) shows, however, the solution is proportional in modulus to $\exp(-\sqrt{(2\epsilon|v|)})$ as $|v|\to\infty$. It is this fact that creates the nonuniformity in the inner expansion, and causes δ to differ from unity, as FOST and the approximate exact theory would have predicted.

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[27]Lerche[2] applied his method also to mirror-symmetric turbulence, and we use this simpler case to make our point. Lerche states that he has spectra of the form $\xi(k) = k^2 \exp(-k^2)$ in mind. For this case, his integral

$$J(k,\kappa) = 2\pi \int_{-1}^{1} (1-\mu^2) \exp[-(k^2+\kappa^2+2k\kappa\mu)]\,d\mu$$

becomes

$$J(k,\kappa) = 2\pi(k\kappa)^{-2}\,[\cosh 2k\kappa - (2k\kappa)^{-1}\sinh 2k\kappa]\exp(-k^2-\kappa^2).$$

An integral that must be evaluated (for $m < M$) is given in Eq. (35) of Ref. 2. It is

$$I = \int_{-\infty}^{\infty} \kappa^2 J(k,\kappa)\,[1 - i\omega k^{-2} + \Lambda_1 J(m,\kappa) + \Lambda_2 J(M,\kappa)]^{-1}\,d\kappa,$$

where Λ_1 and Λ_2 are complex constants. Lerche proposes to close the contour by a semicircle in the upper-half κ-plane, and states that for $k < M$ the integrand is of order $\exp[-(M-k)\,|\,\kappa\,|\,]$ on this semicircle. It may be seen, however, from the explicit form of J above, that the integrand is of order $\exp[-(M-k)\,|R(\kappa)\,|\,]$, and that the contribution to the integral from the neighborhood of $\arg \kappa = \pi/2$ is nonzero, tending to infinity with the radius of the semicircle. It therefore appears that the contour cannot be closed in the way stated, and that the method of solution used in Refs. 2 and 3 requires reconsideration. In view of the unexpected, undeserved but inaccurate acknowledgement at the end of Ref. 2, one of the present authors (PHR) would like to take this opportunity of stating that he informed Lerche only of his general agreement with Ref. 2 up to the end of Sec. III. He was, however, unaware until recently of the objection raised in this footnote.
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Effect of damping on nonlinear three-wave interaction

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We examine the nonlinear evolution of three coherent positive energy waves interacting resonantly in a homogeneous lossy medium. Assuming that only the low-frequency wave is appreciably damped, we establish a necessary and sufficient condition for unidirectional energy transfer from the pump to the two other waves in terms of a critical damping factor. We then find asymptotic solutions and solutions in the weakly and strongly damped regimes. Also, we examine the pump wave depletion time as a function of the damping rate and initial pump wave intensity.

I. INTRODUCTION

To lowest nonlinear order the amplitude—and phase—modulation of three coherent, resonantly interacting, monochromatic, positive energy,[1,2] waves with frequencies $\omega_1 > \omega_2 > \omega_3$ is governed by the equations[3-5]

$$\frac{dE_1}{dt} + \nu_1 E_1 = -C_1 E_2 E_3 \exp(i\Delta\omega t), \tag{1a}$$

$$\frac{dE_2^*}{dt} + \nu_2 E_2^* = C_2 E_1^* E_3 \exp(i\Delta\omega t), \tag{1b}$$

$$\frac{dE_3^*}{dt} + \nu_3 E_3^* = C_3 E_1^* E_2 \exp(i\Delta\omega t). \tag{1c}$$

Here E_j is the complex wave-amplitude, ν_j is its (real) linear damping rate, $C_j > 0$ is a coupling coefficient characteristic of the supporting medium, and the respective wave mode, and $\Delta\omega = \omega_1 - \omega_2 - \omega_3 \ll \omega_j$ is the frequency mismatch.

When all ν_j are equal, analytical solutions of system (1) are known.[3] In particular, when all $\nu_j = 0$, the solutions are Jacobian elliptic functions describing the periodicity of the nonlinear interaction during which the initial pump energy E_{10}^2 is transferred back and forth between the pump and the two other waves. The physically more realistic situation of unequal damping rates leads to the removal of a certain number of invariants of system (1) which is then no longer integrable by quadratures. Indeed, most usually, the lowest frequency wave, E_3, is subject to significant damping whereas the waves $E_{1,2}$ experience mostly nonlinear modification and feel the presence of damping mainly through coupling with the wave E_3. Below we therefore consider the idealized case $\nu_1 = \nu_2 = 0$, $\nu_3 = \nu > 0$.

Due to its physical prominence the case described above has received considerable attention. In particular, the "adiabatic" approximation $\nu_3 E_3^* = C_3 E_1^* E_2 \exp(i\Delta\omega t)$, and the ensuing analytical solutions for $E_{1,2}$, first developed by Tang[6] in connection with the steady state spatial analysis of stimulated scattering in solids, have been widely employed in various applications of nonlinear optics[7,8] and wave interactions in plasmas.[9,10]

In the present paper we first derive a condition for unidirectional energy transfer from the pump, E_1, to the two other waves. A sufficient condition previously derived by Wang[11] under more general conditions appears to be too strong for our case. As a matter of fact in our particular case we are able to obtain a sufficient and necessary condition in terms of a critical damping rate ν_c for which the solutions of (1) cease to oscillate. We then find asymptotic solutions of (1) and solutions in the weakly and strongly damped regimes. In the weakly damped regime approximate solutions are Jacobian elliptic functions with a damped modulus. In the strongly damped regime, $\nu \gg \nu_c$, we show that Tang's[6] approximation corresponds to the degenerate solutions of an equivalent second order overdamped system. Finally, we discuss the pump-wave depletion time as function of the damping rate and the initial wave amplitudes.

II. BASIC CONSIDERATIONS

Let us render system (1) model-free by normalizing to nondimensional quantities

$$\tau = \Omega_0 t, \quad \rho = \nu/\Omega_0, \quad e_j = E_j/RC_j, \tag{2}$$

with

$$\Omega_0^2 = R^2 C_1 C_2 C_3, \quad R^2 = E_{10}^* E_{10}/C_1 + E_{20}^* E_{20}/C_2. \tag{3}$$

Here $E_{j0} \equiv E_j$ $(t=0)$, so that the general invariant of system (1) has the form

$$e_1^* e_1 + e_2 e_2^* = 1. \tag{4}$$

Physically, the quantities $e_j e_j^*$ are normalized actions. Now let the complex amplitudes $e_j = u_j \exp(i\phi_j)$ with u_j and ϕ_j real. By making use of (2) and (3) system (1) becomes

$$u_1' = -u_2 u_3 \cos\phi, \quad u_2' = u_1 u_3 \cos\phi, \quad u_3' + \rho u_3 = u_1 u_2 \cos\phi, \tag{5}$$

$$(u_1 u_2 u_3 \sin\phi)' + \rho u_1 u_2 u_3 \sin\phi = \tfrac{1}{2}(\Delta\omega/\Omega_0)(u_3^2)', \tag{6}$$

where the prime denotes differentiation with respect to τ and $\phi = \phi_2 + \phi_3 - \phi_1 + \Delta\omega\tau/\Omega_0$. Equation (6) results from adding up the imaginary parts of Eqs. (1a,b,c) and multiplying by $u_1 u_2 u_3 \cos\phi$.

We now specify $\Delta\omega = 0$ and $u_{30} = 0$, corresponding to the resonant excitation of u_3 at the beat frequency of waves u_1 and u_2. Then, from (6), it follows that, for $u_1 u_2 u_3$ not to be identically equal to zero for $\tau > 0$, the system must have a second invariant, namely

$$\sin\phi = 0, \quad \tau > 0. \tag{7}$$

Equations (5) and (6) thus reduce finally to

$$u_1' = -u_2 u_3, \tag{8a}$$

$$u_2' = u_1 u_3, \tag{8b}$$

$$u_3' + \rho u_3 = u_1 u_2 \tag{8c}$$

with initial conditions $u_{30}=0$ and u_{10}, u_{20} satisfying the condition $u_{10}^2+u_{20}^2=1$ due to the invariant (4), $u_1^2+u_2^2=1$.

We note that the resonance condition $\Delta\omega=0$ is crucial for the existence of invariant (7), whereas the inital condition $u_{30}=0$ is optional.

We now present, for later reference, the solutions of (8) when $\rho=0$. Using the invariants (4) and $u_1^2-u_3^2=u_{10}^2$, we obtain[12]

$$u_1=k\,\mathrm{cd}(\tau,k),\quad u_2=k_c/\mathrm{dn}(\tau,k),\quad u_3=kk_c\,\mathrm{sd}(\tau,k), \tag{9}$$

where $k=u_{10}$ is the modulus and $k_c=u_{20}$ the complementary modulus of the Jacobian elliptic functions. The interaction period is $4K(k)$, where K is the complete elliptic integral of the first kind.

III. ASYMPTOTIC SOLUTIONS

In this section, we analyze system (8) in phase space. This procedure enables us to find a critical damping rate of system (8) and leads to asymptotic solutions in a very natural way.

Making use of the invariant (4), we introduce a function ψ, such that

$$u_1=\sin\psi,\quad u_2=\cos\psi. \tag{10}$$

Then

$$u_3=-\psi' \tag{11}$$

satisfies the first two equations of (8) identically, whereas Eq. (8c) becomes, for $Y=2\psi$,

$$Y''+\rho Y'+\sin Y=0, \tag{12}$$

with the initial conditions

$$Y(0)=2\arcsin u_{10},\quad Y'(0)=0. \tag{13}$$

The singular points of Eq. (12) in phase space (Y,Y') are $S_m=(\pm m\pi,0)$. For m even, S_m is a focal or nodal point; for m odd, S_m is a saddle point. The solution originates on $Y'=0$ between 0 and π and, since $\rho>0$, it evolves stably, terminating at the point (0, 0). If $\rho>2$, this point is a stable node; if $\rho<2$, it is a stable focal point.[13] We therefore conclude that for the given boundary conditions, if $\rho>2$, Y decreases monotonically to zero; and if $\rho<2$, Y is an attenuated oscillation. We note that the mechanical analog of system (12) is the simple damped pendulum. The interaction is initially strongly nonlinear whenever u_{20} is not much greater than u_{10}, but eventually, since Y systematically decreases, the system enters an asymptotic stage described by $Y''+\rho Y'+Y=0$, and the asymptotic solutions joining the proper initial conditions are simply the following:

$\rho<2$:

$$Y=Y_0\exp(-\rho\tau/2)[\cos(\delta\tau/2)+(\rho/\delta)\sin(\delta\tau/2)], \tag{14a}$$

$$u_3=(Y_0/\delta)\exp(-\rho\tau/2)\sin(\delta\tau/2), \tag{14b}$$

where $\delta=(4-\rho^2)^{1/2}$;

$\rho=2$:

$$Y=Y_0(1+\tau)\exp(-\tau), \tag{15a}$$

$$u_3=(Y_0/2)\tau\exp(-\tau); \tag{15b}$$

$\rho>2$:

$$Y=Y_0\exp(-\rho\tau/2)[\cosh(\Delta\tau/2)+(\rho/\Delta)\sinh(\Delta\tau/2)], \tag{16a}$$

$$u_3=(Y_0/\Delta)\exp(-\rho\tau/2)\sinh(\Delta\tau/2), \tag{16b}$$

where $\Delta=(\rho^2-4)^{1/2}$.

We note that in the strongly overdamped case, $\rho\gg 2$, the relaxation of Y and u_3 reverses with respect to ρ:

$$u_3\approx(Y_0/2\rho)[\exp(-\tau/\rho)-\exp(-\tau\rho+\tau/\rho)]$$
$$=O[\exp(-\tau/\rho)], \tag{17}$$

a fact which will be used later in Sec. V.

The existence of the critical damping rate, $\rho_c=2$, can be understood qualitatively on the physical grounds that when the characteristic absorption time $1/\rho$ for the wave u_3 becomes less than the period of interaction, the transfer of action back to the pump is inhibited.

We stress that, in the weakly nonlinear regime, $u_{20}\gg u_{10}$ (or equivalently $u_{10}\ll 1$), the above solutions are good approximations in the entire range $\tau>0$. In contrast, for strong nonlinearity, $u_{10}>u_{20}$, these solutions break down in the nonasymptotic region. Better approximations are therefore needed, especially for the cases $\rho\ll 2$ and $\rho\gg 2$ characterized by very slow relaxation and long nonasymptotic regions.

IV. WEAKLY DAMPED REGIME, $\rho\ll 2$

An approximate solution of Eq. (12) in this case can be inferred from the known analytical solution

$$\sin(Y/2)=\sin(Y_0/2)\,\mathrm{cd}[\tau,\sin(Y_0/2)] \tag{18}$$

or, according to (10),

$$u_1=u_{10}\,\mathrm{cd}(\tau,u_{10}), \tag{19}$$

of the conservative system

$$Y''+\sin Y=0,$$
$$Y(0)=2\arcsin u_{10},\quad Y'(0)=0 \tag{20}$$

When the absorption is weak, $1/\rho$ much larger than the initial interaction period $4K(u_{10})$, the system may be thought of as evolving through a succession of cycles with systematically decreasing initial amplitudes. We now notice that the initial value problem (20) is characterized by a Jacobian elliptic solution whose modulus is equal to the initial amplitude. The solution is thus constructed as follows. The asymptotic solution (14) leads us to approximate the slow change in amplitude by $u_{10}\exp(-\rho\tau/2)$. The corresponding damped modulus m and its complement m_c are, therefore, respectively

$$m=u_{10}\exp(-\rho\tau/2), \tag{21a}$$

$$m_c=(1-m^2)^{1/2}. \tag{21b}$$

By analogy with (9) we write finally

$$u_1=m\,\mathrm{cd}(\tau,m),\quad u_2=m_c/\mathrm{dn}(\tau,m),\quad u_3=mm_c\,\mathrm{sd}(\tau,m). \tag{22}$$

It can be verified that the solutions (22) satisfy Eqs. (8) to first order in ρ, that is, to the same order of accu-

racy as the first approximation of the Bogoliubov–Mitropolsky–Krylov averaging method,[14] which, however, can be applied to Eq. (12) only in the case of weak pump amplitudes, $u_{10} \ll 1$.

Thus, a weakly damped signal u_3 will catalyse systematic depletion of the pump u_1 whose action is gradually transferred to the idler u_2, while the energy $\nu\int_0^t |E_3|^2\,dt$ is irreversibly lost to the medium. The interaction period $4K(m)$ decreases in time to its asymptotic value 2π, where solutions (22) become $u_1 \approx u_{10}\exp(-\rho\tau/2)\cos\tau$, $u_2 \approx 1$, and $u_3 = u_{10}\exp(-\rho\tau/2)\sin\tau$.

V. OVERDAMPED REGIME, $\rho \gg 2$

When $\rho \gg 2$, the solutions of Eq. (12) are nonoscillatory and slowly changing. Thus, Eq. (12) becomes degenerescent,[13] and an approximate solution is readily found by solving the associated degenerate first order equation

$$\rho Y' + \sin Y = 0, \qquad (23)$$
$$Y(0) = 2\arcsin u_{10}.$$

Going back to (10) and (11), we see immediately that Eq. (23) is equivalent to

$$\rho u_3 = u_1 u_2, \qquad (24)$$

which is the approximation used by Tang [Eq. (2.20) of Ref. 6]. Tang's original procedure, based on writing Eq. (8c) in integral form,

$$u_3 = u_{30}\exp(-\rho\tau) + \exp(-\rho\tau)\int_0^\tau \exp(\rho\tau')u_1u_2\,d\tau', \qquad (25)$$

and taking u_1u_2 out in front of the integral sign, has two disadvantages but one great advantage. It is based on the purely physical assertion that u_1u_2 changes slowly in comparison with $\exp(\rho\tau)$, and, moreover, does not furnish any criterion as to the range of validity of the approximation. However, it avoids the principal difficulty associated with degeneration theory, namely, the discontinuity of Y' at $\tau = 0$.

Now, we will show how both drawbacks of Tang's procedure are easily removed in the overdamped regime. The analysis is carried out to second order in $1/\rho$, revealing the structure of the first approximation.

Let us write Eq. (12) in integral form

$$Y'(\tau) = -\exp(-\rho\tau)\int_0^\tau \exp(\rho\tau')\sin Y(\tau')\,d\tau'. \qquad (26)$$

When $\rho \gg 2$, the asymptotic solution (17) indicates that Y, and therefore also $\sin Y$, relaxes as $\exp(-\tau/\rho)$, which clearly is much slower than $\exp(\rho\tau)$. Since the maximum of $\exp(\rho\tau')$ on $(0,\tau)$ is at τ, we can thus develop $\sin Y(\tau')$ in a Taylor series around $\tau' = \tau$ to obtain $Y'(\tau)$ in the form of an ascending series of the small parameter $1/\rho$. The first two terms are

$$Y' = -(1/\rho)[(1-\exp(-\rho\tau))\sin Y + \tau\exp(-\rho\tau)(\sin Y)'] - (1/\rho^2)(1-\exp(-\rho\tau))(\sin Y)'. \qquad (27)$$

Now, we neglect the rapidly falling exponentials so that finally, to second order in $1/\rho$,

$$Y' = -(1/\rho)\sin Y - (1/\rho^2)Y'\cos Y \qquad (28)$$

This equation is readily integrated, giving a solution in implicit form

$$(\tan Y/2)(\sin Y)^{1/\rho^2} = (\tan Y_0/2)(\sin Y_0)^{1/\rho^2}\exp(-\tau/\rho). \qquad (29)$$

The left-hand side of (29) can be written as

$$2^{1/\rho^2}(\sin Y/2)^{1+1/\rho^2}(\cos Y/2)^{-1-1/\rho^2}, \qquad (30)$$

showing that the first approximation,

$$\tan Y/2 = (\tan Y_0/2)\exp(-\tau/\rho), \qquad (31)$$

equal to the solution of Eq. (23), is sufficient whenever the system is reasonably overdamped.

The first approximation amplitudes u_j are now given by the transformations (10) and (11) of (31) and the subsequent application of (27). We obtain

$$u_1 = f/(1+f^2)^{1/2}, \qquad (32a)$$
$$u_2 = 1/(1+f^2)^{1/2}, \qquad (32b)$$
$$u_3 = [1-\exp(-\rho\tau)]f/\rho(1+f^2), \qquad (32c)$$

where

$$f = (u_{10}/u_{20})\exp(-\tau/\rho). \qquad (33)$$

We see that initially the function u_3 rises sharply to approximately $u_{10}u_{20}/\rho$, within a time interval of the order

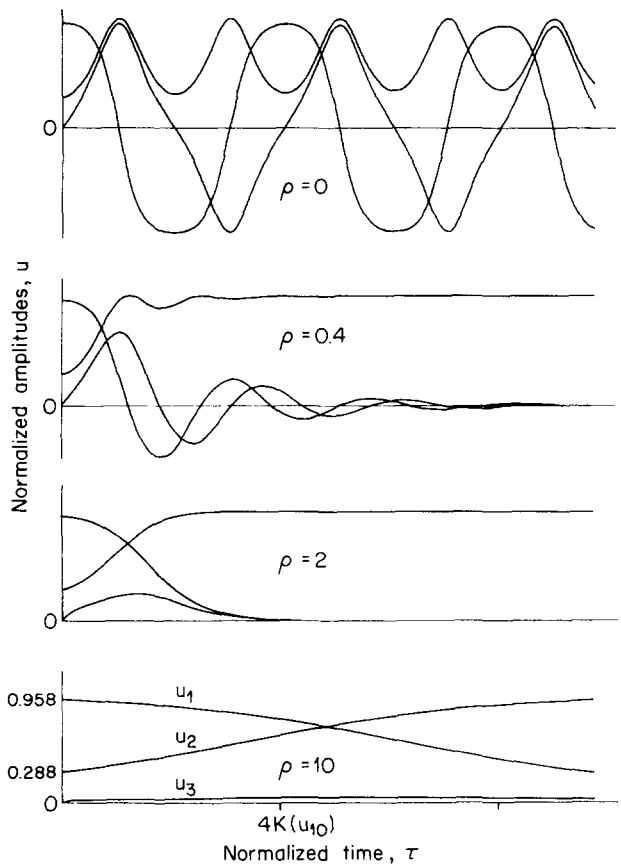

FIG. 1. Analog simulation of system (8) for different damping rates, ρ. The time-scale $K(u_{10})$ is the complete elliptic integral of the first kind, equal to a quarter-period of the undamped waves.

of $1/\rho$ and thereafter, either decreases slowly as $\exp(-\tau/\rho)$ if $u_{10} < u_{20}$ or first passes through a maximum at $\tau_m = \rho \ln(u_{10}/u_{20})$ if $u_{10} > u_{20}$. This behavior is fully confirmed by analog simulations of system (8). For illustration we present on Fig. 1 the traces of a simulation for different damping rates in the strongly nonlinear regime, $u_{10} \gg u_{20}$.

VI. PUMP DEPLETION TIME

An important characteristic of the wave interaction we have studied is the time interval within which the irreversible processes, mentioned at the end of Sec. IV, are practically completed. We will call this time interval the pump depletion time t_d. We define t_d phenomenologically as the relaxation time of the damping agent u_3. As is evident from the solutions (22) and (32), τ_d depends not only on ρ, but also on the initial conditions u_{10}, u_{20}.

(a) When $\rho \ll \min[2, 1/4K(u_{10})]$, the averaging technique employed for obtaining the solution (22) is valid for all times $\tau > 0$, and the relaxation time is simply $\tau_d = 1/\rho$, or according to (2),

$$t_d^{(a)} = 1/\nu. \tag{34}$$

(b) When $\rho \gg 2$, t_d again is long since now the coupling of u_1 and u_2, mediated by the right-hand sides of Eqs. (8a,b), is weak due to strong suppression of the wave u_3. For $u_{10} < u_{20}$, we have $\tau_d = \rho$, or

$$t_d^{(b)}(u_{10} < u_{20}) = \nu/\Omega_0^2. \tag{35}$$

On the other hand, when $u_{10} > u_{20}$, we have to account for the shift in depletion time due to the build-up of u_3 towards its maximum $\tau_m = \rho \ln(u_{10}/u_{20})$. Thus, now, $\tau_d = \rho + \tau_m$, or

$$t_d^{(c)}(u_{10} > u_{20}) = (\nu/\Omega_0^2)[1 + \ln(u_{10}/u_{20})] \tag{36}$$

The logarithmic correction is of purely nonlinear origin and is related to the fact that as $u_{10} \to 1$ even the undamped solutions (9) cease to oscillate, since the interaction period $4K(u_{10})$ tends to a logarithmic singularity, $K(u_{10} \to 1) \to \ln(4/u_{20})$. In physical terms, an increase in u_{10} slows down action transfer, in both undamped and damped cases.

VII. CONCLUDING REMARKS

Although the results of this paper relate to a temporal analysis of a three-wave interaction in the absence of group-velocity dispersion, they are equally applicable to a steady-state spatial analysis of waves propagating in the same direction. The general case is described by the operator[5,7]

$$\left(\frac{d}{dt}\right)_i = \frac{\partial}{\partial t} + v_i \frac{\partial}{\partial x},$$

where v_i is the group velocity of wave E_i. In the presence of damping, and with steady excitation at the boundary, there exists a steady state spatial distribution of amplitudes given by $\partial/\partial t \equiv 0$.

Thus, when all the v_i have the same sign, Eqs. (1) retain their form with new coupling constants $D_i = C_i/v_i$, and absorption coefficients $\kappa_i = \nu_i/v_i$.

On the other hand, when $\mathrm{sgn}v_1 = \mathrm{sgn}v_3 = -\mathrm{sgn}v_2$, which is typical of decay-type processes like Raman and Brillouin backscattering,[6-8] the above analysis would have to be modified to account for the change in sign in Eq. (1b), and, more importantly, because the waves E_1 and E_2 are now specified at opposite boundaries, which leads to an eigenvalue problem. A study of this problem is in preparation.

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The abstract Hilbert space generalization of Feenberg's perturbation theory—A new method of quantum field theory*

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A rigorous generalization of Feenberg's perturbation theory to the calculation of thermodynamic Green's functions is outlined. This method offers an algorithm for calculating correlation functions and propagators for any Hamiltonian, bounded or unbounded, and is exact and tractable in the thermodynamic limit. The method is defined and its use is illustrated by several brief examples.

I. INTRODUCTION

In the last few years there have been many papers[1] attempting to use the exact information which is contained in the moment expansion of various kinds of Green's functions to calculate approximations to the Green's functions themselves. One of the areas of greatest application of the moment expansion has been in the problem of the disordered alloy.[2] Other workers have extended the use of the moment expansion into many different quantum field theoretic models.[3] Of these papers, perhaps the most general and careful from a mathematical point of view has been the paper by Lonke. In this paper I shall attempt to address the same problem as did Lonke, the calculation of thermodynamic, or ground state averaged Green's functions. However, I shall outline a new method of calculating Green's function which has a rigorous foundation, is tractable, has a satisfactory thermodynamic limit, and allows the direct calculation of the self energy. This method is a generalization of a perturbation theory discovered by Feenberg[4] applied to a generalized Hilbert space used by Lonke. While the Feenberg method was originally formulated as primarily a perturbative method, recent work[5] allows the derivation of exact expressions for the Green's functions in the thermodynamic limit which can be evaluated directly. While the exact expressions for the Green's function are not limited to a perturbative regime for their validity, determining approximations to this exact expressions will of necessity still utilize the relative sizes of parameters in any model Hamiltonian.

The paper will be divided into the following sections. Section II will include a short discussion of the current methods of calculating thermodynamic or ground state averaged Green's functions and some of the necessary properties of these functions which will be used later. Section III will describe the essential properties of the Feenberg perturbation theory and detail the abstract Hilbert space generalization of this theory which allows the direct calculation of the Green's function. Section IV will consider some simple applications of this method of calculating Green's functions for various quantum field theory models. Of special emphasis will be those cases where one can rigorously show that the self-energy is represented by only one kind of term. This will be contrasted with the result of most diagrammatic expansions which involve a large number of diagrams.

II. PROPERTIES OF THE GREEN'S FUNCTIONS

This paper will be specialized to the calculation of two different kinds of Green's functions involving fermion operators.

The general form of the retarded Green's function of the sort we will set out to compute is

$$\langle\langle A_\alpha;B_\alpha\rangle\rangle_t = -(i)^{1-\alpha}\theta(t)\langle[A_\alpha(t),\ B_\alpha^\dagger(0)]_\eta\rangle \tag{2.1}$$

where $\alpha = 0, 1$ and $\eta = (-1)^\alpha$ and $\theta(t)$ is a unit step function. Here the brackets will represent some sort of average which is defined by a density matrix ρ such that

$$\langle\cdots\rangle = \mathrm{Tr}(\rho\cdots). \tag{2.2}$$

The only requirement on ρ, besides the usual normalization condition is that only ρ's which commute with the total Hamiltonian H will be considered. That is, it is required that

$$[\rho, H] = 0. \tag{2.3}$$

If the parameter α in (2.1) is zero, then the operators A_α and B_α will be odd numbers of fermion creation and or annihilation operators. The prototypical example of this form will be the one particle function

$$G(\mathbf{k}, t) = -i\theta(t)\langle[c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger]_+\rangle. \tag{2.4}$$

For $\alpha = 1$, the operators A_α and B_α will be restricted to be products of an even number of fermion annihilation or creation operators. The function of most interest of this type is the density—density correlation function

$$\chi(\mathbf{q}, \omega) = -\theta(t)\langle[\rho_{\mathbf{q}}(t), \rho_{\mathbf{q}}^\dagger(0)]_-\rangle \tag{2.5}$$

where

$$\rho_{\mathbf{q}} = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{q}}. \tag{2.6}$$

In particular, the study of this second kind of function will be specialized to operators $A_\alpha = B_\alpha$ such that the equal time commutator vanishes,

$$[A_\alpha, B_\alpha^\dagger] = 0. \tag{2.7}$$

The current methods of calculation of these Green's functions has followed at least three different approaches: (i) a Zubarev[6] decoupling scheme, (ii) a diagrammatic expansion[7] of the interaction representation using a Wick's theorem or its equivalent, or (iii) the analytic continuation of moment expansions as in Lonke's[8] paper.

The Zubarev method has been widely used in thermal physics application. The essential idea was to utilize a factorization of some higher order correlation functions in the hierarchy of equations generated by the Fourier transformed equation of motion

$$\omega\langle\langle A_\alpha;B_\alpha\rangle\rangle_\omega = 2\pi\langle[A_\alpha, B_\alpha]_\eta\rangle + \langle\langle[A_\alpha, H]; B_\alpha\rangle\rangle_\omega, \qquad (2.8)$$

where the subscript ω indicates the Fourier transform of the Green's function (2.1) and ω is a complex energy in the upper half complex energy plane. By approximating some high order correlation functions by products of equal time averages of operators and lower order correlation functions, the infinite hierarchy of equations is made into a closed linear system which can be solved for the desired functions.

One of the nice features of this method is that the derived Green's functions explicitly involve averages of certain operators in the ground state or the equilibrium state of the system. Thus, the excitation spectrum of the particles directly reflects the ground state or vacuum state properties of the interacting system. Usually these expectation values must be determined by the self-consistent solution of a set of equations which are usually quite nonlinear. As demonstrated by Zubarev and by the large number of applications of this method since then this method has been shown to give a good description of such correlated mean field theories as superconductivity, magnetism, and certain phase transitions.

One of the major criticisms of this method has been the ambiguity of the factorization process and the observation[9] that the factorization is only valid if fluctuations of the factorized variable is negligible. The approximation works well if a mean field theory is a good approximation, but higher order approximations have generally not yielded consistent and systematic schemes. Perhaps, the most telling objection to the Zubarev method is the difficulty of controlling the approximations and of deciding which factorizations are important.

The diagrammatic methods in their simplest form determine the causal Green's function by an expansion in powers of the interaction Hamiltonian. The expansion is built up using properties of the ground state of the noninteracting part of the Hamiltonian. The advantage of the expansion is that because of the structure of the diagrams the whole series can be characterized and easily approximated by partial summation of classes of diagrams.

A criticism of the method is that in some cases it can be argued that the expansion is at best asymptotic and the convergence is not guaranteed. Further, since the expansion relies on the ground state properties of the noninteracting Hamiltonian it is not possible, at least, in the simplest form, to achieve a good description of a highly correlated system.[10]

There are many highly sophisticated diagrammatic techniques which have been applied with success to different problems, some of which have been adapted to deal with correlated systems.

The third approach to the calculation of Green's functions to be discussed here is the class of methods using the exact moments of the Green's function. For definiteness in the following $G(\mathbf{k}, t)$ and $\chi(\mathbf{q}, t)$ will be used in the discussion.

The Fourier transform of the one electron Green's function can be shown[11] to have the following formal moment expansion

$$G^{(r)}(\mathbf{k}, \omega) = \sum_{N=0}^{\infty} \frac{1}{\omega^{N+1}} \langle[L^N c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger]_+\rangle, \qquad (2.9)$$

where the operator L is defined as

$$Lc_{\mathbf{k}} = [c_{\mathbf{k}}, H]. \qquad (2.10)$$

If the Hamiltonian H has a bounded spectrum, then this expansion is rigorously convergent for $|\omega|$ larger than the largest energy of H. If the Hamiltonian is an unbounded operator then the moment expansion must be regarded as being only asymptotic and formal.

The method proposed by Lonke for the calculation of $G^{(r)}(k, \omega)$ is effectively to approximate the moment expansion by a Padé approximant or an appropriate generalization thereof and analytically continue the approximation to small $|\omega|$. The desirable attribute of this method is that it uses rigorously exact information, the moments. The major criticism of the method is that it does not yield an acceptable approximation for the thermodynamic limit. This is the limit in which the size of the system goes to infinity in such a way that all intensive quantities remain finite. In this limit the spectrum of the Hamiltonian becomes continuous. Since the moment expansion can yield only countably many values of the moments it cannot yield a continuous spectrum. This is especially true of any approximation using only a finite number of moments.

Since the thermodynamic limit is the only limit which is most often of interest for a quantum field theory model, some sort of method is needed which has a reasonable form in this limit.

In the sections to follow another method of calculating Green's functions which overcomes some of the difficulties listed alone will be discussed. Before proceeding to that discussion, for later reference the moment expansion of the density correlation function could be written as

$$\chi(\mathbf{q}, \omega) = \sum_{S=0}^{\infty} \frac{1}{(\omega^2)^{S+1}} \langle[L^{2S+1}\rho_{\mathbf{q}}, \rho_{\mathbf{q}}^\dagger]_-\rangle \qquad (2.11)$$

where L is defined as before.

III. FEENBERG PERTURBATION THEORY

In 1948, Feenberg[12] was studying the basic problem of all perturbation theories. Namely, given a Hamiltonian $H_0 + V$ and an orthonormal basis set $|n\rangle$ chosen so that H_0 has only diagonal matrix elements

$$E_n = \langle n|H_0|n\rangle \qquad (3.1)$$

with respect to this set, and for which V has only off-diagonal matrix elements

$$V_{nl} = \langle n|V|l\rangle,$$

how can one determine the true energies of the full Hamiltonian?

Feenberg observed that for a Hamiltonian matrix H_{nl} which is finite-dimensional the energies were the zeros of the polynomial

$$\det(\omega\delta_{nl} - H_{nl}) = 0, \qquad (3.2)$$

or equivalently by the poles of the resolvent $R(\omega)$

$$R(\omega)=(\omega-H)^{-1}. \tag{3.3}$$

Feenberg observed that in any term of (3.2) or of the denominator of (3.3) there never was a repeated factor of any of the matrix elements V_{nl}. He then raised the question of why in the Brillouin—Wigner perturbation theory or other methods there was not a similar restriction against repeated factors of the V_{nl} in a particular order of perturbation theory.

Feenberg concluded that the usual methods of perturbation theory were some sort of large $|\omega|$ expansion of $R(\omega)$ and he set about creating an iterative scheme for calculating the perturbed energies which presented the determinantal conditon. His method is equivalent to choosing finite-dimensional Hamiltonian matrices H_N to approximate H and then successively increasing the size N of the subspace which was spanned by H_N. Feshbach[13] was the first to point out that for any finite-dimensional Hamiltonian Feenberg's method finally gave the exact answer.

Recently, Masson[14] has applied the tools of functional analysis to a similar approximation scheme which also approximated the Hamiltonian by finite-dimensional subspaces. He was able to rigorously establish the convergence properties of the theory as the size of the subspace approached the whole infinite-dimensional Hilbert space. One of his results is particularly strong and can be directly applied to the Feenberg formulas to be discussed below.

Masson's central theorem for our purposes says that for any Hamiltonian H, whether bounded or not, the matrix elements of the finite-dimensional resoluents $R_N(\omega)$ converge to the matrix elements of the exact resoluent $R(\omega)$ for any complex value of ω which is not contained in the spectrum of the Hamiltonian. The proof of this theorem can be found in Ref. 14. Note that the result is true for matrix elements of the resolvent and not for the resolvent operator itself.

This result guarantees the convergence of the Feenberg formulas (below) for an extremely wide class of Hamiltonians. Note that convergence is guaranteed irrespective of the size of the coupling parameters of the Hamiltonian.

The Feenberg formulas represent the matrix elements of the resolvent operator in a form which can in principle written down for the limit as the size of the approximating subspace becomes infinite.

The diagonal matrix element of the resolvent is

$$\langle n|(\omega-H)^{-1}|n\rangle=(\omega-E_n-\textstyle\sum(n,\omega))^{-1}, \tag{3.4}$$

where the self energy is defined by

$$\sum(n,\omega)=\sum_{l\neq n}\frac{|V_{ln}|^2}{\omega-e_l(n)}+\sum_{\substack{l_1\neq n\\ l_2\neq l_1 n}}\frac{V_{nl_1}V_{l_1l_2}V_{l_2n}}{(\omega-e_{l_1}(n))(\omega-e_2(n_{l_1}))}$$

$$+\sum_{\substack{l_1\neq n\\ l_2\neq l_1 n\\ l_3=l_1l_2 n}}\frac{V_{nl_1}V_{l_1l_2}V_{l_2l_3}V_{l_3n}}{(\omega-e_{l_1}(n))(\omega-e_{l_2}(nl_1))(\omega-e_{l_3}(nl_1l_2))}+\cdots. \tag{3.5}$$

The reduced energies $e_{l_r}(nl_1l_2,\ldots,l_{r-1})$ are defined as

$$e_{l_r}(nl_1l_2,\ldots,l_r)=E_{l_r}+\textstyle\sum^1(l_r;nl_1l_2\ldots l_{r-1};\omega), \tag{3.6}$$

where the reduced self energy $\sum^1$ is defined by a formula similar to Eq. (3.5), except that in every summation, the sum must not contain any terms involving any of the states $n, l_1, l_2, \ldots, l_{r-1}$, as well. For any finite-dimensional Hamiltonian the restrictions on the summations finally permit no more terms and the expressions truncate. For an infinite-dimensional Hamiltonian the system (3.5) and (3.6) comprise an infinite set of equations.

At first glance, this approach seems totally intractable because of all the summation restrictions. However, as seen below, in the thermodynamic limit these formulas yield several simplifications. Further, it will be shown that there is an intimate relationship between the Feenberg formulas and the thermodynamic Green's functions, and that the strong orthonormality condition expressed by the summation restrictions yields some surprising simplifications for some model Hamiltonians.

For later reference it is useful to write out the Feenberg formula for off-diagonal matrix elements of the resolvent.

$$\langle n|(\omega-H)^{-1}|n'\rangle=\frac{1}{\omega-e_n}\left(V_{nn'}+\sum_{\substack{l\neq n\\ n'}}\frac{V_{nl}V_{ln'}}{\omega-e\,(nn')}\right.$$

$$\left.+\sum_{\substack{l_1\neq nn'\\ l_2\neq nn'l_1}}\frac{V_{nl_1}V_{l_1l_2}V_{l_2n'}}{(\omega-e_{l_1})(\omega-e_{l_2})}+\cdots\right)\frac{1}{(\omega-e_{n'}(n))}. \tag{3.7}$$

Now it is necessary to demonstrate the relationship between the Feenberg formulas and the thermodynamic Green's functions we wish to compute. In the next section we try to demonstrate that the Feenberg formulas generate a tractable calculational scheme.

Note first that the matrix elements of the resolvent taken with respect to the orthonormal basis $|n\rangle$, $|n'\rangle\cdots$ also have a formal moment expansion

$$\langle n|(\omega-H)^{-1}|n'\rangle=\sum_{N=0}^{\infty}\frac{1}{\omega^{N+1}}\langle n|(H)^N|n'\rangle. \tag{3.8}$$

The essential idea by which we shall establish an identification between the Feenberg formulas and the thermodynamic Green's functions is through the use of the moment expansions.

The desired identification will be established if a generalization of a Hilbert space (called an abstract Hilbert space)[15] can be found for which the moments of the Green's functions are matrix elements of a suitably generalized Hamiltonian operator. The two requirements for the determination of the generalized Hilbert space are the definition of a scalar (inner) product on that space and a demonstration that a symmetric (Hermitian) generalization of the Hamiltonian operates on the elements of the abstract Hilbert space. If these two requirements are satisfied, then with respect to that abstract Hilbert space, the thermodynamic Green's functions may be calculated using the Feenberg formulas.

The properties of an abstract Hilbert space are listed

in Ref. 15. Essentially, any set $\mathfrak{H}$ of abstract elements f, g, h, $\cdots$ is called an abstract Hilbert space if it satisfies the following three properties:

A. The space $\mathfrak{H}$ is a linear space. If f, g, $\in \mathfrak{H}$, then $(\alpha f + \beta g) \in \mathfrak{H}$ for arbitrary complex numbers α and β.

B. The space $\mathfrak{H}$ is a metric space whose metric is derived from a scalar product. That is, for every f, g in $\mathfrak{H}$, there is a complex number (f, g) which satisfies the following properties:

(i) $(f, ag) = a(f, g)$ for all numbers a, (3.9)

(ii) $(f+g, h) = (f, h) + (g, h)$, (3.10)

(iii) $(f, g) = (g, f)^*$, (3.11)

(iv) for all f in the space, (3.12)

$(f, f) > 0$ and

$(f, f) = 0$ for the zero element $f = 0$.

C. The space $\mathfrak{H}$ is "complete" in the sense that the limits of sequences of elements in the space are also in the space.

Property A is essentially trivial for any generalization and we will assume that property C is inherited[16] from the underlying Hilbert space of our problem. The essential property for our purposes is the verification of property B and the determination of the generalized Hamiltonian acting on the abstract space.

Lonke has already noted that the space whose elements f_ν are products of odd numbers of Fermion annihilation and or creation operators forms an abstract Hilbert space $\mathfrak{H}_f$. The scalar product[17] on the space

$$((f_1, f_2))_f = \langle [f_2, f_1^\dagger]_+ \rangle. \tag{3.13}$$

Properties (i), (ii), and (iii) are immediate for this inner product, and property (iv) can be easily established by inserting complete sets of states in a representation in which the density matrix is diagonal.

Now by comparing (2.9) with (3.8) we see that if L defined by (2.10) on this new space is Hermitian, the identification is complete. That this is true for

$$[\rho, H] = 0 \tag{3.14}$$

is easily demonstrated.

First, it is clearly the case that

$$((f, Lg))_\rho = \langle gHf^\dagger \rangle - \langle Hgf^\dagger \rangle + \langle f^\dagger gH \rangle - \langle f^\dagger Hg \rangle, \tag{3.15}$$

and

$$((Lf, g))_\rho = \langle gHf^\dagger \rangle - \langle gf^\dagger H \rangle + \langle Hf^\dagger g \rangle - \langle f^\dagger Hg \rangle. \tag{3.16}$$

If H can be commuted through ρ in the middle terms of (3.16), the desired symmetry is established.

Thus we have established that the one electron Green's function has a moment expansion which is the moment expansion of the L operator on an abstract Hilbert space. This allows the identification that

$$G(k, \omega) = \langle\langle c_k; c_k^\dagger \rangle\rangle_\omega = ((c_k, (\omega - L)^{-1} c_k))_f, \tag{3.17}$$

It is worthwhile making several comments about the significance of the identification (3.17). If an orthonormal basis of the abstract Hilbert space can be constructed of which c_k is the initial element, the Feenberg formulas allow an exact formula by which to calculate the Green's function. As will be seen in the examples below the major part of the task is finding the orthonormal basis vectors. This is straightforwardly accomplished by use of the Schmidt orthogonalization procedure.[18]

It is worthwhile emphasizing that these Feenberg formulas for the calculation of the Green's functions are not perturbative in nature, neither are they expansions in terms of some small parameter. The existence of the formulas and their validity has been rigorously established by the mathematical properties of Hilbert spaces and self-adjoint operators. Masson's theorem effectively implies that for any system with a Hamiltonian one can construct the set of Green's functions diagonal and off diagonal with respect to the set of orthonormal elements in the generalized operator Hilbert space. By noting that every energy denominator in the definition of the self energy (3.5) contains a reduced self energy of the appropriate type; these expressions have to be regarded as inherently renormalized. Each intermediate state is "dressed" by the appropriate excitations. This development of the Green's functions differs from the usual Feynman—Dyson expansion in the sense that there all of the intermediate states are specified to be of a particular type (e.g., one electron or one photon propagators), while the Feenberg formulas are expanded in terms of intermediate states which are composites of dressed and interacting groups of elementary excitations. While the Feynman picture is physically more appealing and more intuitive, the dressing of the intermediate states and the inclusion of binding energies or correlation energies between the components of the intermediate states is a much more realistic picture of the underlying physics. This particular feature of the Feenberg formulas could have far reaching consequences for quantum field theory.

The Feenberg formulas share another property of standard matrix theory. By choosing the basis of the space appropriately it is possible to alter the structure of the self energy greatly. Of course in a representation for which the Hamiltonian is diagonal the self energy vanishes. If the Hamiltonian were tridiagonal the self energy would be given by one continued fraction.

In most physical models with momentum conservation, there are only a few matrix elements which connect the one particle subspace of the generalized Hilbert space with other subspaces. This suggests the self energy would not be an infinite series of terms, but could be only finitely many terms, each of which has a denominator with properties similar to a continued fraction. Some of the examples to be studied below will illustrate this behavior. Other examples, notably disordered alloy problems in a momentum representation require an infinite number of self energy terms.

In the examples to follow both the basis dependent features leading to simplification of the self energy and the properties of the Feenberg formulas in the thermodynamic limit will be illustrated.

This effectively accomplishes the goal of the Zubarev program, but in an unambiguous fashion for which corrections can be straightforwardly evaluated.

Before proceeding directly to the examples, let us establish the existence of a different abstract Hilbert space $\mathfrak{H}_b$ and a different generalized Hamiltonian which will allow the similar calculation of $\chi(\mathbf{q}, \omega)$.

We begin as before by examining the moment expansion

$$\chi(\mathbf{q}, \omega) = \sum_{N=0}^{\infty} \frac{1}{(\omega^2)^{N+1}} \langle [L^{2N+1}\rho_{\mathbf{q}}, \rho_{\mathbf{q}}^{\dagger}] \rangle. \tag{3.18}$$

It is desired to find an inner product and a generalized Hamiltonian so that (3.18) looks like (3.8). As will be verified below, the scalar product

$$((\rho_{\mathbf{q}}, \rho_{\mathbf{q}}))_b = \langle [[\rho_{\mathbf{q}}, H], \rho_{\mathbf{q}}^{\dagger}] \rangle \tag{3.19}$$

where these are commutators and the generalized Hamiltonian is

$$\mathcal{L} = L^2, \tag{3.20}$$

where L has been defined in (2.10).

That (3.19) is an inner product and $\mathcal{L}$ is symmetric can be easily verified provided that

$$[\rho, H] = 0.$$

For the Fermion density–density correlation function the elements α_i of this new abstract Hilbert space $\mathfrak{H}_b$ are products of even numbers of Fermion operators with equal numbers of creation and annihilation operators. This boson-like Hilbert space can be applied to other types of operators and the appropriate sets of operators will be elements of the space.

In any of the above cases there is no problem with properties A and C of our Hilbert space properties. Further, properties B(i) and (ii) are trivial. To demonstrate (iii) we want to show that using the line to indicate complex conjugation

$$\overline{((\alpha_i, \alpha_j))_b} = \overline{\langle [[\alpha_j, H], \alpha_i^{\dagger}] \rangle} = \langle [\alpha_i, [H, \alpha_j^{\dagger}]] \rangle \tag{3.21}$$

is the same as

$$((\alpha_j, \alpha_i))_b = \langle [[\alpha_i, H], \alpha_j^{\dagger}] \rangle. \tag{3.22}$$

Writing out (3.21) given

$$\overline{((\alpha_i, \alpha_j))_b} = \langle \alpha_i H \alpha_j^{\dagger} \rangle - \langle \alpha_i \alpha_j^{\dagger} H \rangle - \langle H \alpha_j^{\dagger} \alpha_i \rangle + \langle \alpha_j^{\dagger} H \alpha_i \rangle. \tag{3.23}$$

If H can be commuted through the density matrix in the two middle terms this can be rewritten as

$$\langle [\alpha_i, H] \alpha_j^{\dagger} \rangle - \langle \alpha_j^{\dagger} [\alpha_i, H] \rangle$$

which equals (3.21).

Now we will demonstrate that $((\alpha, \alpha))_b$ is positive. The proof will be for a canonical density matrix, though any density matrix whose diagonal elements are monotonially decreasing functions of energy will give the same result:

$$((\alpha, \alpha))_b = \langle \alpha H \alpha^{\dagger} \rangle - \langle H \alpha \alpha^{\dagger} \rangle - \langle \alpha^{\dagger} \alpha H \rangle + \langle \alpha^{\dagger} H \alpha \rangle.$$

By inserting complete sets of simultaneous eigenstates of the Hamiltonian and the density matrix, we find

$$((\alpha, \alpha))_b = \sum_{n,m} \frac{\exp(-\beta E_n)}{Z} (E_m - E_n) \langle E_n | \alpha | E_m \rangle \langle E_m | \alpha^{\dagger} | E_n \rangle$$

$$+ \sum_{n,m} \frac{\exp(-\beta E_{\ })}{Z} (E_m - E_n) \langle E_n | \alpha^{\dagger} | E_m \rangle \langle E_m | \alpha | E_n \rangle,$$

where $Z = \mathrm{Tr}(\exp(-\beta H))$.

Interchanging the summation variables in the second sum yields

$$Z((\alpha, \alpha))_b = \sum_{n,m} \exp(-\beta E_n)(E_m - E_n) |\langle E_n | \alpha | E_m \rangle|^2$$

$$- \sum_{n,m} \exp(-\beta E_m)(E_m - E_n) |\langle E_m | \alpha^{\dagger} | E_n \rangle|^2.$$

Now

$$|\langle E_m | \alpha^{\dagger} | E_n \rangle|^2 = |\langle E_n | \alpha | E_m \rangle|^2.$$

Combining terms and rearranging slightly yields

$$((\alpha, \alpha))_b = \frac{1}{Z} \sum_{n,m} (E_m - E_n)(1 - \exp[-\beta(E_m - E_n)])$$

$$\times \exp(-\beta E_n) |\langle E_n | \alpha | E_m \rangle|^2. \tag{3.24}$$

A moment's reflection will verify that (3.24) is a sum of terms each of which is positive or zero, so (3.19) does have the properties of an inner product.

It is interesting to note that any operator α which commutes with the Hamiltonian and with its adjoint has a zero norm

$$((\alpha, \alpha))_b = 0,$$

which means that that particular operator is a representation of the zero element of the abstract Hilbert space. This is another way of saying that this operator is not part of the Hilbert space. This is even physically reasonable, for if an operator is an element of the abstract Hilbert space $\mathfrak{H}_b$, then it can have a nonvanishing correlation function at nonzero times. On the other hand, operators which commute with the Hamiltonian are constants of the motion and there should be no time-varying correlation functions for their time behavior.

The proof that $\mathcal{L}$ is Hermitian (symmetric) follows through in essentially the same way as in the previous case, and depends on having ρ and H commute as before. The demonstration will be left to the reader.

IV. APPLICATIONS OF AHGF

In the following several, simple examples will be given to illustrate the AHGF method and to demonstrate the simplifications of some results both due to properties of the thermodynamic limit, but also due to the orthogonalization restrictions of the Feenberg formulas.

A. Diagonal Hamiltonians

Here we study diagonal Hamiltonians both to illustrate the simplest aspect of the AHGF method and to confirm that the correct Green's functions are determined for the free particle case. Accordingly, consider a Hamiltonian of the form

$$H_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}. \tag{4.1}$$

First consider the $c_{\mathbf{k}}$'s as fermion operators. Then $c_{\mathbf{k}}$ is a unit vector of the space $\mathfrak{H}_f$ (Ref. 19)

$$((c_{\mathbf{k}}, c_{\mathbf{k}'})) = \langle\{c_{\mathbf{k}'}, c_{\mathbf{k}}^{\dagger}\}\rangle = \delta_{\mathbf{k},\mathbf{k}'}. \tag{4.2}$$

Note also that $c_{\mathbf{k}}^{\dagger}$ is also a unit vector of the space and that it is orthogonal to $c_{\mathbf{k}}$:

$$((c_k, c_{k'}^{\dagger})) = \langle\{c_{k'}, c_k\}\rangle \tag{4.3}$$

$$= 0. \tag{4.4}$$

To determine the one electron Green's function

$$\langle\langle c_{\mathbf{k}}; c_{\mathbf{k}}^{\dagger}\rangle\rangle = ((c_{\mathbf{k}}, (\omega - L)^{-1} c_{\mathbf{k}})), \tag{4.5}$$

it is necessary to evaluate matrix elements of L. To do this we first evaluate $Lc_{\mathbf{k}}$:

$$Lc_{\mathbf{k}} = \epsilon_{\mathbf{k}} c_{\mathbf{k}}. \tag{4.6}$$

There are no off-diagonal matrix elements, so there will be no self energy [compare (3.5)],

$$((c_{\mathbf{k}}, Lc_{\mathbf{k}}))_f = \epsilon_{\mathbf{k}}. \tag{4.7}$$

Thus,

$$((c_{\mathbf{k}}, (\omega - L)^{-1} c_{\mathbf{k}}))_f = (\omega - ((c_{\mathbf{k}}, Lc_{\mathbf{k}}))_f)^{-1} = (\omega - \epsilon_{\mathbf{k}})^{-1}, \tag{4.8}$$

which is exactly what it should be.

Now consider the density–density correlation function $\chi(\mathbf{q}, \omega)$. This can be written as

$$\chi(\mathbf{q}, \omega) = \sum_{\mathbf{p},\mathbf{p}'} ((c^{\dagger}_{\mathbf{p}} c_{\mathbf{p}+\mathbf{q}}, (\omega^2 - \mathcal{L})^{-1} c^{\dagger}_{\mathbf{p}'} c_{\mathbf{p}'+\mathbf{q}}))_b. \tag{4.9}$$

First, we note that

$$\mathcal{L}\, c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}+\mathbf{q}} = (\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})^2 c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}+\mathbf{q}}. \tag{4.10}$$

Second, we note that $c^{\dagger}_{\mathbf{p}} c_{\mathbf{p}+\mathbf{q}}$ for varying $\mathbf{p}$ form an orthogonal basis of the space, but are not unit vectors,

$$((c_{\mathbf{p}'} c_{\mathbf{p}'+\mathbf{q}}, c_{\mathbf{p}} c_{\mathbf{p}+\mathbf{q}}))_b = \delta_{\mathbf{p},\mathbf{p}'} (\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})(\langle n_{\mathbf{p}}\rangle - \langle n_{\mathbf{p}+\mathbf{q}}\rangle). \tag{4.11}$$

This means that to use the Feenberg formulas to evaluate $\chi(\mathbf{q}, \omega)$ we must be sure to first divide the elements of abstract space by their norms. There are clearly no off-diagonal matrix elements of $\mathcal{L}$ for this Hamiltonian, so there will be no self energy ϵ and we may use (3.4) to evaluate χ. Carefully taking into account the norms of the vectors yields

$$((c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}+\mathbf{q}}, \mathcal{L}\, c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}+\mathbf{q}}))_e = (\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})^2 ((c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}+\mathbf{q}}, c_{\mathbf{p}}^{\dagger}, c_{\mathbf{p}+\mathbf{q}})) \tag{4.12}$$

and

$$\chi(\mathbf{q}, \omega) = \sum_{\mathbf{p}} \frac{(\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})(\langle n_{\mathbf{p}}\rangle - \langle n_{\mathbf{p}+\mathbf{q}}\rangle)}{\omega^2 - (\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})^2}. \tag{4.13}$$

If the c_k are now regarded as boson operators, so that (4.1) might be considered as representing phonons in the Harmonic approximation or a gas of noninteracting bosons, the single particle excitations could presumably be studied through examining

$$\mathcal{D}_0(\mathbf{k}, \omega) = ((\phi_{\mathbf{k}}, (\omega^2 - \mathcal{L})^{-1} \phi_{\mathbf{k}}))_e, \tag{4.14}$$

where

$$\phi_{\mathbf{k}} = c_{\mathbf{k}} + c_{\mathbf{k}}^{\dagger}. \tag{4.15}$$

The relevant matrix elements for this case are

$$((\phi_{\mathbf{k}}, \phi_{\mathbf{k}'})) = 2\epsilon_{\mathbf{k}} \delta_{\mathbf{k}\mathbf{k}'} \tag{4.16}$$

$$((\phi_{\mathbf{k}}, \mathcal{L}\, \phi_{\mathbf{k}})) = \epsilon_{\mathbf{k}}^2 ((\phi_{\mathbf{k}}, \phi_{\mathbf{k}})), \tag{4.17}$$

and the noninteracting Green's function is

$$\mathcal{D}_0(\mathbf{k}, \omega) = 2\epsilon_{\mathbf{k}}/(\omega^2 - \epsilon_{\mathbf{k}}^2). \tag{4.18}$$

Finally, consider the case of a spin I in a magnetic field h_z so that the Hamiltonian is

$$H = -h_z I_z. \tag{4.19}$$

At this point focus interest on $\langle\langle I_x; I_x\rangle\rangle_{\omega}$. In much the same way as before, the requisite matrix elements can be evaluated

$$((I_x, I_x)) = h^z \langle I^z\rangle, \tag{4.20}$$

$$((I_x, \mathcal{L}\, I_x)) = h_z^2 ((I_x, I_x)), \tag{4.21}$$

so that

$$\langle\langle I_x; I_x\rangle\rangle_{\omega} = h_z \langle I_z\rangle/(\omega^2 - h_z^2). \tag{4.22}$$

All of these preceding examples simply show that the AHGF method does not give the incorrect answer. For these cases, we have a much more sophisticated tool than is necessary for the job. In the next example, we study one aspect of the simplification that occurs in the Feenberg formulas in the thermodynamic limit.

B. Single impurity

Koster and Slater[20] first determined the exact solution to the dynamics of a gas of noninteracting electrons scattering from a static impurity potential at the origin. The Hamiltonian for such a model can be written as

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \frac{\delta}{N} \sum_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}'}. \tag{4.23}$$

By the usual equation of motion method this Hamiltonian can be solved for the t-matrix and the self energy $\sum(\mathbf{k}, \omega)$ for the Green's function $\langle\langle c_{\mathbf{k}}; c_{\mathbf{k}}^{\dagger}\rangle\rangle_{\omega}$ can be evaluated exactly[21] in the thermodynamic limit. In this case of studying a single impurity the thermodynamic limit corresponds to keeping only terms which are of order $(1/N)$ is $N \to \infty$. The Koster–Slater self energy is

$$\sum(\mathbf{k}, \omega) = \frac{\delta^2}{N} \frac{F_0(\omega)}{1 - \delta F_0(\omega)}, \tag{4.24}$$

where

$$F_0(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\omega - \epsilon_{\mathbf{k}}}. \tag{4.25}$$

With an eye to the resulting simplification possible in the thermodynamic limit, let us examine the Feenberg formula for this problem. The matrix elements of the Hamiltonian are

$$((c_{\mathbf{k}}, Lc_{\mathbf{k}})) = \epsilon_{\mathbf{k}} + \delta/N,$$

$$((c_{\mathbf{k}}, Lc_{\mathbf{k}'})) = \delta/N, \quad \mathbf{k} \neq \mathbf{k}'. \tag{4.26}$$

The Feenberg formula for the self energy $\sum(k, \omega)$ can be written down as

$$\sum(\mathbf{k},\omega)=\frac{\delta^2}{N}\sum_{\mathbf{k}_1\neq\mathbf{k}}\frac{1}{\omega-\epsilon_{\mathbf{k}_1}}+\frac{\delta^3}{N}\sum_{\substack{\mathbf{k}_1\neq\mathbf{k}\\ \mathbf{k}_2\neq\mathbf{k}_1\mathbf{k}}}\frac{1}{\omega-\epsilon_{\mathbf{k}_1}}\frac{1}{\omega-\epsilon_{\mathbf{k}_2}}$$

$$+\frac{\delta^4}{N}\sum_{\substack{\mathbf{k}_1\neq\mathbf{k}\\ \mathbf{k}_2\neq\mathbf{k}_1\mathbf{k}\\ \mathbf{k}_3\neq\mathbf{k}_1\mathbf{k}_2\mathbf{k}}}\frac{1}{\omega-\epsilon_{\mathbf{k}_1}}\frac{1}{\omega-\epsilon_{\mathbf{k}_2}}\frac{1}{\omega-\epsilon_{\mathbf{k}_3}}+\cdots, \tag{4.27}$$

where in the writing of (4.27) it has been reocgnized that the reduced self energies which should be in each energy denominator [compare (3.5)] are each of order $(1/N)$. To keep only contributions of $(1/N)$ it is permissible to drop these terms. This is not essential for the observations which follow, but it does serve to simplify the resulting expressions.

Even with the simplification of neglecting the reduced self energies, Eq. (4.27) is still quite complicated because of the summation restrictions. It is at this point that the essential simplifying feature of the N/V limit can be used.

To see this quite clearly we must first realize that ω is not real, but is some complex number in the upper half plane. To calculate spectral functions in some approximation we will consider the analytic continuation of the thermodynamic limit of the self energy up to the real axis. This means that at this stage of the calculation none of the factors $(\omega-\epsilon_{\mathbf{k}_\eta})$ is zero. Now as the thermodynamic limit is taken of (4.27) the spectrum $\epsilon_{\mathbf{k}}$ becomes continuous and the sums go over into integrals over $\epsilon_{\mathbf{k}}$. For such integrals the exclusion of countably many points does not give any contribution to the integral[22] and so the summation restrictions of this type can be dropped in the thermodynamic limit.

In the thermodynamic limit then the Feenberg formula can be written as

$$\sum(\mathbf{k},\omega)=\frac{\delta^2}{N}F_0(\omega)\left(1+\delta F_0(\omega)+\delta^2(F_0(\omega))^2+\cdots\right), \tag{4.28}$$

which series can be easily recognized to give exactly the Koster–Slater result.

This example has not been given to show that the Feenberg formula yields an easier solution to this exactly soluble problem, it does not do that. The purpose was to illustrate a situation in which the thermodynamic limit simplifies some aspects of the Feenberg formula. The second point of this example is that in some cases, usually, when there is no translational invariance, the self energy is given as a series and some sort of approximation for this series must be used in any approximation scheme. In some of the situations to be considered below it will be found that the Feenberg formulas truncate and yield some simplifications.

C. The Anderson model

This example will illustrate in an extremely simple case how the orthogonalization and the thermodynamic limit can yield rigorous information about the structure of the self energy of the Green's functions.

The Anderson model[23] attempts to describe the dynamics of a d-orbital on a transition metal impurity atom in a metal. The d-electron states on the impurity are assumed to interact via a Coulomb interaction, while the conduction electrons are assumed to be noninteracting. If $c_{\mathbf{k}}$ is a conduction electron annihilation operator and c_d the impurity orbital operator, the Hamiltonian may be written as

$$H=\sum_{\mathbf{k}_s}\epsilon_{\mathbf{k}_s}c^\dagger_{\mathbf{k}_s}c_{\mathbf{k}_s}+\sum_s E_{ds}c^\dagger_{ds}c_{ds}+Un_{d\uparrow}n_{d\downarrow}$$

$$+\sum_{\mathbf{k}_s}V_{\mathbf{k}d}(c^\dagger_{\mathbf{k}s}c_{ds}+c_{ds}{}^\dagger c_{\mathbf{k}s}). \tag{4.29}$$

Here $\epsilon_{\mathbf{k}s}$ are the conduction electron energies, E_d is the single electron orbital energy, U is the Coulomb integral between two electrons on the impurity site and $V_{\mathbf{k}d}$ is the mixing matrix element between the conduction electrons and the impurity state. Exact solutions exist for this Hamiltonian in several limits. In the atomic limit $V_{\mathbf{k}d}\to 0$, Hubbard[24] was the first to show that the impurity Green's function could be written as

$$\langle\langle c_{d\sigma};c_{d\sigma}{}^\dagger\rangle\rangle=\frac{1-\langle n_{d\bar\sigma}\rangle}{\omega-E_{d\sigma}}+\frac{\langle n_{d\bar\sigma}\rangle}{\omega-E_{d\sigma}-U}. \tag{4.30}$$

The other exact limit is called the resonant level model[25] for which $U=0$ and the exact solution is

$$\langle\langle c_{d\sigma};c_{d\sigma}{}^\dagger\rangle\rangle=\frac{1}{\omega-E_{d\sigma}-\gamma(\omega)}, \tag{4.31}$$

where

$$\gamma(\omega)=\sum_{\mathbf{k}}\frac{|V_{\mathbf{k}d}|^2}{\omega-\epsilon_{\mathbf{k}}}. \tag{4.32}$$

The usual treatment of this model, following Anderson is to treat the Coulomb interaction in the Hartree approximation, which means that $E_{d\sigma}$ in (4.31) is replaced by $E_{d\sigma}+U\langle n_{\bar\sigma}\rangle$ and the number operator expectation values are determined self consistently.

Hewson,[26] among others has observed that the Hartree approximation does not yield the correct atomic limit and used a Zubarev decoupling scheme to derive an approximation which did achieve the correct limit. A simplifying approximation to the AHGF result below recovers the Hewson approximation.

The first step in computing $\langle\langle c_{d\sigma};c_{d\sigma}^\dagger\rangle\rangle$ with the AHGF method is to compute $Lc_{d\sigma}$,

$$Lc_{d\sigma}=E_{d\sigma}c_{d\sigma}+Un_{d\bar\sigma}c_{d\sigma}+\sum_{\mathbf{k}}V_{\mathbf{k}d}c_{\mathbf{k}\sigma}. \tag{4.33}$$

The next step is to use the scalar product and the Schmidt procedure to construct an orthonormal basis for (4.33). Noting that

$$((c_d,\ c_k))=0$$

and

$$((c_{d\sigma},n_{d\bar\sigma}c_{d\sigma}))=\langle n_{d\bar\sigma}\rangle,$$

the orthonormal basis is easily constructed:

$$Lc_{d\sigma}=(E_{d\sigma}+U\langle n_{d\bar\sigma}\rangle)c_{d\sigma}+U\sqrt{\langle n_{d\bar\sigma}\rangle(1-\langle n_{d\bar\sigma}\rangle)}\ \Phi^{(2)}_{d\sigma}+\sum_{\mathbf{k}}V_{\mathbf{k}d}c_{\mathbf{k}\sigma}. \tag{4.34}$$

Here, the orthonormal vector $\Phi^{(2)}_d$ is defined as

$$\Phi^{(2)}_{d\sigma}=\frac{(n_{d\bar\sigma}-\langle n_{d\bar\sigma}\rangle)c_{d\sigma}}{\sqrt{\langle n_{d\bar\sigma}\rangle(1-\langle n_{d\bar\sigma}\rangle)}}. \tag{4.35}$$

Note in passing that the Hartree energy arises in this treatment through the Schmidt orthogonalization procedure. Now L has been proven to be a symmetric operator and if L operating on other elements is studied we must acquire the symmetric matrix elements. For example, the orthonormal expansion of $Lc_{k\tau}$ is

$$Lc_{k\tau} = \epsilon_{k\tau} c_{k\tau} + V_{kd} c_{d\tau}; \tag{4.36}$$

for this study we take V_{kd} to be real.

With the examination of just the two Eqs. (4.34) and (4.35) much can be said about the structure of the impurity self energy and the impurity Green's function. First, by referring to the Feenberg formula (3.5) we see that there will be two types of terms of the form

$$\sum_{l \neq n} \frac{|V_{ln}|^2}{\omega - e_l(n)}$$

for the choice $n = c_{d\tau}$, $l = c_{k\tau}$, and $l = \Phi_d^{(2)}$. Furthermore, because (4.36) has only the off-diagonal matrix element V_{kd}, the summation restrictions on the reduced self energy require that for $l = c_{k\tau}$

$$e_{c_{k\tau}}(c_{d\tau}) = \epsilon_k. \tag{4.37}$$

The interesting question is what about the higher order terms in the Feenberg formula (3.5).

First, we observed that the restrictions require that no matrix element or its transpose may appear in the same factor. Thus in the third order term we need numerators of the form

$$V_{nl_1} V_{l_1 l_2} V_{l_2 n}$$

where $l_1 \neq l_2$. Also both l_1 and l_2 must have matrix elements with n. In this case, the only l_1 and l_2 candidates are $c_{k\tau}$ and $\Phi_d^{(2)}$. However, by looking at (4.36), it is obvious that for the natural choice of orthonormal basis that there is no matrix element of the form $V_{l_1 l_2}$. Therefore, in this natural representation, the impurity self energy can be rigorously written as

$$\sum(d\uparrow, \omega) = \gamma(\omega) + \frac{U^2 \langle n_{\downarrow} \rangle (1 - \langle n_{\downarrow} \rangle)}{\omega - ((\Phi_d^{(2)}, L\Phi_d^{(2)})) - \sum'(\Phi_d^{(2)}, \omega)}. \tag{4.38}$$

If one approximated $((\Phi_d^{(2)}, L\Phi_d^{(2)}))$ by $E_d + U(1 - \langle n_{d\downarrow} \rangle)$ and $\sum'$ by $\gamma(\omega)$, then Hewson's approximation would be recovered. More careful analysis of $L\Phi_d^{(2)}$ and other matrix elements determine $\sum'$ in various approximations.[27] For this paper, the relevant results are that (4.38) is rigorously true for all values of U, in particular for large U, the structure of the Feenberg formula allows one to infer that $\sum'$ can only depend on U through the energy denominators and thus that $\sum'/U \to 0$ a $U \to \infty$.

A more detailed analysis of this model will be given elsewhere. Now we seek to demonstrate that similar simplifications are achieved in other more complicated models. To do this we first examine a model which has been the testing ground for much of many body theory, an interacting electron gas.

D. The Coulomb gas

In this example a gas of electrons interacts via a two particle potential $v(r)$ whose Fourier transform is $v(\mathbf{q})$. The Hamiltonian for this model is taken to be

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{kqk}} v(\mathbf{q}) c_{\mathbf{k}+\mathbf{q}}^{\dagger} c_{\mathbf{k}'-\mathbf{q}}^{\dagger} c_{\mathbf{k}'} c_{\mathbf{k}}. \tag{4.39}$$

It shall be assumed that the gas is translationally invariant, and that $v(\mathbf{q}) = v(-\mathbf{q})$.

As the concern here is to illustrate the AHGF method, we consider only the one electron Green's function $\langle\langle c_{\mathbf{k}}; c_{\mathbf{k}}^{\dagger} \rangle\rangle$, leaving the discussion of $\chi(\mathbf{q}, \omega)$ to another time.

The first task is to compute the necessary matrix elements:

$$Lc_{\mathbf{k}s} = \epsilon_{\mathbf{k}s} c_{\mathbf{k}s} + \sum_{\mathbf{pqs}'} v(\mathbf{q}) c_{\mathbf{p}+\mathbf{q}s'}^{\dagger} c_{\mathbf{p}s'} c_{\mathbf{k}+\mathbf{q}s}. \tag{4.40}$$

We now want to be sure that the second term in (4.40) is orthogonal to the one electron subspace spanned by $c_{\mathbf{k}+\mathbf{q}'s}$, for all $\mathbf{q}'$. This requires the evaluation of

$$((c_{\mathbf{k}+\mathbf{q}'s}, c_{\mathbf{p}+\mathbf{q}s'}^{\dagger} c_{\mathbf{p}s'} c_{\mathbf{k}+\mathbf{q}s})) = \delta_{\mathbf{q},\mathbf{q}'} \langle c_{\mathbf{p}+\mathbf{q}s} c_{\mathbf{p}s'} \rangle - \delta_{\mathbf{p},\mathbf{k}+\mathbf{q}'} \delta_{s',s} \langle c_{\mathbf{p}+\mathbf{q}s}^{\dagger} c_{\mathbf{k}+\mathbf{q}s} \rangle. \tag{4.41}$$

Conservation of momentum shows that there is overlap only if $\mathbf{q}' = 0$, and

$$((c_{\mathbf{k}s}, c_{\mathbf{p}+\mathbf{q}s}^{\dagger} c_{\mathbf{p}s'} c_{\mathbf{k}+\mathbf{q}s})) = \delta_{\mathbf{q},0} \langle n_{\mathbf{p}s'} \rangle - \delta_{\mathbf{p},\mathbf{k}} \langle n_{\mathbf{k}+\mathbf{q}s} \rangle \delta_{s's}. \tag{4.42}$$

Before applying (4.42) to the Schmidt orthogonalization of (4.40), we must realize that elements $c_{-\mathbf{k}-\mathbf{q}'s}^{\dagger}$ are also orthonormal elements of the abstract odd-number-of-fermions Hilbert space. Thus we must require that the rhs of (4.40) must also be orthogonal to $c_{-\mathbf{k}-\mathbf{q}'s}^{\dagger}$. Conservation of momentum again requires that $q' = 0$ and yields

$$((c_{-\mathbf{k}s_1}^{\dagger}, c_{\mathbf{p}+\mathbf{q}s}^{\dagger} c_{\mathbf{p}s'} c_{\mathbf{k}+\mathbf{q}s})) = \delta_{\mathbf{p},-\mathbf{k}-\mathbf{q}} \langle c_{-\mathbf{k}-\mathbf{q}s_1} c_{\mathbf{k}+\mathbf{q}s} \rangle. \tag{4.43a}$$

The first step in the Schmidt procedure is to construct an orthogonal basis for the expansion of $Lc_{\mathbf{k}s}$. Adding and substracting the appropriate contributions yields the following orthogonal expansion—the vectors are not normalized to unity:

$$\begin{aligned} Lc_{\mathbf{k}s} = {} & (\epsilon_{\mathbf{k}s} - \sum_{\mathbf{q}} v(\mathbf{q}) \langle n_{\mathbf{k}+\mathbf{q}s} \rangle) c_{\mathbf{k}s} + \sum_{\mathbf{qs}'} v(\mathbf{q}) \langle c_{-\mathbf{k}-\mathbf{q}s'} c_{\mathbf{k}+\mathbf{q}s} \rangle c_{-\mathbf{k}s'}^{\dagger} \\ & - \sum_{\mathbf{q}} v(\mathbf{q}) (n_{\mathbf{k}+\mathbf{q}s} - \langle n_{\mathbf{k}+\mathbf{q}s} \rangle) c_{\mathbf{k}s} \\ & + \sum_{\mathbf{qs}'} v(\mathbf{q}) c_{-\mathbf{k}s'}^{\dagger} (c_{-\mathbf{k}-\mathbf{q}s'} c_{\mathbf{k}+\mathbf{q}s} - \langle c_{-\mathbf{k}-\mathbf{q}s'} c_{\mathbf{k}+\mathbf{q}s} \rangle) \\ & + \sum_{\substack{\mathbf{qs}' \\ \mathbf{p} \neq \mathbf{k} \\ \mathbf{p} \neq -\mathbf{k}-\mathbf{q}}} v(\mathbf{q}) c_{\mathbf{p}+\mathbf{q}s'}^{\dagger} c_{\mathbf{p}s'} c_{\mathbf{k}+\mathbf{q}s}. \end{aligned} \tag{4.43b}$$

To proceed further requires the normalization of the three-particle operators in (4.43) and then a study of an orthonormal basis of the three-particle subspace. The orthogonalization process done to this point simply guarantees that the one particle and three particle subspaces are orthogonal for fixed k. Before proceeding with the somewhat complicated analysis of the three-particle subspace, let us briefly examine the approximation in which we somewhat arbitrarily restrict (4.43) to the one-particle subspace. Defining

$$E_k = \epsilon_{ks} - \sum_q v(q)\langle n_{k+q\,s}\rangle \tag{4.44}$$

and

$$-\Delta_{ks'} = \sum_q v(q)\langle c_{-k-qs'}\, c_{k+q\,s}\rangle, \tag{4.45}$$

we can write

$$Lc_{ks} = E_{ks}c_{ks} - \Delta_k c^\dagger_{-ks'}. \tag{4.46}$$

The determination of the corresponding equation for $Lc^\dagger_{-ks'}$ and the subsequent evaluation of $\langle c_{-k-q}c_{k+q}\rangle$ using the standard formulas[28] involving the spectral function of the Green's function[29]

$$((c_{ks},(\omega - L)^{-1}c^\dagger_{-ks'}))$$

allows one to see that this is just the BCS model of superconductivity[30] if $v(q)$ is attractive.

From the point of view of the AHGF method, the BCS model of superconductivity is a kind of Hartree–Fock approximation in that it restricts the expansion of the generalized Hamiltonian to the one-particle subspace. This is in agreement, with other field theoretic methods[31] applied to this problem, though here the matrix elements arise from the Schmidt orthonormalization procedure, rather than as initially unknown Hartree potentials. Clearly, the AHGF method yields an unambiguous procedure for calculating self energy corrections to the simplest BCS theory.

For simplicity in the following let us consider only a normal metal and not explicitly orthogonalize with respect to the $c_k^\dagger$ subspace. This will make the subsequent discussion much more transparent.

One of the properties of a normal system which is usually assumed is that there is a sharp Fermi surface. That is, that $\langle n_{ks}\rangle$ has a sharp jump at the Fermi surface if the temperature is zero. The presence of a sharp Fermi surface at low temperatures will be assumed in the following discussion.

The first step in analyzing the three-particle states in (4.43) is to construct an orthonormal basis of the three-particle subspace with a given momentum $-\mathbf{k}$. From Eq. (4.43) we saw that one of the naturally occurring three-particle vectors was

$$\Phi_{k,qs} = (n_{k+qs} - \langle n_{k+q,s}\rangle)c_{ks}. \tag{4.47}$$

The norm of this vector is easily computed to be

$$((\Phi_{k,qs}, \Phi_{k,qs}))^{1/2} = (\langle n_{k+qs}\rangle(1 - \langle n_{k+qs}\rangle))^{1/2}. \tag{4.48}$$

When the metal has a sharp Fermi surface so that the average of n_{k+qs} is approximately 1 or 0 depending on whether $\mathbf{k}+\mathbf{q}$ is below or above the Fermi surface, then the state $\Phi_{k,qs}$ will enter into the calculation only for values of $\mathbf{k}+\mathbf{q}$ on the Fermi surface as $T \to 0$. For these Fermi surface values of $\mathbf{k}+\mathbf{q}$, the state $\Phi_{k,qs}$ has an overlap with the other class of unit vectors

$$\psi^{(2)}(\mathbf{p}+\mathbf{q}, \mathbf{p}s'; \mathbf{k}+\mathbf{q}s) = \frac{c^\dagger_{p+qs'}\, c_{ps'}\, c_{k+qs}}{(\langle n_{p+q\,s'}(1-n_{p\,s'})\rangle + \langle n_{k+q\,s}(n_{ps'} - n_{p+qs'})\rangle)^{1/2}}. \tag{4.49}$$

If $\mathbf{k}+\mathbf{q}$ is not near the Fermi surface, then there is no overlap and the $\psi^{(2)}$ form an orthonormal basis for the rest of the subspace.

In the region of strong overlap of $\psi^{(2)}$ and $\Phi_{k,q}$, the overlaps are of the form

$$\langle c^\dagger_{ks} c^\dagger_{p+qs'}\, c_{p\,s'} c_{k+qs}\rangle$$

which is one of the terms which contribute to the structure factor $S(q)$ of the gas

$$S(q) = \langle \rho^\dagger_q \rho_q\rangle. \tag{4.50}$$

The analysis of the orthonormal "states" in this strongly mixed region of the subspace is very complicated and cannot be adequately examined here. By examining the contribution to the self energy from all of the other states in the three-particle subspace it is still possible to illustrate further properties of the AHGF method. The particular property to be illustrated below is that the self energy contribution of the form

$$\sum_{l\neq n} \frac{|V_{ln}|^2}{\omega - e_l(n)}$$

for state l of the $\psi^{(2)}$ form gives a contribution to the one-electron lifetime which is very close to being the exact expression for the inverse of the dielectric function of the electron gas. This may be seen by examining this approximation to the one-electron Green's function.

We have, approximately,

$$G(\mathbf{k},\omega)^{-1} = \omega - \epsilon_{ks} + \sum_q v(q)\left(\langle n_{k+qs}\rangle - v(q)\sum_{p\neq n}\frac{\langle n_{k+qs}(n_{ps'} - n_{p+qs'})\rangle}{\omega - \epsilon_{k+q} + \epsilon_{p+q} - \epsilon_p - \sum'}\right), \tag{4.51}$$

where the appropriate reduced self energy has been noted symbolically as $\sum'$. Because of the presence of the reduced self energy in the denominator and because the $n_{p's}$ represent the exact number operators, it quite tempting to regard the expression in brackets as being close to the thermal expectation of n_{k+qs} divided by the dielectric function. If one approximates the average $\langle n_{k+qs}(n_{ps'} - n_{p+q\,s'})\rangle = \langle n_{k+qs}\rangle(\langle n_{ps'}\rangle - \langle n_{p+qs'}\rangle)$, then the self energy in (4.51) becomes

$$-\sum_q v(q)\langle n_{k+qs}\rangle\left[1 - v(q)\sum_{\substack{p\neq n\\ s'}}\frac{\langle n_{ps'}\rangle - \langle n_{p+qs'}\rangle}{\omega - \epsilon_{k+q} + \epsilon_{p+q} - \epsilon_p - \sum'}\right]. \tag{4.52}$$

The quantity in brackets now is a very close approximation to the Nozieres and Pines expression[33] for the inverse of the dielectric constant. This identification is not exact and requires much more analysis than has been accomplished at this time. If the expression for the self energy effectively truncates similar to the Anderson model, then the identification of (4.52) as the properly screened Coulomb potential, then the Feenberg method would be a formalism which has already summed the Brueckner–Gellman bubble graphs[32] of the RPA approximation. If this is not the case, then the contribution in (4.52) is the beginning of a series as arose in the Koster–Slater example studied previously. The simplest approximation to the sum of such a series whose first terms are $(1+\alpha)$ is simply $(1-\alpha)^{-1}$ which gives the standard RPA result for the electron lifetime.[34]

The electron gas is an extremely complicated example and much more analysis must be done before the relative merits of the AHGF method in this problem can be evaluated. Unfortunately, the required analysis is not complete at this time. Nevertheless, the preceding discussion has indicated some aspects of the AHGF method for such a many body example.

E. The fermion–boson coupling

In this section a simple model Hamiltonian representing the coupling of the electron to a scalar boson field will be examined from the AHGF method. This model can be thought of as representing the electron phonon interaction or as the simplest field theory model of a fermion–boson coupling. Writing a_q as the annihilation operator of the bosons, the Hamiltonian is

$$H=\sum_k \epsilon_k c_k^\dagger c_k+\sum_{k,q}\lambda_q c_k^\dagger c_{k+q}(a_q+a_q^\dagger)+\sum_q h\omega_q a_q^\dagger a_q \tag{4.53}$$

where λ_q is some coupling parameter. Again we study the one-electron function $(c_k,(\omega-L)^{-1}c_k))$. In the sums over the phonon wavevector q, there is no $q=0$ value.

Because the abstract Hilbert space matrix elements involve the average of groups of operators over the ensemble of states, or over the ground state, the specification of the various expectation values determines the properties of the ground state or most probable state. Within any calculational scheme using AHGF, the self-consistent determination of various expectation values is accomplished using the approximate spectral functions of the various Green's functions.

There are other consistency relations which are generated by the Heisenberg equation of motion and the assumption that the Hamiltonian commutes with the density matrix defining the ensemble average. The simplest of these relations will illustrate the class of equations of this type.

Consider the average value of the Heisenberg operator $a_q(t)$ at time t. Because H commutes with ρ the average value is in fact time independent:

$$\langle a_q(t)\rangle=\langle a_q\rangle. \tag{4.54}$$

One can, however, calculate the time derivative of the expectation value and derive a consistency relation which must be obeyed by various expectation values:

$$0=\frac{i\partial}{\partial t}\langle a_q(t)\rangle=\omega_q\langle a_q\rangle+\lambda_q\sum_{k'}\langle c_{k'}{}^\dagger c_{k'-q}\rangle. \tag{4.55}$$

Note first that this equation only holds for $q\neq 0$, since the mode of uniform displacement is excluded from the Hamiltonian. If momentum conservation is considered, one immediately sees that the second term in (4.55) must vanish unless $(q=0)$. This implies for $q\neq 0$ that

$$\omega_q\langle a_q\rangle=0,$$

and similarly for $a_q^\dagger$.

More complicated relations can obviously be derived and are used to explicitly demonstrate the symmetry of matrix elements of L in the more complicated subspaces of the generalized operator Hilbert space.[35]

The following discussion of the general structure of the AHGF approach to this Hamiltonian will be quite abbreviated. The only intent of this section is to outline some of the differences between this method and the usual diagrammatic methods. The usual method expands the electron self energy in a series of terms involving the exact one-electron propagator and the exact one-phonon propagator. The AHGF method, on the other hand, will involve an expansion in terms of intermediate states in which an interacting electron and phonon are simultaneously present. This difference in the kind of intermediate states could have significant consequences as regards the convergence properties of the theory *per se* and any approximation scheme generated within the theory. Any questions of this sort are beyond the scope of this paper and will not be discussed here. Here it will be enough to indicate the overall structure of the equations.

To determine the one-electron function we need to examine Lc_k,

$$Lc_k=\epsilon_k c_k+\sum_{q\neq 0}\lambda_q\Phi^{(a)}_{k,q}+\sum_{q\neq 0}\lambda_q\Phi^{(b)}_{k,q}, \tag{4.56}$$

where

$$\Phi^{(a)}_{k,q}=a_{-q}c_{k+q} \tag{4.57}$$

and

$$\Phi^{(b)}_{k,q}=a^\dagger{}_q c_{k+q}. \tag{4.58}$$

Here we see that there are only two types of operators which couple into the one-electron states. It is easy to verify that these two elements are orthogonal:

$$((\Phi^{(a)}_{k,q},\Phi^{(b)}_{k,q}))=\delta_{q,q'}\langle a^\dagger{}_q a^\dagger_{-q'}\rangle=0. \tag{4.59}$$

If there were no other vectors spanning the one-electron–one-phonon (1, 1) subspace, and if there were no matrix elements of the sort $((\Phi^{(a)}_{k,q},L\Phi^{(b)}_{k,q'}))$, then the self energy would truncate in much the same way as for the Anderson model. However, a moment's reflection will reveal that the (1, 1) subspace is spanned by two other independent vectors

$$\Phi^{(c)}_{k,q}=a_{-q}c_{-k-q} \tag{4.60}$$

and

$$\Phi^{(d)}_{k,q}=a^\dagger{}_q c^\dagger_{-k-q}. \tag{4.61}$$

While $\Phi^{(c)}$ and $\Phi^{(d)}$ are orthogonal, there is a possibly nonvanishing overlap between (a) and (c) and between (b) and (d),

$$((\Phi^{(a)}_{k,q},\Phi^{(c)}_{kq'}))=-\delta_{qq'}\langle c^\dagger_{k+q}c^\dagger_{-k-q}\rangle. \tag{4.62}$$

All other overlaps between these four vectors are zero. To proceed with the AHGF calculation one needs to first construct an orthonormal basis of this (1, 1) subspace. This can be done in several ways. A natural basis is to choose $\psi^A_{k,q}$ and $\psi^B_{k,q}$ as unit vectors, where

$$\psi^A_{k,q}=a_{-q}c_{k+q}/\sqrt{1+\langle N_q\rangle-\langle n_{k+q}\rangle}\,, \tag{4.63}$$

$$\psi^B_{k,q}=a^\dagger{}_q c_{k+q}/\sqrt{\langle N_q\rangle+\langle n_{k+q}\rangle}\,, \tag{4.64}$$

and to construct a ψ^C and ψ^D using the Schmidt procedure.

This choice of basis maintains the condition that only the two types of functions ψ^A and ψ^B have matrix elements with $c_{\mathbf{k}}$. The expansion of $Lc_{\mathbf{k}s}$ in this basis is

$$Lc_{\mathbf{k}} = \epsilon_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{q}\neq 0}{}' \lambda_{\mathbf{q}} \sqrt{1 + \langle N_{\mathbf{q}}\rangle - \langle n_{\mathbf{k}+\mathbf{q}}\rangle}\, \psi^A_{\mathbf{k},\mathbf{q}} + \sum_{\mathbf{q}\neq 0}{}' \lambda_{\mathbf{q}} \sqrt{\langle N_{\mathbf{q}}\rangle + \langle n_{\mathbf{k}+\mathbf{q}}\rangle}\, \psi^B_{\mathbf{k},\mathbf{q}}. \tag{4.65}$$

It is important to point out here the feature of this method which the normalization of the vectors entails. The sums over q in (4.65) must be restricted to only those values of q for which the vectors of the space have a positive and nonvanishing square of their norm. The primes in (4.65) indicate that the sums are to be so restricted.

The choice of basis leading to (4.65) may not, in many cases, be the most convenient for a particular approximation scheme. If one wants to recover superconductivity from this Hamiltonian it would seem more convenient to choose a basis of this subspace which would bring the pairing amplitude $\langle c^\dagger_{\mathbf{k}+\mathbf{q}} c^\dagger_{-\mathbf{k}-\mathbf{q}}\rangle$ directly into the one-electron self energy expressions; such a basis can be achieved by using the unit vectors derived from $\Phi^{(c)}_{\mathbf{k},\mathbf{q}}$ and $\Phi^{(d)}_{\mathbf{k},\mathbf{q}}$ as basis vectors and constructing the other two using the Schmidt procedure. Such a basis does recover BCS-like Green's functions in various crude approximations.

The exact evaluation of the self energy requires the determination of orthonormal expansions for L operating on the (1, 1) subspace. This can be carried out with the help of various self-consistency conditions[36] which can be derived like (4.55). The orthonormal expansion for a fixed q does involve matrix elements among the ψ^A, ψ^B, ψ^C, and ψ^D, so the self energy does not truncate as simply as found in the Anderson model. The contribution for each q to the one-electron self energy will involve the three V terms in the Feenberg formulas as well as the $|V_{nl}|^2$ terms.

A self-consistent study of this model has as yet been carried out in anything only the simplest of approximations.

It would be of great interest to examine the convergence properties of this sort of development, as it has much more structure than do the usual field theoretic expansions. Such questions are being examined.

The last example of this paper encompasses the interesting question of the breakdown of translational invariance due to substitutional disorder. It is included to illustrate that the averaging procedure which defines the abstract Hilbert space scalar product can also include configuration averaging. This will allow the calculation of configuration averaged Green's functions of various sorts in which the ensemble averaged matrix elements of the self energy expansion can be exactly determined to a given order.

F. Disordered alloy

Much interest has recently been generated in calculating configurationally averaged properties of substitutional alloys. The AHGF method is well adapted for the calculation of configuration averaged Green's functions. As an illustration of the basic application, only enough of the problem will be discussed below to show that the coherent potential approximation for diagonal disorder can be determined. Extensions of this formalism to off-diagonal disorder and approximations beyond the single site approximation will be discussed elsewhere.

The AHGF method could be applied either in the Wannier representation or in a momentum representation. The site representation is somewhat better adapted to extensions beyond the single site approximation, but requires care in truncating the self energy approximations. This occurs partially because the site representation is not amenable to simplification in the N/V limit. In order to utilize the simplifications of the N/V limit, the following discussion will be in the Bloch representation.

Consider a lattice on which n different types of atoms can be randomly distributed on the sites. If the Wannier states of the lattice are created by $c^\dagger_{\mathbf{l}}$ and if the matrix elements in a Wannier representation are ϵ_α and $t_{\alpha\beta}$, where α, β are indices labeling the atom types, the Hamiltonian may be written

$$H = \sum_{\mathbf{l}\alpha} \epsilon_\alpha N_{\mathbf{l}\alpha} c_{\mathbf{l}}{}^\dagger c_{\mathbf{l}} + \sum_{\substack{\mathbf{l}\mathbf{l}'\\ \alpha\beta}} t^{\mathbf{l}\mathbf{l}'}_{\alpha\beta} N_{\mathbf{l}\alpha} N_{\mathbf{l}'\beta} c^\dagger{}_{\mathbf{l}} c_{\mathbf{l}'}. \tag{4.66}$$

Here the $N_{\mathbf{l}\alpha}$ are projection operators on the lattice sites for the αth specie, and have value l if the αth type is present and 0 otherwise.

We set out to determine the configuration averaged Green's function $((c_{\mathbf{k}}, (\omega - L)^{-1} c_{\mathbf{k}}))$ where now the trace includes a configuration average over the ensemble of disordered lattices.

In the Bloch representation the equation for $Lc_{\mathbf{k}}$ is

$$Lc_{\mathbf{k}} = \frac{1}{N} \sum_{\mathbf{l}\alpha\mathbf{q}} \epsilon_\alpha N_{\mathbf{l}\alpha} \exp(i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}})\, c_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}} c_{\mathbf{k}}, \tag{4.67}$$

where for simplicity we have restricted the application to diagonal disorder only and included the band energy $\epsilon_{\mathbf{k}}$.

The first step of the method is to secure an orthonormal expansion of (4.67). The first term in (4.67) is not orthogonal to $c_{\mathbf{k}}$, since

$$\left(\left(c_{\mathbf{k}+\mathbf{q}'}, \frac{1}{N} \sum_{\mathbf{l}\alpha} \epsilon_\alpha N_{\mathbf{l}\alpha} \exp(i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}})\, c_{\mathbf{k}+\mathbf{q}} \right) \right) = \delta_{\mathbf{q},\mathbf{q}'}\, \delta_{\mathbf{q},0} \langle\epsilon\rangle, \tag{4.68}$$

where $\langle\epsilon\rangle = \sum_\alpha \epsilon_\alpha x_\alpha$ and x_α is the concentration of the αth species in the ensemble. The straightforward orthogonalization yields

$$Lc_{\mathbf{k}} = (\epsilon_{\mathbf{k}} + \langle\epsilon\rangle) c_{\mathbf{k}} + \frac{\sqrt{\langle\epsilon^2\rangle - \langle\epsilon\rangle^2}}{\sqrt{N}} \sum_{\mathbf{q}} \psi^{(1)}_{\mathbf{k},\mathbf{q}}, \tag{4.69}$$

where the standard assumption has been made that the occupation of different sites in independent, and where

$$\psi^{(1)}_{\mathbf{k},\mathbf{q}} = \sum_{\mathbf{l}\alpha} \frac{\epsilon_\alpha (N_{\mathbf{l}\alpha} - x_\alpha) \exp(i\mathbf{q}\cdot\mathbf{R}_{\mathbf{l}})}{\sqrt{N}\, \sqrt{\langle\epsilon^2\rangle - \langle\epsilon\rangle^2}}\, c_{\mathbf{k}+\mathbf{q}}. \tag{4.70}$$

The calculation of $L\psi^{(1)}_{\mathbf{k},\mathbf{q}}$ and the determination of the required orthonormal expansion gives the following matrix elements:

$$((\psi^{(1)}_{\mathbf{k},\mathbf{q}}, L\psi^{(1)}_{\mathbf{k},\mathbf{q}})) = \epsilon_{\mathbf{k}} + \langle\epsilon\rangle,$$

$$((c_{\mathbf{k}}, L\psi^{(1)}_{\mathbf{k},\mathbf{q}})) = \frac{1}{\sqrt{N}}\ \sqrt{\langle\epsilon^2\rangle - \langle\epsilon\rangle^2}\,, \tag{4.71}$$

$$((\psi^{(1)}_{\mathbf{k},\mathbf{q}+\mathbf{q}'}, L\psi^{(1)}_{\mathbf{k},\mathbf{q}})) = \frac{1}{N}\ \frac{\langle(\epsilon - \langle\epsilon\rangle)^3\rangle}{\sqrt{\langle\epsilon^2\rangle - \langle\epsilon\rangle^2}}.$$

With just these matrix elements the first two contributions to the one-electron self energy can be determined and they are

$$\sum(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{(\langle\epsilon^2\rangle - \langle\epsilon\rangle^2)}{\omega - e^{(1)}_{\mathbf{k}+\mathbf{q}}(0)} + \frac{1}{N^2}\sum_{\substack{\mathbf{q}\neq 0\\ \mathbf{q}'\neq\mathbf{q},0}}\frac{\langle(\epsilon - \langle\epsilon\rangle)^3\rangle}{(\omega - e^{(1)}_{\mathbf{k}+\mathbf{q}}(0))(\omega - e^{(1)}_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}(0))}, \tag{4.72}$$

where

$$e^{(1)}_{\mathbf{k}+\mathbf{q}}(0) = \langle\epsilon\rangle + \epsilon_{\mathbf{k}+\mathbf{q}} + \sum{}'(\psi_{\mathbf{k},\mathbf{q}}, \omega) \tag{4.73}$$

and $\sum'$ is the reduced self energy for the state $\psi^{(1)}_{\mathbf{k},\mathbf{q}}$. With just these terms, if the reduced self energy is assumed to be the same as the one-electron self energy, the CPA approximation can be obtained as the simplest terminated continued fraction expansion[37] of a series with the first two terms as in (4.73). This is effectively the way that Onodera and Toyozawa[38] first derived the CPA, though they used a diagrammatic expansion to generate the expansion for the self energy. The details of terminated continued fraction interpolation approximations has been discussed in Wall and the work of this author[37] and will not be discussed here.

The value of the AHGF method in application to the disordered alloy problem lies in the fact that for any kind of disorder (diagonal or off-diagonal) with or without correlation between sites the contributions to the self energy could be calculated to almost any degree of complexity. In many cases this still leaves one with the task of seeking a self-consistent approximation, but the AHGF method allows one to calculate the self energy directly and thus is a vast improvement over any scheme which calculates only the moments of the Green's function. Using the AHGF method, the same effort used in calculating moments will determine exact contributions to the self energy in a rigorously established expression which is contained in a very large number of moments.

G. Extension to Bose excitations

The discussion concerning the calculation of density–density correlation functions used the symmetry properties of the density operators to derive the inner product

$$((A, B))_b = \langle[[B, H], A^\dagger]\rangle. \tag{4.74}$$

As such the formulas for calculating functions were strictly only valid for certain symmetric operators. A more general class of retarded Green's functions and correlation functions may be calculated using the following formula for the moment expansion of a general commutator based Green's function:

$$\langle\langle A; B^\dagger\rangle\rangle_\omega = \frac{\langle[A(0), B^\dagger(0)]\rangle}{\omega} + \frac{1}{\omega}\sum_{L=0}^{\infty}\frac{\langle L^N[[A, H], B^\dagger]\rangle}{\omega^{N+1}}. \tag{4.75}$$

Clearly, this is just the formal moment expansion of the following function:

$$\langle\langle A; B^\dagger\rangle\rangle_\omega = \frac{1}{\omega}\langle[A(0), B^\dagger(0)]\rangle + \frac{1}{\omega}((B, (\omega - L)^{-1}A))_b \tag{4.76}$$

where the inner product to be used is (4.74).

Equation (4.76) can be used to compute the properties of magnons in or not in a magnetic field,[39] the properties of the Bose gas, or a general correlation function.[40] In all of these cases the AHGF method allows the study of lifetime effects, and a tool for the self-consistent study of these systems.

One application of interest which these formulae allow is the determination of the conductivity of a disordered alloy. This work will be discussed elsewhere.[41]

V. SUMMARY

This paper has attempted to clearly delineate the rigorous mathematical foundations of a new method of studying quantum field theory models of a wide variety. The basic properties of the method were demonstrated by showing the properties of the Feenberg perturbation theory and detailing its generalization to the operator Hilbert spaces and its simplification in the thermodynamic limit.

The possible breadth of its application and some of the structure of the theory has been sketched in several very brief examples. None of these were in any sense complete, but were intended to illustrate a small aspect of this method and to indicate where this method might yield advantages over other approximation schemes.

Although it has not been thoroughly demonstrated here, this abstract Hilbert space generalization of the Feenberg perturbation theory is a radical departure from the traditional methods of quantum field theory. The Feenberg formulas for matrix elements of the resolvent of L when viewed as representing the limiting case with all states represented is an *exact* expression for the Green's function. It is not an expansion in terms of some small parameter, asymptotic or otherwise. As an exact expression the AHGF formulas allow the possible study of a whole class of strong coupling problems which have not been easily studied before. While the method has been thoroughly outlined as regards its foundations, the particular approximation techniques which will work best are only partially known.

Finally, because the Green's functions involve various expectation values of groups of operators averaged over the ensemble or ground states, the AHGF method offers the possibility of self-consistently determining the properties of the ensemble or ground state.

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Multiple scattering of waves by the doubly periodic planar array of obstacles*

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We analyze the three-dimensional problem of multiple scattering by a doubly periodic planar array of bounded obstacles, and compare the results with those for the grating of parallel cylinders in two dimensions and for the periodic line in three. Plane wave integral forms of the scattered field and of the multiple scattered amplitude lead directly to the array-mode functional representation in terms of the single scattered amplitude and to simple approximations corresponding to array resonances for near-grazing evanescent modes. For the grating and for the periodic line, a grazing mode corresponds to reinforcement of the excitations an obstacle receives from the waves scattered by its neighbors; for the doubly periodic array, to reinforcement of the waves of the lattice lines perpendicular to the mode's direction. We also derive spherical wave (and conical–cylindrical wave) representations of the solution, and exhibit the results for spherically symmetric scatterers as a special case.

INTRODUCTION

In a recent paper[1] we considered multiple scattering of waves by the infinite line of equally spaced identical obstacles, and compared the results with corresponding expressions for the infinite grating of parallel cylinders.[2,3] Now we generalize the development to the analogous doubly periodic planar array of bounded obstacles. The present expressions are closer in form to those for the grating than for the periodic line; similarities will be mentioned and differences will be stressed.

As before,[1,2] there are essentially two classes of multiple scattering phenomena that are of particular interest. The first (analogous to the Wood's anomalies for the grating[4,5]) relates to array resonances associated with near-grazing evanescent modes for spacings moderate or large compared to wavelength, and the second, to multipole coupling for spacings small compared to wavelength. We analyze the first in the present paper, but reserve discussion of the second (which requires detailed consideration of the appropriate lattice sums).

The primary development is based on plane wave integral forms of the scattered field and of the multiple scattered amplitude. These lead directly to the array-mode functional representation in terms of the single scattered amplitude, and to simple approximations for the array resonances. For the grating and for the periodic line, a grazing mode corresponds to reinforcement of the excitation that an obstacle receives from the waves scattered by its neighbors, i.e., for such modes the waves of all neighbors are in phase at the obstacle. For the present case, a grazing mode corresponds to reinforcement of the waves of the lattice lines perpendicular to the mode's direction.

We also derive spherical wave and conical-cylindrical wave representations. Results for spherically symmetric scatterers are exhibited as a special case.

For brevity, we write (1.9) for Eq. 9 of Ref. 1, etc. For concreteness, we use some terminology and illustrations from small-amplitude acoustics.

1. SOLUTION

Consider a plane wave with propagation vector $\mathbf{k}_0 = k\hat{\mathbf{k}}_0$, $0 < \hat{\mathbf{z}}\cdot\hat{\mathbf{k}}_0 \leq 1$,

$$\phi_0 = \exp(i\mathbf{r}\cdot\mathbf{k}_0), \quad \hat{\mathbf{r}} = \hat{\mathbf{r}}(\theta;\varphi) = \hat{\mathbf{z}}\cos\theta + (\hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi)\sin\theta,$$

$$\hat{\mathbf{k}}_0 = \hat{\mathbf{r}}(\theta_0;\varphi_0) \tag{1}$$

incident on a doubly periodic planar distribution of identical obstacles. The center of the smallest sphere (of radius a) circumscribing a scatterer is located in the plane $z=0$ at the lattice site

$$\mathbf{b}_s = \mathbf{b}(s_1, s_2) = s_1 b_1 \hat{\mathbf{x}} + s_2 b_2 \hat{\mathbf{y}}, \quad s_i = 0, \pm 1, \pm 2, \cdots. \tag{2}$$

In the region external to the scatterers, the solution of Helmholtz's equation

$$(\nabla^2 + k^2)\Psi = 0, \quad \Psi = \phi_0 + \mathit{U} \tag{3}$$

subject to any of the usual conditions at the scatterers' surfaces (e.g., for Ψ as the excess pressure in acoustics) is the sum of the excitation ϕ_0 and the total scattered field U. Initially we write U as a set of waves radiating from $\mathbf{b}_s$,

$$\mathit{U} = \sum_s U(\mathbf{r}_s)\exp(i\mathbf{k}_0\cdot\mathbf{b}_s), \quad \mathbf{r}_s = \mathbf{r} - \mathbf{b}_s,$$

$$\sum_s = \sum_{s_1=-\infty}^{\infty}\sum_{s_2=-\infty}^{\infty} = \sum_{s_2}\sum_{s_1}, \tag{4}$$

where the multiple scattered field $U(\mathbf{r}_s)$ of one obstacle is determined essentially by its single scattering analog $U(\mathbf{r}_s)$ (the response of one obstacle in isolation) and by the geometry of the array.[6] In terms of the present $\mathbf{b}_s$, we specify U by its multiple scattering amplitude G as in (6.31), and G by its single scattered analog g as in the functional equation $G[g]$ of (6.34). The equality of the iterates in (4) required by symmetry follows, e.g., if the double series and the row and column series simply converge; however, we may use $k = (2\pi/\lambda) + i\epsilon$ to obtain absolute convergence, and then let $\epsilon = |\epsilon| \to 0$.

We express the direction of incidence $\hat{\mathbf{k}}_0$ as

$$\hat{\mathbf{k}}_0 = \hat{\mathbf{x}}\xi_0 + \hat{\mathbf{y}}\eta_0 + \hat{\mathbf{z}}\zeta_0, \quad \zeta_0 = (1 - \xi_0^2 - \eta_0^2)^{1/2} \tag{5}$$

with ξ_0 and η_0 (or, collectively, ξ_{i0}) regarded as positive, and rewrite the complex integrals in $\int d\Omega(\hat{\mathbf{p}})$ of (6.31) for U as real integrals over the corresponding direction cosines. If $z > a$,

$$U = \int \exp(ik\hat{\mathbf{p}}\cdot\mathbf{r}_s)\, G(\hat{\mathbf{p}}, \hat{\mathbf{k}}_0)\, d\Omega(\hat{\mathbf{p}})/2\pi$$

$$= \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\eta \exp(ik\hat{\mathbf{p}}\cdot\mathbf{r}_s)\, G(\hat{\mathbf{p}}, \hat{\mathbf{k}}_0)/\zeta 2\pi, \tag{6}$$

where $\hat{\mathbf{p}} = \hat{\mathbf{x}}\xi + \hat{\mathbf{y}}\eta + \hat{\mathbf{z}}\zeta$ with $\zeta = (1 - \xi^2 - \eta^2)^{1/2} = |\zeta|$ or $i|\zeta|$ for $\xi^2 + \eta^2 < 1$ or > 1; if $z < -a$, we replace $\hat{\mathbf{p}}$ by $\hat{\mathbf{p}}' = \hat{\mathbf{p}} - 2\zeta\hat{\mathbf{z}}$ (its image in the plane $z = 0$). Substituting into (4), we sum over s_i

$$\sum_{s_i=-\infty}^{\infty} \exp[iks_i b_i(\xi_{i0} - \xi_i)] = \frac{2\pi}{kb_i} \sum_{\nu_i=-\infty}^{\infty} \delta(\xi_i - \xi_{\nu i}),$$

$$\xi_{\nu i} = \xi_{i0} + \frac{2\pi\nu_i}{kb_i}, \quad \nu_i = 0, \pm 1, \pm 2, \cdots \tag{7}$$

and then integrate. Thus, for $z > a$

$$U = 2\sum_{\nu} C_\nu \phi_\nu G_{\nu 0}, \quad G_{\nu 0} = G(\hat{\mathbf{k}}_\nu, \hat{\mathbf{k}}_0), \quad C_\nu = \frac{\pi}{k^2 b_1 b_2 \zeta_\nu},$$

$$\sum_{\nu} = \sum_{\nu_1=-\infty}^{\infty} \sum_{\nu_2=-\infty}^{\infty},$$

$$\phi_\nu = \exp(i\mathbf{r}\cdot\mathbf{k}_\nu), \quad \hat{\mathbf{k}}_\nu = \hat{\mathbf{k}}(\nu_1, \nu_2) = \hat{\mathbf{x}}\,\xi(\nu_1) + \hat{\mathbf{y}}\,\eta(\nu_2) + \hat{\mathbf{z}}\,\zeta(\nu_1, \nu_2) \tag{8}$$

with $\xi(\nu_1) = \xi_{\nu_1}$, $\eta(\nu_2) = \eta_{\nu_2} = \xi_{\nu_2}$ in terms of ξ_{ν_i} of (7). Similarly, for $z < -a$,

$$U = 2\sum_{\nu} C_\nu \phi_{\nu'} G_{\nu' 0}, \quad G_{\nu' 0} = G(\hat{\mathbf{k}}_{\nu'}, \hat{\mathbf{k}}_0),$$

$$\phi_{\nu'} = \exp(i\mathbf{r}\cdot\mathbf{k}_{\nu'}), \quad \hat{\mathbf{k}}_{\nu'} = \hat{\mathbf{x}}\,\xi(\nu_1) + \hat{\mathbf{y}}\,\eta(\nu_2) - \hat{\mathbf{z}}\,\zeta(\nu_1, \nu_2) \tag{9}$$

where $\phi_{\nu'}$ is the image of ϕ_ν in the plane of the array. The forms for U are identical with those for the grating,[3] but now they correspond to a double infinite set of waves.

The images ϕ_ν and $\phi_{\nu'}$ have the identical $x, y, |z|$ dependence, i.e., collectively

$$\phi_\nu(|z|) = \exp[ik(x\xi_{\nu_1} + y\eta_{\nu_2} + |z|\zeta)] \tag{10}$$

represents one mode. If $\xi^2 + \eta^2 = \sin^2\theta < 1$, then $\zeta = \cos\theta = (1 - \xi^2 - \eta^2)^{1/2} = |\zeta|$, and ϕ corresponds to a propagating mode, an outgoing wave along $|z|$; if $\sin^2\theta > 1$, then $\zeta = i|\zeta| = i|\cos\theta|$, and ϕ is an evanescent mode decaying exponentially along $|z|$. The situation $\cos\theta \to \cos\theta_R = 0$, corresponding to a grazing mode

$$\phi_R = \exp[ik(x\xi_{\nu_1} + y\eta_{\nu_2})], \tag{11}$$

is exceptional, and occurs only for special values of k, b_i, and ξ_{i0}; we consider $\cos\theta \to 0$ separately. Although U appears to diverge for a grazing mode, we show subsequently that it does not. The phenomena occurring for near-grazing evanescent modes ($\cos\theta = \cos\theta_N = i|\epsilon| \approx 0$) are analogous to the Wood anomalies for the grating,[4] and the parameters (k_R, ξ_{Ri}) that specify the grazing modes are the analogs of those considered originally by Rayleigh[5] for grating resonances.

The general form of U, say $\sum_\nu Q_{\nu 0}\phi_\nu(|z|)$ follows directly from the geometry of the array. The geometry b_s requires that U/ϕ_0 have periods b_1 in x and b_2 in y, and that U satisfies the radiation condition for an essentially one-dimensional scatterer as $|z| \sim \infty$; this leads immediately to the Fourier expansion in terms of $\phi_\nu(|z|)$. The proportionality of $Q_{\nu 0}$ to $C_\nu G_{\nu 0}$ may be inferred from elementary considerations: the first Fresnel zone corresponding to the propagating mode along $\hat{\mathbf{k}}_\nu$ has area $\pi r\lambda/\cos\theta_\nu$, and $(b_1 b_2)^{-1}$ is the number of scatterers in unit area of array. Asymptotically, the wave scattered by the central obstacle is $U \sim (\exp(ikr)/ikr)G = h(kr)\, G(\hat{\mathbf{r}}, \hat{\mathbf{k}}_0)$, so that $Q_{\nu 0}\phi_\nu$ is proportional to the scattering by the obstacles in the first Fresnel zone. Equivalently, we may obtain the rigorous result (8) by an asymptotic evaluation of the corresponding Fresnel approximation, or by using $U(\mathbf{r}_s) \sim h(kr_s)\, G(\hat{\mathbf{r}}_s, \hat{\mathbf{k}}_0)$ in (4) and evaluating the sum by the method of stationary phase.

From (6.34), we write the multiple scattered amplitude initially as

$$G(\hat{\mathbf{r}}, \hat{\mathbf{k}}_0) = g(\hat{\mathbf{r}}, \hat{\mathbf{k}}_0) + \sum_s{}' \exp(i\mathbf{k}_0\cdot\mathbf{b}_s) \int \exp(-ik\hat{\mathbf{p}}\cdot\mathbf{b}_s)$$

$$\times g(\hat{\mathbf{r}}, \hat{\mathbf{p}}) G(\hat{\mathbf{p}}, \hat{\mathbf{k}}_0)\, d\Omega(\hat{p})/2\pi, \tag{12}$$

where $\sum_s'$ indicates summation over all but the central obstacle $s_1 = s_2 = 0$. (This representation holds at least when the scatterers' projections on $z = 0$ do not overlap.[6]) We replace $\mathbf{b}_s$ by $\mathbf{b}_s - z\hat{\mathbf{z}}$ in the integral to obtain the form $\sum_s' \int d\Omega\, \mathcal{J}_s = \sum_s \int d\Omega \mathcal{J}_s - \int d\Omega \mathcal{J}_0 = \sum_\nu \mathcal{J}(\nu) - \int_\nu \mathcal{J}(\nu)$, where [by (7), etc.] $\sum_\nu = \sum_{\nu_1}\sum_{\nu_2}$ is the set of discrete modes as in (8), and [by (6) in terms of ν_1, ν_2 as continuous variables] $\int_\nu = \int d\nu_1 \int d\nu_2$ is the corresponding set of continuous modes. Proceeding formally, we equate G with the limit for $z = \epsilon = |\epsilon| \to 0$,

$$G_{\alpha 0} = g_{\alpha 0} + \mathbf{S}\, 2C_\nu g_{\alpha\nu} G_{\nu 0},$$

$$\mathbf{S} = \lim_{\epsilon\to 0} \left(\sum_{\nu_1}\sum_{\nu_2} - \int d\nu_1 \int d\nu_2\right) \exp[ik\epsilon\zeta(\nu_1, \nu_2)], \tag{13}$$

where $g_{\alpha\nu} = g(\hat{\mathbf{k}}_\alpha, \hat{\mathbf{k}}_\nu)$, etc., and $\hat{\mathbf{k}}_\alpha$ is in the array set. Since the limit must be the same for $-z = \epsilon \to 0$, we may replace $g_{\alpha\nu}G_{\nu 0}$ by $g_{\alpha\nu'}G_{\nu' 0}$, or use the mean

$$G_{\alpha 0} = g_{\alpha 0} + \mathbf{S}\, C_\nu(g_{\alpha\nu}G_{\nu 0} + g_{\alpha\nu'}G_{\nu' 0}) = G[\mathbf{S}; g] \tag{14}$$

which makes the symmetry of the problem more evident. The form (13) is the same as (1.65) for the periodic line, and (14) the same as (2.32) for the grating, but the operator $\mathbf{S}$ is different.

The factor $\exp[ik\epsilon\zeta(\nu_1, \nu_2)]$, essentially a two-dimensional Abelian convergence factor, approaches zero with increasing $|\nu_1|$ or $|\nu_2|$. As discussed before,[1,2] (12) represents the multiple scattered amplitude G of one obstacle as its response $g(\hat{\mathbf{r}}, \hat{\mathbf{k}}_0)$ to the incident wave $\phi(\hat{\mathbf{k}}_0)$ plus its responses $g(\hat{\mathbf{r}}, \hat{\mathbf{p}})$ to the continuous sets of waves $\phi(\hat{\mathbf{p}})$ corresponding to the radiating fields of all individual neighbors. In (13), $G_{\alpha 0} - g_{\alpha 0}$ consists of the obstacle's responses $g_{\alpha\nu}$ to the discrete set of waves $\phi(\hat{\mathbf{k}}_\nu)$ arising from the array as a whole less the analogous continuous set corresponding to self-excitation responses. We may construct (13) directly from the

superposition principle by writing G as a scatterer's response to $\phi + \mathcal{U} - U$ with $\mathcal{U}[\sum_\nu]$ and $U[\int_\nu]$ represented appropriately in terms of plane waves.

To facilitate obtaining energy conserving approximations of (14) in the absence of presence of near-grazing modes, we first compare the analogous scattering theorems for G and g, and discuss the structure of the array modes.

2. SCATTERING THEOREMS

The theorems for G follow by specializing (7.6) and (7.7), derived for a finite number of equally spaced identical planar lattices,[7] to the case of a single lattice plane. For direct comparison, we rewrite (8) and (9) in terms of transmission (T) and reflection (R) coefficients corresponding to an incident wave $\phi_\alpha = \phi(\hat{\mathbf{k}}_\alpha)$ with $\hat{\mathbf{k}}_\alpha$ in the array set [i.e., the set determined by ξ_{i0}, b_i, and k as in (7)]. For $z > a$, we have the transmitted field

$$\Psi_\alpha = \phi_\alpha + \mathcal{U}(\phi_\alpha) = \sum \phi_\nu T_{\nu\alpha}, \quad T_{\nu\alpha} = \delta_{\nu\alpha} + 2C_\nu G_{\nu\alpha}, \tag{15}$$

and for $z < -a$, the reflected field

$$\mathcal{U}(\phi_\alpha) = \sum \phi_{\nu'} R_{\nu'\alpha}, \quad R_{\nu'\alpha} = 2C_\nu G_{\nu'\alpha}. \tag{16}$$

We can now specialize the earlier theorems by inspection.

From (7.7), G satisfies the reciprocity theorem

$$G(\hat{\mathbf{k}}_\alpha, \hat{\mathbf{k}}_\beta) = G(-\hat{\mathbf{k}}_\beta, -\hat{\mathbf{k}}_\alpha) \tag{17}$$

with $\hat{\mathbf{k}}_\alpha$ and $\hat{\mathbf{k}}_\beta$ (but, in general, not $-\hat{\mathbf{k}}_\alpha$ and $-\hat{\mathbf{k}}_\beta$) in the array set. Equation (17) is the same form as $g(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = g(-\hat{\mathbf{k}}, -\hat{\mathbf{r}})$ for the isolated scattering amplitude, but now restricted to special directions. For lossless scatterers, from (7:6), the propagating amplitudes satisfy the scattering theorem

$$-G_{\beta\alpha} - G^*_{\alpha\beta} = 2\sum_p C_\nu (G_{\nu\alpha} G^*_{\nu\beta} + G_{\nu'\alpha} G_{\nu'\beta}) \tag{18}$$

where $\sum_p$, the sum over the propagating range of ν, consists of the finite number of terms for which $|\sin\theta_\nu| < 1$. (We show subsequently that near-grazing terms which suggest singularities are zero in the limit $\theta_\nu \to \pi/2$, $C_\nu \to \infty$). For lossy scatterers, the right-hand side has the additional term $(k^2/2\pi)\mathcal{S}_A(\hat{\mathbf{k}}_\beta, \hat{\mathbf{k}}_\alpha)$,

$$\mathcal{S}_A(\hat{\mathbf{k}}_\beta, \hat{\mathbf{k}}_\alpha) = -\int (\Psi^*_\beta \nabla \Psi_\alpha - \Psi_\alpha \nabla \Psi^*_\beta) \cdot \hat{\mathbf{n}}\, d\mathcal{A}\, /i2k;$$

here $\Psi_\alpha = \phi_\alpha + \mathcal{U}(\phi_\alpha)$ is the total field of the array resulting from ϕ_α excitation, $\mathcal{A}$ is the surface of the central obstacle, and $\hat{\mathbf{n}}$ is its outward normal.

For an isolated scatterer, the analog of (18) is

$$-g(\hat{\mathbf{k}}_\beta, \hat{\mathbf{k}}_\alpha) - g^*(\hat{\mathbf{k}}_\alpha, \hat{\mathbf{k}}_\beta) = \int_0^{2\pi} d\varphi \int_0^{\pi/2} d\theta \sin\theta [g(\hat{\mathbf{r}}, \hat{\mathbf{k}}_\alpha) g^*(\hat{\mathbf{r}}, \hat{\mathbf{k}}_\beta) + g(\hat{\mathbf{r}}', \hat{\mathbf{k}}_\alpha) g^*(\hat{\mathbf{r}}', \hat{\mathbf{k}}_\beta)]/2\pi,$$

where $\hat{\mathbf{r}}'$ is the image of $\hat{\mathbf{r}}$ in $z = 0$. We rewrite the integral as $\int_{-1}^{1} d\xi \int_{-\gamma}^{\gamma} d\eta[\,]/2\pi\zeta$ with $\gamma = (1-\xi^2)^{1/2}$, and introduce ν_1 and ν_2 of (7) as continuous variables to obtain

$$-g_{\beta\alpha} - g^*{}_{\alpha\beta} = 2\int_p C_\nu (g_{\nu\alpha} g^*_{\nu\beta} + g_{\nu'\alpha} g^*_{\nu'\beta}), \tag{19}$$

$$\int_p = \int_{-n_1^-}^{n_1^+} d\nu_1 \int_{-n_2^-}^{n_2^+} d\nu_2, \quad n_1^\pm = |n_1^\pm| = \frac{kb_1}{2\pi}(1 \mp \xi_0),$$

$$n_2^\pm(\gamma) = |n_2^\pm| = \frac{kb_2}{2\pi}(\gamma \mp \eta_0), \quad \gamma = (1-\xi^2)^{1/2}. \tag{19'}$$

The form (19) differs from (18) only in that the operator is a double integral instead of a double sum. The analogous breakdown of the sum is

$$\sum_p = \sum_{-\nu_1^-}^{\nu_1^+} \sum_{-\nu_2^-}^{\nu_2^+}, \quad \nu_1^\pm = [n_1^\pm] = [kb_1(1 \mp \xi_0)/2\pi], \tag{18'}$$

$$\nu_2^\pm = [n_2^\pm(\gamma_{\nu_1})] = [kb_2(\gamma_{\nu_1} \mp \eta_0)/2\pi], \quad \gamma_{\nu_1} = (1 - \xi_{\nu_1}^2)^{1/2},$$

with $\nu_i^\pm$ as the closest integers from below to $n_i^\pm$.

If the scatterers are lossy, we add $(k^2/2\pi)\sigma_A(\hat{\mathbf{k}}_\beta, \hat{\mathbf{k}}_\alpha)$ to the right-hand side of (19), with σ_A as the form $\mathcal{S}_A$ in terms of the solution $\phi + u$ for the isolated scatterer. For $\beta = \alpha$, the lossy forms of (18) and (19) reduce to the corresponding energy theorems,

$$-\mathrm{Re}\, G_{\alpha\alpha} = \sum_p C_\nu (|G_{\nu\alpha}|^2 + |G_{\nu'\alpha}|^2) + (k^2/4\pi)\mathcal{S}_A, \tag{20}$$

$$-\mathrm{Re} g_{\alpha\alpha} = \int_p C_\nu (|g_{\nu\alpha}|^2 + |g_{\nu'\alpha}|^2) + (k^2/4\pi)\sigma_A \tag{21}$$

with $\mathcal{S}_A$ and σ_A as the respective absorption cross sections. Multiplying through by $4\pi/k^2$ converts these expressions to the usual statement that the total cross section (the energy derived from ϕ_α by interference) is the sum of the scattering and absorption cross sections.

The present forms are identical to those for the grating,[2] and simpler than those for the periodic line[1] (which involved conical instead of plane modes). However, because $\sum_p$ now represents a double sum, the present system of modes has more structure and higher degeneracies arise.

The sum $\sum_p$ represents $(\nu_1^+ + \nu_1^- + 1)(\nu_2^+ + \nu_2^- + 1) = M$ discrete propagating modes (corresponding to fixed k, b_i, and ξ_{i0}), and the integral represents the analogous continuum of modes. If $n_i^\pm \gg 1$ (i.e., if $kb_i \gg 1$), then M is very large and $\sum_p$ approximates $\int_p$. On the other hand, if $n_i^\pm < 1$, then $M = 1$ and $\sum_p$ reduces to the $\alpha-$ mode ($\nu = \alpha$, $\nu' = \alpha'$); for this case, (18) yields $|T_{\alpha\alpha} + R_{\alpha'\alpha}| = 1$ for the corresponding transmission and reflection amplitudes. (See Ref. 7 for discussion of both magnitude and phase effects.)

3. ARRAY MODES

For the incident direction $\hat{\mathbf{k}}_0 = \hat{\mathbf{r}}(\theta_0; \varphi_0)$ as in (1), in terms of $\hat{\boldsymbol{\rho}}(\varphi) = \hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi$, the modes may be specified by θ and φ such that

$$\hat{\boldsymbol{\rho}}(\varphi)\sin\theta = \hat{\boldsymbol{\rho}}(\varphi_0)\sin\theta_0 + \mathbf{v}\lambda = \hat{\boldsymbol{\rho}}_0 \sin\theta_0 + \hat{\mathbf{v}}\lambda/D;$$

$$\mathbf{v} = \hat{\mathbf{x}}\nu_1/b_1 + \hat{\mathbf{y}}\,\nu_2/b_2 = \hat{\mathbf{v}}/D, \quad \hat{\mathbf{v}} = \hat{\boldsymbol{\rho}}(\tau),$$

$$D = [(\nu_1/b_1)^2 + (\nu_2/b_2)^2]^{-1/2} = d/m. \tag{22}$$

Here $\mathbf{v}$ is a lattice vector in the space reciprocal to $\mathfrak{b}$, and d is the separation of the direct lattice lines perpendicular to $\mathbf{v}$, i.e., $\mathfrak{b} \cdot \mathbf{v} = s_1\nu_1 + s_2\nu_2 = (s_1\mu_1 + s_2\mu_2)m$ is constant for variable s_i and fixed $\nu_i = m\mu_i$ with m as

the common integer factor. Because of the sines, the form $(\hat{\rho}\sin\theta - \hat{\rho}_0\sin\theta_0)/\lambda = \mathbf{v}$ differs essentially from that used in the conventional development for Bragg reflection in a two-dimensional crystal[8]; the Bragg relation is appropriate only for grazing incidence ($\theta_0 = \pi/2$) and observation ($\theta = \pi/2$), which we consider only as limits. From (22) we have

$$\sin^2\theta = \sin^2\theta_0 + 2(\lambda/D)\sin\theta_0\cos(\varphi_0 - \tau) + (\lambda/D)^2$$

with $0 \leq \sin\theta_0 < 1$ and $\sin\theta(\nu_1, \nu_2)$ representing a discrete infinite set on the line 0 to ∞.

It is convenient to discuss the propagating modes ($\theta < \pi/2$) in terms of $\hat{\mathbf{k}}_0 = \hat{\mathbf{k}}(\xi_0, \eta_0)$ and

$$\sin^2\theta = \xi_{\nu_1}^2 + \eta_{\nu_2}^2 = \left(\xi_0 + \frac{\nu_1\lambda}{b_1}\right)^2 + \left(\eta_0 + \frac{\nu_2\lambda}{b_2}\right)^2,$$

$$\tan\varphi = \frac{\eta_{\nu_2}}{\xi_{\nu_1}} = \frac{\eta_0 + \nu_2\lambda/b_2}{\xi_0 + \nu_1\lambda/b_1},$$

$$-\nu_1^- \leq \nu_1 \leq \nu_1^+, \quad -\nu_2^-(\nu_1) \leq \nu_2 \leq \nu_2^+(\nu_1) \tag{23}$$

with $\nu_i^\pm = [n_i^\pm]$ as in (18′). We label the modes as follows: The term (0, 0) is the principal mode (the direction of incidence and its image in $z = 0$); the set of terms $\{0, \nu_2\}$ having end points $\nu_2^\pm(0) = [b_2(\gamma_0 \mp \eta_0)/\lambda]$ with $\gamma_0 = (1 - \xi_0^2)^{1/2}$ is the principal ν_2-set, and $\{\nu_1, 0\}$ is the principal ν_1-set. If $b_1(1 \mp \xi_0)/\lambda < 1$, then the principal ν_2-set is the only propagating set; if also $b_2(\gamma_0 \mp \eta_0)/\lambda < 1$, then only the principal mode propagates.

In general, for fixed λ and arbitrary assigned parameters ξ_{i0}, b_i the values of θ and φ as in (23) are all distinct. However, for special values of ξ_{i0} and b_i more than one mode may correspond to the same θ. Thus if $\xi_0 = 0$, then $\xi_{\nu_1} = \nu_1\lambda/b_1 = \pm|\nu_1|\lambda/b_1$ and $\nu_1^\pm = [b_1/\lambda]$; now the principal ν_2-set has end points $[b_2(1 \mp \eta_0)/\lambda]$ and is perpendicular to the x axis, and the other ν_2-sets are paired as images in the plane $x = 0$ with each value of θ corresponding to two modes $(\pm|\nu_1|, \nu_2)$. This applies not only for $\xi_0 = 0$ but also for ξ_0 equal to any value of the set $\nu_1\lambda/b_1$ associated with $\xi_0 = 0$; we call this the $\xi(0)$-set. If in addition $\eta_0 = 0$ (i.e., normal incidence, $\hat{\mathbf{k}}_0 = \hat{\mathbf{z}}$), then $\eta_{\nu_2} = \pm|\nu_2|\lambda/b_2$ and $\nu_2^\pm(\nu_1) = [(b_2/\lambda)(1 - \nu_1^2\lambda^2/b_1^2)^{1/2}]$. Now the mode system is imaged in both axial planes ($y = 0$ as well as $x = 0$), and except for the principal sets ($\{\nu_1, 0\}$ perpendicular to $\hat{\mathbf{y}}$, and $\{0, \nu_2\}$ perpendicular to $\hat{\mathbf{x}}$), each value of θ corresponds to four modes $(\pm|\nu_1|, \pm|\nu_2|)$; for the principal sets, except for the principal mode, each θ corresponds to two modes $(\pm|\nu_1|, 0)$ or $(0, \pm|\nu_2|)$. The same modes as for $\hat{\mathbf{k}}_0 = \hat{\mathbf{z}}$ are also generated by any $\hat{\mathbf{k}}_0$ of the associated set $\hat{\mathbf{k}}(0) = \hat{\mathbf{x}}(\nu_1\lambda/b_1) + \hat{\mathbf{y}}(\nu_2\lambda/b_2) + \hat{\mathbf{z}}\,\zeta$.

The above excludes special values of b_i for which the multiplicities may be higher. Thus for $\hat{\mathbf{k}}_0 = \hat{\mathbf{z}}$, and rational values of b_2/b_1, the same θ may correspond to eight modes $(\pm|\nu_1|, \pm|\nu_2|)$ and $(\pm|\nu_1'|, \pm|\nu_2'|)$ if $(\nu_1 b_2/b_1)^2 + (\nu_2)^2 = (\nu_1' b_2/b_1)^2 + (\nu_2')^2$, or to six if one of the ν_i is zero, or to higher multiplicities if the kb_i are large enough. For the square cell $b_1 = b_2$, the modes are also symmetrical to the diagonal planes $x = \pm y$, and each value of θ corresponds to at least four modes. There are at least four $(\pm\alpha, 0)$ and $(0, \pm\alpha)$ for the axial planes, at least four $(\pm\beta, \pm\beta)$ for the diagonal planes, and at least eight $(\pm\gamma, \pm\delta)$ and $(\pm\delta, \pm\gamma)$ otherwise. If $\alpha^2 = \gamma^2 + \delta^2$ (e.g., $5^2 = 4^2 + 3^2$), there are twelve modes including four in the axial planes; if $2\beta^2 = \gamma^2 + \delta^2$ (e.g., $2 \cdot 5^2 = 1^2 + 7^2$), there are twelve including four in the diagonal planes; if $\gamma^2 + \delta^2 = (\gamma')^2 + (\delta')^2$ (e.g., $1^2 + 8^2 = 4^2 + 7^2$), there are sixteen modes, etc. (For the grating and periodic line, the same λ and θ, measured from the plane normal to the array, are associated with but one or two modes.)

The grazing modes occur for the special values of the parameters corresponding to $\theta = \pi/2$ in (23). Using the definitions $n_i^\pm$ of (19′), we write

$$\xi_{\nu_1} = \mp(-1 + \Delta_1^\pm), \quad \eta_{\nu_2} = \mp(-\gamma_{\nu_1} + \Delta_2^\pm), \quad \Delta_i^\pm = \lambda(n_i^\pm \mp \nu_i)/b_i, \quad 0 \leq \Delta \leq 1,$$

$$\sin^2\theta - 1 = \Delta_2(\Delta_2 - 2\gamma_{\nu_1}) = \Delta_2[\Delta_2 - 2(2\Delta_1 - \Delta_1^2)^{1/2}],$$

and, in general, reserve $R_i^\pm$ to represent integer values of $n_i^\pm$. Discounting special values of b_i, for $n_1^\pm \neq R_1^\pm$, we obtain one grazing mode if either $n_2^+ = R_2^+$ or $n_2^- = R_2^-$, and two if both $n_2^\pm = R_2^\pm$ [corresponding to η in the $\eta(0)$-set]; the number of modes for each case is doubled if ξ is in the $\xi(0)$-set. The cases of either one or both $n_1^\pm = R_1^\pm$ correspond to one or two grazing modes along x, which also require $n_2^- = R_2^-$ for positive η_0. For the last requirement, from (23) for $\xi_{\nu_1}^2 = 1$, we have $\sin^2\theta - 1 = (\eta_{\nu_2})^2 = (\eta_0 + \nu_2\lambda/b_2)^2$, which vanishes for $\eta_0 = -\nu_2\lambda/b_2 = R_2^-\lambda/b_2$ corresponding to $\eta_{\nu_2} = -\Delta_2^- = \lambda(-n_2^- + \nu_2)/b_2 = 0$; both η_0 and η_{R_2} are in the $\eta(0)$-set, but since $\eta_{R_2} = 0$, it represents a single mode.

In general, for arbitrary assigned parameters (λ, b_i, ξ_{i0}) the special conditions for $\sin\theta = 1$ are not fulfilled, and there are no grazing modes. For special wavelengths λ_R, we obtain one, two, or four grazing modes; for special values of the other parameters, the multiplicities are higher for particular λ_R's as discussed before for $\theta < \pi/2$.

For normal incidence, from (22) for $\sin\theta_0 = 0$, the grazing modes satisfy

$$\hat{\mathbf{k}}_R = \hat{\rho}(\varphi) = \hat{\mathbf{v}}\lambda_R/D, \quad \lambda_R = D = d/m,$$

$$\tan\varphi_R = \nu_2 b_1/\nu_1 b_2 = \mu_2 b_1/\mu_1 b_2 \tag{24}$$

with $d = b_1 b_2/[(\mu_1 b_2)^2 + (\mu_2 b_1)^2]^{1/2}$, and $\nu_1 = \pm|\nu_1| = \pm m|\mu_1|$, $\nu_2 = \pm R_2 = m\mu_2$. The grazing modes along the rays φ and $\pi + \varphi$ propagate perpendicular to the lattice lines spaced d apart along $\varphi + \pi/2$. Thus, essentially as for the grating[2] and for the periodic line[1] with scatterer spacing d, the grazing wavelengths satisfy $m\lambda_R = d$: A grazing mode corresponds to reinforcement of the scattered waves of the lattice lines perpendicular to the mode's direction (essentially as discussed before in detail for the grating[2-4,9]).

In order to sequence the occurrence of grazing modes for an incident continuous spectrum in terms of decreasing λ, we assume temporarily that the lattice cell is almost square, with say $b_2 \gtrsim b_1$. The longest wavelength for which grazing modes occur is $\lambda = b_2$ corresponding to the pair $(0, \pm 1)$ propagating along $\pm\hat{\mathbf{y}}$ perpendicular to the lattice lines parallel to $\hat{\mathbf{x}}$. The slightly

shorter wavelength $\lambda = b_1$ corresponds to the pair $(\pm 1, 0)$ propagating along $\pm\hat{\mathbf{x}}$. Next, $\lambda = b_1 b_2/(b_1^2 + b_2^2)^{1/2}$, the distance between parallel diagonals of the rectangles b_1 by b_2, corresponds to four modes $(\pm 1, \pm 1)$; one pair propagates back and forth along $\varphi = \tan^{-1}(b_1/b_2)$, and the other along $\pi - \varphi$. With decreasing wavelength, we get the pair $(0, \pm 2)$ with $\lambda = b_2/2$ along $\pm\hat{\mathbf{y}}$, the pair $(\pm 2, 0)$ with $\lambda = b_1/2$ along $\pm\hat{\mathbf{x}}$, then the four modes $(\pm 1, \pm 2)$ with $\lambda = b_1 b_2/(4b_1^2 + b_2^2)^{1/2}$, two back and forth along $\varphi = \tan^{-1}(2b_1/b_2)$, and two along $\pi - \varphi$, etc.

Dropping the restriction $b_2 \gtrsim b_1$, we see that for irrational values of b_2/b_1, there are essentially two sets of grazing modes: pairs along x and y and quadruples in other directions. However, as discussed for arbitrary θ, the multiplicity may be higher for rational b_2/b_1, and still higher for the square array. If $b_1 = b_2$, then each grazing λ corresponds to at least four modes; at least four for the axial planes ($x = 0$ or $y = 0$) and for the diagonal planes ($x = \pm y$), and at least eight otherwise. There are more for special values of ν_i. Thus the axial wavelength $\lambda = b_1/5$ corresponds to twelve modes, $(\pm 5, 0)$, $(0, \pm 5)$, $(\pm 4, \pm 3)$, $(\pm 3, \pm 4)$; the diagonal wavelength $\lambda = b_1/5\sqrt{2}$ corresponds to twelve, $(\pm 5, \pm 5)$, $(\pm 1, \pm 7)$, $(\pm 7, \pm 1)$; and, similarly, $\lambda = b_1/(65)^{1/2}$ corresponds to sixteen, $(\pm 1, \pm 8)$, $(\pm 8, \pm 1)$, $(\pm 4, \pm 7)$, $(\pm 7, \pm 4)$. The multiplicities increase with increasing b_1/λ. For simplicity, in generalizing the development we consider only the basic multiplicities that do not require special values of b_i.

For the basic cases, for normal incidence, the modes parallel to the sides of the lattice cell are two-fold degenerate, and the rest are four-fold. The degeneracy is removed by changing the angle of incidence from normal; this enables us to consider values of ξ_{i0}, b_i, and λ for which there exist one, two, or four grazing modes. Thus, we eliminate essentially half the degeneracies if we consider incidence normal to only x. Then $\hat{\mathbf{k}}_0 = \hat{\mathbf{z}}\cos\theta_0 + \hat{\mathbf{y}}\sin\theta_0$, and

$$(\nu_1\lambda/b_1)^2 + (\sin\theta_0 + \nu_2\lambda/b_2)^2 = 1,$$

$$\tan\varphi = (\sin\theta_0 + \nu_2\lambda/b_2)b_1/\nu_1\lambda.$$

$$\nu_1 = \pm\,|\,\nu_1\,|, \quad \nu_2 = \pm R_2^{\pm}, \quad R_2^{+} < R_2^{-}. \tag{25}$$

The second order equation for λ together with the four possible values of ν_1, ν_2 has at most two real roots. In general only pair-degeneracy occurs, but exceptions arise because integral values of $(b_1/\lambda)\sin\theta_0 = \mu$ reduce (25) to the forms in (24) and restore full degeneracy. Discounting the exceptions, the simplest set corresponds to the individual modes $(0, \pm R_2^{\pm})$ with wavelengths $\lambda_{\pm} = b_2(1 \mp \sin\theta_0)/R_2^{\pm}$, i.e., to grazing values of the principal ν_2-set which propagate along y. These are the same nondegenerate modes as arise for nonnormal incidence on the corresponding grating[2,3,9] with cylinders parallel to x; they become degenerate[9] if $(b_2/\lambda)\sin\theta_0 = \mu$. All the remaining sets are pairs imaged in the y axis. The simplest set of pairs $(\pm R_1, 0)$ are the grazing values of the principal ν_1-set, with $\lambda = (b_1/R_1)\cos\theta_0$ propagating along $\varphi = \theta_0$ and $\pi - \theta_0$ corresponding to $\tan\varphi = \pm(b_1/R_1\lambda)\sin\theta_0 = \pm\tan\theta_0$. The remaining paired modes form two sets with wavelengths

$$\frac{\lambda_{\pm}}{D_{\pm}} = \left[\left(\frac{D_{\pm}R_2^{\pm}}{b_2}\right)^2 \sin^2\theta_0 + \cos^2\theta_0\right]^{1/2} \mp \frac{D_{\pm}R_2^{\pm}}{b_2}\sin\theta_0,$$

$$D_{\pm} = \left[\left(\frac{\nu_1}{b_1}\right)^2 + \left(\frac{R_2^{\pm}}{b_2}\right)^2\right]^{-1/2} \tag{26}$$

traveling in the directions

$$\hat{\mathbf{k}}_R = \hat{\mathbf{x}}\,\nu_1\lambda_{\pm}/b_1 + \hat{\mathbf{y}}(\sin\theta_0 \pm R_2^{\pm}\lambda_{\pm}/b_2), \quad \nu_1 = \pm\,|\,\nu_1\,|. \tag{27}$$

The shorter wavelength λ_+ travels at larger angles with respect to x, i.e., $|\tan\varphi(\lambda_+)| > |\tan\varphi(\lambda_-)|$.

For arbitrary $\hat{\mathbf{k}}_0$, the grazing modes are in general nondegenerate. [They become as degenerate as (25) if $b_1\xi_0/\lambda = \mu$ and as degenerate as (24) if in addition $b_2\eta_0/\lambda = \mu'$.] In general, there are four positive values of

$$\lambda_R = D\{[(\hat{\mathbf{k}}_0\cdot\hat{\mathbf{v}})^2 + (\hat{\mathbf{k}}_0\cdot\hat{\mathbf{z}})^2]^{1/2} - \hat{\mathbf{k}}_0\cdot\hat{\mathbf{v}}\},$$

$$\hat{\mathbf{k}}_0\cdot\hat{\mathbf{v}} = \left(\frac{\xi_0\nu_1}{b_1} + \frac{\eta_0\nu_2}{b_2}\right)D,$$

$$\hat{\mathbf{k}}_0\cdot\hat{\mathbf{z}} = \zeta \tag{28}$$

with D and $\hat{\mathbf{v}}$ as in (22) in terms of $\nu_2 = \pm R_2^{\pm}$ and different integers for positive and negative ν_1. These represent four different wavelengths traveling along the corresponding nonsymmetrical directions

$$\hat{\mathbf{k}}_R = \hat{\mathbf{x}}(\xi_0 + \nu_1\lambda_R/b_1) + \hat{\mathbf{y}}(\eta_0 + \nu_2\lambda_R/b_2). \tag{29}$$

Thus, discounting special values of b_i (and ξ_{i0}) an assigned incident λ_R generates only one grazing mode.

We shortly consider the array resonances associated with near-grazing modes.

4. THE MULTIPLE SCATTERING AMPLITUDE

In order to reduce the functional equation $G = G[\mathbf{S};g]$ of (14), we decompose the operator $\mathbf{S}$ as

$$\mathbf{S} = \mathbf{S}_p + \mathbf{S}_e, \quad \mathbf{S}_p = \sum_p - \int_p \tag{30}$$

with $\sum_p$ as in (18′) and $\int_p$ as in (19′); $\mathbf{S}_e$ is the corresponding operator over the evanescent range. Proceeding essentially as before,[1,2] we introduce the modified scattering amplitude

$$g''_{\alpha\beta} = g_{\alpha\beta} + \mathbf{S}_p C_\nu (g_{\alpha\nu}g''_{\nu\beta} + g_{\alpha\nu'}g''_{\nu'\beta}) = g''[\mathbf{S}_p;g] \tag{31}$$

and suppress the propagating range in (14):

$$G_{\alpha 0} = g''_{\alpha 0} + \mathbf{S}_e C_\nu (g''_{\alpha\nu}G_{\nu 0} + g''_{\alpha\nu'}G_{\nu' 0}) = G[\mathbf{S}_e;g''\,]. \tag{32}$$

Symbolically, in terms of the radiationless amplitude $g' = g'[-\int_p;g]$, we have $g'' = g''[\sum_p;g']$; the operator $-\int_p$ strips g of radiative loss terms, and $\sum_p$ restores radiation along the propagating modes of the array. Thus if there are no near-grazing modes, then except for small kb_i the leading term

$$G_{\alpha 0} \approx g''_{\alpha 0} \tag{33}$$

should suffice in general. For large kb_i, if the sum $\sum_p$ approximates the integral $\int_p$, then $\mathbf{S}_p = \sum_p - \int_p$ of (30) is negligible, and (33) reduces to the single scattering approximation

$$G_{\alpha 0} \approx g_{\alpha 0}. \tag{34}$$

If kb_i is large, but say mode N is near grazing, then we approximate (13) by

$$G_{\alpha 0} \approx g_{\alpha 0} + 2C_N g_{\alpha N} G_{N0}, \quad C_N = \pi/k^2 b_1 b_2 \cos\theta_N,$$
$$\cos\theta_N = \epsilon \approx 0, \tag{35}$$

where $\epsilon = |\epsilon|$ if N is propagating, and $\epsilon = i|\epsilon|$ if evanescent. Solving for G_{N0}, we obtain

$$G_{N0} \approx g_{N0} + 2C_N g_{NN} G_{N0} = g_{N0}/(1 - 2C_N g_{NN}) \tag{36}$$

which resolves the question of singularities in (8) and (20). The limit of the corresponding term of the solution (8)

$$\phi_N 2C_N G_{N0} \approx \phi_N 2C_N g_{N0}/(1 - 2C_N g_{NN}) \to -(g_{R0}/g_{RR})\phi_R \tag{37}$$

is a plane wave as in (11) traveling in the plane of the array; thus, the solution is finite in the limit. A grazing mode does not transport energy from the array; the corresponding term of the energy theorem (20),

$$2C_N |G_{N0}|^2 \approx |g_{N0}/g_{NN}|^2 / 2C_N \to 0, \tag{38}$$

is zero in the limit $C_N \to \infty$; similarly for (18). However, the near-grazing mode couples the others in (20) and may markedly alter the energy distribution among the propagating modes.

For the nongrazing modes, from (35) in terms of (36),

$$G_{\alpha 0} \approx g_{\alpha 0} + 2C_N g_{\alpha N} g_{N0}/(1 - 2C_N g_{NN}) \tag{39}$$

we see that the effects for a propagating mode near grazing ($\epsilon = |\epsilon|$) are relatively slight. The real part of g_{NN} is negative [from (21)], and C_N is positive in the range $\epsilon = |\epsilon|$ to 0; consequently, the greatest departure of G from g should correspond to the limit

$$G_{\alpha 0} \approx g_{\alpha 0} - g_{\alpha N} g_{N0}/g_{NN} \to (g_{\alpha 0} g_{RR} - g_{\alpha R} g_{R0})/g_{RR} \tag{40}$$

for which case the coupling correction is of the order of magnitude of the single scattered value. For the limit, the effects may be quite pronounced, e.g., for isotropic scatterers ($g_{\alpha 0} = g$) we obtain $G_{\alpha 0} = 0$ and the array becomes transparent.

On the other hand, if N is evanescent ($\epsilon = i|\epsilon|$), then $|G_{\alpha 0}|$ may show a maximum for parameters such that

$$1 - 2C_N i \operatorname{Im} g_{NN} = 1 - 2|C_N| \operatorname{Im} g_{NN} = 0,$$
$$C_N = \pi/k^2 b_1 b_2 i|\epsilon| = -i|C_N|; \tag{41}$$

the corresponding form of (39) is

$$G_{\alpha 0} \approx g_{\alpha 0} - g_{\alpha N} g_{N0}/\operatorname{Re} g_{NN} \tag{42}$$

and the coupling term may be orders of magnitude larger than the single scattered value. For example, for scatterers small compared to wavelength, $|g| \approx i \operatorname{Im} g| = |il|$ is in general very small, and (from the scattering theorem) Reg is of order $|g|^2 \approx l^2$; consequently, $|G/g|^2$ may be of order $l^{-2} \gg 1$. For such scatterers, $|G|$ may also have a minimum at a value $i|\epsilon|$ corresponding to

$$\operatorname{Im} g_{\alpha 0} \approx -2|C_N| \operatorname{Re}(g_{\alpha 0} g_{NN} - g_{\alpha N} g_{N0})$$
$$\approx 2|C_N|(I_{\alpha 0} I_{NN} - I_{\alpha N} I_{N0}),$$
$$I_{\nu\alpha} = \operatorname{Im} g_{\nu\alpha}; \tag{43}$$

then the leading term of the single scattering approximation is cancelled, and (39) is of order l^2 as in (1.59).

To account for a resonance at moderate instead of large values of kb_i, we replace g in (39) by g'', i.e., we use the energy conserving form

$$G_{\alpha 0} \approx g''_{\alpha 0} + 2C_N g''_{\alpha N} g''_{N0}/(1 - 2C_N g''_{NN}) = p_{\alpha 0}. \tag{44}$$

In terms of $p_{\alpha 0}$ we rewrite the complete representation (32) as $G = G[\mathbf{S}_{e(N)}; p]$ where $e(N)$ indicates the exclusion of mode N from $\sum_e$; the first approximation is $G \approx p$, and more complete results may be obtained by iteration.[2] However, for present purposes we continue the development in terms of g.

If there is more than one near-grazing mode, then we replace (35) by the corresponding sum

$$G_{\alpha 0} \approx g_{\alpha 0} + 2\sum_M C_M g_{\alpha M} G_{M0}. \tag{45}$$

As an illustration, we consider the symmetrical case of normal incidence ($\hat{\mathbf{k}}_0 = \hat{\mathbf{z}}$) and scatterers that are rotationally symmetric around $\hat{\mathbf{z}}$; then $C_M = C_N$, $g_{M0} = g_{N0}$, and consequently $G_{M0} = G_{N0}$ for all near-grazing modes. For this special case,

$$G_{N0} \approx g_{N0} + 2C_N G_{N0} \sum_M g_{NM} \approx g_{N0}/(1 - 2C_N \textstyle\sum g_{NM}) \tag{46}$$

and the development carries through essentially as before, but now in terms of

$$G_{\alpha 0} \approx g_{\alpha 0} + 2C_N g_{N0} \textstyle\sum g_{\alpha M}/(1 - 2C_N \sum g_{NM}). \tag{47}$$

See Refs. 2, 3 for detailed development for two near-grazing modes for the general case (and also for the analogous development for arrays of bosses on rigid and pressure release planes).

To emphasize the role of the physical parameters of the scatterers we consider spheres of radius a small compared to the shortest grazing wavelength. For pressure release surfaces, we use the monopole form $g \approx -ika - (ka)^2$, and the corresponding form of (39), $G_{\alpha 0} \approx g/(1 - C_N g)$. If $C_N \to \infty$, then $\mathcal{U} \to -\phi_R$ and the array becomes perfectly transparent if there is a grazing mode; but because (41) cannot be satisfied for $\operatorname{Im} g = -ka$, there are no maxima corresponding to (42). On the other hand, if the monopoles represent small scatterers having the same density as the embedding medium, but different relative compressibility $\mathcal{C}$, then $g \approx id_0 - |d_0|^2$ with $d_0 = (ka)^3(\mathcal{C} - 1)/3$; for this case, (41) may be satisfied for $\mathcal{C} > 1$, and the maximum (42) is $G_{\nu 0} \approx -1 - id_0 \approx -1$. The energy gain of the propagating mode amplitudes $2C_\nu G_{\nu 0} \approx -2C_\nu$ is compensated by a corresponding loss of the central transmitted amplitude $T_{00} = 1 + 2C_0 G_{00} \approx 1 - 2C_0$. The energy theorem (20) for the present case reduces to $-\operatorname{Re} G = |G|^2 \sum_\rho 2C_\nu \approx 2\int_\rho C_\nu = 1$ because we assumed large spacings such that $\sum_\rho \approx \int_\rho$; for moderate spacings, in terms of $g'' \approx id_0 - |d_0|^2 \sum_\rho 2C_\nu$ instead of g, we get $G_{\nu 0} \approx -(\sum_\rho 2C_\nu)^{-1}$.

For rigid scatterers, we use $g(\hat{\mathbf{r}}, \hat{\mathbf{k}}) \approx -iAL(\hat{\mathbf{r}}, \hat{\mathbf{k}}) - A^2 M(\hat{\mathbf{r}}, \hat{\mathbf{k}})$, with $A = \frac{1}{3}(ka)^3$, $L = 1 - \frac{3}{2}\hat{\mathbf{r}} \cdot \hat{\mathbf{k}}$, and $M = 1 + \frac{3}{4}\hat{\mathbf{r}} \cdot \hat{\mathbf{k}}$. Thus, at grazing, from (40) to order A,

$G_{\nu 0} \approx -iA(L_{\nu 0} + 2L_{\nu R}L_{R0})$ with $L_{\nu R} = L(\mathbf{k}_\nu, \mathbf{k}_R)$ $= 1 - \frac{3}{2}\sin\theta_\nu \cos(\varphi_\nu - \varphi_R)$, etc. Since $\mathrm{Im} g_{RR} = \frac{1}{2}A$, the resonance condition (41), $|C_N| A = 1$, is satisfied for near-grazing evanescent modes for which $|\zeta_N| = \pi k a^3/3b_1 b_2$; then, from (42), $G_{\nu 0} \approx -iAL_{\nu 0} - \frac{4}{7}L_{\nu N}L_{N0}$. Similarly the condition for a minimum (43) reduces to

$$|C_N A|^{-1} = \frac{|\zeta| 3b_1 b_2}{\pi k a^3} = 1 + \frac{2L_{\nu N}L_{N0}}{L_{\nu 0}},$$

which can be satisfied for special directions $\hat{\mathbf{k}}_\nu$ for a given $\hat{\mathbf{k}}_0$. For more general scatterers with arbitrary compressibility (ζ) and inverse density (β) parameters, we use $g \approx a_0 + a_1 \hat{\mathbf{k}} \cdot \hat{\mathbf{r}}$ with $a_0 = id_0 - |d_0|^2$ the same as for the monopole, and $a_1 = id_1 - |d_1|^2/3$ in terms of $d_1 = -(ka)^3(\beta - 1)/(\beta + 2)$; the full structure of the anomalies may be obtained for these coefficients.

5. ALTERNATIVE REPRESENTATION

We now consider alternative representations for U and G in which the singularities corresponding to grazing modes are exhibited differently. The representations for G are also convenient for various detailed applications.

A. Spherical waves

We expand G in spherical harmonics[10]

$$G(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = \sum_{nm} A_n{}^m Y_n{}^m(\hat{\mathbf{r}}), \quad \sum_{nm} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \tag{48}$$

with $A_n{}^m(\hat{\mathbf{k}})$ as the corresponding multiple scattering coefficients. Substituting into (6) and using

$$i^n h_n(kr_s) Y_n{}^m(\mathbf{r}_s) = \int \exp(ik\hat{\mathbf{p}} \cdot \mathbf{r}_s)\, Y_n{}^m(\hat{\mathbf{p}})\, d\Omega(\hat{\mathbf{p}})/2\pi = I,$$

$$h_n = h_n{}^{(1)}, \tag{49}$$

we obtain the Hankel–Legendre representation of U; then from (4)

$$U = \sum_s \sum_{nm} A_n^m \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)\, i^n h_n(kr_s)\, Y_n^m(\hat{\mathbf{r}}_s). \tag{50}$$

Thus, at least for $r_s > a$, U consists of spherical waves outgoing from the scatterers at $\mathbf{r}_s = \mathbf{r} - \mathbf{b}_s$. This is the form obtained by separating the reduced wave equation in spherical coordinates, and could have been taken as the starting point of the development for the derivation of (8), the basic representation for the array. Comparing (50) and (8) in terms of (48), we see that for $z > 0$,

$$\sum_s \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)\, i^n h_n(kr_s)\, Y_n^m(\hat{\mathbf{r}}_s) = \sum_\nu 2C_\nu \exp(i\mathbf{r} \cdot \mathbf{k}_\nu) Y_n^m(\hat{\mathbf{k}}_\nu);$$

$$s(s_1, s_2),\ \nu(\nu_1, \nu_2) \tag{51}$$

as follows directly from (49) and

$$I = \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\eta \exp(ik\hat{\mathbf{p}} \cdot \mathbf{r}_s)\, Y_n^m(\hat{\mathbf{p}})/\zeta 2\pi, \qquad z > 0, \tag{49'}$$

by operating with $\sum_s \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)$ and (7); for $z < 0$, we replace $\hat{\mathbf{p}}$ and $\hat{\mathbf{k}}_\nu$ by the images $\hat{\mathbf{p}}'$ and $\hat{\mathbf{k}}_{\nu'}$.

Similarly, we expand the kernel of (12),

$$g(\hat{\mathbf{r}}, \hat{\mathbf{p}})\, G(\hat{\mathbf{p}}, \hat{\mathbf{k}}_0) = F(\hat{\mathbf{p}}) = \sum_{nm} B_n^m Y_n^m(\hat{\mathbf{p}}),$$

$$B_n^m = (-1)^m (2n+1) \int F(\hat{\mathbf{r}})\, Y_n^{-m}(\hat{\mathbf{r}})\, d\Omega(\hat{\mathbf{r}})/4\pi \tag{52}$$

and use (49) to obtain

$$G(\hat{\mathbf{r}}, \hat{\mathbf{k}}_0) = g(\hat{\mathbf{r}}, \hat{\mathbf{k}}_0) + \sum B_n^m H_n^m,$$

$$H_n^m = \sum_s{}' \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)\, i^n h_n(kb_s)\, Y_n^{-m}(-\hat{\mathbf{b}}_s). \tag{53}$$

The functions H_n^m, the basic lattice sums for the doubly periodic planar array, will be discussed subsequently in detail. If we represent G by (48) and use the analogous expansion of g in terms of the isolated scattering coefficients

$$g(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = \sum_{nm} a_n^m(\hat{\mathbf{k}})\, Y_n^m(\hat{\mathbf{r}}), \qquad a_n^m(\hat{\mathbf{k}}) = \sum_{pq} b_{np}{}^{mq} Y_p^{-q}(\hat{\mathbf{k}}), \tag{54}$$

we obtain the corresponding system of algebraic equations

$$A_n^m = a_n^m(\hat{\mathbf{k}}) + \sum_{pq} \sum_{rt} b_{np}{}^{mq} A_r^t \sum_l d_l(^{-q}_{\ p};{}^{\ t}_{r}) H_l^{t-q}. \tag{55}$$

Here $p + r + l$ is even, l changes by steps of 2 from $|p - r|$ (or from $|l - q|$ if it is the larger) to $p + r$, and the numbers d_l arise[11,12] from the expansion $Y_p^{-q} Y_r^t = \sum d_l Y_l^{t-q}$. Equations (50) and (55) comprise the general spherical wave representation of the solution for arbitrary identical scatterers.

For spherically symmetric obstacles, $a_n^m(\hat{\mathbf{k}}) = (-1)^m a_n Y_n^{-m}(\mathrm{k})$, and (55) reduces to

$$A_n^m = (-1)^m a_n [Y_n^{-m}(\hat{\mathbf{k}}) + \sum_{rt} A_r^t \sum_l d_l(^{-m}_{\ n};{}^{\ t}_{r}) H_l^{t-m}] \tag{56}$$

with, e.g., $a_n = -(2n+1) j_n(ka)/h_n(ka)$ for $\phi + u = 0$ at $r_s = a$, etc. Equation (56) may also be constructed by using the spherical function expansion of ϕ and U, and applying boundary conditions at the central sphere (after expanding hY in $\sum'$ by the addition theorem[11]). We apply (56) subsequently.

In general, we take $\hat{\mathbf{z}}$ as the polar axis of the spherical harmonic Y and work with[10]

$$Y_n^m(\zeta; \xi, \eta) = P_n^m(\cos\theta) \exp(im\varphi) = P_n^m(\zeta)(\xi + i\eta)^m/(\xi^2 + \eta^2)^{m/2},$$

$$Y_n^{-m} = P_n^{-m} \exp(-im\varphi), \quad P_n^{-m} = P_n^m (-1)^m (n-m)!/(n+m)! \tag{57}$$

Thus, the special values in (53) correspond to

$$Y_n^m(-\hat{\mathbf{b}}_s) = P_n^m(0) \exp[im(\pi + \beta_s)],$$

$$\exp(i\beta_s) = \frac{s_1 b_1 + i s_2 b_2}{(s_1^2 b_1^2 + s_2^2 b_2^2)^{1/2}},$$

$$P_n^m(0) = \frac{(n+m)!\, \cos[\frac{1}{2}(n-m)\pi]}{2^n (\frac{1}{2}n - \frac{1}{2}m)!\, (\frac{1}{2}n + \frac{1}{2}m)!}. \tag{58}$$

The fact that $n - m$ must be even markedly simplifies the reduction of the corresponding systems of Eqs. (55) and (56), and of the lattice sums H_n^m. In particular, for

normal incidence, $\hat{\mathbf{k}}_0 = \hat{\mathbf{z}}$ (or for any $\hat{\mathbf{k}}_\nu$ in the mode set containing $\hat{\mathbf{z}}$), only the functions $\mathcal{H}_{2n}^{2m}$ are involved; for the square array, only the sums $\mathcal{H}_{2n}^{4m}$ appear.

The plane wave representation (8) for $\mathcal{U}$ suggested difficulties for grazing modes ($\zeta \to 0$, $C \to \infty$), but we showed, from the analogous representation (13) for G that the solution is finite in the limit. The same problem is implicit in $\mathcal{U}$ of (50), and the essentials of the interrelation of the spherical and plane wave representations are given by (51); the right side is singular if $\zeta \to 0$, so $\sum_s$ must then diverge. To investigate this we need consider only large values of s_i. To facilitate discussion, we first substantiate the remark after (11) that the rigorous result (8) also follows from an asymptotic evaluation of (4).

From (4) in terms of the asymptotic form $U(\mathbf{r}_s) \sim h(kr_s)\, G(\hat{\mathbf{r}}_s, \hat{\mathbf{k}}_0)$ for $kr_s \sim \infty$ [obtained, e.g., from the saddle point approximation of (6)], or equivalently, from (50) in terms of $i^n h_n(x) \sim h(x) = \exp(ix)/ix$, we have

$$\mathcal{U} \sim \sum_s \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)\, h(kr_s)\, G(\hat{\mathbf{r}}_s, \hat{\mathbf{k}}_0) = \sum \exp(ikf_s)\, F_s,$$

$$f_s = \hat{\mathbf{k}}_0 \cdot \mathbf{b}_s + r_s = \xi_0 s_1 b_1 + \eta_0 s_2 b_2 + |\mathbf{r}_0 - \mathbf{b}_s|, \quad F_s = G/ikr_s. \tag{59}$$

We relabled the original $\mathbf{r}$ as $\mathbf{r}_0$ in order to replace $s_1 b_1$ and $s_2 b_2$ by x and y in the following; we also use $\mathbf{r}_s = |\mathbf{r}_0 - \mathbf{x} - \mathbf{y}|$. Applying the method of stationary phase, we obtain

$$\mathcal{U} \sim \sum_\nu \frac{\exp[ikf(\nu)]F(\nu)2\pi i}{kb_1 b_2 [f_{xx} f_{yy} - (f_{xy})^2]^{1/2}},$$

$$f = \xi_{\nu_1} x + \eta_{\nu_2} y + |\mathbf{r}_0 - \mathbf{x} - \mathbf{y}| \tag{60}$$

where F and f (and its second derivatives f_{xx}, etc.) are the values at the stationary points specified by $f_x = \xi_{\nu_1} + (x - x_0)/r_s = 0$, $f_y = \eta_{\nu_2} + (y - y_0)/r_s = 0$. We have

$$[\ ]^{1/2} = z_0/r_s^2 = \zeta/r_s,$$

$$f = \xi(x_0 - \xi r_s) + \eta(y_0 - \eta r_s) + r_s = x_0\xi + y_0\eta + |z_0|\,\zeta;$$

thus, (59) and (60) reproduce (8), and all forms exist provided $\zeta = \zeta(\nu_1, \nu_2) \neq 0$.

To investigate the role of the terms $|s_i| \sim \infty$ in the behavior near a singularity $\zeta \approx 0$, we rewrite the rigorous s-sum forms of $\mathcal{U}$ as

$$\mathcal{U} = \mathcal{U}_T + \mathcal{U}_A,$$

$$\mathcal{U}_A = \sum{}^* \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)\, h(kb_s)\, [G(-\hat{\mathbf{b}}_s, \hat{\mathbf{k}}_0) \exp(-ik\mathbf{r}_0 \cdot \hat{\mathbf{b}}_s)], \tag{61}$$

where $\mathcal{U}_T$ is the original s-sum (4) or (50) truncated at some finite large values $|s_i^*|$ corresponding to the smallest values in $\sum^*$ such that $b_s \gg r_0$. In $\mathcal{U}_A$, we have $\hat{\mathbf{r}}_s \approx -\hat{\mathbf{b}}_s$, the direction from the scatterer to the origin. Similarly, from the saddle point approximation of the integral in (12), or from (53) in terms of $i^n h_n \sim h$, we have for large kb_i,

$$G(\hat{\mathbf{r}}, \hat{\mathbf{k}})$$

$$\sim g(\hat{\mathbf{r}}, \hat{\mathbf{k}}) + \sum{}' \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)\, h(kb_s)\, [g(\hat{\mathbf{r}}, -\hat{\mathbf{b}}_s) G(-\hat{\mathbf{b}}_s, \hat{\mathbf{k}}_0)]. \tag{62}$$

For the present purpose, were kb_i small or moderate, we would write $G = G_T + G_A$, with G_T as the form (53) with the s-sum truncated, etc. For either case [as well as for the left side of (51), or for the asymptotic form of $\mathcal{H}$ of (53)], the behavior for large s_i is determined by the form

$$\sum{}^* = \sum{}^* \exp(i\mathbf{k}_0 \cdot \mathbf{b}_s)\, h(kb_s)\, \mathcal{J}(-\hat{\mathbf{b}}_s)$$

$$= \sum{}^* \exp(ikf)\, \mathcal{J}(-\hat{\mathbf{b}}_s)/ikb_s,$$

$$f = \hat{\mathbf{k}}_0 \cdot \mathbf{b}_s + b_s = \xi_0 s_1 b_1 + \eta_0 s_2 b_2 + (s_1^2 b_1^2 + s_2^2 b_2^2)^{1/2} \tag{63}$$

where $\sum^*$ is the remainder of $\sum_s$ after roughly $4|s_1^* s_2^*|$ terms.

We cannot evaluate (63) as we did (59): Because the stationary points of the present $f = \xi x + \eta y + \rho$ with $\rho = (x^2 + y^2)^{1/2}$ are those of (60) for $r_0 = 0$ (i.e., $\xi_{\nu_1} = -x/\rho$ and $\eta_{\nu_2} = -y/\rho$, such that $\xi^2 + \eta^2 = 1$ corresponds to a grazing mode R), we would have to replace $\sum_\nu$ of (60) by the set of singular terms $\sum_R$. Instead we approximate $\sum^*$ by the set of analogous integrals $\sum_N \int^*$ corresponding to the near-grazing modes N. We have $kf = \mathbf{k}_\nu \cdot \mathbf{b}_s + kb_s - 2\pi(s_1\nu_1 + s_2\nu_2)$; dropping the redundant multiples of 2π, and introducing polar coordinates $s_1 b_1 = \rho\cos\beta$, $\xi_{\nu_1} = \sin\theta\cos\varphi$, etc., we write

$$\int^* = (b_1 b_2 ik)^{-1} \int_{\rho^*}^\infty d\rho \int_0^{2\pi} d\beta\, \mathcal{J}|\beta|$$

$$\times \exp\{ik\rho[\sin\theta\cos(\beta - \varphi) + 1]\} \tag{64}$$

with $\theta = \theta(N_1, N_2)$ near $\pi/2$. The phase of the β-integral is stationary at $\beta = \varphi$, $\pi + \varphi$; consequently, since $k\rho\sin\theta \gg 1$,

$$\int^* \sim \frac{1}{ik^2 b_1 b_2} \left(\frac{2\pi}{\sin\theta}\right)^{1/2} \{\mathcal{J}[\varphi] J_+ + \mathcal{J}[\pi + \varphi] J_-\},$$

$$J_\pm = \exp(\mp i\pi/4) k \int_{\rho^*}^\infty \exp[ik\rho(1 \pm \sin\theta)]\, (k\rho)^{-1/2}\, d\rho$$

$$= [\exp(\mp i\pi/4)/(1 \pm \sin\theta)^{1/2}]\, I_\pm,$$

$$I_\pm = \int_{x_\pm}^\infty \exp(ix)\, x^{-1/2}\, dx, \quad x_\pm = k\rho^*(1 \pm \sin\theta), \tag{65}$$

where I is Fresnel's integral. The step from (64) to (65) is the analog of summing the spherical waves of the scatterers on the pair of lattice lines of (63) perpendicular to the rays φ, $\pi + \varphi$ and displaced a distance ρ from the origin. The result (65) shows that the spherical sources on each line add up to a cylindrical source at ρ with axis perpendicular to $\varphi, \pi + \varphi$; the remaining integration is thus the analog of summing the cylindrical waves of the particular set of parallel lattice lines.

Except for $\sin\theta$ very near unity, we have

$$I_\pm \sim i \frac{\exp[ik\rho^*(1 \pm \sin\theta)]}{[k\rho^*(1 \pm \sin\theta)]^{1/2}}, \tag{66}$$

i.e., cylindrical waves which vanish as $\rho^* \sim \infty$. Thus, in general, $\sum_N \int^* \to 0$ as $\rho^* = [(s_1^* b_1)^2 + (s_2^* b_2)^2]^{1/2} \to \infty$.

On the other hand, for $\sin\theta \approx 1$, we use $\int_{\rho*}^{\infty} = \int_0^{\infty} - \int_0^{\rho*}$ to obtain

$$I_- = I_-(\infty) - I_-(\rho^*), \quad I_-(\infty) = \pi^{1/2}\exp(i\pi/4),$$
$$I_-(\rho^*) \approx 2[k\rho^*(1-\sin\theta)]^{1/2}, \tag{67}$$

and similarly (corresponding to $\beta = \pi + \varphi$, $\hat{\mathbf{b}} = -\hat{\mathbf{k}}_N$),

$$\int^* = \int^{\infty} - \int^{\rho*}, \quad \int^{\infty} \approx \frac{\mathcal{J}[\pi+\varphi]\pi}{k^2 b_1 b_2}\left[\frac{2}{\sin\theta(1-\sin\theta)}\right]^{1/2}$$
$$\approx \frac{2\pi\mathcal{J}[\pi+\varphi]}{k^2 b_1 b_2 \cos\theta} = 2C_N\mathcal{J}(\hat{\mathbf{k}}_N), \tag{68}$$

where $\int^{\rho*}$ is finite for $\sin\theta \to 1$. Thus, for near-grazing modes,

$$\sum_s = \sum_1 + \sum_N 2C_N\mathcal{J}(\hat{\mathbf{k}}_N),$$

where $\sum_1$ is finite for $\zeta_N \to 0$, but C_N is singular as $1/\zeta_N$. The near-grazing value $2C_N\mathcal{J}(\hat{\mathbf{k}}_N)$ corresponds to either $2C_N g_{\alpha N} G_{N0}$ of (35) or $\phi_N 2C_N G_{N0}$ of (37).

The same considerations apply for the lattice sums $\mathcal{H}$ of (53). However, just as for $\mathcal{U}$ of (8) and G of (13), the behavior for $\theta \to \pi/2$ follows more directly from the corresponding array mode representation of $\mathcal{H}$ in terms of $\mathbf{S}$ of (13). Specializing the procedure for G, we construct

$$\mathcal{H}_n^m = \lim_{\epsilon\to 0}\left[\sum_s \exp(i\mathbf{k}_0\cdot\mathbf{b}_s)\, i^n h_n(kr_s)Y_n^m(\hat{\mathbf{r}}_s) - i^n h_n(hr_0)Y_n^m(\hat{\mathbf{r}}_0)\right],$$
$$\mathbf{r}_s = \epsilon\hat{\mathbf{z}} - \mathbf{b}_s, \tag{69}$$

where $i^n h_n Y_n^m$ is representable as the integral form (6) with G replaced by $Y_n^m(\hat{\mathbf{p}})$. Proceeding as before for (13), we obtain

$$\mathcal{H}_n^m = \mathbf{S}\, 2C_\nu Y_n^m(\hat{\mathbf{k}}_\nu) = \mathbf{S}\, C_\nu[Y_n^m(\hat{\mathbf{k}}_\nu) + Y_n^m(\hat{\mathbf{k}}_{\nu'})]. \tag{70}$$

Thus, if there are near-grazing modes N, the dominant terms are $2\sum_N C_N Y_n^m(\hat{\mathbf{k}}_N)$, which are singular as $1/\zeta_N$ for $\zeta_N \to 0$.

B. Conical waves

To delineate the relation of the results for the lattice to those of the periodic line[1] (and to develop forms for the reduction of the lattice sums $\mathcal{H}_n^m$ to more rapidly convergent forms) we work with spherical harmonics with polar axis along $\hat{\mathbf{x}}$, instead of along $\hat{\mathbf{z}}$ as in (57), i.e., with

$$Y_n^l(\xi;\zeta,\eta) = P_n^l(\sin\theta\cos\varphi)\exp(il\psi)$$
$$= P_n^l(\xi)(\zeta + i\eta)^l/(\zeta^2+\eta^2)^{l/2}. \tag{71}$$

In applying such forms as (49) and (51), the same choice of polar axis for Y is required on both sides of the equal sign. However, we may also work with mixed forms by using, e.g., $Y_n^m(\zeta;\xi,\eta) = \sum_{l=-n}^{n} D_n^{m,l} Y_n^l(\xi;\zeta,\eta)$, where D is a Wigner coefficient[12] for a 90 degree rotation around $\hat{\mathbf{y}}$.

If we perform only one of the s_i sums in (50) (or sum over one of any equivalent pair of indices) we represent $\mathcal{U}$ by sets of conical cylindrical waves corresponding to the field of the periodic lines we have selected. For convenience, we replace the earlier $s_1 b_1$, $s_2 b_2$ by sb, td, and ν_1, ν_2 by ν, μ. We sum over $s = s_1$ by exploiting our earlier development[1] for the periodic line along $\hat{\mathbf{x}}$.

We rewrite (1.19) as

$$\sum_{s=-\infty}^{\infty}\exp(iksb\xi_0)\, i^n h_n(kr_{st})P_n^l(\xi_s)$$
$$= \frac{\pi}{kb}\sum_{\nu=-\infty}^{\infty}\exp(ikx\xi_\nu)\, i^l H_l(k\rho_t\gamma_\nu)P_n^l(\xi_\nu) \tag{72}$$

with $\gamma_\nu = (1-\xi_\nu^2)^{1/2} = |\gamma_\nu|$ or $i|\gamma_\nu|$ for the corresponding direction sine along $\hat{\mathbf{x}}$, and $\rho_t = [z^2 + (y-td)^2]^{1/2}$ for the distance normal to the line specified by $y = td$ and $z = 0$. Here $H_l(x) = H_l^{(1)}(x)$, and $H_l(i|x|) = -i(i^{-l}/2\pi)K_l(|x|)$. Introducing $\tan\psi_t = (y-td)/z = \eta_t/\xi$, such that ψ and ρ are cylindrical coordinates in the $x=0$ plane, we multiply (72) through by $\exp(il\psi_t)$ and replace $P_n^l(\xi_\nu)\exp(il\psi)$ by $Y_n^l(\xi_\nu;\xi,\eta_t)$. Thus a periodic line of spherical sources is equivalent to a conical cylindrical set of waves as discussed earlier in detail.[1] We obtain (72) most directly by noting that I of (49) in terms of $Y_n^l(\xi;\zeta,\eta)$ also equals

$$I = i^l\exp(il\psi)\int_{-\infty}^{\infty}\exp[ik(x-sb)]P_n^l(\xi)H_l(k\rho\gamma)\,d\xi/2, \tag{73}$$

which together with (49) corresponds to the complete (1.20); multiplying (73) and the first form of the appropriate (49) by $\sum_s \exp(isksb\xi_0)$ we use (7) and get (72). Thus, we may represent (4), (8), or (50) by

$$\mathcal{U} = \frac{\pi}{kb}\sum_t\sum_\nu\sum_{nm}\exp(iktd\eta_0)A_{n,t}\exp(ikx\xi_\nu)\, i^l H_l(k\rho_t\gamma_\nu)$$
$$\times P_n^l(\xi_\nu)\exp(il\psi_t), \tag{74}$$

i.e., the field of a set of periodic lines with axes parallel to $\hat{\mathbf{x}}$ spaced d apart along y.

In (74) we replaced m by l and shifted the index to a subscript on A to emphasize that the values of the coefficients $A(\hat{\mathbf{k}}_0)$ depend on the particular decomposition (57) or (71) for Y. The corresponding systems of algebraic equations (55) and (56) now depend on different lattice sums, say $\mathcal{H}_{n,l}$ representing the functions in (53) expressed in terms of

$$Y_n^l(-\hat{\mathbf{b}}_s) = Y_n^l(-\xi_{st};0,-\eta_{st}) = P_n^l(-sb/B_{st})\exp[-il(\pi/2)\,\mathrm{sgn}\,t],$$
$$B_{st} = [(sb)^2 + (td)^2]^{1/2}. \tag{75}$$

This representation is not as symmetrical as (58), and the corresponding system of algebraic equations (55) and (56) for A_{nl} are about twice as complicated; i.e., the parity requirement that $n-m$ of (58) is even eliminates half the cross terms. On the other hand, the functions $\mathcal{H}_{n,l}$ in terms of (75) are easier to reduce to more convergent forms by exploiting our earlier results for the periodic line[1] and the grating.[2] In the sequel we therefore consider $\mathcal{H}_{n,l}$ in detail, and then use $\mathcal{H}_n^m = \sum D_n^{m,l}\mathcal{H}_{n,l}$ to construct the sums required for the more symmetrical system of equations A_n^m.

Comparison of (74) and (8) rewritten as $U = \sum_{\nu\mu} 2C_{\nu\mu}\,\phi_{\nu\mu} \sum_{n,l} A_{n,l}\, Y_n^l(\xi_\nu;\, \zeta,\, \eta_\mu)$ shows that for $z > 0$,

$$\sum_t \exp(iktd\eta_0) i^l H_l(kp_t\gamma_\nu) Y_n^l(\xi_\nu;\, \zeta,\, \eta_t)$$
$$= 2\sum_\mu \exp[iky\eta_\mu + ikz\zeta(\nu,\mu)]\; Y_n^l(\xi_\nu;\, \zeta,\, \eta_\mu) C'_{\nu\mu} = J,$$
$$C'_{\nu\mu} = [kd\zeta(\nu,\mu)]^{-1}; \tag{76}$$

for $z < 0$, we replace ζ by $-\zeta$. For $\gamma_\nu \neq 0$, this follows directly from the earlier result for the grating, e.g., as in (13.9),

$$\sum_{t=-\infty}^{\infty} \exp(iktd\eta_0) i^l H_l(kp_t\gamma_\nu) \exp(il\psi_t)$$
$$= 2 \sum_{\mu=-\infty}^{\infty} \exp(iky\eta_\mu + ikz\zeta) \exp[il\psi(\nu,\mu)] C'_{\nu\mu}\,; \tag{77}$$

multiplying through by $P_n^m(\xi_\nu)$ gives J of (76). (For $z < 0$, we use $-z$ and $\pi - \psi$.) On the other hand, if $\gamma_\nu \to 0$ (i.e., if $\xi \to 1$ corresponding to a grazing conical mode along $\hat{\mathbf{x}}$), then as shown in detail for (1.31) only the element $l = 0$ of the set $H_l(kp\gamma) P_n^l(\xi)$ becomes singular. For $\gamma_\nu = \gamma_N \approx 0$, we have $\zeta^2 \approx -\eta^2$, and we may use the $l = 0$ case of (76) in the form

$$J \approx \sum_t \exp(iktd\eta_0) H_0(kp_t\gamma_N) \approx 2 \sum_\mu \frac{\exp(iky\eta_\mu - kz|\eta_\mu|)}{kdi|\eta_\mu|},$$
$$\gamma_N \approx 0. \tag{78}$$

If also $\eta_\mu = \eta_\mu \approx 0$, then we are dealing with a grazing plane wave mode.

To analog the development (61) of the spherical representation, except for $\gamma_\nu \approx 0$, we use the asymptotic form

$$i^l H_l(kp_t\gamma_\nu) \sim H(kp_t\gamma_\nu), \quad H(x) = \exp(ix - i\pi/4)(2/\pi x)^{1/2}, \tag{79}$$

and reduce (74) to

$$U \sim (\pi/kb) \sum_\nu \exp(ikx\xi_\nu) V,$$
$$V = \sum_t \exp(iktd\eta_0) H(kp_t\gamma_\nu) G(\hat{\mathbf{r}}_{\nu t}, \hat{\mathbf{k}}_0), \tag{80}$$

where $\hat{\mathbf{r}}_{\nu t} = \hat{\mathbf{x}}\xi_\nu + \hat{\mathbf{y}}\eta_t + \hat{\mathbf{z}}\,\zeta(\nu;t)$ with $\zeta = (\gamma_\nu^2 - \eta_t^2)^{1/2} = |\zeta|$ or $i|\zeta|$. Corresponding to (59) we write

$$V = \sum_t \exp(ikf_t) F_t,$$
$$f_t = td\eta_0 + p_t\gamma_\nu = td\eta_0 + [z_0^2 + (y_0 - td)^2]^{1/2}\gamma_\nu,$$
$$F = G\exp(-i\pi/4)(2/\pi kp_t\gamma_\nu)^{1/2}, \tag{81}$$

where we replaced z, y by z_0, y_0. Using the stationary phase procedure for $\gamma = |\gamma|$,

$$V \sim \sum_\mu \exp[ikf(\mu)]\, \mathcal{G}(\mu), \quad f(\mu) = \eta_\mu y + [z_0^2 + (y_0 - y)^2]^{1/2}\gamma_\nu,$$
$$\mathcal{G}(\mu) = \frac{F(\mu)}{d}\left(\frac{2\pi}{k|f''|}\right)^{1/2} \exp[i(\pi/4)\,\mathrm{sgn} f'')], \tag{82}$$

where $F(\mu)$, $f(\mu)$ and $f'' = f_{yy}$ are the values at the stationary points specified by $f_y = \eta_\mu + (y - y_0)\gamma_\nu/\rho = 0$. We obtain $f'' = \zeta^2/\gamma_\nu\rho$, and consequently, $\mathcal{G}(\mu) = G2/d(k^2\zeta^2)^{1/2} = 2C'_{\nu\mu}\, G_{\nu\mu}$. For the phase, the stationary condition gives $y = y_0 - \rho\eta_\mu/\gamma_\nu$ and $\rho = z_0\gamma/\zeta$; thus $f = \eta y_0 + \rho\zeta^2/\gamma = \eta y_0 + \zeta z_0$. The results are as in (8), even if $\gamma = i|\gamma|$, or in the exceptional case $\gamma_\nu \approx 0$ for which we use (78).

To analog (61) ff., if $\gamma_\nu \not\approx 0$, we use $i^l H_l(kp_t\gamma_\nu) \sim H(k|t|d\gamma_\nu)$ to obtain

$$\sum\nolimits^* = (\pi/kb) \sum_\nu \sum_t{}^* \exp(iktd\eta_0) H(k|t|d\gamma_\nu) \mathcal{J}(-\hat{\mathbf{b}}_{\nu t}),$$
$$\hat{\mathbf{b}}_{\nu t} = -\hat{\mathbf{x}}\xi_\nu + \hat{\mathbf{y}}\eta_t = -\hat{\mathbf{x}}\xi_\nu - \hat{\mathbf{y}}\gamma_\nu \,\mathrm{sgn} t, \tag{83}$$

where $\mathcal{J}$ is the bracketed function of either (61) or (62), and t ranges from $-\infty$ to $-|t^*|$, and from t^* to ∞. For $\gamma = i|\gamma|$, we have $H \propto \exp(-kd|t\gamma_\nu|) \sim \exp(-|t\nu|2\pi d/b)$, and the double sum converges rapidly. For real γ, the phase is $kf = kd(t\eta_0 + |t|\gamma_\nu)$, and the stationary values $\eta_\mu = \pm\gamma_\nu$ [obtained by setting $r_0 = 0$ in (82)] correspond to grazing modes. Proceeding as before for (63), we obtain the analog of (64) and (65),

$$\int^* \sim \frac{\pi}{k^2bd}\left(\frac{2}{\pi\gamma_\nu}\right)^{1/2} \exp(-i\pi/4)\{L_+ + L_-\},$$
$$L_\pm = \frac{\mathcal{J}(\hat{\mathbf{x}}\xi_\nu \mp \hat{\mathbf{y}}\gamma_\nu)}{(\gamma_\nu \pm \eta_\mu)^{1/2}}\, I_\pm \tag{84}$$

with I as in (65) with lower limit $x_\pm = ky^*(\gamma_\nu \pm \eta_\mu)$. In distinction to (65), either term or both terms of (84) may be near-grazing; in (65), only the I_- term may become singular, but φ is a parameter and (84) corresponds essentially to the $I_-(\varphi)$ term of (65) plus an analogous term in $I_-(\pi + \varphi)$. If only η_μ, but not $-|\eta_\mu|$ is near γ_ν, then in terms of I_- of (67),

$$\int^\infty \sim \mathcal{J}(\hat{\mathbf{k}}_{NM})\, \frac{\pi}{k^2bd}\left[\frac{2}{\gamma_N(\gamma_N - \eta_M)}\right]^{1/2} \approx 2\mathcal{J}(\hat{\mathbf{k}}_{NM}) C_{NM} \tag{85}$$

as follows from $2/\gamma(\gamma - \eta) \approx 4/(\gamma^2 - \eta^2) = 4/\zeta^2$. The result $2\mathcal{J}C$ is the same as that obtained from the other representations. [Note that the periodic lines along x are not the resonant lattice lines unless $\gamma_N = 1$, i.e., unless $\xi_N = 0$ corresponding to one of the $\xi(0)$-set.]

On the other hand, if $\gamma_N \approx \eta_M \approx 0$ (i.e., if $\xi_N \approx 1$, as required for grazing along the axes of the periodic lines), then we cannot use the asymptotic form of H_l. We require the analog of (76) for

$$[\mathcal{J}(\hat{\mathbf{x}})\pi/kb] \sum_t{}^* H_0(k|t|d\gamma_\nu) \exp(iktd\eta_0) \tag{86}$$

We evaluated the corresponding $\sum'$ series before[13] for all kd; from (13.42), for $\gamma_N \approx 0$ and $\eta_M \approx 0$,

$$\sum{}' H_0(k|t|d\gamma_N) \exp(iktd\eta_0) \approx 2/kd\gamma_N \cos\psi_{NM} = 2/kd\zeta_{NM} \tag{87}$$

where we used $\gamma_\nu \cos\psi_{\nu\mu} = \zeta_{\nu\mu} = \mathrm{Re}(\zeta^2 + \eta^2)^{1/2}\exp(i\psi)$. Thus, all for cases we obtain $2\mathcal{J}(\hat{\mathbf{k}}_{NM}) C_{NM}$ as before.

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Lattice sums and scattering coefficients for the rectangular planar array*

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We consider the plane wave mode solution for the three-dimensional problem of multiple scattering by a doubly periodic planar array of bounded obstacles. The mode amplitudes are expressed in terms of the multiple scattering coefficients for one obstacle of the array, and these are specified algebraically by the single scattered coefficients and the spherical wave lattice sums that characterize the array. We derive rapidly convergent forms of the lattice sums by exploiting our earlier results for the periodic line of bounded obstacles and for the grating of parallel cylinders. Then we develop closed form approximations for the multiple scattering coefficients for small scatterers which exhibit the effects of the array in coupling the multipole coefficients of the isolated scatterers.

INTRODUCTION

In a previous paper[1] we considered multiple scattering of waves by a doubly periodic planar array of arbitrary obstacles, and derived several representations of the solution in terms of the multiple scattering amplitude G and coefficients A_n^m for one of the obstacles. We emphasized the plane wave array-mode form, and applied the corresponding functional equation for G in terms of its single scattered value to analyze array resonances for near-grazing modes.

Now we consider the system of algebraic equations for the A_n^m in terms of the single scattered coefficients and in terms of the spherical wave lattice sums H_n^m that specify the array. We derive rapidly converging representations for H by exploiting our earlier results for the periodic line[2] of bounded obstacles and for the grating[3] of parallel cylinders. Then we develop closed form approximations for the multiple scattering coefficients for small scatterers to exhibit coupling of the multipole coefficients of the isolated obstacles.

The representations we derive for H apply for an arbitrary rectangular cell d by b, and the size of $d/b = \rho \geq 1$ determines rapidity of convergence of the double Schlömilch series of modified Hankel functions that arise. From symmetry, we express the series for $\rho < 1$ in terms of those for $\rho > 1$, so that the worst case corresponds to the square cell $\rho = 1$. Discounting the resonances considered earlier,[1] convergence is rapid even for $\rho = 1$, for which case about half the lattice sums vanish by symmetry. The development leads to various relations involving the Riemann zeta function, Wigner rotation coefficients, and Bessel functions.

The multipole coupling effects for spacings very small compared to wavelength depend markedly on the boundary conditions of the scatterers. Since the results require detailed physical considerations, we reserve the low frequency region for a sequel.

For brevity, we use the notation (1:9) to indicate Eq. (9) of Ref. 1, etc.

1. SOLUTION

We showed before[1] that, for a plane wave

$$\phi = \exp(i\mathbf{k}\cdot\mathbf{r}), \quad \hat{\mathbf{r}} = \hat{\mathbf{x}}\xi + \hat{\mathbf{y}}\eta + \hat{\mathbf{z}}\zeta = \hat{\mathbf{r}}(\xi,\eta),$$

$$\zeta = (1-\xi^2-\eta^2)^{1/2} = \cos\theta, \quad \eta/\xi = \tan\varphi, \tag{1}$$

$$\hat{\mathbf{k}} = \hat{\mathbf{r}}(\xi_0,\eta_0) = \hat{\mathbf{k}}_{00},$$

incident on a rectangular lattice $sb\hat{\mathbf{x}} + td\hat{\mathbf{y}}$ ($s,t = 0, \pm 1, \pm 2, \cdots$) of identical bounded obstacles, the transmitted scattered field equalled

$$U = 2\sum_{\nu,\mu} C_{\nu\mu} G(\hat{\mathbf{k}}_{\nu\mu}, \mathbf{k}_{00}) \exp(i\mathbf{r}\cdot\mathbf{k}_{\nu\mu}),$$
$$C_{\nu\mu} = \pi/k^2 b\, d\zeta_{\nu\mu}, \qquad \nu,\mu = 0, \pm 1, \pm 2, \cdots, \tag{2}$$

$$\hat{\mathbf{k}}_{\nu\mu} = \hat{\mathbf{x}}\xi_\nu + \hat{\mathbf{y}}\eta_\mu + \hat{\mathbf{z}}\zeta_{\nu\mu}, \quad \xi_\nu = \xi_0 + 2\pi\nu/kb,$$
$$\eta_\mu = \eta_0 + 2\pi\mu/kd, \quad \zeta_{\nu\mu} = (1-\xi_\nu^2-\eta_\mu^2)^{1/2}. \tag{3}$$

Here $\zeta = |\zeta|$ or $i|\zeta|$ for $\sin^2\theta_{\nu\mu} = \xi_\nu^2 + \eta_\mu^2 < 1$ or > 1 (propagating or evanescent modes), and G is the multiple scattered amplitude of one obstacle. For the reflected field, we replace $\hat{\mathbf{k}}_{\nu\mu}$ by its image $\hat{\mathbf{k}}' = \hat{\mathbf{k}} - 2\zeta\hat{\mathbf{z}}$. We expressed G functionally in terms of the single scattered value g in (1:13), and then applied this array-mode form to analyze resonances corresponding to near-grazing modes $\zeta_{\nu\mu} = \zeta_{NM} \approx 0$; although U is not defined for $\zeta_{\nu\mu} = 0$, we obtained the finite limit for $\zeta_{NM} \to 0$.

Now, we work with the spherical harmonic expansion

$$G(\hat{\mathbf{r}},\hat{\mathbf{k}}) = \sum_{nm} A_n^m(\hat{\mathbf{k}}) Y_n^m(\hat{\mathbf{r}}), \quad \sum_{nm} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}, \tag{4}$$

with the multiple scattered coefficients A_n^m expressed algebraically in terms of the corresponding single scattered coefficients and the basic lattice sums H of the array. For general obstacles specified by the isolated scattering amplitude

$$g(\hat{\mathbf{r}},\hat{\mathbf{k}}) = \sum_{nm} a_n^m(\hat{\mathbf{k}}) Y_n^m(\hat{\mathbf{r}}), \quad a_n^m(\hat{\mathbf{k}}) = \sum_{pq} b_{np}^{mq} Y_p^{-q}(\hat{\mathbf{k}}), \tag{5}$$

we have from (1:55)

$$A_n^m = a_n^m(\mathbf{k}) + \sum_{pq}\sum_{\sigma\tau} b_{np}^{mq} A_\sigma^\tau \sum_l d_l \begin{pmatrix} -q & \tau \\ p & \sigma \end{pmatrix} H_l^{\tau-q}, \tag{6}$$

where $p+\sigma+l$ is even, l changes by steps of 2 from $|p-\sigma|$ (or from $|\tau-q|$ if it is the larger) to $p+\sigma$, and the numbers[4,5] d_l arise from the expansion $Y_p^{-q} Y_\sigma^\tau = \sum d_l Y_l^{\tau-q}$. For spherically symmetric obstacles $a_n^m(\hat{\mathbf{k}}) = (-1)^m a_n Y_n^{-m}(\hat{\mathbf{k}})$, and (6) reduces to

$$A_n^m = (-1)^m a_n \left[Y_n^{-m}(\hat{\mathbf{k}}) + \sum_{\sigma\tau} A_\sigma^\tau \sum_l d_l \begin{pmatrix} -m & \tau \\ n & \sigma \end{pmatrix} H_l^{\tau-m} \right], \tag{7}$$

where, e.g., $a_n = -(2n+1)j_n(ka)/h_n(ha)$ if the field equals zero on spheres of radius a.

The lattice sums were represented in (1:53) as sets of spherical waves reaching one obstacle from all neighbors

$$H_n^m = \sum_{st}{}' \exp[ik(sb\xi_0 + t\,d\eta_0)]\, i^n h_n(kb_{st}) Y_n^m(-\hat{\mathbf{b}}_{st}),$$
$$b_{st} = sb\hat{\mathbf{x}} + td\hat{\mathbf{y}}, \quad h_n = h_n^{(1)}, \tag{8}$$

where both s and t range from $-\infty$ to ∞, and the prime means exclusion of the central element $s=t=0$. As will be discussed shortly, the sum does not exist for $\zeta_{\nu\mu}=0$; if $\zeta_{NM}\to 0$, then H becomes singular as $1/\zeta_{NM}$. Otherwise, from symmetry we require $\sum_{st}=\sum_s\sum_t=\sum_t\sum_s$, which follows if the double series and the row and column series simply converge; however, we may use $k=(2\pi/\lambda)+i\epsilon$ to obtain absolute convergence, and then let $\epsilon=|\epsilon|\to 0$. The replacement of ξ_0 and η_0 by ξ_ν and η_μ merely introduces the factor $\exp[i2\pi(s\nu+t\mu)]=1$ into the summand, i.e.,

$$H_n^m(\xi_\nu,\eta_\mu) = H_n^m(\xi_0,\eta_0), \quad H_n^m(\hat{\mathbf{k}}_{\nu\mu}) = H_n^m(\hat{\mathbf{k}}_{00}) = H_n^m(\hat{\mathbf{k}}). \tag{9}$$

Thus, the functions H_n^m for assigned values $\hat{\mathbf{k}}$, b, d, and k are the same if the incident direction $\hat{\mathbf{k}}=\hat{\mathbf{k}}_{00}$ is replaced by any $\hat{\mathbf{k}}_{\nu\mu}$ of the array set (3). We also have $H_n^m(-\hat{\mathbf{k}}_{\nu\mu}) = H_n^m(-\hat{\mathbf{k}}_{00})$ which corresponds to changing the signs of ξ_0 and η_0 in (8); if we then replace s and t by their negatives, and use $Y_n^m(-\hat{\mathbf{r}}) = (-1)^n Y_n^m(\hat{\mathbf{r}})$, it follows that

$$H_n^m(-\hat{\mathbf{k}}_{\nu\mu}) = (-1)^n H_n^m(\hat{\mathbf{k}}), \quad \hat{\mathbf{k}}=\hat{\mathbf{k}}_{00}. \tag{10}$$

Relations (9) and (10) help to demonstrate that approximation for G obtained by truncating the system for A satisfy the required reciprocity and scattering theorems (1:17, 18).

Consideration of the singularities of H may be based on the asymptotic development (1:60)ff and the form

$$H = H_T + H_A, \quad H_A = \sum^{*} \exp(i\mathbf{k}\cdot\mathbf{b}_{st}) h(kb_{st}) Y_n^m(-\mathbf{b}_{st}),$$
$$h(x) = h_0(x) = \exp(ix)/ix, \tag{11}$$

where H_T corresponds to $\sum'$ truncated at finite large values $|s^*|$ and $|t^*|$ satisfying $k[(s^*b)^2+(t^*d)^2]^{1/2} = k\rho^* \gg 1$. The infinite double series H_A (in which we used the asymptotic form $i^n h_n \sim h$) is the remainder after approximately $|4s^*t^*|$ terms. The phase $\mathbf{k}\cdot\mathbf{b}_{st} + kb_{st} = fk$ with $f = \xi x + \eta y + \rho$ is stationary when $\xi_\nu = -x/\rho$ and $\eta_\mu = -y/\rho$, but $\sum^*$ then diverges; this corresponds to $\xi_\nu^2 + \eta_\mu^2 = 1$, i.e., grazing modes $\zeta_{\nu\mu}=0$. If we approximate $\sum^*$ by a set of analogous integrals (1:64) summed over the modes $(\hat{k}_{NM})$ closest to grazing, we obtain the Fresnel integral representation (1:65), $\sum_{NM}\int^*$. Except for $\zeta_{NM}=\cos\theta_{NM}\approx 0$, the approximation for H_A based on (1:66) is a set of cylindrical waves $[e^{iR}R^{-1/2}$, $R = k\rho^*(1\pm\sin\theta_{NM})]$ radiating from the lattice lines through ρ^* perpendicular to φ_{NM}, $\pi+\varphi_{NM}$; thus, in general, $\sum_{NM}\int^* \to 0$ as $\rho^*\to\infty$. On the other hand, if there is one or several near-grazing modes ($\zeta_{NM}\approx 0$), then from (1:68), $\sum' = \sum_1 + 2\sum C_{NM} Y_n^m(\hat{\mathbf{k}}_{NM})$, where $\sum_1$ is finite but C_{NM} becomes singular as $1/\zeta$ as $\zeta\to 0$.

The behavior for near-grazing modes follows more simply from the array-mode representation (1:70) of H. Replacing $-\hat{\mathbf{b}}_{st}$ by $-\hat{\mathbf{b}}_{st}+\epsilon\mathbf{z}$ in (8) and adding and subtracting the missing term, we express H as

$$H_n^m = \mathbf{S}2C_{\nu\mu} Y_n^m(\hat{\mathbf{k}}_{\nu\mu}) = \mathbf{S}C_{\nu\mu}[Y_n^m(\hat{\mathbf{k}}_{\nu\mu}) + Y_n^m(\hat{\mathbf{k}}'_{\nu\mu})],$$
$$\mathbf{S} = \lim_{\epsilon\to 0}\left(\sum_{\nu\mu} - \int d\nu\, d\mu\right)\exp(ik\epsilon\zeta_{\nu\mu}), \tag{12}$$

i.e., as the limit for $\epsilon=|\epsilon|\to 0$ of the field of the complete array less self-excitation responses of one obstacle. The convergence factor $\exp(ik\epsilon\zeta_{\nu\mu}) \sim \exp[-2\pi\epsilon(|\nu/b|^2 + |\mu/d|^2)^{1/2}]$ approaches zero with increasing $|\nu|$, $|\mu|$, and since Y_n^m is a polynomial in ξ and η, the form of the operator as a sum minus the analogous integral indicates rapid convergence except for $\zeta_{\nu\mu}\approx 0$. We decomposed the operator as $\mathbf{S}=\mathbf{S}_p+\mathbf{S}_e$, where $\mathbf{S}_p$ (in which we set $\epsilon=0$ directly) is given by

$$\mathbf{S}_p = \sum_p - \int_p = \sum_{\nu=-\nu^-}^{\nu^+}\sum_{\mu=-\mu^-}^{\mu^+} - \int_{-n^-}^{n^+} d\nu \int_{-m^-}^{m^+} d\mu,$$
$$n^\pm = |n^\pm| = (\mathbf{k}b/2\pi)(1\mp\xi_0), \quad m^\pm(\gamma) = |m^\pm| = (\mathbf{k}d/2\pi)(\gamma\mp\eta_0),$$
$$\gamma = (1-\xi^2)^{1/2}, \tag{13}$$

with $\nu^\pm = [n^\pm]$ and $\mu^\pm = [m^\pm(\gamma_\nu)]$ as the closest integers from below. We exclude integral values of $m^\pm$, $n^\pm$ corresponding to grazing modes ($\zeta_{\nu\mu}=0$) for which H is undefined. For near-grazing modes, $\zeta_{NM}\approx 0$, we see directly that the dominant terms are of the form $2C_{NM}Y_n^m(\hat{\mathbf{k}}_{NM})$. Although H is singular for $\zeta_{NM}\to 0$, we showed that H is finite in the limit.[1] Since we obtained simple approximations for H in terms of g for the array resonances corresponding to $\zeta_{NM}\approx 0$, and indicated how these approximations could be improved, we now exclude discussion of these exceptional cases. However, the alternative more rapidly converging representations H we develop in the following show the required singularities.

Although the scattering amplitudes G and g are invariant to the choice of polar axis for the spherical harmonics, the coefficients A_n^m, etc., are not, i.e., Eqs. (4)—(8) comprise an infinite number of interdependent representations depending on the choice of axis. We consider two, $\hat{\mathbf{z}}$ and $\hat{\mathbf{x}}$. For the first, we write

$$Y_n^m(\xi;\xi,\eta) = P_n^m(\cos\theta)\exp(im\varphi), \quad \cos\theta=\xi,$$
$$\exp(i\varphi) = (\xi+i\eta)/(\xi^2+\eta^2)^{1/2}, \tag{14}$$

and for the second

$$Y_n^l(\xi;\zeta,\eta) = P_n^l(\sin\theta\cos\phi)\exp(il\psi), \quad \sin\theta\cos\varphi=\xi,$$
$$\exp(il\psi) = (\zeta+i\eta)/(\xi^2+\eta^2)^{1/2} = (\zeta+i\eta)/\gamma; \tag{15}$$

in general, we suppress all but the first term of the argument of Y. The sets are related by

$$Y_n^m(\xi) = \sum_{l=-n}^{n} D_n^{m,l} Y_n^l(\xi), \tag{16}$$

where D is a Wigner coefficient[5] for a 90 degree rotation around $\hat{\mathbf{y}}$. The choice $Y(\xi)$ yields a form for H (for which we henceforth reserve H_n^m) retaining the essential symmetries of the lattice in full view: the form involves $P_n^m(0)$ which vanishes unless $n-m$ is even, and there-

fore half the cross-terms are missing in the corresponding simpler system of algebraic equations for A_n^m. However, the choice $Y(\xi)$ enables us to exploit all our earlier results for the periodic line[2] and for the grating[3] to obtain rapidly convergent forms of H; we indicate the $Y(\xi)$ functions by $H_{n,l}$.

In the next section we consider initially H_n^m and discuss the properties that follow directly by inspection of (8) and (12). Then we show how $H_{n,l}$ may be represented in terms of our earlier results,[2,3] and use (16) to obtain $H_n^m = \sum D_n^{m,l} H_{n,l}$. In the last section, we consider the algebraic equations for A_n^m in terms of H_n^m, and develop closed form approximations for small scatterers.

2. THE LATTICE SUMS

A. Initial considerations of H_n^m

From (14), we have

$$Y_n^m(-\hat{\mathbf{b}}_{st}) = P_n^m(0)\exp[im(\pi+\beta_{st})],$$
$$\exp(i\beta_{st}) = \frac{sb+itd}{[(sb)^2+(td)^2]^{1/2}}, \tag{17}$$
$$P_n^m(0) = \frac{(n+m)!\,(-1)^{(n-m)/2}\delta_e(n-m)}{2^n[(n-m)/2]!\,[(n+m)/2]!},$$

where $\delta_e(l) = \frac{1}{2}[1+(-1)^l]$ is a parity factor. Substituting into (8), we obtain

$$H_n^m = (-1)^m P_n^m(0)\sum_{st}{}' \exp(i\mathbf{k}\cdot\mathbf{b}_{st}) i^n h_n(kb_{st})\exp(im\beta_{st})$$
$$= H_n^m \delta_e(n-m), \qquad b_{st} = [(sb)^2+(td)^2]^{1/2}. \tag{18}$$

For the symbolic form $H[\mathbf{S}]$ of (12),

$$Y_n^m(\hat{\mathbf{k}}) + Y_n^m(\hat{\mathbf{k}}') = [P_n^m(\xi) + P_n^m(-\xi)]\exp(im\varphi)$$
$$= 2Y_n^m(\hat{\mathbf{k}})\delta_e(n-m)$$

gives the same parity constraint as in (18). We need consider only m positive in the form $H_n^m = H_n^m(\beta)$ of (18). Since $Y_n^{-m} = P_n^{-m}\exp(-im\beta)$,

$$H_n^{-m} = C_n^m H_n^m(-\beta), \quad C_n^m = (-1)^m(n-m)!/(n+m)!, \tag{19}$$

where $C_n^m = P_n^{-m}/P_n^m$.

Because of the parity factor in (17), we require only

$$H_{2n}^{2m} = (-1)^n P_{2n}^{2m}(0)(\textstyle\sum_{(1)} + i\sum_{(2)}) = H_{(1)}^{2m}(b,\xi;d,\eta) + iH_{(2)}^{2m},$$
$$P_{2n}^{2m}(0) = (2n+2m)!\,(-1)^{n-m}/2^{2n}(n+m)!\,(n-m)!,$$
$$\textstyle\sum_{(1)} = \sum' h_{2n}\cos X\cos Y\cos 2m\beta,$$
$$-\textstyle\sum_{(2)} = \sum' h_{2n}\sin X\sin Y\sin 2m\beta, \tag{20}$$
$$H_{2n+1}^{2m+1} = (-1)^n P_{2n+1}^{2m+1}(0)(\textstyle\sum_{[1]} + i\sum_{[2]}) = H_{[1]}^{2m+1} + iH_{[2]}^{2m+1},$$
$$P_{2n+1}^{2m+1}(0) = (2n+2m+1)P_{2n}^{2m}(0),$$
$$\textstyle\sum_{[1]} = \sum' h_{2n+1}\sin X\cos Y\cos(2m+1)\beta,$$
$$\textstyle\sum_{[2]} = \sum' h_{2n+1}\cos X\sin Y\sin(2m+1)\beta,$$

where $X = skb\xi_0$, $Y = tk\,d\eta_0$, $H_{(1)} \propto \sum_{(1)}$, etc., and where indices have been suppressed for brevity. These forms emphasize the essential symmetries of the problem. If we interchange b, ξ and d, η, then X and Y are interchanged, and β is replaced by $\frac{1}{2}\pi - \beta$. Consequently,

$$H_{(1)}^{2m}(d,\eta;b,\xi) = (-1)^m H_{(1)}^{2m}(b,\xi;d,\eta),$$
$$H_{(2)}^{2m}(d\cdots) = -(-1)^m H_{(2)}^{2m}(b\cdots),$$
$$H_{[1]}^{2m+1}(d\cdots) = (-1)^m H_{[2]}^{2m+1}(b\cdots), \tag{21}$$
$$H_{[2]}^{2m+1}(d\cdots) = (-1)^m H_{[1]}^{2m+1}(b\cdots).$$

Thus for the square unit cell $b=d$, and $\xi=\eta$, it follows that

$$H_{(1)}^{2(2l+1)} = H_{(2)}^{4l} = 0. \tag{22}$$

For the rectangular unit cell and normal incidence $\xi_0 = \eta_0 = 0$ (or for excitation by any mode generated by $\hat{\mathbf{k}} = \hat{\mathbf{z}}$), the problem is characterized by

$$H_{2n}^{2m} = (-1)^n P_{2n}^{2m}(0)\sum_{st}{}' h_{2n}(kb_{st})\cos 2m\beta_{st},$$
$$\cos 2m\beta_{st} = \mathrm{Re}(sb+itd)^{2m}/[(sb)^2+(td)^2]^m. \tag{23}$$

For the square unit cell, we require only

$$H_{2n}^{4m} = (-1)^n P_{2n}^{4m}(0)\sum{}' h_{2n}(kb[s^2+t^2]^{1/2})\frac{\mathrm{Re}(s+it)^{4m}}{(s^2+t^2)^{2m}}, \tag{24}$$

i.e., only the sets H_{2n}^0, H_{2n}^4, H_{2n}^8, etc., are nonvanishing. We consider the general case (18) and then obtain the simpler forms by specialization.

Corresponding to the decomposition $h_n = j_n + in_n$, we write (18) as

$$H_n^m = \mathcal{J}_n^m + i\mathcal{N}_n^m, \quad \mathcal{J}_n^m = \sum{}' \exp(i\mathbf{k}\cdot\mathbf{b}_{st}) i^n j_n(kb_{st}) Y_n^m(-\hat{\mathbf{b}}_{st}), \tag{25}$$

with $\mathcal{N}_n^m$ as the same representation in terms of n_n. From the symbolic form (12), the propagating operator applies for $\mathcal{J}$:

$$\mathcal{J}_n^m = \mathbf{S}_p\, 2C_{\nu\mu}Y_n^m(\hat{\mathbf{k}}_{\nu\mu}) = \textstyle\sum_p 2C_{\nu\mu}Y_n^m(\hat{\mathbf{k}}_{\nu\mu}) - \delta_{n0}, \quad n-m \text{ even}, \tag{26}$$

where we used

$$\textstyle\int_p 2CY_n^m = \oint Y_n^m(\hat{\mathbf{r}})\,d\Omega(\hat{\mathbf{r}})/4\pi = \delta_{n0}$$

(the integral over the unit sphere). Thus, the double infinite series for $\mathcal{J}$ reduces to a finite number of terms (26) representing the propagating modes, in complete analogy with the corresponding earlier results for the grating (3:15) and periodic line (2:100); the essential role of δ_{n0} in the development of energy-conserving approximations of A_n^m and G is the same as discussed before.[2,3] In particular, if there is only one propagating mode (small spacings),

$$\mathcal{J}_n^m = 2C_{00}Y_n^m(\hat{\mathbf{k}}) - \delta_{n0}$$
$$= (2\pi/k^2bd\cos\theta)P_n^m(\cos\theta)\exp(im\varphi) - \delta_{n0}, \tag{27}$$
$$n-m \text{ even}.$$

If we decompose $\mathcal{J}_n^m$ of (26) to correspond to (20), we obtain $\mathcal{J}_n^m = \mathcal{J}_1^m(\cos m\varphi) + i\mathcal{J}_2^m(\sin m\varphi)$; thus interchanging the parameters as before replaces φ by $\frac{1}{2}\pi - \varphi$ and the form shows that the symmetry relations (21) are satisfied by the components. Similarly for the special results for $b=d$, $\xi_0 = \eta_0$.

We obtain (26) directly if we use $j_n(0)=\delta_{n0}$ to rewrite (25) as $\mathcal{J}_n^m=\sum\exp(i\mathbf{k}\circ\mathbf{b}_{st})i^n j_n Y_n^m-\delta_{n0}$, and then introduce

$$i^n j_n(kb)Y_n^m(\hat{\mathbf{b}})=\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\exp(ik\hat{\mathbf{k}}\cdot\mathbf{b})Y_n^m(\hat{\mathbf{k}})\,d\Omega(\hat{\mathbf{k}})$$
$$=\frac{1}{4\pi}\int_{-1}^{1}d\xi\int_{-\gamma}^{\gamma}d\eta\exp(ik\hat{\mathbf{k}}\cdot\mathbf{b})\frac{[Y_n^m(\hat{\mathbf{k}})+Y_n^m(\hat{\mathbf{k}}')]}{\zeta}$$

with $\gamma=(1-\xi^2)^{1/2}$. The resulting sums over s and t are periodic δ functions in $\xi-\xi_\nu$ and $\eta-\eta_\mu$, and integration over the finite intervals reproduces (26).

From (8), (12), (25), and (26), it follows that

$$i\mathcal{N}_n^m=i\sum{}'\exp(i\mathbf{k}\cdot\mathbf{b}_{st})\,i^n n_n(kb_{st})Y_n^m(-\hat{\mathbf{b}}_{st})$$
$$=\mathbf{S}_e\,2C_{\nu\mu}Y_n^m(\hat{\mathbf{k}}_{\nu\mu}),\quad n-m\ \text{even},\tag{28}$$

where, corresponding to $\mathbf{S}_p=\sum_{\nu_p}\sum_{\mu_p}-\int_{\nu_p}\int_{\mu_p}=\mathbf{S}(\nu_p,\mu_p)$, we have, e.g., $\mathbf{S}_e=\mathbf{S}(\nu_p,\mu_e)+\mathbf{S}(\nu_e,\mu_p)+\mathbf{S}(\nu_e,\mu_e)$. In the course of representing $\mathcal{N}$ in terms of the results for the periodic line[2] and for the grating,[3,6] we obtain alternative decompositions of $\mathbf{S}$.

B. The series $\mathcal{H}_{n,l}$

In terms of $Y(\xi)$ of (15), we have

$$Y_n^l(-\hat{\mathbf{b}}_{st})=Y_n^l(-\xi_{st};0,-\eta_{st})$$
$$=P_n^l(-sb/b_{st})\exp(-il(\pi/2)\operatorname{sgn}t)\tag{29}$$

with $\operatorname{sgn}t=1,0,-1$ for $t>0$, $=0,<0$ respectively. The corresponding form of (8) is

$$\mathcal{H}_{n,l}=\sum{}'\exp(i\mathbf{k}\circ\mathbf{b}_{st})i^n h_n(kb_{st})P_n^l(-sb/b_{st})i^{-l\operatorname{sgn}t}$$
$$=\sum{}'f(s,t).\tag{30}$$

Similarly, using (15) in the symbolic form (12), we obtain

$$\mathcal{H}_{n,l}=\mathbf{S}\,C_{\nu\mu}P_n^l(\xi_\nu)\{\exp(il\psi)+\exp[il(\pi-\psi)]\},$$
$$\sin\psi=\eta_\mu/\gamma_\nu=\eta_\mu/(1-\xi_\nu^2)^{1/2}.\tag{31}$$

We express $\mathcal{H}_{n,l}$ in terms of existing results[2,3] (plus a very rapidly converging series) and then construct $\mathcal{H}_n^m$ by superposition.

We decompose (30) into periodic lines along x, sum over s, and then add the contributions of the individual lines by summing over t, i.e.,

$$\mathcal{H}=\sum_{st}{}'f(s,t)=\sum_s{}'f(s,0)+\sum_t{}'\sum_s f(s,t)$$
$$=\mathcal{H}^L+\sum_t{}'\exp(iktd\eta_0)\mathcal{X}(td)\tag{32}$$

with $\mathcal{H}_{n,l}^L=\sum_s' f(s,0)$ as the axial field of the depleted periodic line $t=0$, and $\mathcal{X}(td)$ as the off-axis field of the complete line at $\mathbf{r}=td\hat{\mathbf{y}}$. Thus, since

$$Y_n^l(-\hat{\mathbf{b}}_{s0})=P_n^l(-\operatorname{sgn}s)=\delta_{l0}(\mp1)^n\ \text{ for } s\gtrless0,$$
$$\mathcal{H}_{n,l}^L=\sum_s{}'\exp(iksb\xi_0)i^n h_n(kb|s|)Y_n^l(-\hat{\mathbf{b}}_{s0})$$
$$=\delta_{l0}\sum_{s=1}^{\infty}i^n h_n(skb)[(-1)^n\exp(iskb\xi_0)+\exp(-iskb\xi_0)]$$
$$=\delta_{l0}\mathcal{H}_n^L\tag{33}$$

is the function in (2:94) with the earlier $\sin\theta_0$ replaced by the present ξ_0; see Ref. 2 for detailed discussion. Similarly, from (2:19), $\mathcal{X}$ is a set of conical cylindrical waves

$$\mathcal{X}=\sum_{s=-\infty}^{\infty}\exp(iksb\xi_0)i^n h_n(kb_{st})Y_n^l(-\hat{\mathbf{b}}_{st})$$
$$=i^{-l}\operatorname{sgn}t\frac{\pi}{kb}\sum_{\nu=-\infty}^{\infty}i^l H_l(k|t|d\gamma_\nu)P_n^l(\xi_\nu),\quad H_l=H_l^{(1)},\tag{34}$$

and the remaining sum over t is the form considered earlier for the depleted grating[3]:

$$\sum_t{}'\exp(iktd\eta_0)H_l(k|t|d\gamma_\nu)i^l i^{l\operatorname{sgn}t}$$
$$=\sum_{t=1}^{\infty}H_l(ktd\gamma_\nu)[\exp(itkd\eta_0)(-1)^l+\exp(-itkd\eta_0)]=\mathcal{H}_l^G.\tag{35}$$

For γ_ν real and nonvanishing, $\mathcal{H}_l^G$ is the function in (3:30) and (6:3) with the earlier d replaced by $d\gamma_\nu$ and the earlier $\sin\theta_0$ replaced by η_0/γ_ν; see Refs. 6 and 3 for detailed discussion and mode representations (in which the earlier $\sin\theta_\mu$ now corresponds to $\sin\psi_{\nu\mu}=\eta_\mu/\gamma_\nu$). For imaginary $\gamma=i|\gamma|$ we use $H_l(i|x|)=-i(i^{-l}2/\pi)K_l(|x|)$, and write $\mathcal{H}_l^G(i|x|)=iK_l$:

$$K_{2l}=-(-1)^l\frac{4}{\pi}\sum_{t=1}^{\infty}K_{2l}(ktd|\gamma_\nu|)\cos ktd\eta_0,$$
$$K_{2l+1}=(-1)^l\frac{4}{\pi}\sum_{t=1}^{\infty}K_{2l+1}\sin ktd\eta_0.\tag{36}$$

We do not seek to reduce these series of modified Hankel functions; except for $\gamma_\nu\to0$, they are very rapidly converging.

Thus, we have

$$\mathcal{H}_{n,l}=\mathcal{H}_n^L(\xi_0;b)\delta_{l0}+\frac{(-1)^l\pi}{kb}\sum_\nu P_n^l(\xi_\nu)\mathcal{H}_l^G(\eta_0,\gamma_\nu;d)\tag{37}$$

or, equivalently,

$$\mathcal{H}_{n,l}=\mathcal{H}_{n,l}^L+\mathcal{H}_{n,l}^P+iK_{n,l},\quad \mathcal{H}_{n,l}^L=\mathcal{H}_n^L\delta_{l0},$$
$$\mathcal{H}_{n,l}^P=\frac{(-1)^l\pi}{kb}\sum_{\nu_p}P_n^l\mathcal{H}_l^G,\quad K_{n,l}=\frac{(-1)^l\pi}{kb}\sum_{\nu_e}P_n^l K_l.\tag{38}$$

In this decomposition, a lattice site receives essentially three kinds of fields. The field $\mathcal{H}_{n,l}^L$ represents the net axial effect of all its neighbors on one periodic line, and $\mathcal{H}_{n,l}^P$ and $iK_{n,l}$ represent the net propagating and evanescent fields of all neighboring parallel periodic lines. The finite sum $\sum_{\nu_p}$ specified by the known[3,6] grating function $\mathcal{H}_l^G$ ranges over $-\nu^-\le\nu\le\nu^+$ with $\nu^\pm=[kb(1\mp\xi_0)/2\pi]=[n^\pm]$ as the closest integers from below; thus, $\mathcal{H}_{n,l}^P$ consists essentially of the field of $\nu^++\nu^-+1$ superposed gratings. The infinite series $\sum_{\nu_e}$ ranges from $-\infty$ to $-\nu^{-1}-1$ and ν^++1 to ∞, and the double series $\sum_{\nu_e}\sum_t$ in $K_{n,l}$ corresponds to all evanescent conical modes from all individual neighboring lines. We discuss $K_{n,l}$ after considering the singularities corresponding to integer values of either n^+ or n^- (or of both), i.e., $\gamma_\nu\to0$.

If $\gamma_\nu\to0$, or equivalently, if $|\xi_\nu|\to1$ from either below or above (which also requires $\eta\to0$), we proceed initially as for (2:31). For $l\neq0$, we have $P_n^l(\xi_\nu)H_l(ktd\gamma_\nu)\to-i(n+l)!/\pi(n-l)!\,(ktd)^l$ and the corresponding sums over t reduce to the Fourier series discussed for (2:91). On the other hand, for $l=0$, the terms $P_nH_0\approx H_0$

diverge as $\ln\gamma_\nu$; for the corresponding sum over t we obtain[3] $H_0^G \approx 2/kd\xi$ (and similarly for the K form) which is singular for $\xi = (\gamma^2 - \eta^2)^{1/2} \to 0$. This relates to resonances along the axes of the periodic lines discussed for (1:86). We exclude these in the following.

To analyze $K_{m,l}$, we first consider the behavior of P_n^l and K_l for large ν. In general, with $\gamma_\nu = (1 - \xi_\nu^2)^{1/2}$ and $\xi_\nu = \xi_0 + 2\nu\pi/kb$, we use

$$P_n^l(\xi) = \gamma^l \sum (-1)^\sigma (2n - \sigma - 1)!!\, \xi^{n-l-2\sigma}/2^\sigma \sigma!\,(n - l - 2\sigma)!,$$
$$(2m-1)!! = (2m)!/2^m m! = 1 \cdot 3 \cdot 5 \cdots (2m-1), \tag{39}$$

where, with $(-|m|)! = \infty$, we need not indicate the limits of the summation index σ. For large $|\nu|$ (or small kb) we have $\gamma_\nu = i(\xi_\nu^2 - 1)^{1/2} \approx i|\xi_\nu|$, and

$$P_n^l(\xi_\nu) \approx (\operatorname{sgn}\nu)^{n-l} \rho_n^l(V)[1 + (n\xi_0/V)\operatorname{sgn}\nu],$$
$$\rho_n^l(V) = [(2n-1)!!/(n-l)!]i^l V^n, \tag{40}$$
$$V = 2|\nu|\pi/kb,$$

where we kept up to the first term in ξ_0. Similarly, to first order in ξ_0 for large V,

$$K_l(ktd|\gamma_\nu|) \approx K_l(\alpha) + ktd\xi_0 \operatorname{sgn}\nu \partial_\alpha K_l(\alpha),$$
$$\alpha = 2\pi|t\nu|\rho, \quad \rho = d/b \geq 1, \tag{41}$$

where $\partial_\alpha = d/d\alpha$. We take $\rho = d/b \geq 1$ to promote rapid convergence; with this, we interpret the summation sequence (32) as decomposing the array into periodic lines such that the neighboring sites on each line are closer than the lines, and summing initially over the smaller spacing. For large α, we have asymptotically

$$K_l(\alpha) \sim K(\alpha)[1 + (4l^2 - 1)/8\alpha] \sim K(\alpha),$$
$$K(\alpha) = (\pi/2\alpha)^{1/2} e^{-\alpha}, \quad \alpha = 2\pi|t\nu|\rho, \tag{42}$$

which dominates the polynomial (39). Thus $\sum_{\nu_e}$ decays exponentially with increasing $|\nu|$ independently of k, and $\sum_{\nu_e}\sum_t$ is very rapidly converging in $|\nu|$ and t. The rapidity of convergence is determined by $\rho = d/b \geq 1$; the worst case is the square unit cell $\rho = 1$, but even then a small number of terms suffice since $e^{-2\pi} < 0.002$. Consequently, in general, we need consider only the leading evanescent modes ($|\nu|$ close to $|\nu^\pm + 1|$) from the closer neighboring lines (small integer t).

If $\xi_0 = 0$, then

$$H_{n,l}^L = H_n^L \delta_{l0} \delta_e(n), \quad H_{2n}^L = 2\sum_{s=1}^{\infty} h_{2n}(skb),$$

and since $\xi_\nu = 2\nu\pi/kb = \pm 2|\nu|\pi/kb$, we may pair the corresponding terms of (37) as

$$P_n^l(|\xi_\nu|) + P_n^l(-|\xi_\nu|) = P_n^l(|\xi_\nu|) 2\delta_e(n-l).$$

If, in addition, $\eta_0 = 0$, then

$$H_l^G = H_l^G \delta_e(l), \quad H_{2l}^G = \sum_{t=1}^{\infty} 2H_{2l}(tkd\gamma_\nu).$$

Consequently, for normal incidence, (37) reduces to

$$H_{2n,2l} = H_{2n}^L \delta_{l0} + \frac{\pi}{kb} \sum_\nu P_{2n}^{2l}(\xi_\nu) H_{2l}^G(\gamma_\nu; d), \quad \xi_\nu = 2\nu\pi/kb, \tag{43}$$

which has the same parity constraint as (22). The corresponding form of the original series (30) is

$$H_{2n,2l} = (-1)^{l+n} \sum{}' h_{2n}(kb_{st}) P_{2n}^{2l}(\cos\beta_{st}). \tag{44}$$

To delineate the relation of the results we have obtained from $H(\sum')$ of (30) to the symbolic form $H[\mathbf{S}]$ of (31), we consider initially the propagating ($\mathcal{J}$) part of (37),

$$\mathcal{J}_{n,l} = \mathcal{J}_n^L \delta_{l0} + \frac{(-1)^l \pi}{kb} \sum_{\nu_p} P_n^l(\xi_\nu) \mathcal{J}_l^G. \tag{45}$$

From (2:100) and (3:15),

$$\mathcal{J}_n^L = \frac{\pi}{kb} \sum_{\nu_p} P_n(\xi_\nu) - \delta_{n0},$$

$$\mathcal{J}_l^G = \sum_{\mu_p} \left\{ \frac{\exp(-il\psi) + \exp[il(\pi + \psi)]}{kd\gamma_\nu \cos\psi} \right\} - \delta_{l0}, \quad \psi = \psi_{\nu\mu}, \tag{46}$$

with $\gamma_\nu \cos\psi_{\nu\mu} = \gamma_\nu (1 - \eta_\mu^2/\gamma_\nu^2)^{1/2} = \xi_{\nu\mu}$. Thus

$$\mathcal{J}_{n,l} = \sum_{\nu_p}\sum_{\mu_p} C_{\nu\mu} P_n^l(\xi_\nu) \{\exp(il\psi) + \exp[il(\pi - \psi)]\} - \delta_{n0} \tag{47}$$

as follows directly from the $\mathbf{S}_p$ operation in (31). Similarly, the general reduction (37) is related to the symbolic form (31) by the decomposition

$$\mathbf{S} = \sum_\nu \sum_\mu - \int_\nu \int_\mu = (\sum_\nu - \int_\nu) \int_\mu + \sum_\nu (\sum_\mu - \int_\mu)$$
$$= \mathbf{S}_\nu \int_\mu + \sum_\nu \mathbf{S}_\mu, \tag{48}$$

where the implicit convergence factor is $\exp(ik\epsilon\gamma\cos\psi)$. The $\mathbf{S}_\mu\{\ \}$ operation in (31), with the braces representing the braced function in (46), generates[3] H_l^G, so that $\sum_\nu \mathbf{S}_\mu$ corresponds to the second term of (37). For the first term, we evaluate $\int_\mu \{\ \} \exp(ik\epsilon\gamma\cos x) \propto H_l(\epsilon\gamma kd)$, and thereby reduce $\mathbf{S}_\nu \int_\mu$ to the form considered in (2:67) for the periodic line. Thus (31) decomposed as (48) leads directly to (37).

From (37) and (45), we construct $H - \mathcal{J} = iN$ with

$$N_{n,l} = N_{n,l}^L + N_{n,l}^P + K_{n,l}, \quad N_{n,l}^L = N_n^L \delta_{l0},$$
$$N_{n,l}^P = \frac{(-1)^l \pi}{kb} \sum_{\nu_p} P_n^l N_l^G, \quad K_{n,l} = \frac{(-1)^l \pi}{kb} \sum_{\nu_e} P_n^l K_l. \tag{49}$$

We consider $N_{0,0}$, $N_{1,0}$, and $N_{1,1}$ in some detail, because they are exceptional, and also to provide a guide for using existing results[2,3] to construct (49). We have

$$N_{0,0} = N_0^L + N_{0,0}^P + K_{0,0}, \quad N_0^L = (kb)^{-1} \ln[2|\cos kb - \cos kb\xi_0|],$$
$$N_{0,0}^P = \frac{\pi}{kb} \sum_{\nu_p} N_0^G, \quad N_0^G = -\frac{2}{\pi} \ln \frac{ckd\gamma_\nu}{4\pi} + \frac{1}{\pi} \sum_{\mu_p}{}' \frac{1}{|\mu|}$$
$$- \sum_{\mu_e} \left(\frac{2}{kd|\xi_{\nu\mu}|} - \frac{1}{\pi|\mu|} \right), \tag{50}$$

$$K_{0,0} = \frac{\pi}{kb} \sum_{\nu_e} K_0 = -\frac{4}{kb} \sum_{\nu_e} \sum_t K_0(ktd|\gamma_\nu|) \cos(ktd\eta_0).$$

Here N_0^L was obtained from (2:95) by replacing $\sin\theta_0$ by ξ_0. Similarly, N_0^G is (3:16) in terms of $d\gamma_\nu$ and

$$d|\gamma_\nu \cos\psi_{\nu\mu}| = d|\eta_\mu^2 - \gamma_\nu^2|^{1/2} = d|\xi_{\nu\mu}|$$

with $\gamma_\nu = (1 - \xi_\nu^2)^{1/2} = |\gamma_\nu|$ or $i|\gamma_\nu|$, and $c = 1.781\ldots$ as Euler's constant; the prime means exclude $\mu = 0$, and

μ_p ranges from $-\mu^-$ to μ^+ with $\mu^\pm=[kd(\gamma_{\nu_p}\mp\eta_0)/2\pi]$ as the closest integers from below. In $\mathcal{N}_0^G$, since ν is finite, the summand approximates μ^{-3} for large μ, and convergence is relatively rapid; we could use a similar series for K_0 in terms of $(\eta_\mu^2+|\gamma_\nu|^2)^{1/2}$, and this suffices to show that both $H(|x|)$ and $H(i|x|)$ have the same singularity for γ and $\eta\to 0$. Discounting $\xi\approx 0$, the convergence of the double sum in K_∞ is very rapid; in general we may use the asymptotic form $K_0\sim K$ and restrict consideration to the leading terms $t=1$, and $\nu_e=\pm(\nu^\pm+1)$. The corresponding value of $\mathcal{J}$ is

$$\mathcal{J}_{0,0}=2\sum_p C_{\nu\mu}-1,\quad C_{\nu\mu}=\pi/k^2bd(1-\xi_\nu^2-\eta_\mu^2)^{1/2},\tag{51}$$

which reduces to $(2\pi/k^2bd\cos\theta)-1$ for one propagating mode (small kd).

For small kd from (50), or (2:97′) and (3:77),

$$\mathcal{N}_0^L\approx(2/kb)\{\ln kb\gamma_0-[(kb)^2/4!](1+\xi_0^2)\},$$
$$\mathcal{N}_{0,0}^P\approx-(2/kb)\{\ln(ckd\gamma_0/4\pi)-[(kd)^2/2\pi^3](\tfrac{1}{2}\gamma_0^2+\eta_0^2)\zeta(3)\},$$

where $\zeta(3)$ is a special value of the Riemann zeta function[7] $\zeta(n)=\sum_{s=1}^\infty s^{-n}$. There is only one propagating mode, and to lowest order in k the evanescent sums are symmetrical in $\nu=\pm|\nu|$. Thus, for $k\to 0$,

$$-\tfrac{1}{2}kb\mathcal{N}_{0,0}\to\ln(4\pi/c\rho)-4\textstyle\sum_{\parallel}K_0(\alpha),$$
$$\alpha=t\nu 2\pi\rho,\quad \rho=d/b,\quad \textstyle\sum_{\parallel}=\sum_{\nu=1}^\infty\sum_{t=1}^\infty.\tag{52}$$

In terms of the asymptotic form of K_0,

$$\tfrac{1}{4}kb\mathcal{N}_{0,0}\sim\tfrac{1}{2}\ln(4\pi/c\rho)-\textstyle\sum_{\parallel}\exp(-\nu t2\pi\rho)/(\rho\nu t)^{1/2}.$$

Since $\frac{1}{2}\ln(4\pi/c)\approx 0.977$ and $e^{-2\pi}\approx 1.87\times10^{-3}$, the series affects only the third decimal point.

The next functions of interest are

$$\mathcal{N}_{1,0}=\mathcal{N}_1^L+\mathcal{N}_{1,0}^P+K_{1,0},\quad \mathcal{N}_{1,0}^P=(\pi/kb)\textstyle\sum_{\nu_p}\xi_\nu\mathcal{N}_0^G,$$
$$K_{1,0}=-(4/kb)\textstyle\sum_{\nu_e}\xi_\nu\sum_t K_0\cos(ktd\eta_0),\tag{53}$$

where $\mathcal{N}_1^L$ (which vanishes for $\xi_0=0$) is given in (2:97), and we used $P_1^0=\xi_\nu=\xi_0+2\nu\pi/kb$. The function $\mathcal{N}_{1,0}^P$ consists essentially of two sets of terms: the first equals ξ_0 times $\mathcal{N}_{0,0}^P$, and the terms of the second depend on the sign of ν; both sets vanish for $\xi_0=0$, the second because then $\mathcal{N}_0^G(\gamma_{-\nu})=\mathcal{N}_0^G(\gamma_\nu)$. Similarly for $K_{1,0}$.

For $\mathcal{N}_{1,1}$ we have

$$\mathcal{N}_{1,1}=\mathcal{N}_{1,1}^P+K_{1,1},\quad \mathcal{N}_{1,1}^P=-(\pi/kb)\textstyle\sum_{\nu_p}\gamma_\nu\mathcal{N}_1^G,$$
$$K_{1,1}=-(i4/kb)\textstyle\sum_{\nu_e}|\gamma_\nu|\sum_t K_1\sin(ktd\eta_0),\tag{54}$$

where $\mathcal{N}_1^G$ (which is imaginary) is given in (3:16), and we used $P_1^1=(1-\xi^2)^{1/2}=\gamma$ for ν_p and $i(\xi^2-1)^{1/2}=i|\gamma|$ for ν_e. If $\eta_0=0$, both $\mathcal{N}_1^G$ and $K_{1,1}$ are zero. Thus, as required by (43), both sets of terms $\mathcal{N}_{1,l}$ vanish for normal incidence, $\xi_0=\eta_0=0$. For small kd, from (2:97) and (3:77)

$$\mathcal{N}_1^L\approx(2\xi_0/kb)[\ln(kb\gamma_0)-1]+(kb\xi_0/12)(1-\xi_0^2/3),$$
$$\mathcal{N}_1^G\approx-(i2\eta_0/\pi\gamma_0)\{1+[2(kd)^2\gamma_0^2/4\pi]\zeta(3)\}.$$

For the K sums for small kd, corresponding to (40) and (41), we use

$$\xi_\nu K_0(ktd|\gamma_\nu|)\cos ktd\eta_0$$
$$\approx[\xi_0+(2|\nu|\pi/kb)\operatorname{sgn}\nu][K_0(\alpha)+ktd\xi_0\operatorname{sgn}\nu\partial_\alpha K_0(\alpha)],$$
$$\partial_\alpha K_0=-K_1,$$
$$|\gamma_\nu|K_1(ktd|\gamma_\nu|)\sin ktd\eta_0$$
$$\approx(2|\nu|\pi/kb)\,ktd\eta_0K_1(\alpha)=\eta_0\alpha K_1(\alpha),$$

and combine the corresponding terms for $\nu=|\nu|$ and $\nu=-|\nu|$ in $\sum_{\nu_e}=\sum_\nu'$. Thus the low frequency limits of (53) and (54) are

$$\tfrac{1}{2}kb\mathcal{N}_{1,0}\to\xi_0[\ln(4\pi/c\rho)-1-4\textstyle\sum_{\parallel}(K_0-\alpha K_1)],\quad K_l=K_l(\alpha),\tag{55}$$

$$\tfrac{1}{2}kb\mathcal{N}_{1,1}\to i\eta_0[1-4\textstyle\sum_{\parallel}\alpha K_1].\tag{56}$$

Corresponding to (53) and (54), we have

$$\mathcal{J}_{1,0}=2\textstyle\sum_p C_{\nu\mu}\xi_{\nu\mu},\quad \mathcal{J}_{1,1}=i2\sum_p C_{\nu\mu}\eta_\mu,\tag{57}$$

which reduce to single terms ($\nu=\mu=0$) for small kd.

We see from the above that the low frequency results for $\mathcal{N}_{0,0}$ and $\mathcal{N}_{1,l}$ are of order k^{-1}; these are exceptional in that they are smaller than the one-mode results for the $\mathcal{J}$'s (of order k^{-2} for all n, l). We now construct the leading terms of the low frequency approximations ($kd\approx 0$) for $\mathcal{N}_{n,l}$ of (49) and show that $\mathcal{N}_{2n,l}$ and $\mathcal{N}_{2n+1,l}$ are of order k^{-2n-1}.

From (2:90), or by substituting $n_n(x)\approx-(2n-1)!!/x^{n+1}$ directly into (33),

$$\mathcal{N}_{2n,l}^L\approx-[(-1)^n(4n-1)!!/(kb)^{2n+1}]\,2\zeta(2n+1)\delta_{l0}=\beta_n\delta_{l0},$$
$$\mathcal{N}_{2n+1,l}^L\approx(4n+1)\beta_n\xi_0\delta_{l0},\quad n>0.\tag{58}$$

From (3:78), or by using $N_l(x)\approx-(l-1)!\,2^l/\pi x^l$, $l>0$, directly in (35),

$$\mathcal{N}_{2l}^G\approx-[2(2l-1)!\,2^{2l}/\pi(kd\gamma_0)^{2l}]\,\zeta(2l)=C_l,$$
$$\mathcal{N}_{2l+1}^G\approx-i4lC_l\eta_0/\gamma_0,\quad l>0.$$

The largest values correspond to $l=n$. Thus in the one-mode form of (49), $\mathcal{N}_{n,l}^P=(-1)^l(\pi/kb)P_n^l(\xi_0)\mathcal{N}_l^G$ with $P_n^n(\xi_0)=(2n-1)!!\gamma_0^n$ and $P_n^{n-1}=(2n-1)!!\gamma_0^{n-1}\xi_0$, we keep only the leading terms by writing

$$\mathcal{N}_{2n,2l}^P\approx-\frac{(4n-1)!!}{kb(kd)^{2n}}(2n-1)!\,2^{2n}2\zeta(2n)\delta_{n,l}=\mathcal{D}_n\delta_{nl},\tag{59}$$

$$\mathcal{N}_{2n+1,2l}^P\approx(4n+1)\mathcal{D}_n\xi_0\delta_{nl},\quad \mathcal{N}_{2n+1,2l+1}^P\approx(4n+1)4n\mathcal{D}_n i\eta_0\delta_{nl}.$$

From (36) and (41) to order k,

$$K_{2l}\approx-(-1)^l(4/\pi)\textstyle\sum_t(1+ktd\xi_0\operatorname{sgn}\nu\partial_\alpha)K_{2l}(\alpha),$$
$$K_{2l+1}\approx(-1)^l(4/\pi)kd\eta_0\textstyle\sum_t tK_{2l+1},$$

which we use with (40) for P_n^l to order k^{-n+1} to construct the largest cases for $K_{n,l}=(-1)^l(\pi/kb)\sum_\nu' P_n^l(\xi_\nu)K_l$ of (49). Combining the corresponding terms for $\nu=|\nu|$, and $\nu=-|\nu|$, we obtain

$$K_{2n,2l}\approx-\frac{8(-1)^l}{kb}\textstyle\sum_{\parallel}p_{2n}^{2l}(V)K_{2l}(\alpha)$$
$$\approx-\frac{(4n-1)!!\,8(2\pi)^{2n}}{(kb)^{2n+1}(2n-2l)!}\textstyle\sum_{\parallel}\nu^{2n}K_{2l}(\alpha)=\mathcal{E}_{nl}\sum_{\parallel}\nu^{2n}K_{2l},$$

$$K_{2n+1,2l} \approx -\frac{8(-1)^l}{kb}\xi_0 \sum_{\parallel} \rho^{2l}_{2n+1}\left(\frac{2n+1}{V} + ktd\partial_\alpha\right)K_{2l}$$

$$\approx \frac{4n+1}{2n+1-2l}\mathcal{E}_{nl}\,\xi_0 \sum_{\parallel} \nu^{2n}(2n+1+\alpha\partial_\alpha)\,K_{2l}, \tag{60}$$

$$K_{2n+1,2l+1} \approx -\frac{8(-1)^l}{kb}kd\eta_0 \sum_{\parallel} \rho^{2l+1}_{2n+1}\,tK_{2l+1}$$

$$\approx (4n+1)\mathcal{E}_{nl}\, i\eta_0 \sum_{\parallel} \nu^{2n}\alpha K_{2l+1}.$$

The neglected set $K_{2n,2l+1}$ is only of order k^{-2n}. These relations also apply for $K_{0,0}$, $K_{1,0}$, and $K_{1,1}$ as used in (52), (55), and (56) respectively.

Adding the corresponding terms of (58), (59), and (60), we write

$$-N_{2n,2l}(kb)^{2n+1}/(4n-1)!!(-1)^{n+l} \to \mathcal{L}_{2n,2l},$$

$$-N_{2n+1,2l}(kb)^{2n+1}/(4n+1)!!(-1)^{n+l} \to \xi_0 \mathcal{R}_{2n+1,2l}, \tag{61}$$

$$-N_{2n+1,2l+1}(kb)^{2n+1}/(4n+1)!!(-1)^{n+l} \to i\eta_0 \mathcal{J}_{2n+1,2l+1},$$

where, for $n>0$,

$$\mathcal{L}_{2n,2l} = 2\zeta(2n+1)\delta_{l0} + \frac{(2n-1)!\,2^{2n}}{\rho^{2n}}\,2\zeta(2n)\delta_{nl}$$

$$+\frac{8(-1)^{n+l}}{(2n-2l)!}\sum_{\parallel}(2\pi\nu)^{2n}K_{2l}(\alpha),$$

$$\mathcal{R}_{2n+1,2l} = 2\zeta(2n+1)\delta_{l0} + \frac{(2n-1)!\,2^{2n}}{\rho^{2n}}2\zeta(2n)\delta_{nl}$$

$$+\frac{8(-1)^{n+l}}{(2n-2l)!}\sum_{\parallel}(2\pi\nu)^{2n}\left(K_{2l} - \frac{\alpha K_{2l-1}}{2n+1-2l}\right), \tag{62}$$

$$\mathcal{J}_{2n+1,2l+1} = \frac{(2n)!\,2^{2n+1}}{\rho^{2n}}2\zeta(2n)\delta_{nl}$$

$$+\frac{8(-1)^{n+l}}{(2n-2l)!}\sum_{\parallel}(2\nu\pi)^{2n}\alpha K_{2l+1},$$

$$\mathcal{J}_{2n+1,2l-1} = -\frac{8(-1)^{n+l}}{(2n-2l+2)!}\sum_{\parallel}(2\pi\nu)^{2n}\alpha K_{2l-1}.$$

We used $2lK_{2l} + \alpha\partial_\alpha K_{2l} = -\alpha K_{2l-1}$ in $\mathcal{R}$, and included an additional value of $\mathcal{J}$ to further the development. The limiting forms satisfy the relations

$$(2n+2-2l)\mathcal{J}_{2n+1,2l-1} = -\mathcal{L}_{2n,2l} + \mathcal{R}_{2n+1,2l},$$
$$\mathcal{J}_{2n+1,2l+1} = (2n+1+2l)\mathcal{L}_{2n,2l} - (2n+1-2l)\mathcal{R}_{2n+1,2l}, \tag{63}$$

as may be seen from the recursive relation for the Hankel function $\alpha(K_{m+1} - K_{m-1}) = 2mK_m$.

In analogy with (20), we split (30) into four sets:

$$H_{2n,2l} = (-1)^{l+n}\sum{}' \cos X \cos Y\, h_{2n}P^{2l}_{2n}(\cos\beta),$$

$$H_{2n,2l+1} = -i(-1)^{l+n}\sum{}' \sin X \sin|Y|\, h_{2n}P^{2l+1}_{2n},$$
$$H_{2n+1,2l} = (-1)^{l+n}\sum{}' \sin X \cos Y\, h_{2n+1}P^{2l}_{2n+1}, \tag{64}$$

$$H_{2n+1,2l+1} = i(-1)^{l+n}\sum{}' \cos X \sin|Y|\, h_{2n+1}P^{2l+1}_{2n+1}.$$

The low frequency limits of $H(kb)^{2n+1} \to iN(kb)^{2n+1}$ for $n>0$, normalized as in (62), are the absolutely converging series

$$\mathcal{L}_{2n,2l} = \sum{}' \frac{P^{2l}_n(\cos\beta_{st})}{\gamma^{2n+1}_{st}},\quad \mathcal{R}_{2n+1,2l} = \sum{}' \frac{\cos\beta P^{2l}_{2n+1}}{\gamma^{2n+1}}$$

$$\mathcal{J}_{2n+1,2l+1} = \sum{}' \frac{|\sin\beta|\,P^{2l+1}_{2n+1}}{\gamma^{2n+1}} \tag{65}$$

$$\cos\beta = s/r,\quad \sin\beta = t\rho/r,\quad r = (s^2+t^2\rho^2)^{1/2},\quad \sum{}' = \sum_{st}{}'.$$

The rapidly converging forms of $\sum'$ given in (62) may be constructed by using the Poisson sum formula. The relations in (63) follow directly from (65) and the recursive relations[7] for the Legendre functions,

$$(\nu-\mu+1)(1-x^2)^{1/2}P^{\mu-1}_\nu(x) = -P^\mu_{\nu-1} + xP^\mu_\nu,$$
$$(1-x^2)^{1/2}P^{\mu+1}_\nu = (\nu+\mu)P^\mu_{\nu-1} - (\nu-\mu)xP^\mu_\nu.$$

From (63), except for $l=0$, we may construct $\mathcal{R}$ and $\mathcal{L}$ from $\mathcal{J}$. Thus,

$$4l\mathcal{R}_{2n+1,2l} = \mathcal{J}_{2n+1,2l-1}(2n+2-2l)(2n+1+2l) + \mathcal{J}_{2n+1,2l},$$
$$4l\mathcal{L}_{2n,2l} = \mathcal{J}_{2n+1,2l-1}(2n+2-2l)(2n+1-2l) + \mathcal{J}_{2n+1,2l}.$$

There is only one relation for $l=0$, and we supplement it with the form $\mathcal{L}_{2n,0}$:

$$\mathcal{J}_{2n+1,1} = (2n+1)(\mathcal{L}_{2n,0} - \mathcal{R}_{2n+1,0}),$$

$$\mathcal{L}_{2n,0} = 2\zeta(2n+1) + [8(-1)^n/(2n)!]\sum_{\parallel}(2\pi\nu)^{2n}K_0.$$

Although (62) excludes $n=0$, and the $n=0$ forms of (65) diverge, the limits for $n=0$ in (61) are given in (52), (55), and (56), i.e.,

$$\mathcal{L}_{0,0} = -2\ln(4\pi/c\rho) + 8\sum_{\parallel}K_0,$$

$$\mathcal{R}_{1,0} = -2\ln(4\pi/c\rho) + 2 + 8\sum_{\parallel}(K_0 - \alpha K_1), \tag{66}$$

$$\mathcal{J}_{1,1} = -2 + 8\sum_{\parallel}\alpha K_1.$$

Since $\mathcal{J}_{1,1} = \mathcal{L}_{0,0} - \mathcal{R}_{1,0}$, these exceptional cases also satisfy (63), with $\ln(\pi 4/c\rho) = \ln(kb\gamma_0) - \ln(ckd\gamma_0/4\pi)$ taking the place of the ζ functions.

C. Superposed form of H^m_n

We now express H^m_n in terms of the rapidly converging results for $H_{n,l}$. From (16),

$$Y^m_n(\xi;\xi,\eta) = \sum_{l=-n}^{n} D^{m,l}_n P^l_n(\xi)\exp(il\psi),$$

$$D^{m,l}_n = \frac{(n-l)!}{(n-m)!\,2^n}\sum(-1)^r\binom{n-m}{r}\binom{n+m}{n-l-r}, \tag{67}$$

where $n-m$ is even, and $\sum_r$ terminates with r equal to the smaller of $n-m$ or $n-l$. The present Wigner[5] coefficients D may be written in terms of the Jacobi polynomials of argument zero, as

$$D^{m,l}_n = \frac{(n-l)!\,(-1)^{n-l}}{(n+l)!\,2^l}\,P^{(l-m,l+m)}_{n-l}.$$

For negative l, we introduce a new summation index $r' = n-m-r$; including additional forms for subsequent use, we have

$$\frac{D_n^{m,-l}}{D_n^{m,l}}=\frac{(n+l)!}{(n-l)!}=\frac{(-1)^l P_n^l}{P_n^{-l}}=\frac{H_{n,l}}{H_{n,-l}},$$
$$\frac{D^{m,-l}}{D^{l,-m}}=1,\quad \frac{D^{m,l}}{D^{l,m}}=\frac{(n-l)!\,(n+m)!}{(n+l)!\,(n-m)!}, \tag{68}$$

where the relation for H obtained from (30), also holds for $\mathcal{J}$ and $\mathcal{N}$. Thus

$$Y_n^m(\xi)=D_n^{m,0}P_n^0(\xi)+\sum_{l=1}^{n}D_n^{m,l}P_n^l(\xi)\{\exp(il\psi)+\exp[il(\pi-\psi)]\},$$
$$P_n^m(\xi)\cos m\varphi=\sum_{l=0}^{[n/2]}\epsilon_{2l}D_n^{m,2l}P_n^{2l}(\xi)\cos 2l\psi,$$
$$P_n^m(\xi)\sin m\varphi=\sum\epsilon_{2l+1}D_n^{m,2l+1}P_n^{2l+1}\sin(2l+1)\psi, \tag{69}$$
$$\epsilon_l=1,\ 2 \text{ for } l=,>0,$$

where we use ϵ_{2l+1} instead of 2 and include the redundant $D_n^{0,2l+1}=0$ for uniformity. Since, e.g.,

$$\int \mathrm{Re}Y_n^m\,\mathrm{Re}Y_n^\mu\,dl=(n+m)!\,4\pi\delta_{m\mu}/(n-m)!\,(2n+1)\epsilon_m$$

when integrated over the unit sphere,

$$\sum_{l=0}^{[n/2]}\epsilon_{2l}D_n^{m,2l}D_n^{\mu,-2l}=\sum_{l=0}^{[n/2]}\epsilon_{2l+1}D_n^{m,2l+1}D_n^{\mu,-2l-1}=(n+m)!\,\delta_{m\mu}/(n-m)!\,\epsilon_m=\Delta_{m\mu}. \tag{70}$$

Adding the values for even and odd l, we obtain $\sum_0^n\epsilon_l D_n^{m,l}D_n^{\mu,-l}=\Delta_{m\mu}$; however, the split forms are used subsequently to provide checks. Several values of D may be expressed more simply than in (70),

$$D_n^{m,0}=P_n^m(0),\quad D_n^{0,l}=P_n^l(0)[(n-l)!/(n+l)!\,]\delta_e(l),$$
$$D_n^{n,l}=(2n)!/2^n(n+l)!,\quad D_n^{m,n}=1/2^n(n-m)!, \tag{71}$$
$$D_n^{m,n-1}=2m/2^n(n-m)!.$$

If we apply (67) in reverse to construct $\sum D_n^{m,l}\mathcal{J}_{n,l}$ in terms of $\mathcal{J}_{n,l}$ of (47), we obtain

$$\sum_{l=-n}^{n}D_n^{m,l}\mathcal{J}_{n,l}=D_n^{m,0}\mathcal{J}_{n,0}+2\sum_{l=1}^{n}D_n^{m,l}\mathcal{J}_{n,l}=\mathcal{J}_n^m, \tag{72}$$

where $\mathcal{J}_n^m$ is identically the function derived originally in (26). Similarly,

$$H_n^m=\sum_{l=-n}^{n}D_n^{m,l}H_{n,l}=P_n^m(0)H_{n,0}+2\sum_{l=1}^{n}D_n^{m,l}H_{n,l}, \tag{73}$$

where we used $D_n^{m,0}=P_n^m(0)$ of (71). For subsequent applications, we list the leading values:

$$H_0^0=H_{0,0},\ H_1^1=H_{1,0}+H_{1,1},\ H_2^0=-\tfrac{1}{2}H_{2,0}+\tfrac{1}{4}H_{2,2},$$
$$H_2^2=3H_{2,0}+2H_{2,1}+\tfrac{1}{2}H_{2,2},$$
$$H_3^1=-\tfrac{3}{2}H_{3,0}-\tfrac{1}{4}H_{3,1}+\tfrac{1}{4}H_{3,2}+\tfrac{1}{8}H_{3,3}$$
$$H_3^3=15H_{3,0}+\tfrac{15}{2}H_{3,1}+\tfrac{3}{2}H_{3,2}+\tfrac{1}{4}H_{3,3},$$
$$H_4^0=\tfrac{3}{8}H_{4,0}-\tfrac{1}{24}H_{4,2}+\tfrac{1}{192}H_{4,4}, \tag{74}$$
$$H_4^2=-\tfrac{15}{2}H_{4,0}-\tfrac{3}{2}H_{4,1}+\tfrac{1}{2}H_{4,2}+\tfrac{1}{4}H_{4,3}+\tfrac{1}{16}H_{4,4},$$
$$H_4^4=105H_{4,0}+42H_{4,1}+7H_{4,2}+H_{4,3}+\tfrac{1}{8}H_{4,4}.$$

In terms of $H_{n,l}$ of (37), we rewrite the first form of (73) initially as

$$H_n^m=P_n^m(0)H_n^L+\sum_{l=-n}^{n}D_n^{m,l}\sum_\nu\frac{(-1)^l\pi}{kb}P_n^l(\xi_\nu)H_l^G, \tag{75}$$

where the leading term follows directly from the $\sum_s'$ part of the summation sequence (32), and (18), i.e., $\sum_s' f(s,0)=(-1)^m P_n^m(0)\sum_s'\exp(isk b\xi_0)i^n h_n(|s|kb)\exp(im\beta_{s0})$ with $\beta_{s0}=0$ for $s>0$ and $\beta_{s0}=\pi$ for $s<0$, equals $P_n^m(0)H_n^L$ with H_n^L as in (33), since we require $n-m$ be even. Using the decomposion of H_l^G mentioned after (48), and applying (67) in reverse, enables us to rewrite (75) as

$$H_n^m=P_n^m(0)H_n^L+\textstyle\sum_\nu \mathbf{S}_\mu[2C_{\nu\mu}Y_n^m(\xi_{\nu\mu})] \tag{76}$$

and to identify the first term directly as $\mathbf{S}_\nu\int_\mu[\ ]$ of (48). For the remaining operator, the part $\sum_{\nu_p}\mathbf{S}_{\mu_p}$ generates the rest of $\mathcal{J}_n^m$. In the following, the N^P functions correspond to $\sum_{\nu_p}\mathbf{S}_{\mu_e}$, and the K functions to $\sum_{\nu_e}\mathbf{S}_\mu$.

In working with $\mathcal{J}_n^m$ as in (26), since $n-m$ is even, we may use (39) to reduce Y_n^m to a polynomial in ξ_ν and η_μ, i.e.,

$$\zeta^{n-m-2\sigma}(1-\xi^2)^{m/2}\exp(im\varphi)=(1-\xi^2-\eta^2)^{\tau-\sigma}(\xi+i\eta)^m$$

with $\tau=(n-m)/2$. For $\mathcal{N}_n^m$, from (75) and (49).

$$\mathcal{N}_n^m=P_n^m(0)\mathcal{N}_n^L+\sum_{l=-n}^{n}D_n^{m,l}(\mathcal{N}_{n,l}^P+K_{n,l})=\mathcal{N}_n^{Lm}+\mathcal{N}_n^{Pm}+K_n^m \tag{77}$$

with the individual terms of the first equality as discussed for (49).

From (74), we have $\mathcal{N}_0^0=\mathcal{N}_{0,0}$ in terms of (50), and similarly $\mathcal{N}_1^1=\mathcal{N}_{1,0}+\mathcal{N}_{1,1}$ in terms of (53) and (54). The corresponding functions H_0^0 and H_1^1 are basic for the analytical properties of the general form H_n^m of (18). Since

$$i^n h_n(x)=h(x)\sum[(n+\sigma)!/\sigma!\,(n-\sigma)!\,](i/2x)^\sigma,$$
$$h(x)=h_0(x)=e^{ix}/ix, \tag{78}$$

all but the first two terms ($\sigma=0,1$) correspond to absolutely converging series in $\sum'$ of (18); the behavior of these two terms is determined by h_0 and h_1, and that of the corresponding series in $\sum'$ by H_0^0 and H_1^1. In particular, although the $\sum'$ forms of $k\mathcal{N}_0^0$ and $k\mathcal{N}_1^1$ for $k\to 0$ obtained from (18) diverge, from (52) we have, $-kb\mathcal{N}_0^0=-kb\mathcal{N}_{0,0}\to L_0^0$, with

$$L_0^0(\rho)=-2\ln(4\pi/c\rho)+8\textstyle\sum_{\|}K_0(t\nu 2\pi\rho)=\rho^{-1}L_0^0(\rho^{-1}), \tag{79}$$

and from (55) and (56), $-kb\mathcal{N}_1^1=-kb(\mathcal{N}_{1,0}+\mathcal{N}_{1,1})\to\xi_0R_1^1+i\eta_0I_1^1$, with

$$R_1^1(\rho)=-2\ln(4\pi/c\rho)+2+8\textstyle\sum_{\|}(K_0-\alpha K_1)=\rho^{-1}I_1^1(\rho^{-1}),$$
$$I_1^1(\rho)=-2+8\textstyle\sum_{\|}\alpha K_1=\rho^{-1}R_1^1(\rho^{-1}),\quad L_0^0=R_1^1+I_1^1. \tag{80}$$

The forms in terms of ρ^{-1} follow from the symmetry of the problem, i.e., from the interchange relations (21); this will be discussed further subsequently.

For $n>1$, we construct the low frequency forms of (77) from those derived for $\mathcal{N}_{n,l}$. We express $\mathcal{N}_n^{Lm}=P_n^m(0)\mathcal{N}_{n,0}^L$, in terms of (58),

$$\mathcal{N}_{2n}^{L2m}\approx P_{2n}^{2m}(0)\beta_n,\quad \mathcal{N}_{2n+1}^{L2m+1}\approx P_{2n+1}^{2m+1}(0)\beta_n(4n+1)\xi_0. \tag{81}$$

For $\mathcal{N}_n^{Pm}=\sum D_n^{m,l}\mathcal{N}_{n,l}^P$, from (59) and (71),

$$\mathcal{N}_{2n}^{P2m}\approx 2D_{2n}^{2m,2n}\mathcal{N}_{2n,2n}^P\approx 2D_n/2^{2n}(2n-2m)!,$$

$$\mathcal{N}^{P\,2m+1}_{2n+1} \approx 2D^{2m+1,2n}_{2n+1}\mathcal{N}^{P}_{2n+1,2n} + 2D^{2m+1,2n+1}_{2n+1}\mathcal{N}^{P}_{2n+1,2n+1}$$

$$\approx [2(4n+1)\mathcal{D}_n/2^{2n+1}(2n-2m)!\,]\,[(2m+1)\xi_0 + i2m\eta_0]. \tag{82}$$

For $K^m_n = \sum D^{m,l}_n K_{n,l}$, from (60) and (71),

$$K^{2m}_{2n} \approx \mathcal{E}_n \sum_{l=0}^{n} \sum_{\text{II}} E^{2m,2l}_{2n} K_{2l} \nu^{2n},$$

$$\mathcal{E}_n = \frac{-(4n-1)!\,!\,4(4\pi)^{2n}}{(kb)^{2n+1}}, \tag{83}$$

$$E^{m,l}_n = \frac{2\epsilon_l D^{m,l}_n}{2^n(n-l)!} = \frac{2\epsilon_l D^{m,l}_n D^{n,-l}_n}{(2n)!},$$

$$K^{2n+1}_{2n+1} \approx 2(4n+1)\mathcal{E}_n \sum_{l=0}^{n} \sum_{\text{II}} \{\xi_0 E^{2n+1,2l}_{2n+1}[(2n+1-2l)K_{2l} - \alpha K_{2l-1}]$$

$$+ i\eta_0 E^{2n+1,2l+1}_{2n+1} \alpha K_{2l+1}\}\nu^{2n}.$$

If we may use the asymptotic form $K_l \sim K$ of (42), then since

$$\sum_{l=0}^{[n/2]} E^{m,2l}_n = \sum E^{m,2l+1}_n = \frac{2\delta_{nm}}{\epsilon_m}$$

from (70), we can sum over l in (83) and obtain the leading terms

$$K^{2m}_{2n} \sim K^{2n}_{2n}\delta_{nm} \sim -\delta_{nn}\frac{4(4n-1)!\,!\,(4\pi)^{2n}}{(kb)^{2n+1}} \sum_{\text{II}} \nu^{2n} K(\alpha),$$

$$\alpha = \nu t 2\pi\rho, \quad \sum_{\text{II}} = \sum_{\nu=1}^{\infty}\sum_{t=1}^{\infty}, \tag{84}$$

$$K^{2n+1}_{2n+1} \sim K^{2n+1}_{2n+1}\delta_{nm} \sim \delta_{nm}(\xi_0 - i\eta_0)\frac{8(4n+1)!\,!\,(4\pi)^{2n}}{(kb)^{2n+1}} \sum_{\text{II}} \nu^{2n}\alpha K(\alpha),$$

which also serve to check the numerical values of the coefficients $D^{m,l}_n$.

Adding the corresponding terms of (81)—(83), or applying (77) to (61), we write

$$-\mathcal{N}^{2m}_{2n}(kb)^{2n+1}/(4n-1)!\,!\,(-1)^n P^{2m}_{2n}(0) \to L^{2m}_{2n}(\rho),$$

$$-\mathcal{N}^{2m+1}_{2n+1}(kb)^{2n+1}/(4n+1)!\,!\,(-1)^n P^{2m+1}_{2n+1}(0)$$

$$\to \xi_0 R^{2m+1}_{2n+1}(\rho) + i\eta_0 I^{2m+1}_{2n+1}(\rho), \tag{85}$$

where, for $n > 0$,

$$L^{2m}_{2n}(\rho) = 2\zeta(2n+1) + \frac{4(2n-1)!\,(-1)^n}{(2n-2m)!\,P^{2m}_{2n}(0)}\frac{\zeta(2n)}{\rho^{2n}}$$

$$+ \frac{8(2\pi)^{2n}}{(-1)^n P^{2m}_{2n}(0)} \sum_{\text{II}} \nu^{2n} \sum_{l=0}^{n} \epsilon_l \frac{D^{2m,2l}_{2n} K_{2l}(\alpha)}{(2n-2l)!},$$

$$R^{2m+1}_{2n+1}(\rho) = 2\zeta(2n+1) + \frac{4(2n-1)!\,(2m+1)(-1)^n}{(2n-2m)!\,P^{2m}_{2n}(0)}\frac{\zeta(2n)}{\rho^{2n}}$$

$$+ \frac{8(2\pi)^{2n}}{(-1)^n P^{2m}_{2n}(0)} \sum_{\text{II}} \nu^{2n} \sum_{l} \epsilon_l \frac{D^{2n+1,2l}_{2n+1}}{(2n-2l)!}\left(K_{2l} - \frac{\alpha K_{2l-1}}{2n+1-2l}\right), \tag{86}$$

$$I^{2m+1}_{2n+1}(\rho) = \frac{4(2n)!\,(-1)^n}{(2n-2m)!\,P^{2m+1}_{2n+1}(0)}\frac{\zeta(2n)}{\rho^{2n}}$$

$$+ \frac{8(2\pi)^{2n}}{(-1)^n P^{2m+1}_{2n+1}(0)} \sum_{\text{II}} \nu^{2n} \sum_{l} 2\frac{D^{2n+1,2l+1}_{2n+1}}{(2n-2l)!}\alpha K_{2l+1}.$$

The $n = 0$ terms are given in (79) and (80), and the leading terms of (86) are

$$L^0_2(\rho) = 2\zeta(3) + 4\zeta(2)\rho^{-2} - 4\sum_{\text{II}}(2\pi\nu)^2(K_0 - K_2) = \rho^{-3}L^0_2(\rho^{-1}),$$

$$L^2_2(\rho) = 2\zeta(3) - \tfrac{4}{3}\zeta(2)\rho^{-2} - \tfrac{4}{3}\sum_{\text{II}}(2\pi\nu)^2(3K_0 + K_2)$$

$$= -\rho^{-3}L^2_2(\rho^{-1}),$$

$$R^1_3(\rho) = 2\zeta(3) + \tfrac{4}{3}\zeta(2)\rho^{-2} - \tfrac{4}{3}\sum_{\text{II}}(2\pi\nu)^2(3K_0 - K_2)$$

$$= \rho^{-3}I^1_3(\rho^{-1}),$$

$$I^1_3(\rho) = \tfrac{8}{3}\zeta(2)\rho^{-2} + \tfrac{8}{3}\sum_{\text{II}}(2\pi\nu)^2 K_2 = \rho^{-3}R^1_3(\rho^{-1}),$$

$$R^3_3(\rho) = 2\zeta(3) - \tfrac{4}{5}\zeta(2)\rho^{-2} - \tfrac{4}{15}\sum_{\text{II}}(2\pi\nu)^2(15K_0 + 3K_2 - 8\alpha K_1)$$

$$= -\rho^{-3}I^3_3(\rho^{-1}),$$

$$I^3_3(\rho) = -\tfrac{8}{15}\zeta(2)\rho^{-2} - \tfrac{2}{15}\sum_{\text{II}}(2\pi\nu)^2\alpha(15K_1 + K_3) \tag{87}$$

$$= -\rho^{-3}R^3_3(\rho^{-1}),$$

$$L^0_4(\rho) = 2\zeta(5) + \tfrac{8}{3}\zeta(4)\rho^{-4} + \tfrac{1}{9}\sum_{\text{II}}(2\pi\nu)^4(3K_0 - 4K_2 + K_4)$$

$$= \rho^{-5}L^0_4(\rho^{-1}),$$

$$L^2_4(\rho) = 2\zeta(5) - \tfrac{8}{5}\zeta(4)\rho^{-4} + \tfrac{1}{15}\sum_{\text{II}}(2\pi\nu)^4(5K_0 - 4K_2 - K_4)$$

$$= -\rho^{-5}L^2_4(\rho^{-1}),$$

$$L^4_4(\rho) = 2\zeta(5) + \tfrac{8}{35}\zeta(4)\rho^{-4} + \tfrac{1}{105}\sum_{\text{II}}(2\pi\nu)^4(35K_0 + 28K_2 + K_4)$$

$$= \rho^{-5}L^4_4(\rho^{-1}),$$

$$L^{2m}_{2n} = R^{2n+1}_{2n+1} + I^{2n+1}_{2n+1}.$$

Numerical computations for $\rho = 1$ to 8 keeping at most eight terms of the $K(\rho)$ sums, but over 100 terms for some of the $K(\rho^{-1})$ sums, substantiate the interchanged forms in (79), (80), (87) to at least five significant figures. As required by (84), for $K_l \sim K$, only the $K^{2n}_{2n}[K]$ sums in the L's are nonvanishing; similarly for the $K^{2n+1}_{2n+1}[\alpha K]$ sums, as in R^3_3 and I^3_3.

For the square cell, we require $L^{2(2\sigma+1)}_n(1) = 0$. Thus, from $L^2_{2n}(1) = L^6_{2n}(1) = 0$,

$$3\zeta(3) - 2\zeta(2) = 8\pi^2\sum_{\text{II}}\nu^2(3K_0 + K_2), \quad K_l = K_l(\nu t 2\pi);$$

$$5\zeta(5) - 4\zeta(4) = (8\pi^4/3)\sum_{\text{II}}\nu^4(-5K_0 + 4K_2 + K_4),$$

$$217\zeta(7) - 16\zeta(6) = (8\pi^6/15)\sum_{\text{II}}\nu^6(14K_0 - 17K_2 + 2K_4 + K_6), \tag{88}$$

$$693\zeta(7) - 16\zeta(6) = (8\pi^6/15)\sum_{\text{II}}\nu^6(462K_0 + 495K_2 + 66K_4 + K_6);$$

more generally, with $2m = 2(2\sigma+1) = 2,\ 6,\ 10,\ \cdots$ we obtain

$$\frac{(2n+2m-1)!\,!}{2^{n-m}(n-m)!}\zeta(2n+1) - \frac{2(2n-1)!}{(2n-2m)!}\zeta(2n)$$

$$= -4(2\pi)^{2n}\sum_{l=0}^{n}\epsilon_l\sum_{\nu t}\nu^{2n}D^{2m,2l}_{2n}\frac{K_{2l}(\nu t 2\pi)}{(2n-2l)!}, \tag{89}$$

which relates pairs of values of the Riemann ζ function for successive integers with the Wigner rotation coefficient $D^{m,l}_n$ of (67) and the modified Hankel functions K_l.

D. Direct derivation for low frequencies

The primary purpose of the preceding sections was to represent the slowly converging series for H^m_n of

(18) for all values of k in terms of the known series for the periodic line[2] (H^L) and the grating[3] (H^G) plus a rapidly converging double series (K) of modified Hankel functions. The result (73), in terms of (26) and (49), may be used for numerical computations with the closed form approximations for G of the next section for all kb. We specialized (73) to small kb in (79) to (87), and indicated the roles of H^L, H^G, and K contributions, but except for $n=0$ and 1, the limiting values may be derived more directly.

Thus, if we substitute $n_n(x)\approx -(2n-1)!!/x^{n+1}$ into (20) for $n>1$, and use $H\approx iN$ with N as in (85), the low frequency limits are given by

$$L_{2n}^{2m}(\rho)=\sum{}' \frac{\mathrm{Re}(s+it\rho)^{2m}}{(s^2+t^2\rho^2)^{n+m+1/2}}=\sum{}' \frac{\cos 2m\beta}{r^{2n+1}},$$

$$\beta=\beta_{st},\quad r=(s^2+t^2\rho^2)^{1/2},\quad \rho=|\rho|=d/b;$$

$$R_{2n+1}^{2m+1}(\rho)=\sum{}' \frac{s\,\mathrm{Re}(s+it\rho)^{2m+1}}{(s^2+t^2\rho^2)^{n+m+3/2}}=\sum{}' \frac{\cos\beta\cos(2m+1)\beta}{r^{2n+1}}, \tag{90}$$

$$I_{2n+1}^{2m+1}(\rho)=\sum{}' \frac{t\rho\,\mathrm{Im}(s+it\rho)^{2m+1}}{(s^2+t^2\rho^2)^{n+m+3/2}}=\sum{}' \frac{\sin\beta\sin(2m+1)\beta}{r^{2n+1}}.$$

For $n>0$, these absolutely converging series with ρ as the only parameter are the same as for the potential theory problem ($k=0$); for $n=0$, the series diverge.

Corresponding to the interchange relations (21), we now have

$$\begin{aligned} L_{2n}^{2m}(\rho^{-1})&=(-1)^m\rho^{2n+1}L_{2n}^{2m}(\rho),\\ R_{2n+1}^{2m+1}(\rho^{-1})&=(-1)^m\rho^{2n+1}I_{2n+1}^{2m+1}(\rho),\end{aligned} \tag{91}$$

where we may replace ρ by ρ^{-1} throughout. For the square unit cell,

$$L_{2n}^{2(2l+1)}(1)=0. \tag{92}$$

From the trigonometric versions in (90),

$$R_{2n+1}^{2m+1}=\tfrac{1}{2}(L_{2n}^{2m}+L_{2n}^{2m+2}),\quad I_{2n+1}^{2m+1}=\tfrac{1}{2}(L_{2n}^{2m}-L_{2n}^{2m+2}). \tag{93}$$

Thus, from (93) we require only the L series explicitely, and from (91) we need consider only either $\rho\geq 1$ or $\rho\leq 1$. As before for the general case, we work with $L(\rho)$ such that $\rho=d/b\geq 1$ and sum initially over s (the index for the smaller spacing).

Using the summation sequence (32), we have from (90)

$$L_{2n}^{2m}=M_{2n}+\sum_t{}'\sum_s \cos 2m\beta_{st}/(s^2+t^2\rho^2)^{n+1/2}, \tag{94}$$

where

$$M_{2n}=\sum_s{}'(1/|s|^{2n+1})=2\zeta(2n+1). \tag{95}$$

To convert $\sum_t'\sum_s$ to a more rapidly converging form, we use the Poisson sum formula

$$\sum_{s=-\infty}^{\infty} F(s)=2\int_0^\infty F(x)\,dx+4\sum_{\nu=1}^{\infty}\int_0^\infty F(x)\cos(2\nu\pi x)\,dx$$

and the corresponding decomposition of (94),

$$L_{2n}^{2m}=M_{2n}+N_{2n}^{2m}[\nu=0]+K_{2n}^{2m}\left[\sum_{\nu=1}^{\infty}\right]. \tag{96}$$

In terms of $\cos\beta=x/(x^2+t^2\rho^2)^{1/2}=x/r$, $\sin\beta=t\rho/r$, we have

$$\begin{aligned} N_{2n}^{2m}&=\sum_t{}'2\int_0^\infty \frac{\cos 2m\beta}{r^{2n+1}}\,dx\\ &=4\sum_{t=1}^{\infty}\frac{1}{t^{2n}\rho^{2n}}\int_0^{\pi/2}\cos 2m\beta\sin^{2n-1}\beta\,d\beta\\ &=\frac{\zeta(2n)}{\rho^{2n}}(-1)^m D_{2n}^{2m},\end{aligned} \tag{97}$$

$$\begin{aligned} D_{2n}^{2m}&=\frac{4(2n-1)!\,\pi}{2^{2n}\Gamma(n+m+\tfrac{1}{2})\Gamma(n-m+\tfrac{1}{2})}\\ &=\frac{4(n-1)!}{(2n+2m-1)!!\,(2n-2m-1)!!}\end{aligned}$$

The Γ function[7] version covers N_{2n}^{2n+2}, the special value required to construct R and I for $m=n$. Thus

$$N_{2n}^{2n+2}=\frac{4\zeta(2n)(2n-1)!\,(-1)^{n+1}\pi}{\rho^{2n}2^{2n}\Gamma(2n+\tfrac{1}{2})\Gamma(-\tfrac{1}{2})}=\frac{4\zeta(2n)(2n-1)!\,(-1)^n}{\rho^{2n}(4n+1)!!}. \tag{98}$$

For K_{2n}^{2m}, we expand $\cos 2m\beta$ in powers of $\sin^2\beta$ in order to isolate a standard representation for K_n. Thus, from

$$\begin{aligned} &\cos 2m\beta=\sum_{\sigma=0}^{m}B_\sigma^m\sin^{2\sigma}\beta,\quad B_0^0=1,\\ &B_\sigma^m=\frac{m(-1)^\sigma 2^{2\sigma}(m+\sigma-1)!}{(2\sigma)!\,(m-\sigma)!},\quad \sin^2\beta=\frac{t^2\rho^2}{x^2+t^2\rho^2},\\ &\int_0^\infty\frac{\cos(2\nu\pi x)}{(x^2+t^2\rho^2)^{l+1/2}}\,dx=\left(\frac{2\nu\pi}{t\rho}\right)^l\frac{K_l(2\nu\pi t\rho)}{(2l-1)!!},\end{aligned} \tag{99}$$

we obtain

$$\begin{aligned} &K_{2n}^{2m}=8(2\pi)^{2n}\sum_{\sigma=1}^{m}\frac{B_\sigma^m}{(2n+2\sigma-1)!!}\sum_{\nu}{}'\nu^{2n}\frac{K_{n+\sigma}(\alpha)}{\alpha^{n-\sigma}},\\ &\sum_{\nu}{}'=\sum_{t=1}^{\infty}\sum_{\nu=1}^{\infty},\quad \alpha=t\nu 2\pi\rho.\end{aligned} \tag{100}$$

Equation (96) in terms of (95), (97), (98), and (100), plus the construction relations (93) are equivalent to the earlier set (86). Although we could eliminate $\alpha^{n-\sigma}$ from (100) by successive applications of the recursive relation $(2n/\alpha)K_n=K_{n+1}-K_{n-1}$, the alternate form of K_{2n}^{2m} in (86) obviates the matter. Thus, by comparison,

$$\begin{aligned} &(-1)^nP_{2n}^{2m}(0)\sum_{\sigma=0}^{m}\frac{B_\sigma^m}{(2n+2\sigma-1)!!}\frac{K_{n+\sigma}(\alpha)}{\alpha^{n-\sigma}}\\ &=\sum_{l=0}^{n}\frac{\epsilon_l D_{2n}^{2m,2l}}{(2n-2l)!}K_{2l}(\alpha).\end{aligned} \tag{101}$$

(The special case $m=0$ is given in Ref. 8, p. 71.) The difference in the two forms in (101) corresponds to the two different decompositions for $P_{2n}^{2m}(0)\cos 2m\beta$ that are implicit: For the left side, we used a polynomial in $\sin^2\beta$, and for the right, a set of terms $P_{2n}^{2l}(\cos\beta)$. We may also obtain additional versions from $\cos 2m\beta=(-1)^m\times\sum B_m^\sigma\cos^{2\sigma}\beta$ or $\cos 2m\beta=\sum\binom{2m}{2r}(\cos^2\beta)^{m-r}(-\sin^2\beta)^r$, and the more general integral

$$\int_0^\infty\frac{x^{2l}\cos 2\nu\pi x}{(x^2+t^2\rho^2)^{n+1/2}}\,dx=\frac{(-1)^l\partial_\alpha^{2l}[\alpha^nK_n(\alpha)]}{(t\rho)^{2n-2l}(2n-1)!!},\quad \alpha=2\pi\nu t\rho.$$

Additional relations among K_n series follow from (93) and (100), and the interchange relations (91) provide inversion forms between the series for small and large

values of the argument, e.g.,

$$K_{2r}^{2m}(\rho^{-1}) = [(-1)^m\rho^{2n+1} - 1]2\zeta(2n+1) - [(-1)^m\rho^{2n} - \rho]\, D_{2n}^{2m}\zeta(2n) + (-1)^m\rho^{2n+1}K_{2n}^{2m}(\rho). \tag{102}$$

In particular for $\rho = 1$, we obtain (89) in the form

$$2\zeta(2n+1) - D_{2n}^{2(2l+1)}\zeta(2n) = -K_{2n}^{2(2l+1)}(1). \tag{103}$$

The asymptotic forms of K_{2n}^{2m} implicit in (84) follow directly from (100):

$$K_{2r}^{2m}(\alpha) \sim \delta_{rm}K_{2n}^{2n},$$

$$K_{2r}^{2n} \sim \frac{4(-1)^n(4\pi)^{2n}}{(4n-1)!}\sum_u \nu^{2n}K(\alpha) = K_A^n, \tag{104}$$

$$K_{2r}^{2n+2} \sim \frac{-16(-1)^n(4\pi)^{2n}}{(4n+1)!}\sum_u \nu^{2n}K(\alpha)[\alpha + 2n^2 - \tfrac{1}{8}]$$

$$= K_B^n - \tfrac{1}{2}(4n-1)K_A^n \sim K_B^n, \tag{105}$$

where the next terms are of order K/α. Thus of the functions required for (90), asymptotically, only L_{2n}^{2n}, $R_{2n+1}^{2n\pm1}$, and $I_{2n+1}^{2n\pm1}$ contain K series of order K_A^n or K_B^n. The functions L_{2n}^{2n}, $2R_{2n+1}^{2n-1}$, and $-2I_{2n+1}^{2n-1}$ contain K_A^n; $2R_{2n+1}^{2n+1}$ contains $K_B^n - K_A^n(4n-3)/2 \sim K_B^n$, and $-2I_{2n+1}^{2n+1}$ contains $K_B^n - K_A^n(4n+1)/2 \sim K_B^n$.

3. SCATTERING COEFFICIENTS

The algebraic equations (6) for the multiple scattering coefficients may be reduced in terms of either $H_{n,l}[Y(\xi)]$ or $H_n^m[Y(\xi)]$. We consider the system for A_n^m in terms of H_n^m because it is the simpler, but corresponding results for $A_{n,l}$ in terms of $H_{n,l}$ may be obtained by superposition. The invariant scattering amplitude G may be written $\sum A_n^m Y_n^m(\xi) = \sum A_{n,l}Y_n^l(\xi)$. Substituting $Y_n^m(\xi) = \sum_l D_n^{m,l}Y_n^l(\xi)$ into the first form and using the orthogonality of the $Y_n^l(\xi)$, we obtain $A_{n,l} = \sum_m A_n^m D_n^{m,l}$, from which (by the orthogonality of the $D_n^{m,l}$) we also have $A_n^m = \sum_l A_{n,l}D_n^{l,m}$.

In simplifying (6) it is convenient to work initially with the symbol

$$\left(\begin{smallmatrix}-m\\ n\end{smallmatrix}\middle|\begin{smallmatrix}t\\ r\end{smallmatrix}\right) = \sum_l d_l\left(\begin{smallmatrix}-m\\ n\end{smallmatrix};\begin{smallmatrix}t\\ r\end{smallmatrix}\right)H_l^{t-m} = \left(\begin{smallmatrix}t\\ r\end{smallmatrix}\middle|\begin{smallmatrix}-m\\ n\end{smallmatrix}\right), \tag{106}$$

which, together with

$$Y_n^{-m}Y_r^t = \sum d_l Y_l^{t-m}, \tag{107}$$

makes explicit the spherical modes that are coupling. In particular, in terms of (106), we rewrite (7) initially as

$$A_r^m = (-1)^m a_n[Y_n^{-m}(\hat{\mathbf{k}}) + \sum A_r^t\left(\begin{smallmatrix}-m\\ n\end{smallmatrix}\middle|\begin{smallmatrix}t\\ r\end{smallmatrix}\right)], \quad \sum = \sum_{r=0}^{\infty}\sum_{t=-r}^{r} \tag{108}$$

In (106), the coefficients d_l vanish unless $l+n+r$ is even, and the functions H vanish unless $l-t+m$ is even. Thus, we require that $n+r+t-m$ be even, and (108) reduces to two sets of equations; in one set $n-m$ and $r-t$ are both even, and in the other both odd.

For small scatterers, we truncate the system of equations by retaining only a small number of the isolated scatterer coefficients a_n. Thus, if we retain only the monopole (a_0) and dipole (a_1) terms, (108) reduces to

$$A_0^0 = a_0[1 + A_0^0\left(\begin{smallmatrix}0\\ 0\end{smallmatrix}\middle|\begin{smallmatrix}0\\ 0\end{smallmatrix}\right) + A_1^1\left(\begin{smallmatrix}0\\ 0\end{smallmatrix}\middle|\begin{smallmatrix}1\\ 1\end{smallmatrix}\right) + A_1^{-1}\left(\begin{smallmatrix}0\\ 0\end{smallmatrix}\middle|\begin{smallmatrix}-1\\ 1\end{smallmatrix}\right)], \quad A_1^0 = a_1[Y_1^0 + A_1^0\left(\begin{smallmatrix}0\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}0\\ 1\end{smallmatrix}\right)],$$

$$A_1^{\pm1} = -a_1[Y_1^{\mp1} + A_0^0\left(\begin{smallmatrix}\mp1\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}0\\ 0\end{smallmatrix}\right) + A_1^1\left(\begin{smallmatrix}\mp1\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}\pm1\\ 1\end{smallmatrix}\right) + A_1^{\mp1}\left(\begin{smallmatrix}\mp1\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}\mp1\\ 1\end{smallmatrix}\right)], \tag{109}$$

where the special symbols represent the lattice sums

$$\left(\begin{smallmatrix}0\\ 0\end{smallmatrix}\middle|\begin{smallmatrix}0\\ 0\end{smallmatrix}\right) = H_0^0, \quad \left(\begin{smallmatrix}0\\ 0\end{smallmatrix}\middle|\begin{smallmatrix}1\\ 1\end{smallmatrix}\right) = H_1^1 \equiv H_d^+, \quad \left(\begin{smallmatrix}0\\ 0\end{smallmatrix}\middle|\begin{smallmatrix}-1\\ 1\end{smallmatrix}\right) = -\tfrac{1}{2}H_1^1(-\beta) \equiv H_d^-,$$

$$\left(\begin{smallmatrix}0\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}0\\ 1\end{smallmatrix}\right) = \tfrac{1}{3}(H_0^0 + 2H_2^0) \equiv H_a, \quad \left(\begin{smallmatrix}-1\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}1\\ 1\end{smallmatrix}\right) = -\tfrac{1}{3}(H_0^0 - H_2^0) \equiv -H_b,$$

$$\left(\begin{smallmatrix}1\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}1\\ 1\end{smallmatrix}\right) = \tfrac{1}{3}H_2^2 \equiv H_c^+, \quad \left(\begin{smallmatrix}-1\\ 1\end{smallmatrix}\middle|\begin{smallmatrix}-1\\ 1\end{smallmatrix}\right) = \tfrac{1}{12}H_2^2(-\beta) \equiv H_c^-.$$

We solve the system (109) in a stepwise fashion, to delineate special cases of physical interest.

If we are dealing solely with monopoles, then (109) reduces to

$$A_0^0 = a_0(1 + A_0^0H_0^0) = a_0/(1 - a_0H_0^0) \equiv \mathcal{A}_0, \tag{110}$$

which equals the corresponding multiple scattering amplitude G. For this special case, in view of (9), the multiple scattering coefficient is similar to the single scattered in that it has the same value for all relevent directions $\hat{\mathbf{k}}_{\nu\mu}$.

On the other hand, for pure dipoles, from (109),

$$A_1^0 = a_1(Y_1^0 + A_1^0H_a), \quad A_1^{\pm1} = -a_1(Y_1^{\mp1} - A_1^{\pm}H_b + A_1^{\mp1}H_c^{\mp}), \tag{111}$$

which we reduce to

$$A_1^0 = a_1Y_1^0/(1 - a_1H_a) \equiv \mathcal{A}_1^0Y_1^0, \quad A_1^{\pm} = -\beta Y_1^{\mp1} + \beta\mathcal{A}H_c^{\mp}Y_1^{\pm} \equiv \mathcal{A}_1^{\pm},$$

$$\mathcal{A} \equiv a_1/(1 - a_1H_b), \quad \beta \equiv \mathcal{A}/(1 - \mathcal{A}^2H_c^+H_c^-). \tag{112}$$

The corresponding multiple scattering amplitude, $G = A_1^0Y_1^0(\hat{\mathbf{r}}) + A_1^1Y_1^1 + A_1^{-1}Y_1^{-1}$, may be written

$$G = \mathcal{A}_1^0\cos\theta\cos\theta_0 + \beta\sin\theta\sin\theta_0\{\cos(\varphi - \varphi_0) + \mathcal{A}[H_2^2(-\beta)\exp(i(\varphi + \varphi_0)) + H_2^2(\beta)\exp(-i(\varphi + \varphi_0))]/12\}$$

$$\equiv G_1. \tag{113}$$

The explicit functions of direction are symmetrical in $\hat{\mathbf{r}}$ and $\hat{\mathbf{k}}$ (with both in the set $\hat{\mathbf{k}}_{\nu\mu}$) and from (9), the coefficients which depend implicitely on $H(\hat{\mathbf{k}})$ are also symmetrical to the interchange; thus $G(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = G(\hat{\mathbf{k}}, \hat{\mathbf{r}})$ has the inversion symmetry required by elementary considerations. Because of the inversion symmetry, the reciprocity theorem $G(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = G(-\hat{\mathbf{k}}, -\hat{\mathbf{r}})$ or (1:17) may be written $G(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = G(-\hat{\mathbf{r}}, -\hat{\mathbf{k}})$; from (10), the coefficients are independent of the sign of $\hat{\mathbf{k}}_{00}$, and since $\hat{\mathbf{r}} = \hat{\mathbf{r}}(\theta, \varphi)$ leads to $-\hat{\mathbf{r}} = \hat{\mathbf{r}}(\pi + \theta, \pi + \varphi)$, we see that G_1 fulfills the theorem.

If the isolated scatterers have comparable monopole and dipole coefficients, we again obtain A_1^0 as in (112), but the remaining coefficients are coupled. In terms of the symbols defined in (110) and (112),

$$A_0^0 = \mathcal{A}_0(1 + A_1^1H_d^+ + A_1^{-1}H_d^-),$$

$$A_1^{\pm} = -\mathcal{A}(Y_1^{\pm1} + A_0^0H_d^{\mp} + A_1^{\mp}H_c^{\mp}) = \mathcal{A}_1^{\pm1} + A_0^0C^{\mp}, \tag{114}$$

$$C^{\mp} = -\beta(H_d^{\mp} - \mathcal{A}H_c^{\mp}H_d^{\pm}),$$

where only coupling effects between $n = 0$ and ± 1 are left explicit. Thus

$$A_0^0 = \mathcal{A}_0(1 + H_d^+A_1^1 + H_d^-A_1^{-1})/D = \mathcal{A}_0(1 + Y_1^1C^+ + Y_1^1C^-)/D,$$

$$D \equiv 1 - \mathcal{A}_0(H_d^+C^- + H_d^-C^+), \tag{115}$$

which we also use to eliminate A_0^0 from the final form of $A_1^{\pm1}$ of (114). The present A_0^0 depends on the direction of incidence, and the $A_1^{\pm1}$ also include constant terms. To

emphasize the dependence on directions of incidence, we write

$$A_0^0 = B + B^+Y_1^{-1} + B^-Y_1^1, \quad B = \mathcal{A}_0/D, \quad B^\pm = BC^\pm = \mathcal{A}_0 C^\pm/D,$$
$$A_1^{\pm 1} = B^\mp + B_1 Y_1^{\mp 1} + B_1^\mp Y_1^{\pm 1}, \quad B_1 = -\beta + BC^-C^+, \tag{116}$$
$$B_1^\mp = \beta\mathcal{A}H_c^\mp + B(C^\mp)^2.$$

The corresponding scattering amplitude is

$$G(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = B + B^-(Y_1^1 + Y_1^1) + B^+(Y_1^{-1} + Y_1^{-1}) + A_1^0 Y_1^0 Y_1^0$$
$$+ B_1(Y_1^1 Y_1^{-1} + Y_1^{-1} Y_1^1) + B_1^- Y_1^1 Y_1^1 + B_1^+ Y_1^{-1} Y_1^{-1}, \tag{117}$$

where, for each pair of Y's one Y has argument $\hat{\mathbf{r}}$ and the other $\hat{\mathbf{k}}$ (with both in the set $\hat{\mathbf{k}}_{\nu\mu}$). From the pairing of the Y's and from (9), we see that $G(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = G(\hat{\mathbf{k}}, \hat{\mathbf{r}})$. In addition, $G = (\hat{\mathbf{r}}, \hat{\mathbf{k}}) = G(-\hat{\mathbf{k}}, -\hat{\mathbf{r}}) = G(-\hat{\mathbf{r}}, -\hat{\mathbf{k}})$ is fulfilled; because of (10), only the coefficients of $Y_1^{\pm 1}$ (proportional to $C^\pm[-\hat{\mathbf{k}}] = -C^\pm[\hat{\mathbf{k}}]$) change sign and this is compensated by $Y_n^m(-\hat{\mathbf{r}}) = (-1)^n Y_n^m(\hat{\mathbf{r}})$.

We rewrite (117) as

$$G = G_1 + BF(\hat{\mathbf{r}})F(\hat{\mathbf{k}}), \quad F(\hat{\mathbf{r}}) = 1 + C^- Y_1^1(\hat{\mathbf{r}}) + C^+ Y_1^{-1}(\hat{\mathbf{r}}),$$
$$B = \mathcal{A}_0/D, \tag{118}$$

where G_1 is the pure dipole amplitude as in (113). Since

$$C^+ = -\beta[H_1^1(\beta) + \mathcal{A}H_2^2(\beta)H_1^1(-\beta)/6] \equiv C(\beta), \quad C^- = -\tfrac{1}{2}C(-\beta),$$

we may also work with

$$F(\hat{\mathbf{r}}) = 1 - \tfrac{1}{2}[C(-\beta)\exp(i\varphi) + C(\beta)\exp(-i\varphi)]\sin\theta,$$
$$D = 1 + \tfrac{1}{2}\mathcal{A}_0[H_1^1(\beta)C(-\beta) + H_1^1(-\beta)C(\beta)].$$

For normal incidence, only the lattice sums H_{2p}^{2q} are nonvanishing; thus $t - m$ and l of (106) are even, and consequently $n + r$ of (108) is even. Since $Y_n^{-m}(\hat{\mathbf{z}}) = \delta_{m0}$, we obtain the two independent sets of inhomogeneous equations

$$A_{2n}^{2m} = a_{2n}[\delta_{m0} + \sum A_{2r}^{2t}\left(\begin{smallmatrix} -2m \\ 2n \end{smallmatrix} \middle| \begin{smallmatrix} 2t \\ 2r \end{smallmatrix}\right)],$$
$$A_{2n+1}^{2m} = a_{2n+1}[\delta_{m0} + \sum A_{2r+1}^{2t}\left(\begin{smallmatrix} -2m \\ 2n+1 \end{smallmatrix} \middle| \begin{smallmatrix} 2t \\ 2r+1 \end{smallmatrix}\right)] \tag{119}$$

as well as two sets of homogeneous equations

$$A_n^{2m+1} = -a_n \sum A_r^{2t+1}\left(\begin{smallmatrix} -2m-1 \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 2t+1 \\ r \end{smallmatrix}\right)\delta_e(n-r) \tag{120}$$

corresponding to eigenvalue problems. Thus, for symmetrical excitation, the coefficients decouple, essentially as for the grating and the periodic line.

For small scatterers, if we retain only a_0 and a_1 we obtain simply the uncoupled pair, (110) for $A_0^0 = \mathcal{A}_0$ and (112) for $A_1^0 = \mathcal{A}_1^0$. The missing coefficients $A_1^{\pm 1}$ and A_1^{-1} correspond to the homogeneous system (120), i. e., $A_1^{\pm 1} = a_1(A_1^{\pm 1}H_b - A_1^{\mp 1}H_c^\mp)$; unless $(1 - a_1/H_b)^2 = a_1^2 H_c^- H_c^+$, the only solution is $A_1^{+1} = A_1^{-1} = 0$.

For lossless scatterers, from theorem (1:18) with $G = \mathcal{A}_0 + A_1\cos\theta$, we require

$$-\mathrm{Re}\mathcal{A}_0 = 2C_0|\mathcal{A}_0|^2 \sum_p \sec\theta_{\nu\mu},$$
$$-\mathrm{Re}\mathcal{A}_1^0 = 2C_0|\mathcal{A}_1^0|^2 \sum_p \cos\theta_{\nu\mu}, \quad C_0 = \pi/k^2 bd. \tag{121}$$

Using $-\mathrm{Re}a_n = |a_n|^2/(2n+1)$ and $\mathcal{G}_n^0 = \mathrm{Re}H_n^0$, we demonstrate directly that the present explicit results satisfy these relations. Thus, from $\mathcal{A}_0 = a_0/(1 - a_0 H_0^0)$, we have

$$\mathrm{Re}\mathcal{A}_0 = \mathrm{Re}[a_0(1 - a_0 H_0^0)^*]/|1 - a_0 H_0^0|^2$$
$$= -|\mathcal{A}_0|^2(1 + \mathcal{G}_0^0)$$

with $\mathcal{G}_0^0 = 2C_0 \sum_p \sec\theta_{\nu\mu} - 1$; similarly, from $\mathcal{A}_1^0 = a_1/[1 - a_1(H_0^0 + 2H_2^0)/3]$, we have $\mathrm{Re}\mathcal{A}_1^0 = -|\mathcal{A}_1^0|^2(1 + \mathcal{G}_0^0 + 2\mathcal{G}_2^0)/3$ with $\mathcal{G}_n^0 = 2C_0 \sum_p P_n \sec\theta_{\nu\mu}$ and $P_0 + 2P_2 = 3\cos^2\theta$.

To consider higher order coupling effects in detail, we rewrite $G = \sum A_n^m Y_n^m$ as

$$G = \sum_{n=0}^{\infty} A_n^0 P_n^0 + \sum_{n=1}^{\infty}\sum_{m=1}^{n} B_n^m P_n^m \cos m\varphi,$$
$$B_m^n = A_m^n + C_n^m A_n^{-m}, \quad C_n^m = (-1)^m(n-m)!/(n+m)!. \tag{122}$$

The terms in $(A_n^m - C_n^m A_n^{-m})\sin m\varphi$ were dropped because, from (120), they satisfy a homogeneous system. If we write $A_n^0 = B_n^0$, then either set of equations in (119) may be reduced to the system

$$B_n^0 = a_n[1 + \sum B_r^{2t}\left(\begin{smallmatrix} 0 \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 2t \\ r \end{smallmatrix}\right)\delta_e(n-r)],$$
$$B_n^{2m} = a_n \sum B_r^{2t}\left\{\begin{smallmatrix} 2m \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 2t \\ r \end{smallmatrix}\right\}\delta_e(n-r), \tag{123}$$
$$\left\{\begin{smallmatrix} m \\ n \end{smallmatrix} \middle| \begin{smallmatrix} t \\ r \end{smallmatrix}\right\} = C_n^m\left(\begin{smallmatrix} m \\ n \end{smallmatrix} \middle| \begin{smallmatrix} t \\ r \end{smallmatrix}\right) + \left(\begin{smallmatrix} -m \\ n \end{smallmatrix} \middle| \begin{smallmatrix} t \\ r \end{smallmatrix}\right), \quad \left\{\begin{smallmatrix} m \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ r \end{smallmatrix}\right\} = 2C_n^m\left(\begin{smallmatrix} m \\ n \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ r \end{smallmatrix}\right).$$

To include all terms up to a_2, we retain A_1^0 as in (111), but replace (110) by

$$B_0^0 = a_0[1 + B_0^0\left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right) + B_0^0\left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right) + B_2^0\left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right)],$$
$$B_0^0 = a_2[1 + B_0^0\left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right) + B_2^0\left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right) + B_2^2\left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right)], \tag{124}$$
$$B_2^2 = a_2[B_0^0\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right\} + B_2^0\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right\} + B_2^2\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right\}],$$

where the symbols represent the lattice sums

$$\left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right) = H_0^0, \quad \left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right) = H_2^0, \quad \left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right) = H_2^2, \quad \left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right\} = 2H_2^2/4!,$$
$$\left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right) = \tfrac{1}{5}H_0^0 + \tfrac{2}{7}H_2^0 + \tfrac{18}{35}H_4^0 \equiv H_e,$$
$$\left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right) = -\tfrac{2}{7}H_2^2 + \tfrac{3}{35}H_4^2 = H_f, \quad \left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right\} = 2H_f/4!,$$
$$\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right\} = \tfrac{3}{35}H_4^4/4! + \tfrac{1}{5}H_0^0 - \tfrac{2}{7}H_2^0 + \tfrac{3}{35}H_4^0.$$

Suppressing self-coupling in B_2^2, we rewrite (122) as

$$B_0^0 = a_0(1 + B_0^0 W + B_2^0 X), \quad B_2^0 = a_2(1 + B_0^0 Y + B_2^0 Z),$$
$$B_2^2 = \mathcal{A}_2(B_0^0\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right\} + B_2^0\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right\}), \quad \mathcal{A}_2 = a_2/(1 - a_2\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right\}), \tag{125}$$
$$W = \left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right)\mathcal{A}_2\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right\}, \quad X = \left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 \\ 0 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right)\mathcal{A}_2\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right\},$$
$$Y = \left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right)\mathcal{A}_2\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right\} = X, \quad Z = \left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 2 \end{smallmatrix}\right)\mathcal{A}_2\left\{\begin{smallmatrix} 2 \\ 2 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right\}.$$

We obtain

$$B_0^0 = a_0[1 + a_2(X - Z)]/D, \quad B_2^0 = a_2[1 + a_0(Y - W)]/D,$$
$$D = 1 - a_0 W - a_2 Z + a_0 a_2(WZ - XY), \tag{126}$$

and B_2^2 follows by superposition.

Similarly, to include all terms to a_3, we replace (111) by the analog of (124) for n odd,

$$B_1^0 = a_1[1 + B_1^0\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right) + B_3^0\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 3 \end{smallmatrix}\right) + B_3^2\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 3 \end{smallmatrix}\right)],$$
$$B_3^0 = a_3[1 + B_1^0\left(\begin{smallmatrix} 0 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right) + B_3^0\left(\begin{smallmatrix} 0 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 3 \end{smallmatrix}\right) + B_3^2\left(\begin{smallmatrix} 0 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 3 \end{smallmatrix}\right)], \tag{127}$$
$$B_3^2 = a_3[B_1^0\left\{\begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right\} + B_3^0\left\{\begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 3 \end{smallmatrix}\right\} + B_3^2\left\{\begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 3 \end{smallmatrix}\right\}]$$
$$= \mathcal{A}_3[B_1^0\left\{\begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right\} + B_3^0\left\{\begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 0 \\ 3 \end{smallmatrix}\right\}], \quad \mathcal{A}_3 = a_3/(1 - a_3\left\{\begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \middle| \begin{smallmatrix} 2 \\ 3 \end{smallmatrix}\right\}),$$

from which we obtain corresponding closed forms by inspection of (125) and (126).

In particular, for the square cell ($b = d$) all H_n^2 terms

vanish. For this case, reverting to $A_n^0 = B_n^0$, we reduce (123) to

$$A_0^0 = a_0[1 + A_0^0(\begin{smallmatrix}0\\0\end{smallmatrix}) + A_2^0(\begin{smallmatrix}0\\2\end{smallmatrix})], \quad A_2^0 = a_2[1 + A_0^0(\begin{smallmatrix}0\\0\end{smallmatrix}) + A_2^0(\begin{smallmatrix}0\\2\end{smallmatrix})]. \tag{128}$$

In terms of self-coupling coefficients $\mathcal{A}_0$ and $\mathcal{A}_2$, we have

$$\begin{aligned} &A_0^0 = \mathcal{A}_0(1 + \mathcal{A}_2 H_2^0)/D, \quad A_2^0 = \mathcal{A}_2(1 + \mathcal{A}_0 H_2^0)/D, \\ &\mathcal{A}_0 = a_0/(1 - a_0 H_0^0), \quad \mathcal{A}_2 = a_2/(1 - a_2 H_g), \\ &D = 1 - \mathcal{A}_0 \mathcal{A}_2 (H_2^0)^2. \end{aligned} \tag{129}$$

These forms emphasize the symmetry of the monopole–quadrupole effects. Similarly, for dipole–octupole coupling, from (127),

$$\begin{aligned} &A_1^0 = a_1[1 + A_1^0(\begin{smallmatrix}0\\1\end{smallmatrix}) + A_3^0(\begin{smallmatrix}0\\1\end{smallmatrix})], \quad A_3^0 = a_3[1 + A_1^0(\begin{smallmatrix}0\\3\end{smallmatrix}) + A_3^0(\begin{smallmatrix}0\\3\end{smallmatrix})], \\ &(\begin{smallmatrix}0\\1\end{smallmatrix}\,|\,\begin{smallmatrix}0\\3\end{smallmatrix}) = \tfrac{3}{7}H_2^0 + \tfrac{4}{7}H_4^0 \equiv H_g, \\ &(\begin{smallmatrix}0\\3\end{smallmatrix}\,|\,\begin{smallmatrix}0\\3\end{smallmatrix}) = \tfrac{1}{7}H_0^0 + \tfrac{4}{21}H_2^0 + \tfrac{18}{77}H_4^0 + \tfrac{100}{231}H_6^0 \equiv H_h. \end{aligned} \tag{130}$$

In terms of self-coupling coefficients, $\mathcal{A}_1$ and $\mathcal{A}_3$,

$$\begin{aligned} &A_1^0 = \mathcal{A}_1(1 + \mathcal{A}_3 H_g)/D, \quad A_3^0 = \mathcal{A}_3(1 + \mathcal{A}_1 H_g)/D, \\ &\mathcal{A}_1 = a_1/(1 - a_1 H_a), \quad \mathcal{A}_3 = a_3/(1 - a_3 H_h), \\ &D = 1 - \mathcal{A}_1 \mathcal{A}_3 (H_g)^2. \end{aligned} \tag{131}$$

For detailed applications we rewrite the algebraic results for A_n^m in terms of the coefficients a_n' of the radiation-stripped amplitude g' discussed after (1:32). We have

$$g'(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = g(\hat{\mathbf{r}}, \hat{\mathbf{k}}) - \int g(\hat{\mathbf{r}}, \hat{\mathbf{r}}') g'(\hat{\mathbf{r}}', \hat{\mathbf{k}})\, d\Omega(\hat{\mathbf{r}}'), \tag{132}$$

where $\hat{\mathbf{r}}'$ is over the real unit sphere. Substituting the general form for spherically symmetric scatterers,

$$g(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = \sum_{nm} a_n (-1)^m Y_n^m(\hat{\mathbf{r}}) Y_n^{-m}(\hat{\mathbf{k}}) = g[a], \tag{133}$$

and its analog $g' = g[a']$ into the integral equation (132), we obtain

$$a_n' = \frac{a_n}{1 + a_n/(2n+1)} \tag{134}$$

and the inverse

$$a_n = \frac{a_n'}{1 - a_n'/(2n+1)}\,. \tag{135}$$

Corresponding to the a_n given after (7), we have $a_n' = i(2n+1) j_n / n_n$.

For lossless scatterers, from $-\mathrm{Re}g(\mathbf{r}, \mathbf{k}) = \int g(\hat{\mathbf{r}}, \hat{\mathbf{r}}') \times g^*(\hat{\mathbf{r}}', \hat{\mathbf{k}})\, d\Omega(\hat{\mathbf{r}}')/4\pi$ and (133), we obtain $-\mathrm{Re}a_n = |a_n|^2/(2n+1)$. Similarly, from $\mathrm{Re}g' = 0$, it follows that $-\mathrm{Re}a_n' = 0$. We now show that the role of δ_{n0} in the lattice function $\mathcal{G}_n^m$ of (26) is essentially to replace a_n by a_n' in A_n^m. The stripped coefficients show no radiative losses corresponding to omnidirectional scattering, and their use in A_n^m makes more evident that the only radiations losses (as determined by $\mathcal{G}_n^m - \delta_{n0}$) are along the propagating modes of the array. See analogous detailed discussion for the grating.

We convert (7) and (108) and all subsequent results stated in terms of a_n and $H_n^m = \mathcal{G}_n^m + i\mathcal{N}_n^m$ to the corresponding results in terms of a_n' and

$$H_n'^m = H_n^m + \delta_{n0} = \mathcal{G}_n'^m + i\mathcal{N}_n^m, \quad \mathcal{G}_n'^m = \sum_p 2C_{\nu\mu} Y_n^m(\hat{\mathbf{k}}_\nu). \tag{136}$$

Thus with

$$d_0(\begin{smallmatrix}-m;m\\n;n\end{smallmatrix}) H_0^0 = d_0(H_0'^0 - 1), \quad (\begin{smallmatrix}-m\\n\end{smallmatrix}\,|\,\begin{smallmatrix}t\\\tau\end{smallmatrix})' = \sum d_l(\begin{smallmatrix}-m;t\\n;\tau\end{smallmatrix}) H_l'^{t-m}$$

we rewrite (108) originally as

$$\begin{aligned} A_n^m &= (-1)^m a_n[Y_n^{-m} - A_n^m d_0(\begin{smallmatrix}-m;m\\n;n\end{smallmatrix}) + \sum A_\tau^t(\begin{smallmatrix}-m\\n\end{smallmatrix}\,|\,\begin{smallmatrix}t\\\tau\end{smallmatrix})'] \\ &= \left\{\frac{(-1)^m a_n}{1 + (-1)^m a_n d_0}\right\}[Y_n^{-m} + \sum A_\tau^t(\begin{smallmatrix}-m\\n\end{smallmatrix}\,|\,\begin{smallmatrix}t\\\tau\end{smallmatrix})']. \end{aligned} \tag{137}$$

To evaluate d_0, we consider the special case of (107) corresponding to $Y_n^{-m} Y_n^m$. If we integrate both sides of

$$P_n^{-m}(\zeta) P_n^m(\zeta) = \sum d_l(\begin{smallmatrix}-m;m\\n;m\end{smallmatrix}) P_l^0(\zeta)$$

over $\int_{-1}^{1} d\zeta$, then only the d_0 term survives, and we have

$$d_0(\begin{smallmatrix}-m;m\\n;m\end{smallmatrix}) = (-1)^m/(2n+1). \tag{138}$$

Using this value in (137), we identify the function in braces as a_n' of (134), and thereby reduce A_n^m to

$$A_n^m = (-1)^m a_n'[Y_n^{-m} + \sum A_\tau^t(\begin{smallmatrix}-m\\n\end{smallmatrix}\,|\,\begin{smallmatrix}t\\\tau\end{smallmatrix})'], \tag{139}$$

i. e., to the original form (108) in terms of the stripped functions. Similarly all the explicit results for A_n^m, in terms of a_n and H in (110)ff, hold equally in terms of a_n' and H'.

The results (110)–(131) for the coefficients A_n^m and the corresponding scattering amplitude G of (4) enable us to construct the associated transmission and reflection amplitudes of (1:15) and (1:16), i. e.,

$$T_\tau = 2C_\tau G(\hat{\mathbf{k}}_\tau) + \delta_{\tau 0}, \quad R_\tau = 2C_\tau G(\hat{\mathbf{k}}_\tau'), \quad C_\tau = \pi/k^2 b d\zeta_\tau \tag{140}$$

with $\tau = \tau(\nu, \mu)$, and $\hat{\mathbf{k}}_0$ suppressed in G.

We may also apply the results to the related problem of the corresponding array of protuberances on a rigid (+) or free (−) plane. The symmetry components of $2G$ with respect to reflection in the plane of the array provide the corresponding amplitudes for the bosses,

$$F_\tau^\pm = G(\hat{\mathbf{k}}_\tau) \pm G(\hat{\mathbf{k}}_\tau'), \quad \hat{\mathbf{k}}' = \hat{\mathbf{k}} - 2\zeta\hat{\mathbf{z}}. \tag{141}$$

For an incident wave $\pm\phi(\hat{\mathbf{k}}_0')$, the reflection amplitudes for the embossed plane equal

$$R_\tau^\pm = 2C_\tau[G(\hat{\mathbf{k}}_\tau) \pm G(\hat{\mathbf{k}}_\tau')] + \delta_{\tau 0} \tag{142}$$

as discussed in detail for the two-dimensional problem.[3] For a rigid base plane, we work with R^+; however, the bosses may be free or rigid or general.

The present closed form representations (110)–(131) in terms of H_n^m of (73) allow for more detailed development of the resonances for near-grazing modes than (1:37). However, since (1:39) suffices for the essentials, and since we have considered the additional details obtained from the closed form approximations of A for the analogous[3] two-dimensional problem, we restrict the sequel to the novel low-frequency coupling effects for small spacings.

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Low frequency coupling in the planar rectangular lattice*

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The solution for the three-dimensional problem of multiple scattering by a doubly periodic planar array of bounded obstacles is specialized to consider low frequency coupling effects for spheres. For all of the usual boundary conditions, we derive closed form approximations for the transmission and reflection amplitudes explicitly in terms of the physical parameters of the isolated scatterers, lattice spacings, and direction of incidence. The results are compared with those obtained earlier for the grating of parallel cylinders and for the periodic line (and planar random distribution) of spheres. We show, for example, that the pseudo-Brewster effects are anisotropic for the rectangular lattice cell, and that the leading effects of close packing for a square array of rigid spheres may be approximated by single scattering by an equivalent spheroid representing elongation in the plane of the array and contraction along the normal. For dense packing at very low frequencies, we obtain explicit closed form approximations including up to octupole–octupole coupling effects.

INTRODUCTION

In previous papers[1,2] we consider multiple scattering of waves by a doubly periodic planar array of obstacles. In the first[1] we emphasized the plane wave array-mode representations for the solution and for the multiple scattering amplitude, and investigated the resonances corresponding to near-grazing evanescent modes. In the second[2] we derived rapidly convergent representations of the spherical wave lattice sums that characterize the array, and obtained closed form approximations for the multiple scattered coefficients of small scatterers in terms of their single scattered values.

Now we consider the second major class of interaction effects which invalidate a single-scattering approximation: low frequency coupling of the multipole moments of the component scatterers. We take the obstacles to be spheres subject to the usual boundary or transition conditions; for concreteness, we use the terminology of small amplitude acoustics. We derive closed-from approximations for the corresponding transmitted and reflected fields (explicitly in terms of the physical parameters of the isolated scatterers, lattice spacings, and direction of incidence) and compare with earlier results for the grating of parallel cylinders, and for the periodic line (and random planar distribution) of spheres.

We show, for example, that the pseudo-Brewster effects are anisotropic for the rectangular lattice cell, and that the leading effects for a square array of rigid spheres are described in terms of a multiple scattering amplitude approximating the single scattering function for a spheroid elongated in the plane of the array and contracted along the normal. For dense packing at very low frequencies, we obtain explicit closed form approximations including up to octupole-octupole coupling effects.

For brevity we use the notation (1 : 9) to indicate Eq. (9) of Ref. 1, etc. We start by stating several results derived earlier[1,2] and then go directly to physical applications, and generalizations.

1. TRANSMISSION AND REFLECTION COEFFICIENTS

The radiation field for a plane wave $\phi(\hat{\mathbf{k}}) = \exp(i\mathbf{k}\cdot\mathbf{r})$ incident on a planar lattice of obstacles with spacings b and d (along x and y) small compared to wavelength is specified by the transmission and reflection amplitudes

$$T = 1 + 2CG, \quad R = 2CG', \quad C = \pi/k^2 bd\zeta. \tag{1}$$

Here $G = G(\hat{\mathbf{k}}, \hat{\mathbf{k}})$ is the forward multiple scattering amplitude for direction of incidence $\hat{\mathbf{k}} = \zeta\hat{\mathbf{z}} + \xi\hat{\mathbf{x}} + \eta\hat{\mathbf{y}} = \hat{\mathbf{z}}\cos\theta + (\hat{\mathbf{x}}\cos\varphi + \hat{\mathbf{y}}\sin\varphi)\sin\theta$; similarly, $G' = G(\hat{\mathbf{k}}', \hat{\mathbf{k}})$, with $\hat{\mathbf{k}}' = -\zeta\hat{\mathbf{z}} + \xi\hat{\mathbf{x}} + \eta\hat{\mathbf{y}}$ as the image of $\hat{\mathbf{k}}$ in $z = 0$ (the plane of the array). We have

$$G(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = \sum_{n,m} A_n^m(\hat{\mathbf{k}}) Y_n^m(\hat{\mathbf{r}}), \quad \sum = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \tag{2}$$

with the multiple scattered coefficients A_n^m expressed algebraically[2] in terms of their single scattered analogs, and in terms of the basic lattice sums $\mathcal{H}_n^m = \mathcal{J}_n^m + i\mathcal{N}_n^m = \mathcal{H}_n'^m + \delta_{n0}$ for the array.[1,2] For spherically symmetric obstacles, in terms of the coefficients a_n of the isolated scattering amplitude,

$$g(\hat{\mathbf{r}}, \hat{\mathbf{k}}) = \sum_{n,m} a_n(-1)^m Y_n^m(\hat{\mathbf{r}}) Y_n^{-m}(\hat{\mathbf{k}}),$$

$$a_n = \frac{a_n'}{1 - a_n'/(2n+1)}, \tag{3}$$

we considered the algebraic system $A = A[a, \mathcal{H}]$ as in (2:7) and (2:108), as well as the form, $A = A[a', \mathcal{H}']$ of (2:139), in terms of the radiation-stripped coefficients a' and the sums $\mathcal{H}'$. Now we specialize the closed form approximations for A_n^m and the rapidly converging representations for $\mathcal{H}$ developed earlier,[2] and construct explicit low-frequency practical approximations for T and R for the usual acoustic conditions[3] at the obstacles. In addition, we obtain more complete closed forms than before[2] in order to investigate higher-order multipole coupling at dense packing, and generalize some of the results to ellipsoids.

We also apply the results to the related problem of the corresponding array of protuberances on a rigid (+) or free (−) plane. For an incident wave $\pm\phi(\hat{\mathbf{k}}')$, the reflection amplitudes equal

$$\mathcal{R}_\pm = T \pm R = 1 + 2CF_\pm = (1 + Z_\pm)/(1 - Z_\pm), \quad F_\pm = G \pm G', \tag{4}$$

as discussed in detail for the two dimensional problem[4]; F_+ and F are the symmetrical and antisymmetrical com-

ponents of $2G$ for reflection in the plane of the array. In using (4) say, for a rigid base plane, we work with R_+; however, the bosses need not be rigid, but may correspond to other boundary conditions. The impedance $Z = CF/(1+CF)$ facilitates comparison with related results for the random distribution[5] (rough surface).

For the small spacings of present interest, the scattering theorems[1] for G are particularly simple. For lossless scatterers ($\mathrm{Re}a_n' = 0$),

$$-\mathrm{Re}G = C(|G|^2 + |G'|^2), \quad -\mathrm{Re}G' = 2CG'G^*, \tag{5}$$

or, equivalently,

$$|T|^2 + |R|^2 = 1, \quad \mathrm{Re}R^*T = 0, \quad |T \pm R| = 1. \tag{6}$$

Similarly,

$$-\mathrm{Re}F_\pm = C|F_\pm|^2, \quad Z_\pm = i|Z_\pm|\,\mathrm{sgn}Z_\pm, \quad |R_\pm|^2 = 1. \tag{7}$$

We use these forms as checks to insure the development of energy conserving approximations.

All cases we consider are based essentially on (2:139) in the form

$$A_n^m = (-1)^m a_n' \left[Y_n^{-m}(\hat{\mathbf{k}}) + \sum_{r,t} A_r^t \begin{pmatrix} -m & t \\ n & r \end{pmatrix}' \right],$$
$$\begin{pmatrix} -m & t \\ n & r \end{pmatrix}' = \sum_l d_l \begin{pmatrix} -m, & t \\ n, & r \end{pmatrix} H_l'^{t-m} \tag{8}$$

where the numbers d_l arise[6] in the expansion $Y_n^{-m}Y_n^t = \sum d_l Y_n^{t-m}$. For $n+r>1$, the largest terms of $\binom{m}{n}\binom{t}{r}$ are of order $k^{-2(n+r)-1}$. We begin by listing the long wavelength (small $k = 2\pi/\lambda$) approximations of the coefficients a_n' and of the lattice sums $H_m'^n$ that we require. Then we proceed directly to obtain explicit results for R and T.

A. Stripped coefficients

The leading terms of the following approximations are based on the small x values of the spherical Bessel and Newmann functions,

$$j_n(x) \approx \frac{x^n}{(2n+1)!!}, \quad n_n(x) \approx -\frac{(2n-1)!!}{x^{n+1}},$$
$$(2n-1)!! = \frac{(2n)!}{2^n n!} = 1\cdot 3\cdot 5\cdots(2n-1), \quad (\pm 1)!! = 1.$$

If the field ψ vanishes on the surface $r=a$, i.e., pressure release (free surface) scatterers, we have[3] $a_n' = i(2n+1)j_n(x)/h_n(x)$, $x = ka$:

$$a_0' \approx -ix(1+\tfrac{1}{3}x^2), \quad a_1' \approx -ix^3(1-\tfrac{3}{5}x^2), \quad a_n' \approx \frac{-ix^{2n+1}}{[(2n-1)!!]^2}. \tag{9}$$

The next term of a_n' (here, and in all subsequent illustrations) are of order x^{2n+2}. For rigid scatterers, $\partial_r\psi = \partial\psi/\partial r = 0$ at $r=a$ gives the same form for a_n' in terms of $\partial_x j_n$ and $\partial_x n_n$; consequently,

$$a_0' \approx -i\tfrac{1}{3}x^3(1-\tfrac{3}{5}x^2), \quad a_1' \approx i\tfrac{1}{2}x^3(1-\tfrac{3}{10}x^2),$$
$$a_n' \approx \frac{ix^{2n+1}n}{[(2n-1)!!]^2(n+1)}. \tag{10}$$

More generally, ψ is continuous and $\partial_r\psi$ is discontinuous at $r=a$, and the propagation constant differs from k for $r<a$. From (3:46) in terms of an inverse relative density parameter β and a compressibility parameter C, such that $(C/\beta)^{1/2} = \mu$ is the scatterer's relative index of refraction, we have

$$a_0' \approx -i\tfrac{1}{3}x^3(1-C), \quad a_1' \approx ix^3(1-\beta)/(2+\beta) = ix^3\mathcal{E},$$
$$a_n' \approx i\frac{x^{2n+1}(1-\beta)n}{[(2n-1)!!]^2(n+1+\beta)} = \frac{ix^{2n+1}\mathcal{E}_n}{[(2n-1)!!]^2}, \tag{11}$$

where the next terms in a_0' and a_1' are of order x^5. If $C=\beta=0$, then (11) reduces to (10). The monopole coefficient dominates for free surfaces or if the scatterers have the same density ($\beta=1$) as the embedding space, and the dipole dominates, if $C=1$. For rigid scatterers, or for the general case (11), the monopole and dipole terms are of the same order of magnitude. We also consider other scatterers in the course of the development, but the above shows the essentials of the dependence on the parameters.

B. Low frequency lattice sums

The original lattice sums (2:8) in terms of outgoing (h_n) spherical waves were slowly converging, but we developed alternative representations. In terms of the decomposition

$$H_n'^m = H_n^m + \delta_{n0} = \mathcal{J}_n'^m + i\mathcal{N}_n^m, \quad \mathcal{J}_n'^m = \mathcal{J}_n^m + \delta_{n0}, \quad n-m \text{ even}, \tag{12}$$

we obtain $\mathcal{J}'(j_n)$ from the one-mode case (2:27),

$$\mathcal{J}_n'^m = 2CY_n^m(\hat{\mathbf{k}}) = (2\pi/k^2bd\xi)P_n^m(\xi)\exp(im\varphi),$$
$$\xi = \cos\theta, \quad \eta/\xi = \tan\varphi. \tag{13}$$

For $\mathcal{N}(n_n)$, we work with small kd approximations based on the limiting values

$$\frac{-\mathcal{N}_{2n}^{2m}(kb)^{2n+1}}{(4n-1)!!(-1)^n P_{2n}^{2m}(0)} \to L_{2n}^{2m}(\rho),$$
$$\frac{-\mathcal{N}_{2n+1}^{2m+1}(kb)^{2n+1}}{(4n+1)!!(-1)^n P_{2n+1}^{2m+1}(0)} \to \xi_0 R_{2n+1}^{2m+1}(\rho) + i\eta_0 L_{2n+1}^{2m+1}(\rho), \tag{14}$$
$$P_{2n}^{2m}(0) = \frac{(2n+2m)!(-1)^{n-m}}{2^{2n}(n+m)!(n-m)!} = \frac{(2n+2m-1)!!(-1)^{n-m}}{2^{n-m}(n-m)!},$$
$$P_{2n+1}^{2m+1}(0) = (2n+2m+1)P_{2n}^{2m}(0)$$

where $\rho = d/b \geq 1$.

The $n=0$ terms were given in (2:79) and (2:80):

$$L_0^0 = -2\ln(4\pi/\gamma\rho) + 8\sum K_0(\alpha),$$
$$\gamma = 1.781\cdots, \quad \alpha = \nu t 2\pi\rho, \quad \sum = \sum_{\nu=1}^{\infty}\sum_{t=1}^{\infty}, \tag{15}$$
$$R_1^1 = -2\ln(4\pi/\gamma\rho) + 2 + 8\sum(K_0 - \alpha K_1),$$
$$I_1^1 = -2 + 8\sum \alpha K_1. \tag{16}$$

From (2:87),

$$L_2^0 = 2\zeta(3) + 4\zeta(2)\rho^{-2} - 4\sum(2\pi\nu)^2(K_0 - K_2),$$
$$L_2^2 = 2\zeta(3) - \tfrac{4}{3}\zeta(2)\rho^{-2} - \tfrac{4}{3}\sum(2\pi\nu)^2(3K_0 + K_2); \tag{17}$$

$$R_3^1 = 2\zeta(3) + \tfrac{4}{3}\zeta(2)\rho^{-2} - \tfrac{4}{3}\sum(2\pi\nu)^2(3K_0 - K_2),$$
$$I_3^1 = \tfrac{8}{3}\zeta(2)\rho^{-2} + \tfrac{8}{3}\sum(2\pi\nu)^2 K_2, \tag{18}$$
$$R_3^3 = 2\zeta(3) - \tfrac{4}{5}\zeta(2)\rho^{-2} - \tfrac{4}{15}\sum(2\pi\nu)^2(15K_0 + 3K_2 - 8\alpha K_1),$$

$$I_3^3 = -\tfrac{8}{15}\zeta(2)\rho^{-2} - \tfrac{2}{15}\sum(2\pi\nu)^2\alpha(15K_1 + K_3);$$

$$L_4^0 = 2\zeta(5) + \tfrac{8}{3}\zeta(4)\rho^{-4} + \tfrac{1}{9}\sum(2\pi\nu)^4(3K_0 - 4K_2 + K_4),$$
$$L_4^2 = 2\zeta(5) - \tfrac{8}{5}\zeta(4)\rho^{-4} + \tfrac{1}{15}\sum(2\pi\nu)^4(5K_0 - 4K_2 - K_4), \quad (19)$$
$$L_4^4 = 2\zeta(5) + \tfrac{8}{35}\zeta(4)\rho^{-4} + \tfrac{1}{105}\sum(2\pi\nu)^4(35K_0 + 28K_2 + K_4).$$

We also require L_6^{2m}, which we obtain from the general form (2:86)

$$L_6^{2m} = 2\zeta(7) + \frac{(-1)^m}{(5-2m)!!\,(5+2m)!!}\left(4(5!)\frac{\zeta(6)}{\rho^6} + \tfrac{1}{4}\sum(2\pi\nu)^6 S_6^{2m}\right),$$

$$S_6^0 = -10K_0 + 15K_2 - 6K_4 + K_6,$$
$$S_6^2 = 14K_0 - 17K_2 + 2K_4 + K_6,$$
$$S_6^4 = -42K_0 + 15K_2 + 26K_4 + K_6, \quad (20)$$
$$S_6^6 = 462K_0 + 495K_2 + 66K_4 + K_6.$$

From the results for $\rho \geq 1$ we can construct the values for $\rho < 1$ by using the interchange relations (2:91)

$$L_{2n}^{2m}(\rho^{-1}) = (-1)^m\rho^{2n+1}L_{2n}^{2m}(\rho),$$
$$R_{2n+1}^{2m+1}(\rho^{-1}) = (-1)^m\rho^{2n+1}I_{2n+1}^{2m+1}(\rho), \quad (21)$$

where we may replace ρ by ρ^{-1} throughout. For the square unit cell ($\rho = 1$), $L_{2n}^2(1) = L_{2n}^6(1) = L_{2n}^{2(2l+1)}(1) = 0$. We may construct the R's and I's from the L's by using (2:93), i. e., $R_{2n+1}^{2m+1} = \frac{1}{2}(L_{2n}^{2m} + L_{2n}^{2m+2})$ and $I_{2n+1}^{2m+1} = \frac{1}{2}(L_{2n}^{2m} - L_{2n}^{2m+2})$. From (2:86, 98) we write

$$L_{2n}^{2m} = Z_{2n}^{2m} + K_{2n}^{2m}, \quad Z_{2n}^{2m} = 2\zeta(2n+1) + (-1)^m D_{2n}^{2m}\zeta(2n)/\rho^{2n},$$
$$D_{2n}^{2m} = \frac{4(2n-1)!}{(2n-2m-1)!\,(2n+2m-1)!!}, \quad 0 \leq m \leq n, \quad (22)$$
$$D_{2n}^{2n+2} = -\frac{4(2n-1)!}{(4n+1)!!};$$

the exceptional case K_{2n}^{2n+2} follows most directly from (2:96), and the rest from (2:86). For $\rho \geq 1$, the infinite series in K_{2n}^{2m} are very rapidly converging. Numerical computations for $\rho = 1$ to 10 show that to 6 significant figures, we need at most 9 terms of the K-series; the largest number of terms are required for $\rho = 1$ and $2m = 2(2l+1)$, but if $\rho \geq 2, 3$ the series do not affect the first 2, 5 significant figures. For many practical purposes we may use the asymptotic form for the modified Hankel function, $K_n(x) \sim K(x) = e^{-x}(\pi/2x)^{1/2}$ and approximate the rapidly converging sums by the leading terms. If $K_n \sim K$ is adequate, then except for $m = n$, the K-series vanish in the L's; similarly, only R_{2n+1}^{2n+1} and I_{2n+1}^{2n+1} contain series in αK.

2. MONOPOLES

For pure monopoles, from (2:110),

$$G = A_0^0 = \frac{a_0}{1 - a_0\mathcal{H}_0} = \frac{a_0'}{1 - a_0'\mathcal{H}_0'} \equiv \mathcal{A}_0^0,$$
$$\mathcal{H}_0'^0 = 2C + i\mathcal{N}_0^0 \approx 2C - iL_0^0/kb \quad (23)$$

with $C = \pi/k^2bd\zeta$, and L_0^0 as in (15). For lossless scatterers, $\mathrm{Re}\,a_0' = 0$, we obtain $-\mathrm{Re}A_0^0 = 2C|A_0^0|^2$ as required by (5).

For the free surface case, we neglect all but the leading term of (9), i. e.,

$$R = T - 1 = 2CA_0^0 = \frac{-1}{1 - i\mathcal{L}},$$
$$\mathcal{L} = \frac{kd\zeta}{2\pi}\left(\frac{b}{a} + L_0^0\right) = \frac{kd\zeta}{2\pi}\left(\frac{b}{a} - 2\ln\frac{4\pi b}{\gamma d} + 8\sum K_0\right). \quad (24)$$

The contribution of K_0^0 is minor: Even for the worst case ($\rho = 1$), K_0^0 effects only the fourth significant figure. This can be seen from, e. g.,

$$\mathcal{L} \approx \frac{kd\zeta}{2\pi}\left(\frac{b}{a} - 3.908 + 2\ln\rho + \frac{4}{\rho^{1/2}}\exp(-2\pi\rho)\right),$$
$$\rho = \frac{d}{b} \geq 1, \quad e^{-2\pi} \approx 1.87\times10^{-3}.$$

For the compressible monopoles, from (11) with $\beta = 1$, we may neglect $\mathcal{N}_0^0$ and work with

$$2CA_0^0 \approx \frac{-iQ_0}{1 + iQ_0}, \quad Q_0 = 2Ca_0' = \frac{2\pi ka^3}{3bd\zeta}(1 - \mathcal{C}) = \frac{\mathcal{V}k}{2bd\zeta}(1 - \mathcal{C}), \quad (25)$$

where we introduced $\mathcal{V}$ for the volume of the scatterer. Equation (25) also holds for ellipsoids with $\mathcal{V} = 4\pi a_1a_2a_3/3$, provided that the semi-axes $a_i \ll \lambda$, etc.; similarly, for (24) with the radius a representing some appropriate length parameter of the scatterer. For either case the array becomes perfectly reflecting at grazing incidence, i. e., $R \to -1$ as $\zeta = \cos\theta \to 0$.

We may also use (23) for small resonant scatterers,

$$a_0' \approx -i(ka)^2\frac{\mathcal{T} + ka/3}{1 + \mathcal{T}ka}, \quad \mathcal{T} = \frac{\mathcal{C}}{\mu}\left(\cot\mu ka - \frac{1}{\mu ka}\right), \quad (26)$$

such that $g = a_0 = -1$ for the resonance condition $ka\mathcal{T} = -1$; if $ka\mu$ is also small, resonance occurs for $(ka)^2 \approx 3/\mathcal{C}$. Using (26) in (23) for $G = A_0^0$, we get the resonance value $G = -1/2C$, and consequently $R = 2CA_0^0 = -1$ and $T = 0$ for frequencies specified by

$$ka(\mathcal{T} - ka\mathcal{N}_0^0) = -1 + (ka)^2\mathcal{N}_0^0/3 \approx -1. \quad (27)$$

If $ka\mu$ is small, then

$$(ka)^2 \approx 3/\mathcal{C}(1 - ka\mathcal{N}_0^0) \approx 3/\mathcal{C}\left[1 - \frac{2a}{b}\left(\ln\frac{4\pi}{\gamma\rho} - 4\sum K_0\right)\right] \quad (28)$$

gives the frequency shift for resonance arising from coupling effects.

For the analogous boss problems of (4), we have $F_- = 0$ and $F_+ = 2G$. Thus

$$\mathcal{R}_- = 1, \quad \mathcal{R}_+ = 1 + 4CG = (1 + Z_+)/(1 - Z_+). \quad (29)$$

The reflection amplitude is unity for a free base surface, but not for a rigid base. Corresponding to the free monopoles of (24), we now have

$$\mathcal{R}_+ = (1 - i/\mathcal{L})/(1 + i/\mathcal{L}), \quad Z = -i/\mathcal{L} \quad (30)$$

and for the compressible monopoles of (25)

$$\mathcal{R}_+ = (1 - iQ)/(1 + iQ), \quad Z = -iQ. \quad (31)$$

More generally, to include the resonant monopoles, we use

$$\mathcal{R}_+ = 1 + 4CA_0^0 = \frac{1 + a_0'(2C - i\mathcal{N}_0^0)}{1 - a_0'(2C + i\mathcal{N}_0^0)} \qquad Z = \frac{2Ca_0'}{1 - ia_0'\mathcal{N}_0^0} \tag{32}$$

with a_0' as in (26). At resonance, we get $\mathcal{R} = -1$.

3. DIPOLES

For pure dipoles, corresponding to $\mathcal{C} = 1$ and a_1' of (11) dominant, we work with the symmetry components of (2:113) in the form

$$G = G_A + G_S = \tfrac{1}{2}F_- + \tfrac{1}{2}F_+, \qquad G' = -G_A + G_S. \tag{33}$$

We have

$$\begin{aligned} G_A &= \mathcal{A}_1^0\zeta^2 = a_1'\zeta^2/(1 - a_1'H_a'), \\ H_a' &= \tfrac{1}{3}(H_0'^0 + 2H_2^0) \approx 2C\zeta^2 - iL_2^0/(kb)^3, \end{aligned} \tag{34}$$

where we used $\mathcal{G}_2'^0 + 2\mathcal{G}_2^0 = 2C(1 + 2P_2^0)$ with $P_2^0 = (3\zeta^2 - 1)/2$, and neglected $\mathcal{N}_0^0$ compared to $\mathcal{N}_2^0$. Similarly, in terms of $\mathcal{G}_2^2(\pm\varphi) = 2CP_2^2(\zeta)\exp(\pm i2\varphi)$ with $P_2^2 = 3(1 - \zeta^2)$,

$$\begin{aligned} &G_s = a_1'(1 - \zeta^2)\,N/D, \\ &N = 1 - a_1'H_b' + (a_1'/12)[H_2^2(-\varphi)\exp(i2\varphi) + H_2^2(\varphi)\exp(-i2\varphi)], \\ &D = 1 - 2a_1'H_b' + (a_1')^2[(H_b')^2 - H_2^2(\varphi)H_2^2(-\varphi)/36], \\ &H_b' = \tfrac{1}{3}(H_0'^0 - H_2^0) \approx C(1 - \zeta^2) + iL_2^0/2(kb)^3, \\ &H_2^2(\pm\varphi) \approx 6C(1 - \zeta^2)\exp(\pm i2\varphi) + i9L_2^2/(kb)^3, \end{aligned} \tag{35}$$

where $\mathcal{N}_0^0$ was neglected compared to $\mathcal{N}_2^m$.

In terms of a_1' of (11),

$$G_A \approx \frac{a_1'\zeta^2}{V - iQ_1\zeta^2}, \quad Q_1 = i2Ca_1' \approx \frac{\pi ka^3 2\mathcal{E}}{bd\zeta}, \quad V = 1 - v, \qquad v = \frac{a_1'L_2^0}{i(kb)^3} \approx \frac{a^3}{b^3}\mathcal{E}L_2^0. \tag{36}$$

The K-sum in L_2^0 of (17) vanishes if the asymptotic form of K_l is used; more generally, to two significant figures, $L_2^0 \approx 2.4 + 6.6/\rho^2$. In reducing G_s, the $\mathcal{G}$ terms of N and of D cancel, and we obtain

$$\begin{aligned} &N = 1 + \tfrac{1}{2}v - \tfrac{1}{2}v'\cos 2\varphi, \\ &D = (1 + \tfrac{1}{2}v + \tfrac{1}{2}v')(1 + \tfrac{1}{2}v - \tfrac{1}{2}v') - iQ_1(1 - \zeta^2)\,N, \\ &v' = \frac{3a_1'L_2^2}{i(kb)^3} = \frac{a^3}{b^3}3\mathcal{E}L_2^2. \end{aligned} \tag{37}$$

Using $(1 - \zeta^2)\cos 2\varphi = \sin^2\theta(\cos^2\varphi - \sin^2\varphi) = \xi^2 - \eta^2$, etc., we write

$$G_s = \frac{a_1'(\xi^2 V_- + \eta^2 V_+)}{V_+V_- - iQ_1(\xi^2 V_- + \eta^2 V_+)}, \quad V_\pm = 1 + \tfrac{1}{2}v \pm \tfrac{1}{2}v'. \tag{38}$$

For the square cell, $L_2^2(1)$ of (17) vanishes, and v' drops out of the forms.

The approximations (36) and (38) are energy conserving forms. For lossless scatterers, from (36), we have $-\mathrm{Re}G_A = 2C|G_A|^2$; similarly, from (38) $-\mathrm{Re}G_s = 2C|G_s|^2$. In view of (33), these correspond to $-\mathrm{Re}F_\mp = C|F_\mp|^2$ in accord with the energy theorem (7).

We specify the direction of observation by ξ_r, η_r, ζ_r and combine (36) and (38) as

$$\frac{G}{a_1'} = \frac{\zeta_r\zeta}{V - iQ_1\zeta^2} + \frac{\xi_r\xi V_- + \eta_r\eta V_+}{V_+V_- - iQ_1(\xi^2 V_- + \eta^2 V_+)}, \tag{39}$$

where $Q_1 \propto k$, but the V's are independent of k. The cases involved in T and R correspond to $\zeta_r = \pm\zeta$, $\xi_r = \xi$, $\eta_r = \eta$; however, the present form facilitates various considerations.

Initially, we consider the low frequency limit. For $k \to 0$, we have $Q_1 \to 0$, and, consequently,

$$\begin{aligned} &\frac{G}{a_1'} \to \frac{\zeta_r\zeta}{1 - v} + \frac{\xi_r\xi}{1 + \frac{1}{2}v + \frac{1}{2}v'} + \frac{\eta_r\eta}{1 + \frac{1}{2}v - \frac{1}{2}v'}, \\ &G \approx ik^3a^3\,\frac{(1 - \beta)}{2 + \beta}\sum\frac{\zeta_{ri}\zeta_i}{V_i}, \end{aligned} \tag{40}$$

where ζ_i stands for ζ, ξ, η, and V_i for the respective denominators V, V_+, V_-. The analogous result for an isolated ellipsoid[8] with semi-axes a_i in the form (3:88), is

$$\begin{aligned} &g_e \approx ik^3a_1a_2a_3\,\frac{(1 - \beta)}{3}\sum\frac{\zeta_{ri}\zeta_i}{1 + (\beta - 1)q_i}, \quad \sum q_i = 1, \\ &q_i = (a_1a_2a_3/2)\int_0^\infty (a_i^2 + u)^{-1}[(a_1^2 + u)(a_2^2 + u)(a_3^2 + u)]^{-1/2}\,du. \end{aligned} \tag{41}$$

This approximation corresponds to the leading terms $g_e \approx \sum a_{1i}'\zeta_{ri}\zeta_i = g_e'$; for energy conservation, we replace a_{1i}' by $a_{1i} = a_{1i}'/(1 - \frac{1}{3}a_{1i}')$ as in (3:140).

We compare (40) to (41) for

$$\begin{aligned} &a_1a_2a_3 = a^3, \quad (2 + \beta)\,V_i = 3[1 + (\beta - 1)q_i], \\ &3q_i - 1 = \frac{2 + \beta}{\beta - 1}(V_i - 1) = -(V_i - 1)/\mathcal{E}. \end{aligned} \tag{42}$$

If we sum over i and use $\sum q_i = 1$, we require $\sum V_i = 3[3 + (\beta - 1)\sum q_i]/(2 + \beta) = 3$, as is fulfilled by the denominators V_i in (40). Thus at very low frequencies, the sphere of volume $V = 4\pi a^3/3$ in a rectangular lattice is equivalent to an isolated ellipsoid of volume V and semi-axes determined by (42). The analogous monopole term a_{e0}' for the ellipsoid in (3.38) is the same as a_0' in terms of V; consequently, the equal volume condition in (42) also insures that (25) corresponds to $A_0^0 \approx a_0' \approx a_{e0}'$.

For a nearly spherical ellipsoid we approximate q_i by using $a_i = a(1 + \epsilon_i)$ with $\epsilon_i \approx 0$. To first order in ϵ, we have, e.g., $q_1 = \frac{1}{3} + \frac{1}{15}(-4\epsilon_1 + 2\epsilon_2 + 2\epsilon_3)$, and similarly for the others; these approximations satisfy $\sum q_i = 1$. The equal volume condition requires $\sum\epsilon_i = 0$, and consequently $3q_i = 1 - 6\epsilon_i/5$. Substituting into (42), we obtain

$$\begin{aligned} &\epsilon_2 = \frac{5}{12}\frac{v + v'}{\mathcal{E}} = \frac{5}{12}\left(\frac{a}{b}\right)^3(L_2^0 + 3L_2^2) > 0, \\ &\epsilon_3 = \frac{5}{12}\frac{v - v'}{\mathcal{E}} = \frac{5}{12}\left(\frac{a}{b}\right)^3(L_2^0 - 3L_2^2) < \epsilon_2, \\ &\epsilon_1 = -\frac{5}{6}\frac{v}{\mathcal{E}} = -\frac{5}{6}\left(\frac{a}{b}\right)^3 L_2^0 = -(\epsilon_1 + \epsilon_2) < 0, \quad a_i = a(1 + \epsilon_i), \end{aligned} \tag{43}$$

where ϵ_3 changes sign at $\rho \approx 1.65$ (for which $L_2^0 \approx 3L_2^2 \approx 4.8$). We assume $\epsilon_3 > 0$ to facilitate discussion; thus $a_1 < a$ and $a_2 > a_3 > a$, i.e., the equivalent ellipsoid corresponds to flattening of the sphere along the array normal and to broadening in the plane of the array, the elongation being greatest perpendicular to the closest spaced lattice lines (the lines spaced $b < d$ apart along x). For the square cell,

$$\frac{G}{a_1'} \to \frac{\zeta_r\zeta}{V} + \frac{\xi_r\xi+\eta_r\eta}{V_0}, \quad V=1-v, \quad V_0=1+\tfrac{1}{2}v, \tag{44}$$

corresponds to an oblate spheroid with symmetry axis $a_1 < a_2 = a_3$ along the array normal,

$$a_2=a_3=a(1+\epsilon), \quad a_1=a(1-2\epsilon),$$
$$\epsilon=\frac{5}{12}\left(\frac{a}{b}\right)^3 L_2^0(1) \approx \frac{15}{4}\left(\frac{a}{b}\right)^3. \tag{45}$$

On the other hand, if $\rho \to \infty$ in (43) then $L_2^0 \to L_2^2 \to 2\zeta(3)$, and the general results reduce to those for a single periodic line along x, i. e., $a_1=a_3=a(1-\epsilon)$, $a_2=a(1+2\epsilon)$, $\epsilon=(5/3)(a/b)^3\zeta(3)$, which corresponds to a prolate sphere elongated along the axis of the line. See (4:143) for the analogous comparison of a circular cylinder in a grating with an isolated elliptic cylinder. These low frequency effects are independent of $\hat{\mathbf{k}}$, λ or β; the ϵ's depend only on scatterer radius and spacing.

For the square cell, from (39),

$$R=-iQ_1(V_0\cos^2\theta - V\sin^2\theta)/\mathit{\Delta}, \tag{46}$$
$$\mathit{\Delta}=(V-iQ_1\cos\theta)(V_0-iQ_1\sin^2\theta),$$

$$T=(VV_0+Q_1^2\cos^2\theta)/\mathit{\Delta}. \tag{47}$$

The reflection amplitude vanishes at the pseudo-Brewster's angle

$$\tan^2\theta_B=V_0/V=(1+\tfrac{1}{2}v)/(1-v)\approx 1+\tfrac{3}{2}v, \quad \theta_B\approx 45^0+\tfrac{3}{8}v \tag{48}$$

with v depending only on a/b and the relative density β^{-1}. Corresponding to $R_B=0$, the transmission amplitude is

$$T_B=(V+iQ_1\zeta_B^2)/(V-iQ_1\zeta_B^2). \tag{49}$$

For lossless scatterers, Q_1 is real; then $|T_B|^2=1$ as required. On the other hand, for grazing incidence, $\theta \to \pi/2$ in (46), we again obtain perfect reflection $|R|^2 \to 1$.

For the general rectangular lattice, from (39),

$$R=-iQ_1[\xi^2V_+V_- - V(\xi^2V_- + \eta^2V_+)]/\mathit{\Delta},$$
$$\mathit{\Delta}=(V-iQ_1\zeta^2)[V_+V_- - iQ_1(\xi^2V_- + \eta^2V_+)], \tag{50}$$
$$T=[VV_+V_- + Q^2\zeta^2(\xi^2V_- + \eta^2V_-)]/\mathit{\Delta}.$$

The reflection amplitude vanishes, and we again obtain T_B of (49), if

$$\zeta^2/V=(\xi_B^2/V_+)+(\eta_B^2/V_-) \tag{51}$$

corresponding to an anisotropic Brewster's effect. We have

$$\cot^2\theta_B=(V/V_+V_-)(V_-\cos^2\varphi + V_+\sin^2\varphi)$$
$$\approx 1-\tfrac{3}{2}v-\tfrac{1}{2}v'\cos 2\varphi,$$
$$\theta_B\approx 45^\circ+\tfrac{3}{8}v+\tfrac{1}{8}v'\cos 2\varphi \tag{52}$$

which indicates the essential effects of anisotropy. If $\varphi=0$ (incidence perpendicular to the longer spacing d), then $\tan^2\theta_B=V_+/V$, $\theta_B\approx 45^\circ+(3v+v')/8$; If $\varphi=\pi/2$ (incidence perpendicular to b), then $\tan^2\theta_B=V_-/V$, $\theta_B\approx 45^\circ+(3v-v')/8$. Thus zero reflection occurs at a larger angle with the normal for incidence perpendicular to the larger spacing if $\beta<1$.

For the analogous protuberances on free and rigid surfaces we have $F_-=2G_A$ of (36) and $F_+=2G_s$ of (38). The corresponding reflection amplitudes $R_\pm=(1+Z_\pm)/(1-Z_\pm)$ are given by

$$Z_-=iQ_1\zeta^2/V=a_1'2\pi\zeta/k^2bdV, \quad V=1-v=1-a_1'L_2^0/i(kb)^3,$$
$$a_1'=i(ka)^3(1-\beta)/(2+\beta), \tag{53}$$

$$Z_+=iQ_1[(\xi^2/V_+)+(\eta^2/V_-)], \quad V_\pm=1+\tfrac{1}{2}v\pm\tfrac{1}{2}v',$$
$$v'=3a_1'L_2^2/i(kb)^3. \tag{54}$$

For grazing incidence ($\zeta \to 0$) we have $Z_- \to 0$ and $Z_+ \to \infty$ (as shown before[5] for arbitrary scatterers); consequently, $R_- \to 1$ and $R_+ \to -1$.

For the square cell, $v'=0$, we obtain

$$F_-=\frac{2a_1'\cos^2\theta}{V-iQ_1\cos^2\theta}, \quad F_+=\frac{2a_1'\sin^2\theta}{V_0-iQ_1\sin^2\theta} \tag{55}$$

as well as the more symmetrical impedances

$$Z_-=iQ_1\cos^2\theta/V, \quad Z_+=iQ_1\sin^2\theta/V_0. \tag{56}$$

In terms of the corresponding symmetry components for an isolated scatterer, $f_\pm=g(\hat{\mathbf{r}},\hat{\mathbf{k}})\pm g(\hat{\mathbf{r}},\hat{\mathbf{k}}')$ (or, equivalently, the scattering amplitude for a single protuberance), we obtain functional equations $F[f]$ for the multiple scattered amplitude (and for the associated scattering coefficients) with no cross-coupling terms between the symmetry components.[4] Thus, we may generalize (55) directly to small spheroids with isolated scattering amplitudes determined by inspection of (41):

$$f_-=2a_{11}\zeta_r\zeta, \quad f_+=2a_{12}(\xi_r\xi+\eta_r\eta),$$
$$a_{1i}=\frac{a_{1i}'}{1-\frac{1}{3}a_{1i}'}, \quad a_{1i}'=\frac{ik^3a_1a_2^2(1-\beta)}{3[1+(\beta-1)q_i]}. \tag{57}$$

We obtain

$$F_-=\frac{2a_{11}'\cos^2\theta}{V_1-iQ_{11}\cos^2\theta}, \quad Q_{11}=-i2Ca_{11}'=\frac{2\pi a_{11}'}{(kb)^2i\zeta}, \tag{58}$$
$$V_1=1-v_1=1-\frac{a_{11}'L_2^0}{i(kb)^3}$$

$$F_+=\frac{2a_{12}'\sin^2\theta}{V_2-iQ_{12}\sin^2\theta}, \quad Q_{12}=-i2Ca_{12}', \tag{59}$$
$$V_2=1+\tfrac{1}{2}v_2, \quad v_2=\frac{a_{12}'L_2^0}{i(kb)^3}.$$

The functions $q_1=1-2q_2$ are given, e. g., in (3:91) and (3:93) for the elongated and flattened spheroid respectively. For the elongated near sphere we have

$$q_1=\frac{(1-e^2)}{e^3}\left(\tfrac{1}{2}\ln\frac{1+e}{1-e}-e\right), \quad e^2=1-(a_2/a_1)^2,$$
$$q_1\approx\tfrac{1}{3}-\tfrac{2}{15}e^2=\frac{1}{3}-\frac{2}{15}\frac{(a_1^2-a_2^2)}{a_1^2}, \quad a_1\gtrsim a_2, \tag{60}$$

and for the near needle

$$q_1\approx\frac{a_2^2}{a_1^2}\left(\ln\frac{2a_1}{a_2}-1\right), \quad a_1\gg a_2. \tag{61}$$

For the flattened near sphere,

$$q_1=e^{-2}-e^{-3}(1-e^2)^{1/2}\sin^{-1}e, \quad e^2=1-(a_1/a_2)^2,$$
$$q_1\approx\tfrac{1}{3}+\tfrac{2}{15}e^2=\tfrac{1}{3}+\tfrac{2}{15}\frac{(a_2^2-a_1^2)}{a_2^2}, \quad a_2\gtrsim a_1; \tag{62}$$

for the near disk

$$q_1 \approx 1 - \frac{\pi a_1}{2a_2} + \frac{2a_1^2}{a_2^2}, \quad a_1 \ll a_2. \tag{63}$$

We may obtain more complete results for ellipsoidal scatterers by using the general algebraic system (2:6) in terms of the isolated ellipsoid coefficients[9] a_{nm} and the present lattice sums H.

4. MONOPOLES PLUS DIPOLES

If the monopole and dipole terms of the isolated scatterer are comparable, then for arbitrary angles of incidence we work with G of (2:118). For normal incidence, the two different multipoles are uncoupled and G equals the sum of the $\zeta_0 = 1$ results for A_0^0 of (25) and G_A of (34). Thus

$$G = \frac{a_0'}{1 + iQ_0} + \frac{\zeta a_1'}{1 - iQ_1 - v} = G(\zeta), \quad G' = G(-\zeta). \tag{64}$$

For the penetrable scatterers of (11),

$$CF_+ = \frac{-iQp_0}{1 + iQp_0}, \quad CF_- = \frac{iQp_1}{1 - iQp_1 - v}, \quad Q = \frac{2\pi ka^3}{3bd} = \frac{4\pi^2 a^3}{3\lambda bd}, \tag{65}$$

$$p_0 = 1 - \mathcal{E}, \quad p_1 = \frac{3(1-\beta)}{2+\beta}$$

with corresponding $R = C(F_+ - F_-)$ and $T = 1 + C(F_+ + F_-)$. For the boss problem,

$$\mathcal{R}_+ = \frac{1 - iQp_0}{1 + iQp_0}, \quad \mathcal{R}_- = \frac{1 + iQp_1/(1-v)}{1 - iQp_1/(1-v)}, \tag{66}$$

$$v = \frac{a^3}{b^3}\frac{(1-\beta)}{(2+\beta)} L_2^0(\rho)$$

from which we may also construct $R = \frac{1}{2}(\mathcal{R}_+ - \mathcal{R}_-)$, $T = \frac{1}{2}(\mathcal{R}_+ + \mathcal{R}_-)$. In particular, for rigid scatterers ($\beta = C = 0$), we have $p_0 = 1$ and $p_1 = 3/2$. Thus for the embossed surface

$$\mathcal{R}_+ = \frac{1 - iQ}{1 + iQ}, \quad \mathcal{R}_- = \frac{1 - i3Q/2(1-v)}{1 + i3Q/2(1-v)}, \quad v = \frac{a^3}{b^3}\frac{L_2^0}{2} \tag{67}$$

and for the complete lattice,

$$R = \frac{-iQ}{1 + iQ} - \frac{i3Q/2}{1 - i3Q/2 - v}, \quad T = 1 - \frac{iQ}{1 + iQ} + \frac{i3Q/2}{1 - i3Q/2 - v}. \tag{68}$$

For lossless scatterers, these approximations satisfy $|\mathcal{R}_\pm|^2 = 1$ and $|T \pm R| = 1$ as required.

The expressions for R and T have the same forms as for the grating given in (4:129); for the two-dimensional case we had 2 instead of 3/2 and the corresponding Q and v equalled $Q_G = \pi^2 a^2/\lambda d$ and $v_G = \pi^2 a^2/d^2 3$. We now have $Q = Q_G 4a/3b$, and for the square array $v \approx v_G 4a/3b$. For comparison with the results for the periodic line, we note that the present

$$2CA_0^0 = -iQ/(1 + iQ), \quad 2CA_1^0 = i(3Q/2)/[1 - i3Q/2 - v] \tag{69}$$

are the same forms as in (7:131); there we had 3/4 instead of 3/2, and the corresponding Q and v equalled $Q_L \approx 4\pi^3 a^3/3\lambda^2 b$ and $v_L = (a/b)^3 \zeta(3) \approx 1.2(a/b)^3$, i. e., $Q = Q_L \lambda/\pi d$ and $v \approx v_L(1 + 3.3b^2/1.2d^2)$.

For pressure release scatterers, if we keep both monopole and dipole terms of (9), we supplement $2CA_0^0$ of (24) with (34) in terms of $a_1' = -i(ka)^3$, i. e., with the smaller coefficient

$$2CA_1^0 \approx -i3Q/(1 + i3Q + 2v) \tag{70}$$

which differs from the corresponding result for the periodic line (7:134) in terms of Q_L and v_L in containing 3 instead of 3/2. Although this coefficient is negligible compared to $2CA_0^0$, it provides the leading departure from unity for reflection from the corresponding protuberances on a free surface. Thus instead of $\mathcal{R}_- = 1$ of (29) obtained for the pure monopoles, we now have

$$\mathcal{R}_- = \frac{1 + 2v - i3Q}{1 + 2v + i3Q}. \tag{71}$$

From this expression we get the corresponding impedance Z_- for reflection from an embossed pressure release surface and, similarly, Z_+ of $\mathcal{R}_+$ of (67) provides the mate for an entirely rigid surface. For these homogeneous surfaces we have

$$Z_- = -i3Q/(1 + 2v), \quad Z_+ = -iQ, \tag{72}$$

which we compare with the imaginary parts of the analogous expressions in (5:86) for the corresponding random distributions used to model rough surfaces. (The real parts of the earlier Z's correspond to incoherent scattering, and are therefore absent for the present periodic array.) Except for the dipole packing factor $1 + 2v$ in (72) the results are the same: The earlier function $Q_R = \nu 2\pi ka^3/3$ with ν as the number of scatterers in unit area gives identical values as Q of (65), since $db = 1/\nu$ is the area of unit cell of the periodic array.

For arbitrary angle of incidence, if we neglect Q^2 and smaller terms in the numerators and denominators of the individual coefficients $2CA_n^m$ obtained from (2:116), then

$$G \approx \frac{a_0'}{1 + iQ_0} + \frac{a_1'\zeta_r\zeta}{V - iQ_1\zeta^2} + \frac{a_1'(\xi^2 V_- + \eta^2 V_+)}{V_+ V_- - iQ_1(\xi^2 V_- + \eta^2 V_+)} \tag{73}$$

in terms of the symbols given in (25) and (39). This approximation neglects monopole-dipole coupling effects and is merely a superposition of the results we have already discussed.

In particular, for the homogeneous reflection problems, the pressure release surface is specified by

$$CF_- = \frac{-i3Q\zeta}{1 + i3Q\zeta + 2v}, \quad Q = \frac{2\pi ka^3}{3bd} \tag{74}$$

and the rigid surface by

$$CF_+ = \frac{-iQ/\zeta}{1 + iQ/\zeta} + \frac{i(3Q/2\zeta)[(\xi^2/V_+) + (\eta^2/V_-)]}{1 - i(3Q/2\zeta)[(\xi^2/V_+) + (\eta^2/V_-)]}. \tag{75}$$

For the square array, instead of (72), now

$$Z_- = \frac{-i3Q\zeta}{1 + 2v}, \quad Z_+ = -\frac{iQ}{\zeta}\left(1 + \frac{3\sin^2\theta}{2(1 + v/2)}\right) \tag{76}$$

where we dropped Q^2 in Z_+. Except for the packing factors in v these are the same as the imaginary parts of (5:86) for the corresponding random distributions.

The sum of (25) and (47) is the corresponding transmission amplitude for the full array, and similarly (25) plus (46) is the reflection amplitude. To first order

in Q in the numerator, for the square cell in the notation of (65),

$$R \approx -i(Q/\zeta)[pVV_0 + p_1(V_0\cos^2\theta - V\sin^2\theta)]/D,$$
$$D = (1+iQ_0)(V - iQ_1\cos^2\theta)(V_0 - iQ_1\sin^2\theta) \qquad (77)$$
$$\approx VV_0 + [p_0 - p_1(V_0\cos^2\theta + V\sin^2\theta)]iQ/\zeta.$$

For the single scattering approximation, R vanishes when $\cos 2\theta_B = -p_0/p_1$, e.g., for rigid scatterers, when $\cos 2\theta = -2/3$. Now, however, the Brewster angle depends on v through $V = 1 - v$ and $V_0 = 1 + v/2$, i.e.,

$$\cos 2\theta_B \approx -(p_0/p_1)(1 - v/4) + 3v/4 \qquad (78)$$

which reduces to $\cos 2\theta_B \approx -\frac{2}{3} - \frac{7}{12}v$ for rigid scatterers.

To include monopole-dipole coupling effects, from (2:118),

$$G = G_1 + G_0(1+p)^2/D, \quad p = -\tfrac{1}{2}[C(-\varphi)e^{i\varphi} + C(\varphi)e^{-i\varphi}]\sin\theta,$$
$$D = 1 + \tfrac{1}{2}G_0[H_1^1(\varphi)C(-\varphi) + H_1^1(-\varphi)C(\varphi)], \qquad (79)$$
$$C(\varphi) = -(a_1'/D)[H_1^1(\varphi)(1 - a_1'H_b') + a_1'H_2^2(\varphi)H_1^1(-\varphi)/6],$$

where G_1 is the dipole form of Sec. 3, and $G_0 = A_0^0$ is the monopole coefficient of Sec. 2. For the general scatterers in (11), we neglect N_0^0 and specify G_0 by (25), and $G_1 = G_A + G_s$ by (39). Similarly, if we neglect $N_1' \propto k^{-1}$ to obtain $H_1^1(\pm\varphi) \approx g_1^1(\pm\varphi) + 2CP_1^1(\zeta)e^{\pm i\varphi}$ with $P_1^1 = \sin\theta$, then

$$D \approx 1 + CG_0\sin\theta[e^{i\varphi}C(-\varphi) + e^{-i\varphi}C(\varphi)] = 1 - MP,$$
$$M = 2CG_0, \qquad (80)$$

and

$$C(\varphi) \approx -(a_1'/D)2C\sin\theta[e^{i\varphi}(1 - a_1'H_b') + e^{-i\varphi}H_2^2(\varphi)/6];$$

consequently,

$$p \approx (2Ca_1'\sin^2\theta)N/D = 2CG_s = CF_+ \qquad (81)$$

with G_s as in (38). Thus, we may write

$$2CG \approx 2CG_A + P + M(1+P)^2/(1 - MP) = S_A + S_s = S \qquad (82)$$

with $S_A = 2CG_A = CF_-$ as the asymetrical component in terms of G_A of (36). If we neglect monopole-dipole interactions, we obtain $S \approx S_A + P + M = 2C(G_0 + G_1)$ of (73). Since $M \propto Ca_0'$ and $P \propto Ca_1'$ are of order k, the first interaction term MP is of order k^2 as compared to the leading quadrupole term $Ca_2' \propto k^3$.

A simple way to construct (82) once we have obtained M for pure monopoles, and P for the symmetric part of pure dipoles, is to consider the system appropriate to coupling solely between M and P, i.e.,

$$S_s = M + P, \quad M = M(1+P), \quad P = P(1+M). \qquad (83)$$

Here the total monopole response M consists of two terms corresponding to multiple scattering by coupled monopoles (M) of essentially two exciting fields, the incident wave (represented by 1) and the total symmetrical dipole response P. Similarly, P is the coupled dipole factor (P) times the incident wave plus total monopole response M. Solving (83) we obtain

$$M = \frac{M(1+P)}{1 - MP}, \quad P = \frac{P(1+M)}{1 - MP},$$
$$S_s = \frac{M + P + 2MP}{1 - MP} = M + P + \frac{MP(2 + M + P)}{1 - MP}, \qquad (84)$$

as well as the less symmetrical form in (82).

We may use (82) to derive more complete versions of (73) ff, but as they stand they show the essentials.

5. HIGHER ORDER PACKING EFFECTS

For normal incidence $\hat{\mathbf{k}} = \hat{\mathbf{z}}$, we have $P_n^m(\pm 1) = (\pm 1)^n\delta_{m0}$. From (2), we require only

$$G = \sum_{n=0}^{\infty} A_n^0, \quad G' = \sum_{n=0}^{\infty} A_n^0(-1)^n, \qquad (85)$$

with A_n^0 determined by A_n^m as in (8) expressed in terms of a_n' and H' [i.e., although only A_n^0 appears in (86), these are in general coupled by the A_n^m, $m \neq 0$]. All lattice sums except H_{2n}^{2m} vanish, and (8) reduces to (2:119) in terms of a_n', H':

$$A_n^{2m} = a_n'[\delta_{m0} + \sum A_r^{2t}\left(\begin{smallmatrix} -2m & 2t \\ n & r \end{smallmatrix}\right)'\delta_e(n-r)] \qquad (86)$$

where $\delta_e(n-r)$ means that $n-r$ is even. Thus the system consists of two uncoupled sets corresponding to even or odd values of n.

Initially we consider the square cell $\rho = 1$; then only the sums H_{2n}^{4m} are nonvanishing and the results are relatively simple. To include up to octupole-octupole coupling effects, we use (2:128) in the form

$$A_0^0 = a_0'(1 + A_0^0H_0'^0 + A_2^0H_2^0), \quad A_2^0 = a_2'(1 + A_0^0H_2^0 + A_2^0H_e),$$
$$H_0'^0 = \left(\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right)', \quad H_2^0 = \left(\begin{smallmatrix} 0 & 0 \\ 2 & 0 \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 & 0 \\ 2 & 0 \end{smallmatrix}\right), \qquad (87)$$
$$H_e' = \left(\begin{smallmatrix} 0 & 0 \\ 2 & 0 \end{smallmatrix}\right)' = \tfrac{1}{5}H_0'^0 + \tfrac{2}{7}H_2^0 + \tfrac{18}{35}H_4^0,$$

and, similarly, from (2:130),

$$A_1^0 = a_1'(1 + A_1^0H_a' + A_3^0H_g), \quad A_3^0 = a_3'(1 + A_1^0H_g + A_3^0H_h'),$$
$$H_a' = \left(\begin{smallmatrix} 0 & 0 \\ 1 & 0 \end{smallmatrix}\right)' = \tfrac{1}{3}H_0'^0 + \tfrac{2}{3}H_2^0, \quad H_g' = \left(\begin{smallmatrix} 0 & 0 \\ 1 & 3 \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 & 0 \\ 3 & 1 \end{smallmatrix}\right) = \tfrac{3}{7}H_2^0 + \tfrac{4}{7}H_4^0, \qquad (88)$$
$$H_h' = \left(\begin{smallmatrix} 0 & 0 \\ 3 & 3 \end{smallmatrix}\right)' = \tfrac{1}{7}H_0'^0 + \tfrac{4}{21}H_2^0 + \tfrac{18}{77}H_4^0 + \tfrac{100}{231}H_6^0.$$

The first pair takes into account all monopole-monopole, monopole-quadrupole, and quadrupole-quadrupole interactions. Explicitly,

$$A_0^0 = a_0'(1 - a_2'H_e)/D_{02}, \quad A_2^0 = a_2'(1 - a_0H_0'^0)/D_{02},$$
$$D_{02} = (1 - a_0'H_0'^0)(1 - a_2'H_e') - a_0'a_2'(H_2^0)^2. \qquad (89)$$

Similarly, for the dipole and octupole effects,

$$A_1^0 = a_1'(1 - a_3'H_h')/D_{13}, \quad A_3^0 = a_3'H_a')/D_{13},$$
$$D_{13} = (1 - a_1'H_a')(1 - a_3'H_h') - a_1'a_3'(H_g)^2. \qquad (90)$$

These forms may be applied for numerical computations for all kd by using the complete H's of (2:73) and the complete a_n' of (3:46). However, we specialize them to determine the higher order low frequency closed packing effects.

For the pressure release scatterers as in (9), we retain only

$$A_0^0 = \frac{a_0'}{1 - a_0'H_0'^0 - M}, \quad M = \frac{a_0'a_2'(H_2^0)^2}{1 - a_2'H_e'} \qquad (91)$$

which differs from (23) by containing M. For $k \approx 0$, we have

$$M \approx \frac{ikar^5 4\pi/3 + r^6(L_2^0)^2/4}{1 + r^5L_4^0 9/4} \to \frac{r^6(L_2^0)^2/4}{1 + r^5L_4^0 9/4} = M_0,$$

$$r=a/b,\quad L_2^0(1)\approx 9.03,\quad L_4^0(1)\approx 5.09, \tag{92}$$

in terms of $L_2^0(1)$ of (17) and $L_4^0(1)$ of (19). Since $\mathcal{N}_0$, the limit for $k\to 0$, is a frequency-independent packing factor, its inclusion in (24) does not alter the original form, i. e.,

$$R=T-1=-1/(1-i\mathcal{L}'),\quad \mathcal{L}'=\frac{kb}{2\pi}\left(\frac{b}{a}(1-\mathcal{N}_0)+L_0^0\right),$$

$$L_0^0(1)\approx -3.90 \tag{93}$$

with the term in b/a decreased by the closer packing. Similarly, for the resonant scatterers, we replace $\mathcal{N}_0^0$ of (27), (28), and (32) by $\mathcal{N}_0^0+\mathcal{N}_0/ka$.

For the general scatterers of (11), or the rigid scatterers of (10), both a_0' and a_1' are of order k^3, and we retain A_1^0 as well as A_0^0. For these cases, $\mathcal{N}$ of (91) is of order k^2, and is negligible compared to $\mathcal{N}_0^0$ which we dropped to obtain (25). Thus.

$$A_0^0/a_0'\to 1,\quad k\to 0, \tag{94}$$

and the monopole terms shows no frequency independent packing effects.

The situation is quite different for the dipole coefficient. From (90),

$$A_1^0/a_1'=[1-a_1'\mathcal{H}_a'-\mathcal{M}']^{-1},\quad \mathcal{M}'=a_1'a_3'(\mathcal{H}_g)^2/(1-a_3'\mathcal{H}_h') \tag{95}$$

with

$$a_1'\mathcal{H}_a'\approx a_1'i2\mathcal{N}_2^0/3\to r^3L_2^0\mathcal{E}_1=r^3d_1=v,\quad \mathcal{E}_1=\mathcal{E}=\frac{1-\beta}{2+\beta} \tag{96}$$

as in (36). Similarly

$$\mathcal{M}'\approx\frac{a_1'a_3'(i\mathcal{N}_4^0 4/7)^2}{1-a_3'i\mathcal{N}_6^0(100/231)}\to\frac{r^{10}\mathcal{E}_1\mathcal{E}_3(L_4^0 3/2)^2}{1-r^7\mathcal{E}_3L_6^0 25/4}=\frac{r^{10}d_2}{1-r^7d_3}=\mathcal{M}_1,$$

$$\mathcal{E}_3=\frac{3(1-\beta)}{4+\beta},\quad L_6^0\approx 4.42. \tag{97}$$

Thus

$$A_1^0/a_1'\to S=[1-v-\mathcal{M}_1]^{-1}=\frac{1-r^7d_3}{1-r^3d_1-r^7d_3-r^{10}d_4},$$

$$d_4=d_2-d_1d_3, \tag{98}$$

where v corresponds to the dipole-dipole coupling as before in (36), and $\mathcal{M}_1$ to the dipole-octupole coupling effects. For rigid scatterers, $\mathcal{E}_1=\frac{1}{2}$ and $\mathcal{E}=\frac{3}{4}$.

Although we could expand S in powers of r, or work with the expansion

$$S^{-1}\approx 1-r^3d_1-r^{10}d_2+r^{17}d_2d_3, \tag{99}$$

we expect the closed form to be more accurate (as indicated before for the analogous problem of the grating[4]). The form for S^{-1} as a polynomial in r is the same as that obtained by Rayleigh[10] for the related problem of the three-dimensional cubical lattice of spheres; however, the numerical coefficients are different. (In a subsequent paper we consider the three-dimensional lattice and discuss the interrelations of the coefficients.)

The generalization to the rectangular lattice is provided by (2:123) ff. In particular, to obtain the analogous form of (96) for anisotropic packing effects, we use (2:127) in the matrix equation

$$(I-\alpha H)A=a,\quad I=(\delta_{ij}),$$

$$\alpha=(\alpha_{ii}\delta_{ij}),\quad \alpha_{11}=a_1',\quad \alpha_{22}=\alpha_{33}=a_3', \tag{100}$$

$$A=[A_{i1}]=[A_1^0,A_3^0,A_3^2+A_3^{-2}/5!],\quad a=[a_{i1}]=[a_1',a_3',0].$$

Here $H=(H_{ij})$ is the matrix whose elements are the sets of lattice sums

$$H_{11}=\left(\begin{smallmatrix}0\\1\end{smallmatrix}\middle|\begin{smallmatrix}0\\1\end{smallmatrix}\right)'=\mathcal{H}_a'\approx\tfrac{2}{3}\mathcal{H}_2^0,\quad H_{12}=H_{21}=\left(\begin{smallmatrix}0\\1\end{smallmatrix}\middle|\begin{smallmatrix}0\\3\end{smallmatrix}\right)=\mathcal{H}_g\approx\tfrac{4}{7}\mathcal{H}_4^0,$$

$$H_{22}=\left(\begin{smallmatrix}0\\3\end{smallmatrix}\middle|\begin{smallmatrix}0\\3\end{smallmatrix}\right)'=\mathcal{H}_h'\approx\tfrac{100}{231}\mathcal{H}_6^0,\quad H_{13}=(5!/2)H_{31}\approx\left(\begin{smallmatrix}0\\1\end{smallmatrix}\middle|\begin{smallmatrix}2\\3\end{smallmatrix}\right)\approx\tfrac{2}{7}\mathcal{H}_4^2,$$

$$H_{23}=(5!/2)H_{32}=\left(\begin{smallmatrix}0\\3\end{smallmatrix}\middle|\begin{smallmatrix}2\\3\end{smallmatrix}\right)\approx\tfrac{60}{7}\mathcal{H}_6^2, \tag{101}$$

$$H_{33}=\left(\begin{smallmatrix}2\\3\end{smallmatrix}\middle|\begin{smallmatrix}2\\3\end{smallmatrix}\right)(1/5!)+\left(\begin{smallmatrix}-2\\2\end{smallmatrix}\middle|\begin{smallmatrix}2\\3\end{smallmatrix}\right)\approx\tfrac{10}{231}[(1/5!)\mathcal{H}_6^4+3\mathcal{H}_6^0]$$

We kept only the largest value of $n+r$ for a given entry with the understanding that we use $\mathcal{H}\approx i\mathcal{N}$. Solving for A_1^0, we write

$$A_1^0=(M_{11}a_1'+M_{21}a_3')/\Delta \tag{102}$$

with Δ as the determinant of $(I-\alpha H)$ and M_{ij} as the corresponding minors. We see that M_{11}, M_{21}, and Δ are of order k^0, and since a_3'/a_1' is of order k^2 we obtain

$$A_1^0/a_1'\to M_{11}/\Delta=S,\quad k\to 0, \tag{103}$$

where M_{11} and Δ now represent the limiting values. Thus, we require only the low frequency limits of the first minor and of the determinant of the system [and this holds even if we include a_5', etc. in the n-odd system of (86)].

Corresponding to (101), we obtain

$$S=\frac{1-r^7c_1-r^{14}c_2}{1-r^3c_3-r^7c_1-r^{10}c_4-r^{14}c_2-r^{17}c_5},\quad r=a/b \tag{104}$$

where the numbers $c_n(\rho)$ will be given directly. The expansion

$$S^{-1}\approx 1-r^3c_3-r^{10}(c_4+c_3c_1)-r^{17}(c_5+c_4c_1+c_3c_2+c_3c_1^2) \tag{105}$$

contains no terms in r^7 or r^{14}.

Using braces to indicate the limit for $k\to 0$, we construct the c_n as follows:

$$c_3=\{a_1H_{11}/r^3\}=\mathcal{E}_1L_2^0,$$

$$c_1=\{a_3(H_{22}+H_{33})/r^7\}=\mathcal{E}_3(65L_6^0+63L_6^4)/8,$$

$$c_2=\{(a_3)^2(H_{23}H_{32}-H_{22}H_{33})/r^{14}\}$$

$$=3(\mathcal{E}_3/4)^2[(3465L_6^2)^2/5-L_6^0(21L_6^4+5L_6^0)25/2],$$

$$c_4=\{a_1a_3[H_{12}H_{21}+H_{13}H_{31}-H_{11}(H_{22}+H_{33})]/r^{10}\}$$

$$=(\mathcal{E}_1\mathcal{E}_3/4)[9(L_4^0)^2+15(L_4^2)^2-L_2^0(65L_6^0+63L_6^4)/2], \tag{106}$$

$$c_5=\{a_1a_3^2[(H_{11}H_{22}-H_{12}H_{21})H_{33}+2H_{12}H_{13}H_{32}-H_{11}H_{23}H_{32}$$

$$-H_{22}H_{13}H_{31}]/r^{17}\}$$

$$=\mathcal{E}_1(\mathcal{E}_3)^2(3/32)[25L_2^0L_6^0-9(L_4^0)^2](5L_6^0+21L_6^4)$$

$$+\mathcal{E}_1(\mathcal{E}_3)^2(15/16)[6(693)L_4^0L_4^2L_6^2-(693)^2L_2^0(L_6^2)^2$$

$$-25L_6^0(L_4^2)^2].$$

For the square array, $L_n^2(1)=0$; then $1-r^7\mathcal{E}_3(3/8)(5L_6^0$

$+21L_6^4$) factors out of both numerator and denominator of (104), and the result reduces to (98) as required. The numbers $L_n^m(\rho)$ for (106) are given in (17)—(20). If we may use the asymptotic form $K_n(\alpha) \sim K(\alpha)$, then all the K-sums vanish and $L_{2n}^{2m} \sim Z_{2n}^{2m}$ as in (22). If $\rho \to \infty$, then $L_{2n}^{2m} \to 2\zeta(2n+1)$, and the results reduce to those for a single periodic line along x.

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Reversible dynamics in a proposition-state structure

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We propose an intrinsic definition of reversible dynamical evolution of a physical system based on a unified formulation of the principle of superposition within an axiomatic approach to quantum mechanics.

1. INTRODUCTION

The fundamental role played by the superposition principle in physics and its distinguishing properties in classical and quantum theories are well known. Recently, several possible definitions of this principle have been proposed within the axiomatic approaches to quantum mechanics,[1–5] some of which have the advantage of providing a unified formulation of both the quantum and classical concepts of superposition.[2–5]

In Ref. 1 a formulation in terms of atomic propositions has been given, which shows that the quantum superposition principle is in fact a consequence of the non-Boolean structure of the proposition system. This has also been emphasized in Refs. 2 and 3, in which the superposition principle has been given a unified formulation in terms of the states of the logic. Specifically, it was shown, for example, in Ref. 3 that if a superposition principle holds, then the quantum logic is a complete atomic lattice, and if the latter is Boolean, then the only nontrivial superpositions are the statistical mixtures of states.

In Ref. 4 a treatment of the facial aspect of the superposition principle has been given within the framework of algebraic quantum theory. The formulation contained therein is shown to satisfy the definition of Ref. 2 when applied to the logic of decision effects.[6]

In Ref. 5 we proposed a formulation of the superposition principle which is based on the concept of maximal state in a proposition-state structure (pss). This formulation has been given in terms of principal ideals of the logic,[7] and it can be shown to be equivalent to the definition of Ref. 2. However, in our scheme, additivity of states has not been assumed.

In this note, the superposition principle is employed in order to give an intrinsic definition of reversible dynamics within a pss scheme. Precisely, we introduce the dynamics in terms of a one parameter group of permutations of the states preserving superposition and complementation. Our main result is the proof that these conditions univocally define a corresponding one parameter group of automorphisms of the lattice of propositions in such a way that the standard equivalence between the Schrödinger and Heisenberg pictures can be made to hold (Sec. 3). The proof is based on the existence of a natural closure operation on the subsets of states, which is discussed in Sec. 2. In the Hilbert model, which is a pss by the Gleason theorem, one recovers the standard evolution in terms of a one parameter unitary group using the Kadison–Sirugue theorem (Sec. 4). The generalization of the dynamical scheme to include the description of irreversible processes will be the object of a future paper.

2. A CLOSURE OPERATION

Let L be a complete orthocomplemented lattice. By an automorphism of L we mean a bijection $\mu: L \to L$ such that (i) $a \leq b \Leftrightarrow \mu(a) \leq \mu(b)$ and (ii) $\mu(a') = \mu(a)'$, where a' denotes the complement of a. Then, μ^{-1} is also an automorphism and if $\{a_\alpha\}$ is any family of elements of L, $\mu(\bigwedge_\alpha a_\alpha) = \bigwedge_\alpha \mu(a_\alpha)$ and $\mu(\bigvee_\alpha a_\alpha) = \bigvee_\alpha \mu(a_\alpha)$ (Ref. 1, Lemma 9.4.1).

Definition 2.1[5]: A *proposition-state structure* (pss) is a pair (L, S), where L is a complete, orthocomplemented, atomic lattice and S is a family of maps s: $L \to [0, 1]$ such that:

A1. $a, b \in L$, $a \leq b \Leftrightarrow S_1(a) \subset S_1(b)$, where $S_1(a) = \{s \mid s \in S, s(a) = 1\}$.

A2. $S_1(a) = S_0(a')$ $\forall\, a \in L$, where $S_0(a) = \{s \mid s \in S, s(a) = 0\}$.

A3. $S_1(\mathbb{1}) = S$, where $\mathbb{1} = \bigvee_{\alpha \in L} a$.

A4. $S_1(\bigwedge_\alpha a_\alpha) = \bigcap_\alpha S_1(a_\alpha)$ $\forall\, \{a_\alpha\} \subset L$.

A5. S is convex, i.e., $\forall\, s_1, s_2 \in S$ and $\forall\, \gamma \in (0, 1)$ $\exists\, s \in S$ such that $s(a) = \gamma s_1(a) + (1 - \gamma)\, s_2(a)$, $\forall\, a \in L$. We write $s = \gamma s_1 + (1 - \gamma)\, s_2$.

A6. (Maximality axiom). If μ is an automorphism of L, define $S_\mu = \{\tilde{s} \mid \tilde{s}: L \to [0, 1],\ \tilde{s}(a) = s(\mu(a))$ $\forall\, s \in S, \forall\ a \in L\}$. Then, $S_\mu \subset S$.

Remark: The pair (L, S_μ) satisfies A1–A5 and $S_\mu \subset S \Rightarrow S_\mu = S$.

To every physical system Σ we associate a pss (L, S), where L represents the set of classes (propositions) of equivalent yes–no experiments on Σ, and S the set of preparing procedures (states) pertaining to Σ. The number $s(a)$ $(s \in S,\ a \in L)$ is interpreted as the probability of the outcome "yes" for a test of the class a when Σ has been prepared according to the procedure corresponding to s.

The physical motivations for axioms A1–A5 were discussed in Ref. 8. A condition for the atomicity of L was provided therein by the requirement of existence of sufficiently many characteristic states. Actually, in this paper we do not make use of the atomicity condition. However, the latter has been included in the axioms to ensure the existence of maximal (nontrivial) superpositions of maximal states for non-Boolean lattices (see Ref. 5, Proposition 2). As to axiom A6, it will be seen in Sec. 3 that it ensures the stability of the states under dynamical evolution.

Apart from axiom A6, the scheme based on Definition 2.1 is similar to the one proposed by Pool in Ref. 9, where, however, the problem of the dynamical evolution of the system was not treated.

For every family D of elements of S define

$$\overline{D}=\cap_{S_1(a)\supset D}S_1(a).$$

The map $D\to\overline{D}$ is a closure operation[10] on the subsets of S, namely, it satisfies C1. $D\subset\overline{D}$, C2. $\overline{\overline{D}}=\overline{D}$, and C3. $D\subset E\Rightarrow\overline{D}\subset\overline{E}$. The corresponding family of closed sets is $\mathcal{J}=\{S_1(a): a\in L\}$. These assertions follow from Theorem 1, Chap. V of Ref. 7, $\mathcal{J}$ being a Moore family of subsets of S (Ref. 10) by A3 and A4. Under set inclusion, $\mathcal{J}$ is a complete lattice which, by A1, is isomorphic to L. The lub and glb of a family $\{S_1(a_\alpha)\}\subset\mathcal{J}$ are, respectively, $\overline{\cup_\alpha S_1(a_\alpha)}$ and $\cap_\alpha S_1(a_\alpha)$.[11] If $D\subset S$ define $L(D)=\{a\,|\,a\in L,\ s(a)=1\ \ s\in D\}\equiv\{a\,|\,a\in L,\ S_1(a)\supset D\}$. Then $L(D)$ is a dual principal ideal in L.[5,7] We denote

$$\wedge L(D)=\wedge_{b\in L(D)}b.$$

Definition 2.2: A state s is said to be a superposition of the states in D if $L(s)\supset L(D)$.[5]

Lemma 2.1: $\forall\, D\subset S$, $\overline{D}=\{s\,|\,s\in S,\ L(s)\supset L(D)\}$.

Proof: First note the identity $a=\wedge L(S_1(a))$ $\forall\, a\in L$. Indeed, $s\in S_1(\wedge L(s))\subset S_1(\wedge L(S_1(a)))$ $\forall\ s\in S_1(a)$. Hence, by A1, $a\leq\wedge L(S_1(a))$. On the other hand, $a\geq\wedge L(S_1(a))$ because a is an element of $L(S_1(a))$. If $L(s)\supset L(D)$, then $s\in S_1(\wedge L(s))\subset S_1(\wedge L(D))$. On the other hand, if $s\in S_1(\wedge L(D))$, then $\wedge L(s)\leq\wedge L(S_1(\wedge L(D)))=\wedge L(D)$ by the previous identity. Since $L(s)$ and $L(D)$ are dual principal ideals, this implies $L(s)\supset L(D)$. Hence

$$\{s\,|\,s\in S, L(s)\supset L(D)\}=S_1(\wedge L(D))$$
$$=\bigcap_{a\in L(D)}S_1(a)=\bigcap_{S_1(a)\supset D}S_1(a)=\overline{D}.$$

By definition, a state s belongs to $\overline{D}$ iff any proposition (and hence the smallest) which is true on the elements of D is also true on s. Lemma 2.1 states that for a state to belong to $\overline{D}$ it is necessary and sufficient that it is a superposition of states of D. Therefore, we can refer to the map $D\to\overline{D}$ as *closure under superposition*.

The following lemma will be used in the next section.

Lemma 2.2: Let α be a permutation of S. Then the following conditions are equivalent:

(i) $L(s)\supset L(D)\Leftrightarrow L(\alpha s)\supset L(\alpha D)$, $s\in S$, $D\subset S$.

(ii) $\alpha\overline{D}=\overline{\alpha D}$ $\forall\, D\subset S$.

Proof: Use Lemma 2.1.(i)$\Rightarrow$ (ii): $s\in\overline{D}\Leftrightarrow L(s)\supset L(D)$ $\Leftrightarrow L(\alpha s)\supset L(\alpha D)\Leftrightarrow\alpha s\in\overline{\alpha D}$. (ii) $\Rightarrow$ (i): $L(s)\supset L(D)$ $\Leftrightarrow s\in\overline{D}\Leftrightarrow\alpha s\in\alpha\overline{D}=\overline{\alpha D}\Leftrightarrow L(\alpha s)\supset L(\alpha D)$.

3. THE TIME EVOLUTION

Definition 3.1: A *pseudodynamical group* of a pss (L,S) is a one parameter group of permutations of $S: t\to\alpha_t$, $t\in\mathbb{R}$, $\alpha_{t+t'}=\alpha_t\alpha_{t'}$ such that

(i) $L(s)\supset L(D)\Rightarrow L(\alpha_t s)\supset L(\alpha_t D)$ $\forall\, t\in\mathbb{R}$ $(s\in S,\ D\subset S)$

and

(ii) $\wedge\ L(\alpha_t S_1(a))=(\wedge L(\alpha_t S_1(a')))'$ $\forall\, a\in L$ and $\forall\, t\in\mathbb{R}$.

Lemma 3.1: Conditions (i) and (ii) of Definition 3.1 are jointly equivalent to the following condition: (iii) $\forall\, a\in L$ and $\forall\, t\in\mathbb{R}\ \exists\, b\in L$ such that $\alpha_t S_1(a)=S_1(b)$ and $\alpha_t S_1(a')=S_1(b')$.

Proof: (i) + (ii) $\Rightarrow$ (iii). Since $S_1(a)$ is closed, by the group property, by (i) and by Lemma 2.2 we have that $\alpha_t S_1(a)$ is closed, hence $\exists\, b\in L$ such that $\alpha_t S_1(a)=S_1(b)$. By the identity $b=\wedge L(S_1(b))$ and by (ii) it follows that $b'=\wedge L(\alpha_t S_1(a'))$. Therefore, $S_1(b')=\alpha_t S_1(a')$.

(iii) $\Rightarrow$ (i) + (ii). By hypothesis, we have $b=\wedge L(\alpha_t S_1(a))$ and $b'=\wedge L(\alpha_t S_1(a'))$ which proves (ii). By Lemma 2.2 in order to demonstrate (i) it is enough to prove that $\alpha_t\overline{D}=\overline{\alpha_t D}$ $\forall\, t\in\mathbb{R}$ and $\forall\, D\subset S$. By hypothesis, α_t maps closed sets to closed sets. Therefore, from $\alpha_t\overline{D}\supset\alpha_t D$ there follows $\alpha_t\overline{D}\supset\overline{\alpha_t D}$ $\forall\, D\subset S$ and $\forall\, t\in\mathbb{R}$. Moreover, from $\alpha_{-t}(\overline{\alpha_t D})\supset D$ by taking closures we get $\alpha_{-t}(\overline{\alpha_t D})\supset\overline{D}$ and hence $\overline{\alpha_t D}\supset\alpha_t\overline{D}$.

Given a pseudodynamical group $t\to\alpha_t$, by Lemma 3.1 for every $t\in\mathbb{R}$ we can define a map μ_t^α of L into itself by $\alpha_{-t}S_1(a)=S_1(\mu_t^\alpha(a))$. Then the following proposition is a straightforward consequence of axiom A1 and of Lemma 3.1.

Proposition 3.1: The map $t\to\mu_t^\alpha$ is a one parameter group of automorphisms of L.

We refer to $t\to\mu_t^\alpha$ as the group induced on L by the pseudodynamical group $t\to\alpha_t$. On the set of pseudodynamical groups of a pss (L,S) there exists a canonical equivalence relation defined by $\{t\to\alpha_t\}\sim\{t\to\beta_t\}$ if $\mu_t^\alpha=\mu_t^\beta$, $\forall\ t\in\mathbb{R}$. Conversely, the following proposition shows by construction that every one parameter group of automorphisms of L is induced by at least one pseudodynamical group.

Proposition 3.2: Let $t\to\mu_t$ be a one parameter group of automorphisms of L. $\forall\ t\in\mathbb{R}$ define $\rho_t: S\to S$ by $(\rho_t s)(a)=s(\mu_t(a))$. Then (i) $t\to\rho_t$ is a pseudodynamical group and (ii) $\forall\ t\in\mathbb{R}$ the map ρ_t is affine.

Proof: Note first that ρ_t is indeed a map of S into itself by axiom A6. (i) $s\in S_1(\mu_{-t}(a))\Leftrightarrow s(\mu_{-t}(a))=1\Leftrightarrow$ $(\rho_{-t}s)(a)=1\Leftrightarrow\rho_{-t}s\in S_1(a)\Leftrightarrow s\in\rho_t S_1(a)$ whence $\rho_t S_1(a)$ $=S_1(\mu_{-t}(a))$. Moreover, $\rho_t S_1(a')=S_1(\mu_{-t}(a'))=S_1([\mu_{-t}(a)]')$. Therefore, by Lemma 3.1, $t\to\rho_t$ is a pseudodynamical group.

(ii) If $s=\sum_{i=1}^n\alpha_i s_i$ with $\alpha_i\in(0,1)$ $(i=1,2,\ldots n)$ and $\sum_{i=1}^n\alpha_i=1$, we have $\forall\, t\in\mathbb{R}$ and $\forall\ a\in L$

$$(\rho_t s)(a)=s(\mu_t(a))=\sum_{i=1}^n\alpha_i s_i(\mu_t(a))=\sum_{i=1}^n\alpha_i(\rho_t s_i)(a)$$

whence

$$\rho_t s=\sum_{i=1}^n\alpha_i(\rho_t s_i).$$

Definition 3.2: A *dynamical group* of a pss (L,S) is a pseudodynamical group $t\to\alpha_t$ of (L,S) such that $(\alpha_t s)(a)=s(\mu_t^\alpha(a))$, $\forall\ t\in\mathbb{R}$, $a\in L$, $s\in S$.

Proposition 3.2 shows that every equivalence class of pseudodynamical groups contains exactly one dynamical group. In order to ensure the standard equivalence between Heisenberg and Schrödinger picture, we assume a reversible time evolution of the states of a physical system characterized by a pss (L,S) to be described by

a dynamical group of (L, S). Accordingly, we refer to a dynamical group $t \to \alpha_t$ as a (reversible) Schrödinger dynamics and to $t \to \mu_t^\alpha$ as the corresponding (reversible) Heisenberg dynamics. With the further assumption of continuity of the map $t \to (\alpha_t s)(a), \forall\, s \in S$, $a \in L$ which has to be required on physical grounds, such a reversible dynamics could possibly be ascribed to the idealized situation of the time behavior of a strictly isolated system. If the system interacts with its surroundings it evolution is irreversible and the above scheme is not adequate for the description of its time behavior.[12,13] In a forthcoming paper, we propose a generalization of the present dynamical framework to accommodate the description of irreversible processes as well. The new feature introduced by such a generalization and which is connected with the dispersion of information taking place in an irreversible process is that the lattice of propositions is no longer stable under the Heisenberg dynamics. Rather, the latter acts on the set of all effects, of which the propositions form the subset of the so-called decision effects.[6]

4. THE HILBERT MODEL

Let $L = \mathcal{L}(\mathfrak{H})$ be the complete, orthocomplemented, atomic, weakly modular lattice of the closed subspaces of a separable complex Hilbert space $\mathfrak{H}$ of dimension ≥ 3 (possibly infinite)[14] and let S be the set of maps $s: L \to [0, 1]$ such that (i) $s(\mathbb{1}) = 1$, $\mathbb{1} \equiv \mathfrak{H}$ and (ii) $s(\bigvee_i a_i) = \sum_i s(a_i)$ if $a_i \leq a_j'$ for $i \neq j$ (σ-additivity). It follows from the weak modularity and from (ii) that $s(0) = 0$, where 0 denotes the null subspace of $\mathfrak{H}$ ($0 = \mathbb{1}'$). The Gleason theorem[15] implies that there exists an affine isomorphism $\rho \to s_\rho$ of the convex set $K(\mathfrak{H})$ of positive trace 1 operators on $\mathfrak{H}$ (density operators) onto S, such that $s_\rho(a) = \mathrm{Tr} P^a \rho$, $\forall\ \rho \in K(\mathfrak{H})$ and $\forall\ a \in L$, where P^a is the orthogonal projection whose range is a. Using the spectral decomposition of a density operator $\rho = \sum_i \gamma_i P^{a_i}$ ($\gamma_i \neq 0$), where the a_i's are the eigenspaces of ρ in the range of the latter, one gets $S_1(a) = \{s_\rho \mid \rho \in K(\mathfrak{H}),\ P^a \rho = \rho\}$ and $S_0(a) = \{s_\rho \mid \rho \in K(\mathfrak{H}),\ P^a \rho = 0\}$ whence it readily follows that the pair (L, S) satisfies axioms A1—A5. As to axiom A6, it holds since σ-additivity is preserved under an automorphism of L. Therefore, (L, S) is a pss. We have the following formulas (see Lemma 1 of Ref. 5 and Lemma 2.1): (1) $L(s_\rho) = \{a \mid a \in L,\ P^a \rho = \rho\}$; (2) $\bigwedge L(s_\rho) = \bigvee_i a_i \not\perp [\rho] \equiv$ the range of ρ; (3) if $D \subset S$, $\bigwedge L(D) = \bigvee_{s_\rho \in D} [\rho]$; (4) if $D \subset S$, $\overline{D} = S_1(\bigwedge L(D)) = \{s_\rho \mid \rho \in K(\mathfrak{H}),\ P^{\bigwedge L(D)} \rho = \rho\}$. Moreover, if $D \subset S$, $L(s_\rho) \supset L(D)$ iff the range of ρ is contained in the closure of the linear span of the ranges of all density operators σ such that $s_\sigma \in D$.

Let now $t \to \alpha_t$ be a dynamical group of (L, S). Since α_t is affine (see Proposition 3.2), $\forall\ t \in \mathbb{R}$ there exists a unitary or antiunitary operator U_t^α on $\mathfrak{H}$ such that

$$\alpha_t s_\rho = s_{U_t^\alpha \rho U_t^{\alpha *}},\ \forall\ \rho \in K(\mathfrak{H}).^{16}$$

Antiunitary operators are ruled out by the group property. Therefore, with the further assumption of continuity, a reversible dynamics is described by a weakly (hence strongly[17]) continuous one parameter group of unitary operators on $\mathfrak{H}$[18] whose generator can be interpreted as the Hamiltonian of the system.[19]

5. CONCLUDING REMARKS

In this paper we have tried to give an intrinsic characterization of a reversible time evolution of a physical system within a possible exiomatic approach to quantum mechanics based on Definition 2.1. This characterization is based on Definition 3.1 and 3.2, whose physical motivations are plausible. In this connection, there arise some interesting problems. First of all, one might ask whether, in the general scheme as well as in the Hilbert model, there exist pseudodynamical groups which are not dynamical. Secondly, the question arises whether axiom A6 is independent of A1—A5 and whether in Definition 3.1 condition (ii) is independent of (i). Indeed, if one defines a pseudodynamical group $t \to \alpha_t$ in terms of condition (i) of Definition 3.1 alone, it is still possible to prove, using the property of closure under superposition, that $t \to \alpha_t$ induces a one parameter group $t \to \mu_t^\alpha$ of partial order preserving permutations of L, but there is no guarantee that μ_t^α preserves complementation. Furthermore, if we relax A6, there might *a priori* exist equivalence classes of pseudodynamical groups which do not contain any dynamical group and one parameter groups of automorphisms of L which are not induced by corresponding pseudodynamical groups. Besides the situation in the Hilbert model, another problem of interest is the study of conditions for the existence of nontrivial ($\neq \mathbb{1}, \mathbb{1}'$) constants of motion ($\mu_t^\alpha(a) = a$, $\forall\ t \in \mathbb{R}$) and of invariant states ($\alpha_t s = s$, $\forall\ t \in \mathbb{R}$). These problems are currently under investigation.

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The Cauchy problem in general relativity. I. Metrics containing arbitrary functions

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This paper develops a Lagrangian formalism (the y_A-formalism) for use in investigating the Cauchy problem in general relativity. In particular it will be used in a subsequent paper to present a Lagrangian formulation of the characteristic initial-value problem in general relativity. The formalism enables one to define "field equations" and "Bianchi identities" for metrics containing arbitrary functions in the case when the arbitrary functions are treated as the field variables.

I. INTRODUCTION

This work was instigated by a discovery of A. Held[1] (private communication) in which he found that a variation of the Einstein Lagrangian of Bondi's radiating metric[2] with respect to the four arbitrary functions contained in the metric resulted in Bondi's so-called "main equations" up to unimportant factors. This paper develops a formalism, the y_A-formalism, for investigating variations with respect to arbitrary functions contained in a metric. In Paper II the formalism will be used to present a Lagrangian formulation of the characteristic initial-value problem of general relativity.

Sections II and III contain a short development of Noether's basic identity together with some of the resulting expressions in the context of general relativity. Section IV develops the y_A-formalism in some generality and Sec. V applys the formalism to metrics containing arbitrary functions. After a brief discussion of special coordinate systems in Sec. VI, the formalism is applied to a derivation of Bianchi identities. A final section collects together the more important formulas.

II. THE BASIC IDENTITY

We start by considering the Lagrangian density

$$L(x;y(x)) \equiv L(y_A(x^a), y_{A,b}(x^a), y_{A,bc}(x^a), x^c) \tag{2.1}$$

where $y_{A,b} = \partial y_A/\partial x^b$, etc., x^a are local coordinates defined on an n-dimensional differentiable manifold, and the y_A are A field variables. If we consider an infinitesimal symmetry transformation[3]

$$x^{a'} = x^a - \xi^a \tag{2.2}$$

which leaves the Lagrangian density form-invariant, then integration over an arbitrary volume Ω of R^n leads to

$$0 \equiv \int_{\Omega'} L(x'; y'(x'))d^n x' - \int_\Omega L(x; y(x))d^n x$$

$$= \int_\Omega (L^A \bar{\delta} y_A + t^a{}_{,a}) d^n x, \tag{2.3}$$

where

$$L^A = \frac{\delta L}{\delta y_A} = \frac{\partial L}{\partial y_A} - \left(\frac{\partial L}{\partial y_{A,a}}\right)_{,a} + \left(\frac{\partial L}{\partial y_{A,ab}}\right)_{,ab}, \tag{2.4}$$

$$\bar{\delta} y_A = y'_A(x) - y_A(x), \tag{2.5}$$

and

$$t^a = -L\xi^a + \frac{\partial L}{\partial y_{A,a}} \bar{\delta} y_A + \frac{\partial L}{\partial y_{A,ab}} \bar{\delta} y_{A,b} - \left(\frac{\partial L}{\partial y_{A,ab}}\right)_{,b} \bar{\delta} y_A. \tag{2.6}$$

Since Ω is arbitrary, we obtain Noether's basic identity

$$L^A \bar{\delta} y_A + t^a{}_{,a} \equiv 0. \tag{2.7}$$

In particular, if we consider the case when $\xi^a = 0$ and the variations $\bar{\delta} y_A$ and $\bar{\delta} y_{A,b}$ vanish at the surface $\partial\Omega$, then (2.6) leads to the field equations

$$L^A = 0. \tag{2.8}$$

III. THE EINSTEIN LAGRANGIAN

The Einstein Lagrangian

$$L = \sqrt{-g}\, R \tag{3.1}$$

remains form-invariant under an infinitesimal coordinate transformation since it remains so under a general coordinate transformation. Taking the field variables y_A to be g_{ab}, the field equations (2.7) become the Einstein (vacuum) field equations

$$-\sqrt{-g}\, G^{ab} = 0. \tag{3.2}$$

Under an infinitesimal coordinate transformation of the form (2.2)

$$\bar{\delta} g_{ab} = \underset{\xi}{\mathcal{L}} g_{ab} = \xi_{a;b} + \xi_{b;a}, \tag{3.3}$$

where $\mathcal{L}$ denotes Lie derivative, so that the basic identity becomes

$$-2\sqrt{-g}\, G^{ab} \xi_{a;b} + t^a{}_{,a} = 0. \tag{3.4}$$

A long but straightforward calculation reveals that

$$t^a = 2\sqrt{-g}\, G^{ab} \xi_b + (2\sqrt{-g}\, \xi^{[a;b]})_{,b}. \tag{3.5}$$

The second term in this equation is an interesting quantity since it is the same term as A. Komar[4] constructed and which gives rise to an infinite number of conservation laws since clearly its divergence vanishes identically. The quantity becomes Møller's energy–momentum tensor for the choice $\xi^a = \delta^a_0$ in an appropriate coordinate system.

IV. LAGRANGIAN DEPENDING ON TWO SETS OF FIELD VARIABLES

We now restrict attention to a Lagrangian density which may be considered simultaneously to be on the one hand a functional of the field variables y_A their first and second derivatives and the coordinates x^a and on the other hand a functional of the M field variables z_M, say, and their first and second derivatives only. Thus we assume

$$L(y_A, y_{A,a}, y_{A,ab}, x^c) = K(z_M, z_{M,a}, z_{M,ab}) \tag{4.1}$$

where L depends explicitly on x^c whereas K does not

(in the next section we shall take the z_M to be g_{ab}). We also assume that the z_M are functionals of the y_A and the coordinates only, i.e.,

$$z_M = z_M(y_A, x^a). \tag{4.2}$$

We define

$$X^A_M = \frac{\partial z_M}{\partial y_A} \tag{4.3}$$

and so by (4.2)

$$X^A_M = X^A_M(y_B, x^a).$$

In this section only we let $\partial/\partial x^a$ denote the partial derivative keeping the y_A and the z_M fixed, whereas comma or D/Dx^a denote total or implicit derivative,[5] so that, for instance,

$$\frac{D}{Dx^a} = \frac{\partial}{\partial x^a} + y_{A,a}\frac{\partial}{\partial y_A} + y_{A,ab}\frac{\partial}{\partial y_{A,b}} + y_{A,abc}\frac{\partial}{\partial y_{A,bc}}. \tag{4.4}$$

Now, in addition to the basic identity (2.7) for the y_A we also have the basic identity for the z_M

$$K^M \bar{\delta} z_M + s^a{}_{,a} = 0 \tag{4.5}$$

where the quantities involved are defined in an analogous manner to the definitions of Sec. II. We wish to prove that

$$s^a = t^a. \tag{4.6}$$

Some key formulas needed and which follow directly from Eqs. (4.1)–(4.4) are given in the Appendix. If we now contemplate an arbitrary variation of the y_A, the resulting variation of the z_M is given by

$$\begin{aligned}\bar{\delta} z_M &= z_M(y'_A(x), x) - z_M(y_A(x), x)\\ &= z_M(y_A(x) + \bar{\delta} y_A(x), x) - z_M(y_A(x), x)\\ &= X^A_M \bar{\delta} y_A\end{aligned} \tag{4.7}$$

to first order, where we have used (2.5) and (4.3). Using these relationships and the fact that $\bar{\delta}$ and total differentiation commutes, we find

$$\begin{aligned}s^a &= -K\xi^a + \left[\frac{\partial K}{\partial z_{M,a}} - \left(\frac{\partial K}{\partial z_{M,ab}}\right)_{,b}\right]\bar{\delta} z_M + \frac{\partial K}{\partial z_{M,ab}}\bar{\delta} z_{M,b}\\ &= -K\xi^a + \left[\frac{\partial K}{\partial z_{M,a}} - \left(\frac{\partial K}{\partial z_{M,ab}}\right)_{,b}\right] X^A_M \bar{\delta} y_A\\ &\quad + \frac{\partial K}{\partial z_{M,ab}}(X^A_M \bar{\delta} y_{A,b} + X^A_{M,b}\bar{\delta} y_A)\\ &= -K\xi^a + \left[\left(X^A_M \frac{\partial K}{\partial z_{M,a}} + 2X^A_{M,b}\frac{\partial K}{\partial z_{M,ab}}\right)\right.\\ &\quad \left. - \left(X^A_M \frac{\partial K}{\partial z_{M,ab}}\right)_{,b}\right]\bar{\delta} y_A\\ &\quad + \left(X^A_M \frac{\partial K}{\partial z_{M,ab}}\right)\bar{\delta} y_{A,b}\\ &= -L\xi^a + \left[\frac{\partial L}{\partial y_{A,a}} - \left(\frac{\partial L}{\partial y_{A,ab}}\right)_{,b}\right]\bar{\delta} y_A + \frac{\partial L}{\partial y_{A,ab}}\bar{\delta} y_A\\ &= t^a.\end{aligned}$$

We have used the fact that $K \equiv L$ when considered solely as a function of x^a. Using the above result together with (2.7) and (4.5), it follows that

$$L^A \bar{\delta} y_A = K^M \bar{\delta} z_M = (X^A_M K^M)\bar{\delta} y_A$$

and since the $\bar{\delta} y_A$ are arbitrary

$$L^A = X^A_M K^M. \tag{4.8}$$

This relates the A field equations $L^A = 0$ to the M field equations $K^M = 0$. The result can be proved directly by substituting the expression (2.4) for L^A in terms of K using the above relationships. J. Stachel has pointed out that (4.8) is virtually immediate since in the variational notation it follows in a straightforward manner that

$$\frac{\delta L}{\delta y_A} = \frac{\delta K}{\delta z_M}\frac{\partial z_M}{\partial y_A}.$$

V. METRICS CONTAINING ARBITRARY FUNCTIONS

We now apply the theory of the last section to the case when z_M is g_{ab}, $L = K = \sqrt{-g}\,R$, g_{ab} contains A arbitrary functions y_A, and satisfies (4.2), namely

$$g_{ab} = g_{ab}(y_A, x^c) \quad \text{only.} \tag{5.1}$$

Considering K as a functional of g_{ab} (or equivalently g^{ab}) and its derivatives, then the field equations $K^M = 0$ are the Einstein field equations (3.2). If on the other hand we consider the Lagrangian density as a functional of the y_A and its derivatives, we obtain the A field equations $L^A = 0$ and from (4.8)

$$L^A = X^A_{ab}(-\sqrt{-g}\,G^{ab}) = \frac{\partial g_{ab}}{\partial y_A}(-\sqrt{-g}\,G^{ab}) \tag{5.2}$$

or equivalently in terms of g^{ab}

$$L^A = \frac{\partial g^{ab}}{\partial y_A}(\sqrt{-g}\,G_{ab}) = X^{ab}_A \sqrt{-g}\,G_{ab}. \tag{5.3}$$

In applications A is less than ten and so the equations $L^A = 0$ are only a restricted set of the Einstein field equations, or rather *combination* of the field equations.

Under an infinitesimal symmetry transformation Eq. (4.7) requires

$$\bar{\delta} g_{ab} = \underset{\xi}{\mathcal{L}} g_{ab} = \xi_{a;b} + \xi_{b;a} = X^A_{ab}\bar{\delta} y_A. \tag{5.4}$$

These equations do two things, they impose differential conditions on ξ_a and also serve to determine $\bar{\delta} y_A$ in terms of ξ_a. More precisely the role of Eq. (5.4) is to restrict the infinitesimal coordinate transformation to a transformation which preserves the functional form of the metric assumed in (5.1). In many cases (5.4) allows a determination of ξ_a and $\bar{\delta} y_A$. In such cases given (5.1) and (2.1) we can calculate t^a since

$$t^a = s^a = -L\xi^a + \frac{\partial L}{\partial y_{A,a}}\bar{\delta}y_A + \frac{\partial L}{\partial y_{A,ab}}(\bar{\delta}y_A)_{,b} - \left(\frac{\partial L}{\partial y_{A,ab}}\right)_{,b}\bar{\delta}y_A. \tag{5.5}$$

The resulting expression will be equivalent to that given in (3.5). The formalism developed in this section forms the essential component of what we shall term the y_A formalism.

VI. SPECIAL COORDINATE SYSTEMS

From Eq. (3.5) t^a differs from $2\sqrt{-g}\,G^{ab}\xi_b$ by

$$(2\sqrt{-g}\,\xi^{[a;b]})_{,b} = (2\sqrt{-g}\,g^{ac}g^{bd}\,\xi_{[c,d]})_{,b} \tag{6.1}$$

which vanishes in particular if

$$\xi_a = \phi_{,a}. \tag{6.2}$$

A particular solution of this equation in a given coordinate system is any coordinate $x^{(c)}$ for which

$$\underset{\delta^{(c)}_d}{\mathcal{L}}\, g_{ab} = -2\Gamma^{(c)}_{ab} = X^A_{ab}\,\bar{\delta}y_A. \tag{6.3}$$

In general of course these equations will not form a consistent set.

We may solve (5.4) directly for ξ_a and $\bar{\delta}y_A$ when the metric does not depend explicity on a coordinate $x^{(c)}$, i.e., when

$$\frac{\partial}{\partial x^{(c)}} g_{ab} = 0 \tag{6.4}$$

where the partial derivative is to be taken in the sense of Sec. IV. For taking $\xi^a = \delta^a_{(c)}$ we find

$$\begin{aligned}\underset{\xi}{\mathcal{L}}\, g_{ab} = g_{ab,(c)} &= \frac{D}{Dx^{(c)}} g_{ab} \\ &= \frac{\partial}{\partial x^{(c)}} g_{ab} + y_{A,(c)}\frac{\partial g_{ab}}{\partial y_A} = y_{A,(c)}\frac{\partial g_{ab}}{\partial y_A} \\ &= X^A_{ab}\, y_{A,(c)}.\end{aligned}$$

Thus

$$\bar{\delta}y_A = y_{A,(c)} \tag{6.5}$$

and

$$t^a = 2\sqrt{-g}\,G^a{}_{(c)} + (2\sqrt{-g}\,g^{ad}g^{be}g_{(c)[d,e]})_{,b}. \tag{6.6}$$

If ξ^a is a Killing vector field, i.e.,

$$\underset{\xi}{\mathcal{L}}\, g_{ab} = 0,$$

then

$$\bar{\delta}y_A = 0$$

and (5.5) and (3.5) result in

$$2\sqrt{-g}\,G^a{}_b\,\xi^b = -L\xi^a - (2\sqrt{-g}\,\xi^{[a;b]})_{,b} \tag{6.7}$$

or equivalently

$$R^a{}_b\,\xi^b = g^{c[a}\xi^{b]}{}_{;cb}. \tag{6.8}$$

Finally, if the metric does not depend explicitly or implicitly on a coordinate $x^{(c)}$, then $\xi^a = \delta^a_{(c)}$ is a Killing field and so combining (6.6) and (6.7) we find

$$2\sqrt{-g}\,G^a{}_{(c)} = -L\delta^a_{(c)} - (2\sqrt{-g}\,g^{ad}g^{be}g_{(c)[d,e]})_{,b}. \tag{6.9}$$

VII. BIANCHI IDENTITIES

In general, the Bianchi identities are derived from (2.3) by assuming that ξ^a and its derivatives vanish on the boundary and by assuming that $\bar{\delta}y_A$ satisfies an equation of the form[3]

$$\bar{\delta}y_A = \gamma_{Aa}\,\xi^a - \gamma^a_{Ab}\,\xi^b{}_{,a}. \tag{7.1}$$

For then (2.3) becomes

$$0 = \int_\Omega [L^A\gamma_{Aa} + (L^A\gamma^b_{Aa})_{,b}]\,\xi^a d^4x + \text{vanishing surface terms}$$

and since Ω is arbitrary

$$[L^A\gamma_{Aa} + (L^A\gamma^b_{Aa})_{,b}]\,\xi^a = 0. \tag{7.2}$$

Finally, since ξ^a is arbitrary the expression in square brackets vanishes and these are then the so-called Bianchi identities. In particular, in the case of the Einstein Lagrangian, Eq. (3.3) is of the form (7.1) and the above procedure results in the (contracted) Bianchi identities

$$G^{ab}{}_{;b} = 0. \tag{7.3}$$

In order to develop these identities in the y_A-formalism it is necessary to solve (5.4) for $\bar{\delta}y_A$. We start by considering the y_A as functionals of the g_{ab} and the coordinates, i.e.,

$$y_A = y_A(g_{ab}, x^c). \tag{7.4}$$

It is emphasized that these equations are not unique. However, proceeding as before a variation in the g_{ab} results in

$$\begin{aligned}\bar{\delta}y_A &= y_A(g_{ab} + \bar{\delta}g_{ab},\ x^c) - y_A(g_{ab}, x^c) \\ &= \frac{\partial y_A}{\partial g_{ab}}\,\bar{\delta}g_{ab}\end{aligned} \tag{7.5}$$

to first order. We define

$$Y^{ab}_A = \frac{\partial y_A}{\partial g_{ab}} \tag{7.6}$$

where the matrix Y^{ab}_A is assumed symmetrized, but unlike X^A_{ab} it is not unique. Nonetheless we may work with Y^{ab}_A since, in a sense, the nonuniqueness is factored out in the following equations by multiplicative expressions. Combining (5.4) and (7.6) leads to

$$X^A_{ab}\,Y^{ab}_A = \delta^A_B. \tag{7.7}$$

This allows inversion of some of the previous formulas, for example (5.2) becomes

$$-\sqrt{-g}\,G^{ab}\bar{\delta}g_{ab} = L^A\bar{\delta}y_A = L^A\,Y^{ab}_A\bar{\delta}g_{ab},$$

so that

$$(L^A\,Y^{ab}_A + \sqrt{-g}\,G^{ab})\,\bar{\delta}g_{ab} = 0.$$

If for a particular choice of the variations $\bar{\delta}y_A$ there exists values of a and b such that $\bar{\delta}g_{ab} \neq 0$, then for these values

$$L^A\,Y^{ab}_A = -\sqrt{-g}\,G^{ab}. \tag{7.8}$$

Now for an infinitesimal symmetry transformation (5.4) gives

$$\bar{\delta}y_A = 2Y^{ab}_A\,\xi_{a;b} \tag{7.9}$$

which is of the form (7.1). We cannot proceed exactly as before because although we can obtain an expression of the form (7.2) the ξ^a are no longer arbitrary but must in fact satisfy (5.4). Of course since the ξ^a must therefore be of a particular form, this will result in certain relationships among the terms in the square brackets of (7.2). However the expressions so derived do not lend themselves very well to the y_A-formalism and so we proceed in a slightly different (but equivalent) manner.

Again, starting from (2.3)

$$\begin{aligned} 0 &\equiv \int_\Omega (L^A \bar{\delta} y_A + t^a{}_{,a})\, d^4x \\ &= \int_\Omega [2 L^A Y^{ab}_A (\xi_{a,b} - \Gamma^c_{ab} \xi_c) + t^a{}_{,a}] d^4x \\ &= \int_\Omega \{ - [2 L^A Y^{ab}_A \Gamma^c_{ab} \xi_c + 2(L^A Y^{ac}_A)_{,a} \xi_c] \\ &\quad + [t^a + 2 L^A Y^{ab}_A \xi_b]_{,a} \} d^4x. \end{aligned}$$

The second term in square brackets can be converted into a vanishing surface integral and so since Ω is arbitrary we get

$$[2 L^A Y^{ab}_A \Gamma^c_{ab} \xi_c + 2(L^A Y^{ac}_A)_{,a} \xi_c] = 0.$$

However since the integrand in the above integral is identically zero this last expression is identical to the simpler expression

$$[t^a + 2 L^A Y^{ab}_A \xi_b]_{,a} = 0. \tag{7.10}$$

This is the expression we choose to define as the "Bianchi identities" in the y_A-formalism. Substituting the solution for ξ^a of (5.4) in (7.10) results in differential constraints on the full field equations (3.2). If the field equations $L^A = 0$ are assumed to hold, then (7.10) reduces to

$$t^a{}_{,a} = 0. \tag{7.11}$$

VIII. SUMMARY OF BASIC FORMULAS

Starting from a metric of the form

$$g_{ab} = g_{ab}(y_A, x^c)$$

where y_A denote A arbitrary functions, we can calculate the Einstein Lagrangian

$$L = L(y_A, y_{A,b}, y_{A,bc}, x^a) = \sqrt{-g} R.$$

The y_A formalism allows us to define the "field equations"

$$0 = L^A = \frac{\partial L}{\partial y_A} - \left(\frac{\partial L}{\partial y_{A,a}}\right)_{,a} + \left(\frac{\partial L}{\partial y_{A,ab}}\right)_{,ab}$$

or equivalently from a knowledge of the Einstein tensor

$$0 = L^A = \frac{\partial g_{ab}}{\partial y_A}(-\sqrt{-g}\, G^{ab}) = \frac{\partial g^{ab}}{\partial y_A}(\sqrt{-g}\, G^{ab}).$$

Next we attempt to find a solution of the differential equations

$$\underset{\xi}{\pounds} g_{ab} = g_{ab,c} \xi^c + g_{ac} \xi^c{}_{,b} + g_{bc} \xi^c{}_{,a} = \frac{\partial g_{ab}}{\partial y_A} \bar{\delta} y_A$$

for both ξ^a and $\bar{\delta} y_A$. From a solution we can calculate t^a either in the y_A-formalism using

$$t^a = -L\xi^a + \frac{\partial L}{\partial y_{A,a}} \bar{\delta} y_A + \frac{\partial L}{\partial y_{A,ab}} \bar{\delta} y_{A,b} - \left(\frac{\partial L}{\partial y_{A,ab}}\right)_{,b} \bar{\delta} y_A$$

or equivalently using

$$t^a = 2\sqrt{-g}\, G^{ab} \xi_b + (2\sqrt{-g}\, \xi^{[a;b]})_{,b}.$$

In special coordinate systems we have in addition the results of Sec. VI.

Finally, we calculate the nonunique symmetrized expression

$$Y^{ab}_A = \frac{\partial y_A}{\partial g_{ab}}$$

and from it the "Bianchi identities"

$$[t^a + 2 L^A Y^{ab}_A \xi_b]_{,a} = 0.$$

In Paper II we shall describe how these results can be used to help devise an integration scheme for the Einstein field equations.

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APPENDIX

The key formulas referred to in Sec. IV are

$$\frac{\partial z_{M,a}}{\partial y_{A,c}} = X^A_M \delta^c_a,$$

$$\frac{\partial z_{M,ab}}{\partial y_{A,c}} = 2X_{M,(a} \delta^c_{b)},$$

$$\frac{\partial z_{M,ab}}{\partial y_{A,cd}} = X^A_M \delta^c_{(a} \delta^d_{b)},$$

$$\frac{\partial L}{\partial y_{A,a}} = X^A_M \frac{\partial K}{\partial z_{M,a}} + 2X^A_{M,b} \frac{\partial K}{\partial z_{M,ab}},$$

$$\frac{\partial L}{\partial y_{A,ab}} = X^A_M \frac{\partial K}{\partial z_{M,ab}}.$$

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The Cauchy problem in general relativity. II. Main and constraint equations in the characteristic initial-value problem

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This paper applies the "y_A-formalism" of a previous paper (Paper I) to a Lagrangian formulation of the characteristic initial-value problem in general relativity. The essential content of the paper is the respective identifications of the "field equations" and "Bianchi identities" of the y_A-formalism with the "main equations" and "constraint equations" of a metric in a Bondi coordinate system. The identifications are developed in detail in the case of Bondi's (axially symmetric) radiating metric.

I. INTRODUCTION

In paper I (Ref. 1) a Lagrangian formalism, called the y_A-formalism, was developed and "field equations" and "Bianchi identities" were defined in terms of it—the field variable y_A corresponding to arbitrary functions contained in a metric. Extensive reference to paper I will be made throughout this sequel. Although the formalism can be applied quite generally to any metric containing arbitrary functions, it is used in this paper to present a Lagrangian formulation of the characteristic initial-value problem in general relativity (or more precisely it identifies those equations which can be employed to construct an integration scheme for the Einstein field equations).

In Sec. II Bondi's solution[2] of the problem is outlined (other formulations due to Sachs[3] and Tamburino and Winicour[4] follow essentially similar lines). The disadvantages of such solutions are that on the one hand they are somewhat ad hoc and on the other they are couched in coordinate-dependent language. The y_A-formalism goes someway to meet these criticisms. Section III contains the essential point of the paper, namely the respective identifications are made of Bondi's so called "main" and "constraint" equations of a metric in a Bondi coordinate system[2,3,4] with the field equations and Bianchi identities mentioned above.

The remainder of the paper is concerned specifically with developing the equations in the case of Bondi's radiating metric[2] which is axially symmetric. There is little loss in generality in assuming axial symmetry, since the procedure is quite analogous in general, but there is a considerable simplification in the expressions involved in this case. Section IV develops the main equations and Sec. V the constraint equations in the y_A-formalism. A final section presents an alternative derivation of the constraint equations by directly employing an integration procedure.

II. BONDI'S SOLUTION OF THE CHARACTERISTIC INITIAL-VALUE PROBLEM

Bondi's radiating metric[2] has the form

$$ds^2=(Vr^{-1}e^{2\beta}-U^2r^2e^{2\gamma})\,du^2+2e^{2\beta}du dr+2Ur^2e^{2\gamma}du d\theta$$
$$-r^2(e^{2\gamma}d\theta^2+e^{-2\gamma}\sin^2\theta d\phi^2) \tag{2.1}$$

where the coordinates are[5]

$$(x^a)=(x^0,x^1,x^2,x^3)=(u,r,\theta,\phi)$$

and V, U, β, and γ are four arbitrary functions of u, r, and θ. The null coordinate u is the "retarded time," r is a luminosity distance along null rays, and θ and ϕ are the usual colatitude and azimuth coordinates (as defined on a 2-sphere Σ on future null infinity $\mathcal{J}^+$). The metric is both axially symmetric, i.e., $\xi^a=\delta^a_3$ is a Killing field and so

$$g_{ab,3}=0,$$

and azimuth reflection invariant, i.e., the transformation

$$x^{0'}=x^0,\quad x^{1'}=x^1,\quad x^{2'}=x^2,\quad x^{3'}=-x^3$$

is an isometry and hence

$$g_{\alpha 3}=0.$$

The two symmetries are often referred to simply as axial symmetry and we shall use this terminology in the rest of the paper. The contravariant form of the metric is given by

$$g^{ab}=\begin{pmatrix} 0 & e^{-2\beta} & 0 & 0 \\ \cdot & -Ve^{-2\beta}r^{-1} & Ue^{-2\beta} & 0 \\ \cdot & \cdot & -e^{-2\gamma}r^{-2} & 0 \\ \cdot & \cdot & \cdot & -e^{2\gamma}r^{-2}\sin^{-2}\theta \end{pmatrix} \tag{2.2}$$

and

$$\sqrt{-g}=e^{2\beta}r^2\sin\theta.$$

Bondi splits the Einstein vacuum field equations $R_{ab}=0$ into various groups which he and others have given various names. The axial symmetry leads immediately to

(0) three symmetry conditions

$$R_{03}=R_{13}=R_{23}=0. \tag{2.3}$$

The remaining equations are

(i) four main equations

$$R_{11}=R_{1X}=R_{XY}=0; \tag{2.4}$$

(ii) one trivial equation

$$R_{01}=0; \tag{2.5}$$

(iii) two supplementary conditions (or subsidiary equations)

$$R_{00}=R_{0X}=0. \tag{2.6}$$

The main equations are split further and *combined* to give

(ia) three hypersurface equations

$$R_{11}=R_{1X}=g^{WZ}R_{WZ}=0; \tag{2.7}$$

(ib) one dynamical (standard, propagating) equation

$$R_{XY}-\tfrac{1}{2}g_{XY}g^{WZ}R_{WZ}=0. \tag{2.8}$$

[There is only one independent equation in (2.8) as contraction with g^{XY} and use of (2.1) and (2.3) will reveal.] This last important breakup is made since the dynamical equations are the only equations involving derivatives with respect to the retarded time u. We have written the equations in a slightly more general form to that given in Bondi since if we wish to drop the symmetry assumptions we simply ignore (2.3) and the break-up is then as given in Eqs. (2.4)—(2.8), although the numbers of equations involved are now 6, 1, 3, 4, and 2, respectively. In some contexts it is slightly more convenient to use the Einstein tensor in which case the above equations are equivalent to

$$\text{(0) } G_{\alpha 3}=0, \tag{2.9}$$

$$\text{(ia) } G_{1a}=0, \tag{2.10}$$

$$\text{(ib) } G_{XY}-\tfrac{1}{2}g_{XY}g^{WZ}G_{WZ}=0, \tag{2.11}$$

$$\text{(ii) } g^{WZ}G_{WZ}=0, \tag{2.12}$$

$$\text{(iii) } G_{0\alpha}=0. \tag{2.13}$$

The contracted Bianchi identities $G^{ab}{}_{;b}=0$ can now be used to prove the following lemma[3]: The trivial equation is an algebraic consequence of the main equations, and the supplementary conditions hold everywhere if they hold on a hypersurface $r=\text{const}$ and the main equations hold everywhere. There last consequences are called the constraint equations and they are

$$R_{01}=0, \tag{2.14}$$

$$\text{(iv) } R_{00}=j(u,x^W)r^{-2}, \tag{2.15}$$

$$R_{0Z}=k_Z(u,x^W)r^{-2} \tag{2.16}$$

or more precisely, if the main equations hold, then

$$R_{01}=0, \tag{2.17}$$

$$R_{01}=0\Rightarrow(r^2R_{0Z})_{,1}=0, \tag{2.18}$$

$$R_{01}=R_{0Z}=0\Rightarrow(r^2R_{00})_{,1}=0, \tag{2.19}$$

where of course Eqs. (2.18) and (2.19) lead immediately to Eqs. (2.16) and (2.15), respectively.

It now becomes a straightforward matter (in principle) to specify the initial data and integrate the field equations thus solving the characteristic initial-value problem. In particular, Bondi and Sachs adopt the boundary conditions that space—time is asymptotically flat and proceed to expand all quantities in inverse powers of r. This allows an investigation of the asymptotic properties of a bounded radiative source. Although the procedure outlined above solves the characteristic initial-value problem, as we have pointed out, it suffers on the one hand from being rather ad hoc (where does the particular break-up of the field equations come from?) and on the other from being formulated in a non covariant manner. The y_A-formalism goes some way to satisfying these objections.

III. THE y_A-FORMULATION

We start off by assuming that we have in a Bondi coordinate system a metric containing A arbitrary functions y_A. We now identify the main and constraint equations with the field equations and Bianchi identities of paper I. Thus employing the formalism of I and the numbering of the last section we define

(i) main equations[6]

$$L^A=0; \tag{3.1}$$

(iv) constraint equations

$$[t^a+2L^AY^{ab}_A\xi_b]_{,a}=0. \tag{3.2}$$

The dynamical equations are contained in (3.1) and are those equations which correspond to the y_A defining the so-called "conformal 2-structure," which for example is defined by the arbitrary function γ in (2.1). (This result will be elaborated in a paper with J. Stachel.) The hypersurface equations are the remaining main equations, hence we define

(ib) dynamical equations

$L^A=0$ corresponding to y_A defining conformal 2-structure (e.g., in Bondi $y_A\sim\gamma$, in Sachs $y_A\sim\gamma$, δ, and Tamburino and Winicour $y_A\sim g_{XY}$);

(ia) hypersurface equations

remaining main equations $L^A=0$. (3.4)

In addition, in the axially symmetric case $\xi^a=\delta^a_3$ is a Killing vector in which case equation (6.9) of paper I holds and this reduces to Eq. (2.3), namely

(0) three symmetry conditions

$$2\sqrt{-g}\,G^{\alpha}_{\ 3}=-L\delta^{\alpha}_{\ 3}-(2\sqrt{-g}\,g^{\alpha e}g^{bd}g_{3[e,d]})_{,b}. \tag{3.5}$$

Altogether we have reexpressed the following equations of Sec. II in the y_A-formalism:

(0) (3.5), (i) (3.1), (ia) (3.3), (ib) (3.4), (ii) included in (3.2), (iv) (3.2).

However the author has been unable so far to formulate the supplementary conditions (iii) in the y_A-formalism. Of course it may be that such a reformulation is not possible. One way out of this problem is the adoption of the following viewpoint: our starting point is Einstein's equations $\sqrt{-g}\,G^{ab}=0$, the above formalism allows us to extract a great deal of information contained in these equations directly applicable to the characteristic initial-value problem, any information not so gained is still contained in them and it follows from inspection that the only additional information they provide is precisely the supplementary conditions. It might be mentioned that some of the above formalism has been used by Chellone and Williams[6] (private communication) to help solve the characteristic inital-value problem for a radiating perfect fluid. The remainder of this paper is concerned with the application of the formalism to the case of Bondi's metric (2.1).

IV. THE MAIN EQUATIONS

Adopting Bondi's metric we find first of all that equation (3.5) leads to the symmetry conditions

$$G^{\alpha}{}_{3}=0 \Rightarrow G_{\alpha 3}=R_{\alpha 3}=0. \tag{4.1}$$

We now take

$$y_A=(y_0, y_1, y_2, y_3)=(V, U, \beta, \gamma) \tag{4.2}$$

and then using (2.2) a direct calculation of

$$X^{ab}_{A}=\frac{\partial g^{ab}}{\partial y_A}$$

leads to

$$\left.\begin{aligned} &X^{11}_{0}=-e^{-2\beta}r^{-1}\\ &X^{12}_{1}=X^{21}_{1}=e^{-2\beta}\\ &X^{01}_{2}=X^{10}_{2}=-2e^{-2\beta}\\ &X^{01}_{2}=X^{10}_{2}=-2e^{-2\beta},\quad X^{11}_{2}=2Ve^{-2\beta}r^{-1}\\ &X^{12}_{2}=X^{21}_{2}=-2Ue^{-2\beta}\\ &X^{22}_{3}=2e^{-2\gamma}r^{-2},\ X^{33}_{3}=-2e^{2\gamma}r^{2}\sin^{-2}\theta \end{aligned}\right\}\ \text{rest zero.} \tag{4.3}$$

Hence

$$L^A=X^{ab}_{A}\sqrt{-g}\,G_{ab}=0$$

gives as the four main equations

$$L^0=-\sqrt{-g}\,e^{-2\beta}r^{-1}G_{11}=-r\sin\theta R_{11}=0, \tag{4.4}$$

$$L^1=2e^{-2\beta}\sqrt{-g}\,G_{12}=2r^2\sin\theta R_{12}=0, \tag{4.5}$$

$$\begin{aligned} L^2&=-4e^{-2\beta}\sqrt{-g}\,G_{01}+2Ve^{-2\beta}r^{-1}\sqrt{-g}\,G_{11}-4e^{-2\beta}U\sqrt{-g}\,G_{12}\\ &=2\sqrt{-g}\,(g^{22}R_{22}+g^{33}R_{33})=0, \end{aligned} \tag{4.6}$$

$$L^3=2\sqrt{-g}\,(g^{33}G_{33}-g^{22}G_{22})=2\sqrt{-g}\,(g^{33}R_{33}-g^{22}R_{22})=0, \tag{4.7}$$

where in the second equality in (4.6) use has been made of the identity

$$R=g^{ab}R_{ab}=2g^{01}R_{01}+g^{11}R_{11}+2g^{12}R_{12}+g^{22}R_{22}+g^{33}R_{33}.$$

The first three of the main equations are the hypersurface equations and (4.7) is the dynamical equation (since $y_3=\gamma$). The four main equations given above are equivalent to the main equations as given by Bondi, which with our sign conventions are

$$-R_{11}=0,$$

$$2r^2R_{12}=0,$$

$$\sin^{-1}\theta\sqrt{-g}\,(g^{22}R_{22}+g^{33}R_{33})=0,$$

$$\sin^{-1}\theta\sqrt{-g}\,(g^{33}R_{33})=0.$$

The first three of each set of equations are the same (apart from unimportant factors) and the last equations is equivalent to L^2+L^3, where in each case the last equation alone contains retarded time derivatives. Of course we could calculate L^A directly from $L=\sqrt{-g}R$ using

$$L^A=\frac{\delta L}{\delta y_A},$$

but the above procedure relates the results more easily to those of Bondi.

In a similar manner to the above we can calculate

$$X^{A}_{ab}=\frac{\partial g_{ab}}{\partial y_A}$$

(the results are given in the Appendix) and hence obtain the main equation in terms of G^{ab} using

$$L^A=-X^{A}_{ab}\sqrt{-g}\,G^{ab}.$$

They then become

$$L^0=-r^{-1}e^{2\beta}\sqrt{-g}\,G^{00}=0, \tag{4.8}$$

$$L^1=2Ur^2e^{2\gamma}\sqrt{-g}\,G^{00}-2r^2e^{2\gamma}\sqrt{-g}\,G^{02}=0, \tag{4.9}$$

$$L^2=-2Vr^{-1}e^{2\beta}\sqrt{-g}\,G^{00}-4e^{2\beta}\sqrt{-g}\,G^{01}=0, \tag{4.10}$$

$$\begin{aligned} L^3=&2U^2r^2e^{2\gamma}\sqrt{-g}\,G^{00}-4Ur^2e^{2\gamma}\sqrt{-g}\,G^{02}\\ &-2\sqrt{-g}\,(g_{22}G^{22}-g_{33}G^{33})=0. \end{aligned} \tag{4.11}$$

Hence the main equations are equivalent to

$$G^{00}=G^{01}=G^{02}=(g_{22}G^{22}-g_{33}G^{33}). \tag{4.12}$$

This form of the main equations will be used in the next two sections.

V. THE CONSTRAINT EQUATIONS

In order to find the ξ_b in Eq. (3.2) we need to solve Eq. (5.4) of paper I, namely

$$\bar{\delta}g_{ab}=g_{ab,c}\xi^c+g_{ac}\xi^c{}_{,b}+g_{bc}\xi^c{}_{,a}=X^{A}_{bc}\bar{\delta}y_A. \tag{5.1}$$

This is a straightforward procedure as long as the equations are integrated in the correct order; for example, since $X^{A}_{11}=0$ (see Appendix)

$$0=\bar{\delta}g_{11}=2g_{1c}\xi^c{}_{,1}=2g_{01}\xi^0{}_{,1}=2e^{2\beta}\xi^0{}_{,1}$$

and hence

$$\xi^0=f(u,\theta)$$

where f is an arbitrary function of u and θ. Proceeding in this manner, we find

$$\xi^0=f(u,\theta), \tag{5.2}$$

$$\xi^1=\tfrac{1}{2}r[uf_{,2}-(\xi^2\sin\theta)_{,2}\sin^{-1}\theta], \tag{5.3}$$

$$\xi^2=h(u,\theta)+f_{,2}I, \tag{5.4}$$

$$\xi^3=c, \tag{5.5}$$

where

$$I=I(u,\theta)=\int_{\infty}^{r}r^{-2}e^{2(\beta-\gamma)}dr.$$

Thus ξ^a involves two arbitrary functions f and h and a constant c. These equations determine the descriptors ξ^a of the infinitesimal coordinate transformations which preserve the coordinate conditions used in deriving Bondi's metric.

We next need to construct the nonunique matrix

$$Y^{ab}_{A}=\frac{\partial y_A}{\partial g_{ab}}.$$

For example, when $y_A=\beta$ then using $g_{01}=e^{2\beta}$ (the only covariant metric component involving β alone) we can write

$$\beta=\tfrac{1}{2}\ln g_{01}$$

and so

$$\frac{\partial\beta}{\partial g_{01}}=\frac{1}{2g_{01}}=\tfrac{1}{2}e^{-2\beta},$$

$$\frac{\partial\beta}{\partial g_{ab}}=0 \quad \text{for } a\neq 0,\quad b\neq 1.$$

Since we require Y^{ab}_{A} to be symmetrized, we take

$$Y^{01}_{2}=Y^{10}_{2}=\tfrac{1}{4}e^{-2\beta},$$

or alternatively we could have obtained this by writing

$$\beta = \tfrac{1}{2}\ln(g_{01} + g_{10}).$$

The nonuniqueness shows itself in the fact that we can take γ to be defined in terms of g_{22}, or g_{33}, or g_{22} and g_{33}, but this does not materially affect the ensuing calculations. One choice of Y_A^{ab} is

$$\left.\begin{aligned} &Y_0^{00} = re^{-2\beta}, \quad Y_0^{01} = Y_0^{10} = -\tfrac{1}{2}Ve^{-2\beta} \\ &Y_0^{02} = Y_0^{20} = rUe^{-2\beta} \\ &Y_1^{02} = Y_1^{20} = \tfrac{1}{2}r^{-2}e^{-2\gamma} \\ &Y_1^{33} = -Ue^{2\gamma}r^{-2}\sin^{-2}\theta \\ &Y_2^{01} = Y_2^{10} = \tfrac{1}{4}e^{-2\beta} \\ &Y_3^{33} = \tfrac{1}{2}r^{-2}\sin^{-2}\theta e^{2\gamma} \end{aligned}\right\} \text{rest zero.} \qquad (5.6)$$

From this and from Eqs. (4.8)—(4.11) we can calculate $L^A Y_A^{ab}$ in terms of G^{ab}, say, to get

$$\left.\begin{aligned} &L^A Y_A^{00} = -\sqrt{-g}\,G^{00} \\ &L^A Y_A^{01} = -\sqrt{-g}\,G^{01} \\ &L^A Y_A^{02} = -\sqrt{-g}\,G^{02} \\ &L^A Y_A^{33} = -r^{-2}e^{2\gamma}\sin^{-2}\theta\sqrt{-g}\,(g_{22}G^{22} - g_{33}G^{33}) \end{aligned}\right\} \text{rest zero,} \qquad (5.7)$$

[compare with (4.12)]. The first three equations are particular instances of Eq. (7.8) of Paper I.

The constraint equations are

$$[t^a + 2L^A Y_A^{ab}\xi_b]_{,a} = [2\sqrt{-g}\,G^{ab}\xi_b + 2(\sqrt{-g}\,\xi^{[a;b]})_{,b} + 2L^A Y_A^{ab}\xi_b]_{,a} \equiv 0$$

where we have used Eq. (3.5) of Paper I. Since the middle term in the second square brackets vanishes identically when its divergence is taken, we can write the equation in the form

$$b^a{}_{,a} \equiv 0,$$

where

$$\begin{aligned} b^a &= 2\sqrt{-g}\,G^{ab}\xi_b + 2L^A Y_A^{ab}\xi_b \\ &= 2\sqrt{-g}\,[0, (G^{11}\xi_1 + G^{12}\xi_2), (G^{12}\xi_1 + G^{22}\xi_2), e^{4\gamma}\sin^{-2}\theta G^{22}]. \end{aligned}$$

Hence

$$b^a{}_{,a} = [2\sqrt{-g}\,(G^{11}\xi_1 + G^{12}\xi_2)]_{,1} + [2\sqrt{-g}\,(G^{12}\xi_1 + G^{22}\xi_2)]_{,2} \equiv 0. \qquad (5.8)$$

Using (5.2)—(5.5) we can find $\xi_a = g_{ab}\xi^b$ and in particular

$$\xi_1 = e^{2\beta}f,$$

$$\xi_2 = Ur^2e^{2\gamma}f - r^2e^{2\gamma}(h + f_{,2}I).$$

Substituting in (5.8) gives

$$\begin{aligned} b^a{}_{,a} = {} & 2[\sqrt{-g}\,G^{11}e^{2\beta}f + \sqrt{-g}\,G^{12}(Ur^2e^{2\gamma}f - r^2e^{2\gamma}h - r^2e^{2\gamma}f_{,2}I)]_{,1} \\ & + 2[\sqrt{-g}\,G^{12}e^{2\beta}f + \sqrt{-g}\,G^{22}(Ur^2e^{2\gamma}f - r^2e^{2\gamma}h \\ & - r^2e^{2\gamma}f_{,2}I)]_{,2} \equiv 0. \end{aligned} \qquad (5.9)$$

Since this expression vanishes identically the coefficients of algebraically independent terms must vanish. The coefficient of $h_{,2}$ is

$$-e^{2(\beta+\gamma)}r^4\sin\theta G^{22} \Rightarrow G^{22} = 0.$$

But

$$L^A = 0 \text{ and } G^{22} = 0 \Rightarrow R = 0 \Rightarrow R_{01} = 0$$

which gives the constraint equation (2.17). Similarly, assuming $L^A = 0$ and the algebraic consequence $R_{01} = 0$ then the coefficient of h in (5.9) reduces to

$$[(r^2R_{02})_{,1}]\sin\theta = 0$$

which gives (2.18). Finally, assuming $L^A = R_{01} = R_{02} = 0$, the coefficient of f in (5.9) reduces to

$$[(r^2R_{00})_{,1}]\sin\theta = 0$$

which gives (2.19). So collecting the results together we obtain the constraint equations

$$\begin{aligned} &L^A = 0 && \Rightarrow R_{01} = 0, \\ &L^A = R_{01} = 0 && \Rightarrow R_{02} = k(u, \theta)r^2, \\ &L^A = R_{01} = R_{02} = 0 && \Rightarrow R_{00} = j(u, \theta)r^{-2}. \end{aligned}$$

VI. AN INTEGRATION PROCESS FOR THE CONSTRAINT EQUATIONS

We finally show how the constraint equations may be derived directly by the integration process described in Sec. VII of I for obtaining Bianchi identities. The integration will be taken over the region D lying between two null hypersurfaces on which u = constant, called s_T (top) and s_B (bottom), and two time-like hypersurfaces, exterior to any source, on which r + constant, called s_I (inside) and s_O (outside), (see Fig. 1). The basic identity

$$L^A\bar{\delta}y_A + t^a{}_{,a} \equiv 0$$

implies that when the main equations hold

$$t^a{}_{,a} = (2\sqrt{-g}\,G^a{}_b\xi^b)_{,a} \equiv 0$$

so that

$$\int_D t^a{}_{,a}\,d^4x = \int_{\partial D} 2\sqrt{-g}\,G^{ab}\xi_b n_a\,d^3x \equiv 0. \qquad (6.1)$$

Now on s_T, s_B, s_O, and s_I the normal vector field n_a is given by δ_a^0, $-\delta_a^0$, δ_a^1, and $-\delta_a^1$, respectively. Assuming the main equations (4.12) then the integrand in the second integral in (6.1) vanishes on s_T and s_B. Hence Eq. (6.1) reduces to

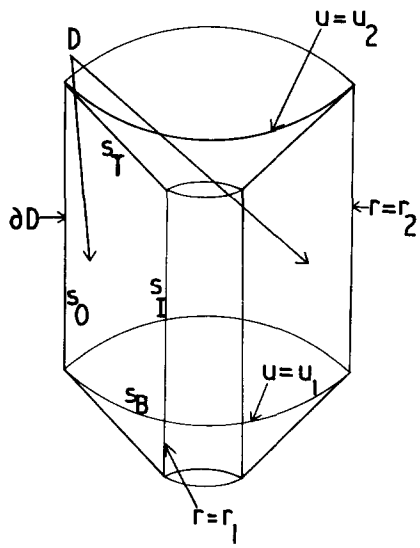

FIG. 1. The region of integration D.

$$\int_{s_I} 2\sqrt{-g}G^{1b}\xi_b d^3x = \int_{s_0} 2\sqrt{-g}G^{1b}\xi_b d^3x$$

and since s_I and s_O are arbitrary, this implies

$$\frac{\partial}{\partial r}\int_{s_I} \sqrt{-g}G^{1b}\xi_b d^3x \equiv 0. \tag{6.2}$$

However,

$$\int_{s_I} \sqrt{-g}G^{1b}\xi_b d^3x = \int_{s_I} \sqrt{-g}G^{1b}\xi_b du d\theta d\phi = 2\pi J$$

where

$$J = \int_{u=u_1}^{u_2}\int_{\theta=0}^{2\pi} \sqrt{-g}(G^{11}\xi_1 + G^{12}\xi_2)\, du d\theta,$$

so that Eq. (6.2) becomes

$$J_{,1} \equiv 0. \tag{6.3}$$

We now evaluate J for two choices of ξ_1 and ξ_2. In Eqs. (5.2)—(5.5) we let

(a) $f = 0$,

$h = \delta(u-u_0)\delta(\theta-\theta_0)$ where $u_1 < u_0 < u_2$, $0 < \theta_0 < \pi$,

$c = 0$.

Then using the main equations we find

$$J = [r^2 R_{02}]_{\substack{u=u_0 \\ \theta=\theta_0}} \sin\theta_0$$

and so Eq. (6.3) leads to Eq. (2.18), the second constraint equation. Similarly, the choice

(b) $f = \delta(u-u_0)\delta(\theta-\theta_0)$ where $u_1 < u_0 < u_2$, $0 < \theta_0 < \pi$,

$g = 0$,

$c = 0$,

leads to Eq. (2.19), the third constraint equation. We do not obtain the trivial constraint equation $R_{01} = 0$ with this approach, but as its name implies the equation contains *no* additional information being merely an algebraic consequence of the main equations.

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APPENDIX

The quantities X^A_{ab} for Bondi's metric are

$$\left.\begin{aligned} &X^0_{00} = r^{-1}e^{2\beta}, \\ &X^1_{00} = -2Ur^2e^{2\gamma}, \quad X^1_{02} = X^1_{20} = r^2e^{2\gamma}, \\ &X^2_{00} = 2Vr^{-1}e^{2\beta}, \quad X^2_{01} = X^2_{10} = 2e^{2\beta}, \\ &X^3_{00} = -2U^2r^2e^{2\gamma}, \quad X^3_{02} = X^3_{20} = 2Ur^2e^{2\gamma}, \\ &X^3_{22} = -2r^2e^{2\gamma}, \quad X^3_{33} = 2r^2e^{-2\gamma}\sin^2\theta \end{aligned}\right\} \text{rest zero.}$$

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The Weyl and Dirac equations in terms of functions over the group SU_2*

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Carmeli's approach to Maxwell's equations, in which the field variables are considered as functions of the group SU_2, is extended to two-component Weyl spinors and four-component Dirac spinors. The Weyl and Dirac equations are formulated over the group SU_2, the relevent functions are shown to be "quantities of spin-weight $s = \pm 1/2$"; they are expanded in a generalized Fourier series and the equations for the coefficients are derived. The "quantities of spin-weight s" are shown to be closely related to eigenvectors and eigenspinors of the radial spin operator $\hat{n} \cdot \mathbf{s}$.

1. INTRODUCTION

A method for writing vector fields as functions over the elements u of the group SU_2 (the group of all unitary matrices of order two and determinant unity) was recently developed by Carmeli.[1,2] He utilized the method to write down and solve Maxwell's equations without sources.[3] Instead of describing the electromagnetic field in terms of electric and magnetic vector fields, or a vector potential, he introduced three complex functions $\eta_\pm$, η_0, whose independent variables are t, r, u, (t—the time, r—the radius in polar coordinates, u—an element of the group SU_2), rather than the customary variables t, r, θ, ϕ. The exact definitions of functions $\eta_\pm$, η_0 is given in Sec. 2. The elements $u \in SU_2$ depend on three parameters, θ, ϕ_1, ϕ_2, and one obtains the physical field functions by setting $\phi_2 = 0$.

It was shown by Carmeli that the problem of solving Maxwell's equations reduces to the solution for one scalar complex function only, namely η_0, and the other two functions, η_+ and η_-, are uniquely determined by η_0. Since the electromagnetic field has, in fact, two degrees of freedom, this formulation is free of all gauge problems. This formulation was subsequently extended to include Maxwell's equations with sources.[4] In the same paper Carmeli quantized the wave equation for η_0 for the case without charges, the canonical quantization procedure being entirely gauge-free.

Barut, Carmeli, and the present author have subsequently applied Carmeli's approach to the general formulation of scattering of eletromagnetic waves.[5] In particular, the differential cross section was obtained as a sum of two noninterfering spherical waves, which can be considered as the spherical wave analog of the positive and negative helicities of plane waves.

In the present paper Carmeli's method is further developed by writing spinor fields as functions of the elements u of the group SU_2. After summarizing previous results in Sec. 2 we derive in Sec. 3 the Weyl equation over the group SU_2. This derivation features the so-called "quantities of spin-weight s" which were first introduced by Newman and Penrose in their spinor formulation of the Einstein equations of general relativity, as "spin-s spherical harmonics"[6] and subsequently used and investigated by Moses,[7] Goldberg *et al.*,[8] and Carmeli.[1] These quantities are expanded in Sec. 4 in a generalized Fourier series[9] and the equations for the coefficients are obtained.

Section 5 includes the expression of four-component Dirac spinors as functions of the elements of the group SU_2, derivation of the Dirac equation within this framework, the corresponding generalized Fourier expansion, and the equation for the coefficients.

The physical interpretation of "quantities of spin-weight s" is derived in Section 6. They are shown to be closely related to the eigenvectors and eigenspinors of the radial spin operator $\hat{n} \cdot \mathbf{s}$ ($\hat{n}$ is the unit vector in the radial direction, $\mathbf{s}$ is the spin operator).

2. CARMELI'S GROUP ANALYSIS OF MAXWELL EQUATIONS

Consider Maxwell's equations with or without sources and introduce the complex vector field

$$\mathbf{V} = \mathbf{E} + iB. \tag{2.1}$$

Using the notation

$$V_\pm = -2^{-1/2}(V_\phi \pm V_\theta), \quad V_0 = V_r, \tag{2.2}$$

we introduce the functions

$$\eta_\pm = V_\pm \exp(\mp i\phi_2), \quad \eta_0 = V_0, \tag{2.3}$$

where ϕ_2, together with the usual angular variables ϕ, θ, is such that with any value of the variables ϕ, θ, ϕ_2 we can associate a rotation $g \in O_3$, whose Euler angles are $(\pi/2) - \phi, \theta, \phi_2$. The functions $\eta_\pm, \eta_0$ can be considered, therefore, as functions over the group O_3 for each value of the time t and the radius r in polar coordinates. It turns out to be more convenient to consider the functions $\eta_\pm, \eta_0$ over SU_2, the covering group of O_3, rather than O_3 itself. Euler angles are again employed to describe an element $u \in SU_2$,

$$u = \begin{pmatrix} \cos\tfrac{1}{2}\theta \exp[\tfrac{1}{2}i(\phi_1 + \phi_2)] & i\sin\tfrac{1}{2}\theta \exp[-\tfrac{1}{2}i(\phi_1 - \phi_2)] \\ i\sin\tfrac{1}{2}\theta \exp[\tfrac{1}{2}i(\phi_1 - \phi_2)] & \cos\tfrac{1}{2}\theta \exp[-\tfrac{1}{2}i(\phi_1 + \phi_2)] \end{pmatrix}, \tag{2.4}$$

where $\phi_1 = \pi/2 - \phi$.

It was shown by Carmeli[3] that Maxwell's equations in free space are equivalent to the following set of equations for the η functions:

$$\begin{aligned} &\frac{1}{\sqrt{2}}\frac{1}{r}\left(\frac{\partial}{\partial r} \pm \frac{\partial}{\partial t}\right)(r^2\eta_0) \mp K_\pm \eta_\mp = 0, \\ &\left(\pm\frac{\partial}{\partial r} + \frac{\partial}{\partial t}\right)(r\eta_\pm) + \frac{1}{\sqrt{2}}K_\pm \eta_0 = 0, \end{aligned} \tag{2.5}$$

where the operators $K_\pm$ are defined by

$$K_\pm = \exp(\pm i\phi_2)\left(\pm \cot\theta \frac{\partial}{\partial \phi_2} + i\frac{\partial}{\partial\theta} \mp \csc\theta \frac{\partial}{\partial \phi_1}\right). \tag{2.6}$$

These operators, along with

$$K_3 = i\frac{\partial}{\partial \phi_2}, \tag{2.7}$$

are well known from the theory of representations of SU_2. They satisfy the following relations[1]:

$$\begin{aligned} K_\pm T^j_{mn} &= [(j \pm m + 1)(j \mp m)]^{1/2} T^j_{m\pm1,n}, \\ K_3 T^j_{mn} &= m T^j_{mn}, \end{aligned} \tag{2.8}$$

where $T^j_{mn}(u)$ are the matrix elements of the irreducible representation of weight j of the group SU_2.

The functions $\eta_\pm$ and η_0 can be expanded in the following way:

$$\begin{aligned} \eta_\pm(t, r, u) &= \sum_{j=1}^{\infty} \sum_{n=-j}^{j} \alpha^j_{\pm1,n}(t, r) T^j_{\pm1,n}(u), \\ \eta_0(t, r, u) &= \sum_{j=0}^{\infty} \sum_{n=-j}^{+j} \alpha^j_{0,n}(t, r) T^j_{0,n}(u), \end{aligned} \tag{2.9}$$

where the coefficients are given by

$$\begin{aligned} (2j+1)^{-1}\alpha^j_{\pm1,n}(t, r) &= \int \eta_\pm(t, r, u)\overline{T^j_{\pm1,n}(u)}\, du, \\ (2j+1)^{-1}\alpha^j_{0,n}(t, r) &= \int \eta_0(t, r, u)\overline{T^j_{0,n}(u)}\, du, \end{aligned} \tag{2.10}$$

and $du = (1/16)\pi^{-2}\sin\theta\, d\phi_1\, d\theta\, d\phi_2$ is the invariant measure over SU_2, normalized so that $\int du = 1$.

Substitution of Eq. (2.9) in Eq. (2.5) yields the partial differential equations for $\alpha^j_{\pm1,m}$, $\alpha^j_{0,m}$:

$$\frac{1}{\sqrt{2}}\frac{1}{r}\left(\frac{\partial}{\partial r} \pm \frac{\partial}{\partial t}\right)(r^2\alpha^j_{0,m}) \mp [j(j+1)]^{1/2}\alpha^j_{\pm1,m} = 0, \tag{2.11}$$

$$\left(\pm\frac{\partial}{\partial r} + \frac{\partial}{\partial t}\right)(r\alpha^j_{\pm1,m}) + \left(\frac{j(j+1)}{2}\right)^{1/2}\alpha^j_{0,m} = 0, \tag{2.12}$$

where $j = 1, 2, 3, \cdots$ for $\alpha^j_{\pm1,m}$ and $j = 0, 1, 2, 3, \cdots$ for $\alpha^j_{0,m}$, and $m = -j, -j+1, \ldots, j$ for both cases. By elimination we get a separate partial differential equation for $\alpha^j_{0,m}$ and expression of $\alpha^j_{\pm1,m}$ in terms of $\alpha^j_{0,m}$:

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial r^2}\right)(r^2\alpha^j_{0,m}) + j(j+1)\alpha^j_{0,m} = 0,$$

$$j = 0, 1, 2, \cdots, \quad m = -j, \ldots, +j, \tag{2.13}$$

$$\alpha^j_{\pm1,m} = \pm 1/[2j(j+1)]^{1/2}\frac{1}{r}\left(\frac{\partial}{\partial r} \pm \frac{\partial}{\partial t}\right)(r^2\alpha^j_{0,m}),$$

$$j = 1, 2, \cdots, \quad m = -j, \ldots, j. \tag{2.14}$$

We thus arrive at the conclusion that the functions $\alpha^j_{0,m}(t, r)$ determine $\alpha^j_{\pm1,m}$ completely, through substitution in Eq. (2.14). The problem of solving Maxwell's equations reduces, therefore, to the solution of Eq. (2.13) for a single scalar complex function $\eta_0(t, r, u)$.

3. THE WEYL EQUATION

The Weyl equation in the natural system of units $\hbar = c = 1$,

$$i\frac{\partial}{\partial t}\psi = (\boldsymbol{\sigma}\cdot\mathbf{p})\psi, \tag{3.1}$$

where $\mathbf{p} = (-i\,\partial/\partial x, -i\,\partial/\partial y, -i\,\partial/\partial z)$ and $\sigma_1, \sigma_2, \sigma_3$ are the usual Pauli matrices, can be expressed in spherical coordinates using the following relationships[10,11]:

$$\mathbf{p} = \hat{n}(\hat{n}\cdot\mathbf{p}) - \hat{n}\times(\hat{n}\times\mathbf{p}) = \hat{n}(\hat{n}\cdot\mathbf{p}) - \hat{n}\times\mathbf{L}/r, \tag{3.2}$$

$$(\boldsymbol{\sigma}\cdot\mathbf{p}) = (\boldsymbol{\sigma}\cdot\hat{n})(\hat{n}\cdot\mathbf{p}) - (1/r)(\boldsymbol{\sigma}\cdot\hat{n})(\boldsymbol{\sigma}\cdot\mathbf{L}). \tag{3.3}$$

where $\hat{n}$ is the unit vector in the radial direction. One then obtains the equation

$$\frac{\partial}{\partial t}\psi = \left[-(\boldsymbol{\sigma}\cdot\hat{n})\frac{\partial}{\partial r} + \frac{1}{r}(\boldsymbol{\sigma}\cdot\hat{n})(\boldsymbol{\sigma}\cdot\mathbf{L})\right]\psi \tag{3.4}$$

for the two-component spinor $\psi(t, r, \theta, \phi)$, where t is the time and r, θ, ϕ are spherical coordinates in Euclidean space. Defining now, in each point of space–time, the fundamental two-component spinors

$$q_+ = \begin{pmatrix} i\cos\frac{1}{2}\theta\exp(-i\varphi/2) \\ i\sin\frac{1}{2}\theta\exp(i\varphi/2)\end{pmatrix}, \quad q_- = \begin{pmatrix} -\sin\frac{1}{2}\theta\exp(-i\varphi/2) \\ \cos\frac{1}{2}\theta\exp(i\varphi/2)\end{pmatrix} \tag{3.5}$$

we expand the given spinor ψ in terms of q_+ and q_- as follows:

$$\psi(t, r, \theta, \phi) = f_+(t, r, \theta, \phi)\cdot q_+ + f_-(t, r, \theta, \phi)\cdot q_-, \tag{3.6}$$

where

$$f_\pm(t, r, \theta, \phi) = \psi^\dagger(t, r, \theta, \phi)\cdot q_\pm(\theta, \phi)\ . \tag{3.7}$$

$\psi^\dagger$ is the Hermitian conjugate of ψ. Equation (3.7) is derived using the orthogonality relationships

$$\begin{aligned} q^\dagger_+(\theta, \phi)q_+(\theta, \phi) &= q^\dagger_-(\theta, \phi)q_-(\theta, \phi) = 1, \\ q^\dagger_+(\theta, \phi)q_-(\theta, \phi) &= q^\dagger_-(\theta, \phi)q_+(\theta, \phi) = 0. \end{aligned} \tag{3.8}$$

The fundamental two-component spinors q_+ and q_- are eigenspinors of the radial spin operator $\boldsymbol{\sigma}\cdot\hat{n}$:

$$(\boldsymbol{\sigma}\cdot\hat{n})q_\pm = \begin{pmatrix}\cos\theta & \sin\theta\exp(-i\phi) \\ \sin\theta\exp(i\phi) & -\cos\theta\end{pmatrix}q_\pm = \pm q_\pm. \tag{3.9}$$

A straightforward calculation yields, furthermore,

$$\begin{aligned} (\boldsymbol{\sigma}\cdot\mathbf{L})q_\pm &= \begin{pmatrix} -i\frac{\partial}{\partial\varphi} & \exp(-i\varphi)\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) \\ \exp(i\varphi)\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) & i\frac{\partial}{\partial\varphi}\end{pmatrix}\cdot q_\pm \\ &= -q_\pm + \tfrac{1}{2}i\cot\theta\ q_\mp. \end{aligned} \tag{3.10}$$

Substituting the expansion (3.6) in the Weyl equation (3.4), one obtains

$$\begin{aligned} \frac{\partial f_+}{\partial t}q_+ + \frac{\partial f_-}{\partial t}q_- &= -\frac{\partial f_+}{\partial r}q_+ + \frac{\partial f_-}{\partial r}q_- \\ &\quad + \frac{1}{r}(\boldsymbol{\sigma}\cdot\hat{n})\{[(\boldsymbol{\sigma}\cdot\mathbf{L})f_+]q_+ + f_+(\boldsymbol{\sigma}\cdot\mathbf{L})q_+ \\ &\quad + [(\boldsymbol{\sigma}\cdot\mathbf{L})f_-]q_- + f_-(\boldsymbol{\sigma}\cdot\mathbf{L})q_-\}. \end{aligned} \tag{3.11}$$

The two-component spinors $[(\boldsymbol{\sigma}\cdot\mathbf{L})f_+]q_+$ and $[(\boldsymbol{\sigma}\cdot\mathbf{L})f_-]q_-$ can be expanded in the form (3.6) as follows:

$$\begin{aligned} [(\sigma\cdot L)f_+]q_+ &= a_{++}q_+ + a_{+-}q_-, \\ [(\sigma\cdot L)f_-]q_- &= a_{-+}q_+ + a_{--}q_-, \end{aligned} \tag{3.12}$$

where, by Eq. (3.7),

$$a_{++} = q^\dagger_+[(\boldsymbol{\sigma}\cdot\mathbf{L})f_+]q_+ = 0,$$

$$a_{+-} = q^\dagger_-[(\boldsymbol{\sigma}\cdot\mathbf{L})f_+]q_+ = \left(i\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right)f_+,$$

$$a_{-+} = q_+^\dagger[(\sigma\cdot\mathbf{L})f_-]q_- = \left(i\frac{\partial}{\partial\theta} - \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right)f_-, \tag{3.13}$$

$$a_{--} = q_-^\dagger[(\sigma\cdot\mathbf{L})f_-]q_- = 0.$$

Substitution of Eqs. (3.9), (3.10), (3.12), (3.13) in Eq. (3.11) and equating the coefficient of q_+ and q_- to zero yields the wave-equations for f_+ and f_-:

$$\left(\frac{\partial}{\partial t} \pm \frac{\partial}{\partial r} \pm \frac{1}{r}\right)f_\pm \mp \frac{1}{r}\left(i\frac{\partial}{\partial\theta} \pm \frac{1}{\sin\theta}\frac{\partial}{\partial\phi} + \frac{i}{2}\cot\theta\right)f_\mp = 0. \tag{3.14}$$

To write Eqs. (3.14) over the group SU_2, we express the polar angle ϕ in terms of one of the Euler angles $\phi_1 = \frac{1}{2}\pi - \phi$; $\partial/\partial\phi$ will be replaced, therefore, by $-\partial/\partial\phi_1$. Furthermore, defining now the functions

$$\xi_\pm = f_\pm \exp(\mp i\phi_2/2) \tag{3.15}$$

and introducing the operators (2.6) and (2.7), namely,

$$K_\pm = \exp(\mp i\phi_2/2)\left(i\frac{\theta}{\partial\theta} \mp \frac{1}{\sin\theta}\frac{\partial}{\partial\phi_1} \mp \cot\theta\frac{\partial}{\partial\phi_2}\right), \tag{3.16}$$

$$K_3 = i\frac{\partial}{\partial\phi_2},$$

we can write Eq. (3.14) in the form

$$\left(\frac{\partial}{\partial t} \pm \frac{\partial}{\partial r}\right)(r\xi_\pm) \mp K_\pm\xi_\mp = 0. \tag{3.17}$$

Equation (3.17) is the Weyl equation written partially over the group SU_2. The functions ξ_+ and ξ_- are functions of the space–time coordinates t and r as well as the three parameters θ, ϕ_1, ϕ_2 of the group SU_2. As pointed out in the previous section the operators $K_\pm$ and K_3 are the infinitesimal operators of SU_2.

4. QUANTITIES OF SPIN WEIGHT $s = \pm\frac{1}{2}$

In their spinor formulation of the equations of general relativity Newman and Penrose[6] introduced a class of functions ${}_sY_{jm}(\phi,\theta)$, defined on the surface of a sphere and called spin-s spherical harmonics. These and related functions were subsequently discussed by other authors[7,8] and were shown to be related to the matrix elements T^j_{mn} of the representations of the rotation group. The group theoretical and geometrical interpretation of these functions was established by Carmeli.[1] He has shown, in particular, that functions $f(u)$ defined over the group SU_2 are quantities of spin-weight s if and only if they satisfy the equation

$$f(\chi u) = \exp(is\alpha)f(u) \tag{4.1}$$

where

$$\chi = \begin{pmatrix}\exp(-i\alpha/2) & 0\\ 0 & \exp(i\alpha/2)\end{pmatrix}, \quad \alpha \text{ real}, \tag{4.2}$$

is an element of the group SU_2.

Since the matrix elements $T^j_{mn}(u)$ of all the irreducible representations of the group SU_2 form a complete orthogonal set over the group, any function $f(u)$, $u \in SU_2$, which satisfies

$$\int |f(u)|^2\,du < \infty \tag{4.3}$$

can be uniquely expanded in the $T^j_{sm}(u)$:

$$f(u) = \sum_j \sum_{m=-j}^{j}\sum_{n=-j}^{j} \beta^j_{mn}T^j_{mn}(u), \tag{4.4}$$

where

$$\beta^j_{mn} = (2j+1)\int f(u)\overline{T^j_{mn}(u)}\,du. \tag{4.5}$$

$\overline{T^j_{mn}(u)}$ is the complex conjugate of $T^j_{mn}(u)$. Equation (4.5) follows from the orthogonality relations of the T^j_{sm}:

$$\int T^j_{mn}(u)\overline{T^{j'}_{s'm'}(u)}\,du = \frac{1}{2j+1}\delta_{jj'}\delta_{ss'}\delta_{mm'}. \tag{4.6}$$

Carmeli has shown that if the function $f(u)$ is a quantity of spin weight s then the triple sum (4.4) reduces to a double sum as follows:

$$f(u) = \sum_{j=|s|}^{\infty}\sum_{n=-j}^{j} \beta^j_{sn}T^j_{sn}(u). \tag{4.7}$$

It follows from Eqs. (2.4), (4.1), and (4.2) that the functions $\xi_\pm(t,r,u)$, introduced in the last section, are quantities of spin $\pm\frac{1}{2}$. Consequently, they can be expanded in the series (4.7):

$$\xi_\pm(t,r,u) = \sum_{j=\frac{1}{2}}^{\infty}\sum_{n=-j}^{j} \beta^j_{\pm1/2,n}(t,r)T^j_{\pm1/2,n}(u), \tag{4.8}$$

where

$$\beta^j_{\pm1/2,n}(t,r) = (2j+1)\int \overline{T^j_{\pm1/2,n}(u)}\,\xi_\pm(t,r,u)\,du. \tag{4.9}$$

substituting Eq. (4.8) in the Weyl Equation (2.8) and making use of Eq. (3.16), we obtain the equations for the coefficients $\beta^j_{\pm1/2,n}(t,r)$:

$$\left(\frac{\partial}{\partial t} \pm \frac{\partial}{\partial r}\right)(r\beta^j_{\pm1/2,n}) \mp (j+\tfrac{1}{2})\beta^j_{\mp1/2,n} = 0, \tag{4.10}$$

where $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots$ and $n = -j, -j+1, \ldots, j$. For each value of (j,n) we obtained a separate set of two partial differential equations for $\beta^j_{+1/2,n}(t,r)$ and $\beta^j_{-1/2,n}(t,r)$.

By elimination we can obtain a separate partial differential equation for $\beta^j_{+1/2,n}$ and express $\beta^j_{-1/2,n}$ in terms of $\beta^j_{+1/2,n}$:

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial r^2}\right)(r\beta^j_{+1/2,n}) - \left(\frac{\partial}{\partial t} - \frac{\partial}{\partial r}\right)(r\beta^j_{+1/2,n}) + (j+\tfrac{1}{2})^2\beta^j_{+1/2,n} = 0, \tag{4.11}$$

$$\beta^j_{-1/2,n} = \frac{1}{j+\frac{1}{2}}\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial r}\right)(r\beta^j_{+1/2,n}).$$

Or, equivalently, one can solve for $\beta^j_{-1/2,n}$ and express $\beta^j_{+1/2,n}$ in terms of $\beta^j_{-1/2,n}$:

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial r^2}\right)(r\beta^j_{-1/2,n}) + \left(\frac{\partial}{\partial t} + \frac{\partial}{\partial r}\right)(r\beta^j_{-1/2,n}) + (j+\tfrac{1}{2})^2\beta^j_{-1/2,n} = 0,$$

$$\beta^j_{+1/2,n} = -\frac{1}{j+\frac{1}{2}}\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial r}\right)(r\beta^j_{-1/2,n}). \tag{4.12}$$

If the solution of Eq. (10) is expanded in the form

$$\beta^j_{+1/2,n}(t,r) = (1/r)\int Q^j_{+1/2,n}(k,r)\exp(-ikt)\,dk, \tag{4.13}$$

we obtain for $Q^j_{+1/2,n}(k,r)$ the following pair of ordinary differential equations:

$$\left(-\frac{ik}{r} \pm \frac{\partial}{\partial r}\right)Q^j_{\pm1/2,n} \mp (j+\tfrac{1}{2})\,Q^j_{\mp1/2,n} = 0. \tag{4.14}$$

5. THE DIRAC EQUATION

In Dirac theory the four-component wavefunctions ψ

satisfy the equation

$$i\frac{\partial}{\partial t}\psi=\left[-i\hbar\left(\alpha_1\frac{\partial}{\partial x}+\alpha_2\frac{\partial}{\partial y}+\alpha_3\frac{\partial}{\partial z}\right)+m\beta\right]\psi, \tag{5.1}$$

the natural system of units $\hbar=c=1$ is used again and α_1, α_2, α_3, and β are 4×4 matrices satisfying the anti-commutation relations

$$\begin{aligned}&\alpha_i\alpha_j+\alpha_j\alpha_i=2\delta_{ij}I,\\&\beta\alpha_i+\alpha_i\beta=0,\\&\beta^2=I,\end{aligned} \tag{5.2}$$

I being the unit matrix. The derivations of the present section will be carried out in Pauli's representation of the matrices α_i, β.[12] Defining the 2×2 matrices

$$\rho_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \rho_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \rho_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{5.3}$$

the 4×4 matrices α_i, β are given in Pauli's representation by

$$\alpha_i=\rho_1\sigma_i=\begin{pmatrix}0&\sigma_i\\\sigma_i&0\end{pmatrix},\quad \beta=\rho_3 I=\begin{pmatrix}I&0\\0&-I\end{pmatrix} \tag{5.4}$$

where the σ_i are Pauli's spin matrices.

Dirac equation in spherical coordinates is given in Pauli's representation as follows[10,11]:

$$\frac{\partial}{\partial t}\psi=\left(-\rho_1(\boldsymbol{\sigma}\cdot\hat{n})\frac{\partial}{\partial r}+\frac{1}{r}\rho_1(\boldsymbol{\sigma}\cdot\hat{n})(\boldsymbol{\sigma}\cdot\mathbf{L})-im\rho_3 I\right)\psi. \tag{5.5}$$

Consider now the following four-component spinors:

$$y_\pm^{(1)}=\begin{pmatrix}q_\pm\\0\end{pmatrix},\quad y_\pm^{(2)}=\begin{pmatrix}0\\q_\pm\end{pmatrix}, \tag{5.6}$$

where $q_\pm$ are the fundamental two-component spinors (3.5). It follows from Eqs. (3.9), (3.10), and (5.3) that the four-component spinors $y_\pm^{(1,2)}$ satisfy the following equations[13]:

$$(\boldsymbol{\sigma}\cdot\hat{n})y_\pm^{(1,2)}=y_\pm^{(1,2)}, \tag{5.7}$$

$$\rho_1 y_\pm^{(1,2)}=y_\pm^{(2,1)}, \tag{5.8}$$

$$\rho_3 y_\pm^{(1)}=y_\pm^{(1)},\quad \rho_3 y_\pm^{(2)}=-y_\pm^{(2)}, \tag{5.9}$$

$$(\boldsymbol{\sigma}\circ\mathbf{L})\,y_\pm^{(1,2)}=-y_\pm^{(1,2)}+\tfrac{1}{2}i\cot\theta y_\mp^{(1,2)}. \tag{5.10}$$

Furthermore, because of Eqs. (3.12), (3.13), and (5.10), given any function $f=f(t,r,\theta,\phi)$,

$$\begin{aligned}&(\boldsymbol{\sigma}\circ\mathbf{L})(fy_\pm^{(1,2)})\\&\quad=[(\boldsymbol{\sigma}\cdot\mathbf{L})f]y_\pm^{(1,2)}+f\circ(\boldsymbol{\sigma}\cdot\mathbf{L})y_\pm^{(1,2)}\\&\quad=-y_\pm^{(1,2)}+\left[\left(i\frac{\partial}{\partial\theta}\mp\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}+\tfrac{1}{2}i\cot\theta\right)f\right]y_\mp^{(1,2)}.\end{aligned} \tag{5.11}$$

In analogy with Eqs. (3.6), (3.7) for two-component spinors, any four-component Dirac spinor $\psi(t,r,\theta,\phi)$ can be uniquely expanded in $y_\pm^{(1)}$ and $y_\pm^{(2)}$ as follows:

$$\psi(t,r,\theta,\phi)=\sum_{i=1}^{2}\left[g_+^{(i)}y_+^{(i)}(\theta,\phi)+g_-^{(i)}y_-^{(i)}(t,r)\right], \tag{5.12}$$

where

$$g_\pm^{(i)}(t,r,\theta,\phi)=\psi^\dagger(t,r,\theta,\phi)\,y_\pm^{(i)}(\theta,\phi). \tag{5.13}$$

The orthogonality relations

$$\begin{aligned}&y_+^{(i)\dagger}y_+^{(j)}=y_-^{(i)\dagger}y_-^{(j)}=\delta_{ij},\\&y_+^{(i)\dagger}y_-^{(j)}=y_-^{(i)\dagger}y_+^{(j)}=0\end{aligned} \tag{5.14}$$

are used in deriving Eq. (5.13).

Substituting the expansion (5.13) in the Dirac equation (5.5) and equating the coefficient of $y_\pm^{(1)}$ and $y_\pm^{(2)}$ to zero, we obtain, by virtue of Eqs. (5.7)–(5.10), the wave equations for the $g_\pm^{(1)}$ and $g_\pm^{(2)}$:

$$\begin{aligned}&\frac{\partial}{\partial t}g_\pm^{(1)}\pm\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)g_\pm^{(2)}-mg_\pm^{(1)}\\&\quad\mp\frac{1}{r}\left(i\frac{\partial}{\partial\theta}\pm\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}+\tfrac{1}{2}i\cot\theta\right)g_\mp^{(2)}=0,\\&\frac{\partial}{\partial t}g_\pm^{(2)}\pm\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)g_\pm^{(1)}mg_\pm^{(2)}\\&\left(\mp\tfrac{1}{2}\;i\frac{\partial}{\partial\theta}\pm\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}+\tfrac{1}{2}i\cot\theta\right)g_\mp^{(1)}=0.\end{aligned} \tag{5.15}$$

Equations (5.15) will now be written partially over the group SU_2. Expressing the polar angle ϕ in terms of the Euler angle $\phi_1=\frac{1}{2}\pi-\phi$, and, furthermore, defining the functions

$$\zeta_\pm^{(1,2)}=g_\pm^{(1,2)}\exp(\mp i\phi_2/2), \tag{5.16}$$

we can write Eqs. (5.15) in terms of the SU_2 infinitesimal operators K_+ and K_- [see Eqs. (2.6)] as follows:

$$\begin{aligned}&\left(\frac{\partial}{\partial t}-m\right)\zeta_\pm^{(1)}\pm\frac{1}{r}\frac{\partial}{\partial r}(r\zeta_\pm^{(2)})\mp\frac{1}{r}K_\pm\zeta_\mp^{(2)}=0,\\&\left(\frac{\partial}{\partial t}+m\right)\zeta_\pm^{(2)}\pm\frac{1}{r}\frac{\partial}{\partial r}(r\zeta_\pm^{(1)})\mp\frac{1}{r}K_\pm\zeta_\mp^{(1)}=0.\end{aligned} \tag{5.17}$$

Equations (5.17) are the Dirac equations, written partially over the group SU_2. The functions $\zeta_\pm^{(1)}$ and $\zeta_\pm^{(2)}$ are functions of t and r as well as the elements u of the group SU_2.

It follows from Eqs. (5.16), (4.1), and (4.2) that the functions $\zeta_+^{(1)}$ and $\zeta_+^{(2)}$ are quantities of spin weight $s=\frac{1}{2}$, while $\zeta_-^{(1)}$ and $\zeta_-^{(2)}$ are quantities of spin weight $s=-\frac{1}{2}$. The ζ functions can be expanded, therefore, in the $T^j_{\pm1/2,n}(u)$ [Eqs. (4.5) and (4.6)]:

$$\zeta_\pm^{(1,2)}=\sum_{j=1/2}^{\infty}\sum_{m=-j}^{j}\mu_{\pm1/2,n}^{j(1,2)}T^j_{\pm1/2,n}(u), \tag{5.18}$$

where

$$\mu_{\pm1/2,n}^{j(1,2)}(t,r)=(2j+1)\int\zeta_\pm^{(1,2)}\overline{T^j_{\pm1/2,n}(u)}\,du. \tag{5.19}$$

Substituting Eqs. (5.18) in the Dirac equations (5.17), and making use of Eq. (3.16), we obtain the equations for the coefficients $\mu_{\pm1/2,n}^{j(1)}$ and $\mu_{\pm1/2,n}^{j(2)}$:

$$\begin{aligned}&\left(\frac{\partial}{\partial t}-m\right)\mu_{\pm1/2,n}^{j(1)}\pm\frac{1}{r}\frac{1}{\partial r}(r\mu_{\pm1/2,n}^{j(2)})\mp\frac{1}{r}(j+\tfrac{1}{2})\mu_{\mp1/2,n}^{j(2)}=0,\\&\left(\frac{\partial}{\partial t}+m\right)\mu_{\pm1/2,n}^{j(2)}\pm\frac{1}{r}\frac{\partial}{\partial r}(r\mu_{\pm1/2,n}^{j(1)})\mp\frac{1}{r}(j+\tfrac{1}{2})\mu_{\mp1/2,n}^{j(1)}=0.\end{aligned} \tag{5.20}$$

Defining the functions

$$\begin{aligned}&\nu_{\pm1/2,n}^{j(+)}=2^{-1/2}(\mu_{\pm1/2,n}^{j(1)}+\mu_{\pm1/2,n}^{j(2)}),\\&\nu_{\pm1/2,n}^{j(-)}=2^{-1/2}(\mu_{\pm1/2,n}^{j(1)}-\mu_{\pm1/2,n}^{j(2)}),\end{aligned} \tag{5.21}$$

we obtain the equations

$$\begin{aligned}&\left(\frac{\partial}{\partial t}\pm\frac{\partial}{\partial r}\right)(r\nu_{\pm1/2,n}^{j(+)})\mp(j+\tfrac{1}{2})\nu_{\mp1/2,n}^{j(+)}-m\nu_{\pm1/2,n}^{j(-)}=0,\\&\left(\frac{\partial}{\partial t}\pm\frac{\partial}{\partial r}\right)(r\nu_{\mp1/2,n}^{j(-)})\mp(j+\tfrac{1}{2})\nu_{\pm1/2,n}^{j(-)}-m\nu_{\mp1/2,n}^{j(+)}=0,\end{aligned} \tag{5.22}$$

$j=\frac{1}{2},\frac{3}{2},\frac{5}{2},\cdots$ and $n=-j,-j+1,\ldots,j$.

Equations (5.22) are a generalization of the Weyl equations (4.10). They reduce to Eqs. (4.10) in the limit $m \to 0$. For each value of (j,n) Eqs. (5.22) form a set of four partial differential equations for the four functions $\nu^{j(\pm)}_{\pm 1/2,n}(t,r)$.

The functions $\nu^{j(\pm)}_{\pm 1/2,n}$ can be expanded in a Fourier integral. The energy spectrum of the Dirac equation is

$$-\infty < E \leq -m, \quad m \leq E < \infty,$$

and therefore the Fourier integral of the functions $\nu^{j(\pm)}_{\pm 1/2,n}$ is

$$\nu^{j(\pm)}_{\pm 1/2,n}(t,r) = \frac{1}{r}\left[\int_{-\infty}^{-m} + \int_{+m}^{\infty}\right][P^{j(\pm)}_{\pm 1/2,n}(r,k)\exp(-ikt)\,dk]. \tag{5.23}$$

Substitution of Eq. (5.23) in Eq. (5.22) yields the four ordinary differential equations for the functions $P^{j(\pm)}_{\pm 1/2,n}(r,k)$:

$$\left(-ik \pm \frac{\partial}{\partial r}\right)P^{j(+)}_{\pm 1/2,n} \mp \frac{1}{r}(j+\tfrac{1}{2})P^{j(+)}_{\pm 1/2,n} - \frac{m}{r}P^{j(-)}_{\pm 1/2,n} = 0, \tag{5.24}$$

$$\left(-ik \pm \frac{\partial}{\partial r}\right)P^{j(-)}_{\mp 1/2,n} \mp \frac{1}{r}(j+\tfrac{1}{2})P^{j(-)}_{\pm 1/2,n} - \frac{m}{r}P^{j(+)}_{\mp 1/2,n} = 0.$$

6. PHYSICAL INTERPRETATION

Theorem: In three-dimensional Euclidean space the vectors

$$\chi_\pm = (1/\sqrt{2})(\hat{e}_\theta \pm i\hat{e}_\phi), \quad \chi_0 = \hat{e}_2 \tag{6.1}$$

are the eigenvectors of the radial spin operator $\hat{n}\cdot\mathbf{S}$ with the eigenvalue ± 1 and 0 respectively.

Proof: The spin matrices in three-dimensions are given by[14]

$$S_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -i & 0 \\ i & 0 & 0 \end{pmatrix}, \quad S_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{6.2}$$

Therefore, the operator $\hat{n}\cdot\mathbf{S}$ is given by

$$\hat{n}\cdot\mathbf{S} = i\begin{pmatrix} 0 & -n_z & n_y \\ n_z & 0 & -n_x \\ -n_y & n_x & 0 \end{pmatrix} = i\begin{pmatrix} 0 & -\cos\theta & \sin\theta\sin\varphi \\ \cos\theta & 0 & -\sin\theta\cos\varphi \\ -\sin\theta\sin\varphi & \sin\theta\cos\varphi & 0 \end{pmatrix}. \tag{6.3}$$

On the other hand the vectors $\chi_\pm, \chi_0$ are given in Carterean coordinates by

$$\chi_\pm = \frac{1}{\sqrt{2}}\begin{pmatrix} \cos\theta\cos\varphi \mp i\cos\varphi \\ \cos\theta\sin\varphi \pm i\cos\varphi \\ -\sin\theta \end{pmatrix}, \quad \chi_0 = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}. \tag{6.4}$$

A straightforward calculation yields

$$(\hat{n}\cdot\mathbf{S})\chi_\pm = \pm\chi_\pm, \quad (\hat{n}\cdot\mathbf{S})\cdot\chi_0 = 0. \tag{6.5(QED)}$$

If the complex vector field $\mathbf{V} = \mathbf{E} + i\mathbf{B}$ is expanded in terms of the radial helicity eigenvectors $\chi_\pm, \chi_0$, one obtains

$$\mathbf{V} = (-i)V_+\chi_+ + iV_-\chi_- + V_0\chi_0, \tag{6.6}$$

where $V_\pm, V_0$ are defined by Eqs. (2.2). The quantities of spin weight s, $\eta_\pm$, and η_0 [Eqs. (2.3)] are obtained, therefore, as functions over the group SU_2 through the following procedure: The complex field V is expanded in the eigenvectors of the operator $\hat{n}\cdot\mathbf{S}$; the coefficients of the expansions are then multiplied by the phase factors $\exp(is\phi_2)$, where s is the corresponding eigenvalue.

We conclude that the functions $\eta_\pm, \eta_0$ are, up to a phase factor, the coefficients of the eigenvectors of the radial spin operator $\hat{n}\cdot\mathbf{S}$, and the infinitesimal operators K_+ and K_- [Eq. (2.6)] are the raising and lowering operators for these coefficients.

The physical interpretation for the Weyl equation (3.17) and the Dirac equation (5.17) is the same. The quantities q_+ and q_- [Eqs. (3.5)] and $y^{(1)}_+$, $y^{(1)}_-$, $y^{(2)}_+$, $y^{(2)}_-$ [Eqs. (5.6)] are, again, eigenspinors of the radial spin operator $\sigma\cdot\hat{n}$,[15] and the ξ and ζ functions over the group SU_2 are obtained by multiplying the coefficients in the expansions (3.6) and (5.12) by $\exp(is\phi_2)$, where s is the corresponding eigenvalue.

When the η, ξ, or ζ functions were expanded in the matrix elements $T^j_{mn}(u)$ of the group SU_2, we obtained a separate set of partial differential equations for each pair of the eigenvalues (j,n) of the total angular momentum operator and its projection along the z axis. By using the Fourier integral, each "partial wave" was written as a superposition of energy eigenstates [Eqs. (4.13), (5.24)]. Since the radial spin operator $\sigma\cdot\hat{n}$ does not commute with the Hamiltonian, Eqs. (4.10) and (5.25) cannot be further decoupled into separate equations for the different quantities of spin s.

What is the physical meaning of a solution consisting of a single representation of the group SU_2? For the case of the electromagnetic field it was shown by Barut, Carmeli, and Malin[5] that if the α^l_{0m}, $\alpha^l_{\pm 1m}$ are nonzero only for one given value of (l,m), then the electromagnetic field contains just an electric multipole of order (l,m) and a magnetic multipole of the same order. For a detailed derivation of the relationship between the usual multipole expansion and the expansion in the T^j_{sm}, the reader is referred to Ref. 5. The corresponding analysis for the case of the Weyl and Dirac equations can be carried out in complete analogy. The usual multipole expansions of the Weyl and Dirac wavefunctions is carried out in the eigenfunctions of the operators $J^2 J_z$ and K, where J is the total angular momentum operators and K is defined by[10]

$$K = L\cdot\sigma + \hbar \quad \text{for a Weyl spinor,}$$
$$K = \rho_3(L\cdot\sigma + \hbar) \quad \text{for a Dirac Spinor.} \tag{6.7}$$

By comparison, expansion in terms of the T^j_{sm} are expansions in the eigenfunctions of the operators J^2, J_2, and $\sigma\cdot\mathbf{n}$. Therefore, if a solution of the Weyl or Dirac equations consists of a single representation (j,m) of the group SU_2, the corresponding multipole expansion will contain terms of the order (j,m) only.

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Phase shifts as functions of the cross section

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We show that an elastic scattering amplitute may be defined as an implicit function of the differential cross section. A practical method is given for a numerical investigation of this dependence, both in the elastic and in the inelastic regions. In particular, we consider the case of a polynomial amplitude, and we show that the Crichton ambiguity is not isolated.

1. INTRODUCTION

In recent years our understanding of the nature of the unitarity constraint upon scattering amplitudes has greatly improved.[1–32] In particular, sufficient conditions under which an elastically unitary scattering amplitude is unique, once the differential cross section is specified, have been given.[4–7] Further, the existence of a continuum ambiguity in the inelastic region has been investigated in detail.[7–17] Some preliminary investigations of spin and isospin complications have also been made.[12,13,24,25,29,30]

In this paper we investigate a different, but mathematically similar problem: given the differential cross section *and* a set of phase shifts that fit it, we show that in general one may change the cross section by a small increment, and find the correspondingly altered phase shifts that fit the new cross section. This is interesting (if not wholly unexpected) from an epistomological point of view; and it is also of importance practically, for it means that we can explore systematically the uncertainty in the phase shifts that is generated by the experimental error associated with a measurement of the differential cross section. In this paper we limit our attention for simplicity to spinless, isospinless scattering.

The basic result of the present work is set out and proved in Sec. 2. Here we use the Hildebrandt—Graves theorem to show that the unitarity equation defines the amplitude as an implicit function of the cross section. We employ a certain set of Hilbert spaces of functions that are analytic in the $\cos\theta$-plane, and the key of the proof is the demonstration that the Fréchet derivative of the unitarity mapping is compact. For the singular situation in which unity belongs to the point spectrum of this derivative, we show by means of bifurcation theory that the amplitude is still defined (though in general no longer unique). The precise nature of the solution manifold in the vicinity of a singular point depends on the number of real solutions of the bifurcation equation.

In Sec. 3 we show how to prevent zeros of the dispersive part from turning into unwanted square-root branch points, and in Sec. 4 we sketch the Newton—Kantorovich method that can be used for a numerical investigation. In Sec. 5 we generalize the method to the inelastic region, where we now have the choice of varying the inelastic term, or the cross section, or both. Finally, in Sec. 6 we use our methods to investigate the case of a polynomial amplitude. In particular, it is shown that a continuation away from both of the Crichton amplitudes is in general possible.

2. IMPLICIT FUNCTION THEOREM

Suppose that we know an elastically unitary scattering amplitude, $F_0(z)$, that is analytic in the small Martin ellipse, $\epsilon(z_0)$. Suppose that F_0 fits the given cross section, $\sigma_0(x)$, i.e.,

$$|F_0(x)|^2 = \sigma_0(x), \tag{2.1}$$

for $-1 \leq x \leq 1$. As in Ref. 11, one continues this equation into $\epsilon(z_0)$ by writing

$$\sigma_0(z) = F_0(z)F_0^*(z^*) = D_0^2(z) + A_0^2(z), \tag{2.2}$$

where D_0 and A_0 are the dispersive and absorptive parts of F_0, respectively. We wish to find sufficient conditions under which we may change $\sigma_0(z)$ to $\sigma_0(z) + \delta\sigma(z)$, and find a corresponding unitary amplitude $F_0(z) + \delta F(z)$.

In this general demonstration, we allow $D_0(z)$ to have zeros in $\epsilon(z_0)$. However, for the given $D_0(z)$, we can certainly find $\zeta_0' < z_0$, such that $|D_0(z)|$ does not vanish on $\partial\epsilon(\zeta_0')$. We shall define a set of real Hilbert spaces, $\mathcal{H}(\zeta)$, parametrized by the real number $\zeta > 1$, by means of the inner product,

$$(f,g)_\zeta = \sum_{l=0}^{\infty} (2l+1) f_l g_l [Q_l(\zeta)]^{-2}, \tag{2.3}$$

on the set of functions, $f(z)$, that are real-analytic within $\epsilon(\zeta)$. Here

$$f_l = \tfrac{1}{2}\int_{-1}^{1} dz f(z) P_l(z), \tag{2.4}$$

and similarly for g. P_l and Q_l are the Legendre functions of the first and second kinds.

Note that an arbitrary function that is real-analytic in $\epsilon(\zeta)$ does not necessarily belong to $\mathcal{H}(\zeta)$, but it does belong to $\mathcal{H}(\eta)$, for any $\eta < \zeta$. Since $\sigma_0(z)$ is real-analytic in $\epsilon(z_0)$, it belongs to $\mathcal{H}(\zeta_0'')$, $\zeta_0'' < z_0$, and for later convenience we choose ζ_0'' so that $\zeta_0' < \zeta_0'' < z_0$. Because of the unitarity condition, we know that $A_0(z)$ is real-analytic in the *large* Martin ellipse, $\epsilon(2z_0^2 - 1)$. Hence it belongs to $\mathcal{H}(\zeta_1)$, where

$$\zeta_1 = 2\zeta_0^2 - 1, \tag{2.5}$$

where $\zeta_0 < z_0$. For convenience we choose $\zeta_0 < \zeta_0'$. Let us summarize the foregoing:

$$1 < \zeta_0 < \zeta_0' < \zeta_0'' < z_0, \tag{2.6}$$

$$\sigma_0 \in \mathcal{H}(\zeta_0''); \; D_0 \in \mathcal{H}(\zeta_0''); \; A_0 \in \mathcal{H}(\zeta_1). \tag{2.7}$$

We may define

$$n_0 = \inf_{z \in \partial\epsilon(\zeta_0')} |D_0(z)|, \tag{2.8}$$

where it will be recalled that ζ_0' was chosen specifically to ensure that n_0 is strictly positive. We can arrange without difficulty that

$$\zeta_1 > \zeta_0''. \tag{2.9}$$

Let us define, for each pair

$$(A,\sigma) \in \mathcal{H}(\zeta_1)\times\mathcal{H}(\zeta_0''), \tag{2.10}$$

the following two sequences:

$$D_l = \tfrac{1}{2}\int_{-1}^{1} dx P_l(x)[\sigma(x) - A^2(x)]^{1/2}, \tag{2.11}$$

$$\overline{D}_l = \frac{1}{2\pi i}\oint_{\partial\epsilon(\zeta_0')} dz Q_l(z)[\sigma(z) - A^2(z)]^{1/2}, \tag{2.12}$$

$l = 0, 1, 2, \cdots$. In order to give a precise meaning to the integral (2.12), we must explain how to treat possible zeros of $\sigma(z) - A^2(z)$ within or upon the contour of integration, $\partial\epsilon(\zeta_0')$. Odd-order zeros will give rise to square-root branch points of the integrand of (2.12). In the case that the number of odd-order zeros in $\epsilon(\zeta_0')$ is even, suitable cuts may be drawn within the ellipse, and the integrand is then continuous around $\partial\epsilon(\zeta_0')$. If the number of odd-order zeros is odd, at least one such zero must lie on the real axis. In this case, we draw a cut from the rightmost real odd-order zero towards $+\infty$ along the real axis. Suitable cuts may be drawn within the ellipse between the other odd-order zeros. In this case the contour is open, but the integral is still well-defined, and moreover $\overline{D}_l$ is always purely real or purely imaginary. Hence $\overline{D}_l^2$ is well-defined and real.

The necessary and sufficient condition for the P_l-transform (2.11) and the Q_l-transform (2.12) to be equal is that there should be *no* odd-order zeros in $\epsilon(\zeta_0')$, so that the surd in (2.12) is analytic in $\epsilon(\zeta_0')$. We know from (2.7) that $D_0(z)$ is analytic in $\epsilon(\zeta_0')$, and from (2.2) that

$$D_0(z) = [\sigma_0(z) - A_0^2(z)]^{1/2}; \tag{2.13}$$

hence certainly

$$D_{0l} = \overline{D}_{0l}. \tag{2.14}$$

Let us define the nonlinear operator

$$M(A,\sigma;z) = \sum_{l=0}^{\infty}(2l+1)P_l(z)(A_l^2 + \overline{D}_l^2), \tag{2.15}$$

where $\overline{D}_l$ is given by (2.12), and where

$$A_l = \tfrac{1}{2}\int_{-1}^{1} dx P_l(x)A(x). \tag{2.16}$$

We will also use the operator

$$S(A,\sigma;z) = A(z) - M(A,\sigma;z). \tag{2.17}$$

Because $F_0(z)$ is an elastically unitary amplitude, and because of the equivalence (2.14), we know that

$$S(A_0,\sigma_0) = 0, \tag{2.18}$$

where we have suppressed the variable z. In this section, we shall use the Hildebrandt—Graves theorem to show that

$$S(A,\sigma) = 0 \tag{2.19}$$

defines $A(\sigma)$, as an implicit function of σ, for σ in some neighborhood of σ_0, such that

$$A(\sigma_0) = A_0. \tag{2.20}$$

This is not in itself enough to show that there exist unitary amplitudes, $F(\sigma)$, for σ in some neighborhood of σ_0, since in general

$$\overline{D}_l(\sigma) \neq D_l(\sigma). \tag{2.21}$$

We shall postpone until the next section the proof that there is an infinite-dimensional subset of the neighborhood of σ_0, in which indeed $\overline{D}_l$ and D_l are the same, so that unitarity is satisfied. For the present, we consider only Eq. (2.19), so we treat $\overline{D}_l$ only, and temporarily forget about D_l.

The form of the Hildebrandt—Graves theorem that we shall use, adapted to our particular case, is as follows (Ref. 33):

Let S be an operator taking pairs $(A,\sigma) \in \mathcal{H}(\zeta_1)\times\mathcal{H}(\zeta_0'')$ into $\mathcal{H}(\zeta_1)$. Suppose that $S(A_0,\sigma_0) = 0$, and that S is continuous with respect to (A,σ), in some neighborhood of (A_0,σ_0). Suppose also that $S_A(A,\sigma)$, the partial Fréchet derivative of S with respect to A, exists as a bounded linear operator on $\mathcal{H}(\zeta_1)$, and that it is continuous with respect to (A,σ) (in the operator topology) in the above neighborhood of (A_0,σ_0). Lastly, suppose that $S_A(A_0,\sigma_0)$ has an inverse, as a bounded linear operator on $\mathcal{H}(\zeta_1)$. Then $S(A,\sigma) = 0$ has a unique, continuous solution, $A(\sigma)$, for σ in some neighborhood of σ_0, with $A(\sigma_0) = A_0$.

This theorem is usually stated for Banach spaces rather than for Hilbert spaces. We understand that $\mathcal{H}(\zeta)$ is to be regarded as a Banach space, by means of the usual norm $(f,f)_\zeta^{1/2}$. We could have worked with the Banach space of Ref. 11, instead of $\mathcal{H}$, but we shall in fact find it very convenient to have a Hilbert space at our disposal, when we come to consider the singular case at the end of this section.

We need to check all the conditions of this theorem. Let us first prove that

$$(A,\sigma) \in \mathcal{H}(\zeta_1)\times\mathcal{H}(\zeta_0'') \Rightarrow M(A,\sigma) \in \mathcal{H}(\zeta_1). \tag{2.22}$$

Now $\sigma(z) - A^2(z)$ is analytic in $\epsilon(\zeta_0'')$, and hence

$$N^2 = \sup_{z\in\partial\epsilon(\zeta_0')} |\sigma(z) - A^2(z)| \tag{2.23}$$

is finite. We can deduce from (2.12) (see Ref. 11) that

$$|\overline{D}_l| \leq \frac{LN}{2\pi} Q_l(\zeta_0') \tag{2.24}$$

where L is the circumference of $\epsilon(\zeta_0')$. Also the fact that $\|A\|_{\zeta_1}$ exists implies that

$$|A_l| \leq \|A\|_{\zeta_1} Q_l(\zeta_1) < \|A\|_{\zeta_1} Q_l(\zeta_0'). \tag{2.25}$$

Hence

$$A_l^2 + \overline{D}_l^2 \leq \kappa[Q_l(\zeta_0')]^2 \leq \kappa\Omega(\zeta_1')Q_l(\zeta_1'), \tag{2.26}$$

where

$$\kappa = \frac{L^2N^2}{4\pi^2} + \|A\|_{\zeta_1}^2, \tag{2.27}$$

where

$$\zeta_1' = 2\zeta_0'^2 - 1 > \zeta_1, \tag{2.28}$$

and where

$$\Omega(\zeta_1') = [Q_0(\zeta_1')]^2/Q_1(\zeta_1'), \tag{2.29}$$

as in Ref. 11. Hence

$$\|M(A,\sigma)\|_{\zeta_1}^2 = \sum_{l=0}^{\infty}(2l+1)[A_l^2 + \overline{D}_l^2][Q_l(\zeta_1)]^{-2}$$

$$\leq [\kappa\Omega(\zeta_1')]^2 \sum_{l=0}^{\infty} (2l+1)[Q_l(\zeta_1')/Q_l(\zeta_1)]^2. \tag{2.30}$$

This norm exists, since the series on the right converges exponentially, thanks to the inequality (2.28). This concludes the proof of (2.22).

Since $F_0(z)$ is analytic in $\epsilon(z_0)$, the zeros of $\sigma_0(z) - A_0^2(z)$ in $\epsilon(\zeta_0')$ are certainly of even order, and there can only be a finite number of them. If we change σ_0 to $\sigma_0 + \delta\sigma$, and wish to induce a change A_0 to $A_0 + \delta A$, consistent with Eq. (2.19), the zeros will in general move, and may split up into zeros of lower, and possibly odd order. Thus the surd $[\sigma(z) - A^2(z)]^{1/2}$ in (2.12) may no longer be analytic in $\epsilon(\zeta_0')$. This does not affect the applicability of the Hildebrandt—Graves theorem, provided we ensure that some neighborhood of $\partial\epsilon(\zeta_0')$ remains zero-free and is not intersected by square-root branch cuts. We will show that there is a neighborhood of (A_0, σ_0) in $\mathcal{H}(\zeta_1) \times \mathcal{H}(\zeta_0'')$, say Ξ, for which $\sigma(z) - A^2(z)$ does not vanish on $\partial\epsilon(\zeta_0')$. In fact, we shall take any n, such that $0 < n < n_0$, and show that a neighborhood Ξ exists, such that

$$n^2 \leq \inf_{\substack{z\in\partial\epsilon(\zeta_0') \\ (A,\sigma)\in\Xi}} |\sigma(z) - A^2(z)|. \tag{2.31}$$

Since $\sigma(z) - \sigma_0(z) \in \mathcal{H}(\zeta_0'')$, we see that for $z \in \epsilon(\zeta_0')$,

$$|\sigma(z) - \sigma_0(z)|^2 = \Big|\sum_l (2l+1)P_l(z)[\sigma_l - \sigma_{0l}]\Big|^2$$

$$\leq \sum_l (2l+1)\frac{|\sigma_l - \sigma_{0l}|^2}{[Q_l(\zeta_0'')]^2} \times \sum_l (2l+1)[P_l(\zeta_0')Q_l(\zeta_0'')]^2 \tag{2.32}$$

by the Schwarz inequality. The first sum here is $\|\sigma - \sigma_0\|^2_{\zeta_0''}$, and the second sum converges exponentially. Hence we have shown the existence of a constant, κ_1, such that

$$\sup_{z\in\epsilon(\zeta_0')} |\sigma(z) - \sigma_0(z)| \leq \kappa_1 \|\sigma - \sigma_0\|_{\zeta_0''}. \tag{2.33}$$

Similarly, we may show that there is a constant, κ_2, such that

$$\sup_{z\in\epsilon(\zeta_0')} |A(z) - A_0(z)| \leq \kappa_2 \|A - A_0\|_{\zeta_1}, \tag{2.34}$$

so that

$$\sup_{z\in\epsilon(\zeta_0')} |A^2(z) - A_0^2(z)|$$

$$\leq \sup_{z\in\epsilon(\zeta_0')} \{[|A(z) - A_0(z)| + 2|A_0(z)|]|A(z) - A_0(z)|\}$$

$$\leq \kappa_2^2[\|A - A_0\|_{\zeta_1} + 2\|A_0\|_{\zeta_1}]\|A - A_0\|_{\zeta_1}. \tag{2.35}$$

Hence

$$\sup_{z\in\epsilon(\zeta_0')} |[\sigma(z) - A^2(z)] - [\sigma_0(z) - A_0^2(z)]| \tag{2.36}$$

is bounded by the sum of the right-hand sides of (2.33) and (2.35). By making $\|\sigma - \sigma_0\|_{\zeta_0''}$ and $\|A - A_0\|_{\zeta_1}$ small enough, we may make (2.36) smaller than $n_0^2 - n^2$, and in view of (2.8) this suffices to demonstrate (2.31).

There is therefore a neighborhood, Ξ, of (A_0, σ_0), such that $\sigma(z) - A^2(z)$ remains zero-free for $z \in \partial\epsilon(\zeta_0')$. We may therefore assert, by the theorem of Rouché (Ref. 34), that the number of zeros of $\sigma(z) - A^2(z)$ inside $\partial\epsilon(\zeta_0')$ is the same as that of $\sigma_0(z) - A_0^2(z)$ (the zeros being counted according to their multiplicity). Any splitting of even-order zeros into odd-order zeros may be accommodated by cuts that do not intersect $\partial\epsilon(\zeta_0')$.

Let us now consider the Fréchet derivative

$$S_A(A, \sigma) = 1 - M_A(A, \sigma), \tag{2.37}$$

where

$$M_A(A, \sigma)\delta A = \sum_{l=0}^{\infty} (2l+1)P_l(z)\phi_l, \tag{2.38}$$

with

$$\phi_l = \frac{1}{i\pi} \oint_{\partial\epsilon(\zeta_0')} dt Q_l(t)\left(A_l - \frac{\overline{D}_l A(t)}{[\sigma(t) - A^2(t)]^{1/2}}\right)\delta A(t) \tag{2.39}$$

for any $\delta A \in \mathcal{H}(\zeta_1)$. We will now show that $M_A(A, \sigma)$ is a bounded linear operator on $\mathcal{H}(\zeta_1)$, if (A, σ) belongs to the neighborhood Ξ of (A_0, σ_0). In view of (2.24), (2.25) (2.31), and

$$\sup_{t\in\epsilon(\zeta_0')} |\delta A(t)| \leq \kappa_2 \|\delta A\|_{\zeta_1}, \tag{2.40}$$

which one can prove as in Eq. (2.34), we see that there is a constant, say κ_3, such that

$$|\phi_l| \leq \kappa_3[Q_l(\zeta_0')]^2 \|\delta A\|_{\zeta_1} \leq \kappa_3\Omega(\zeta_1')Q_l(\zeta_1')\|\delta A\|_{\zeta_1}, \tag{2.41}$$

ζ_1' being defined in (2.28). Hence [much as in Eq. (2.30)]

$$\|M_A(A, \sigma)\delta A\|^2_{\zeta_1} = \sum (2l+1)|\phi_l|^2[Q_l(\zeta_1)]^{-2} \leq \{\kappa_3\Omega(\zeta_1')\|\delta A\|_{\zeta_1}\}^2 \sum_l (2l+1)[Q_l(\zeta_1')/Q_l(\zeta_1)]^2. \tag{2.42}$$

The series converges, and so we have proved that $M_A(A, \sigma)$ is a bounded linear operator. By similar, but somewhat longer calculations, it may be shown that $M_A(A, \sigma)$, and $S(A, \sigma)$ itself, are continuous with respect to (A, σ), for $(A, \sigma) \in \Xi$.

We have now verified all the conditions for the applicability of the Hildebrandt—Graves theorem, except the existence of an inverse linear operator $S_A^{-1}(A_0, \sigma_0)$. We show first that $M_A(A_0, \sigma_0)$ is compact, which we do by a method due to Johnson (Ref. 8). Let us define a ball of radius r in $\mathcal{H}(\zeta_1)$:

$$T_r = \{\alpha(z) : \|\alpha\|_{\zeta_1} \leq r, r > 0\}. \tag{2.43}$$

We prove that, for every $\epsilon > 0$, and any r, there exists a finite ϵ-net for the set $M_A(A_0, \sigma_0)T_r$, which means that it is totally bounded. For any $\delta A \in T_r$, we see from (2.41) that there is a constant, say κ_4, such that

$$|\phi_l| \leq \kappa_4 Q_l(\zeta_1'). \tag{2.44}$$

Hence, given any $\epsilon > 0$, we may find an L such that

$$\sum_{l=L}^{\infty} (2l+1)|\phi_l|^2[Q_l(\zeta_1)]^{-2} < \epsilon. \tag{2.45}$$

The L-tuples $(\phi_0, \phi_1, \ldots, \phi_{L-1})$, corresponding to all $\delta A \in T_r$, constitute a bounded set in the locally compact space $\mathbb{R}^L$, and so the set can be covered by a finite ϵ-net, which clearly also serves as a finite net for $M_A(A_0, \sigma_0)T_r$, in view of (2.45). Hence $M_A(A_0, \sigma_0)$ is a compact linear operator on $\mathcal{H}(\zeta_1)$, and we may apply the Riesz—Schauder theory (Ref. 35). In particular, the spectrum is a point set, and if unity does not belong to it, $S_A(A_0, \sigma_0)$ has a bounded inverse, and the Hildebrandt—Graves theorem applies. If unity *is* an eigen-

value of $M_A(A_0,\sigma_0)$, nevertheless the corresponding eigenspace is only finite-dimensional, by Riesz–Schauder, and we will show that Eq. (2.19) can still be used in general to define an implicit function, $A(\sigma)$.

We attack the singular case, when unity is an eigenvalue of $M_A(A_0,\sigma_0)$, by a modification of bifurcation theory (Ref. 36). We define

$$U(\delta A,\delta\sigma)=S(A,\sigma)-S_A(A_0,\sigma_0)\delta A, \tag{2.46}$$

where

$$\delta A=A-A_0, \tag{2.47a}$$

$$\delta\sigma=\sigma-\sigma_0. \tag{2.47b}$$

Again we start from (2.18), and we wish to demonstrate the existence of a solution, $A(\sigma)$, of Eq. (2.19), for $\sigma\neq\sigma_0$. At such a solution,

$$S_A(A_0,\sigma_0)\delta A=-U(\delta A,\delta\sigma), \tag{2.48}$$

but now we assume that unity is in the spectrum of $M_A(A_0,\sigma_0)$, so that $S_A(A_0,\sigma_0)$ has no inverse. We will show nevertheless that there does exist a so-called pseudoinverse. We know that $M_A(A_0,\sigma_0)$ is compact, and this allows us to assert two things:

(a) the nullspace of $S_A(A_0,\sigma_0)$, say N, is a linear subspace of $H(\xi_1)$ of finite dimension, say n;

(b) the range of $S_A(A_0,\sigma_0)$, say R, is strongly closed.

These results follow from the Riesz–Schauder theory.

We define the quotient space

$$H_N(\xi_1)=H(\xi_1)/N \tag{2.49}$$

in the standard way. This is a Banach space, normed by

$$\|\delta A_N\|_N=\inf_{\alpha\in N}\|\delta A+\alpha\|_{\xi_1} \tag{2.50}$$

where δA_N is the equivalence class, modulo N, that contains δA (i.e., $\delta A\in\delta A_N$ and $x\in\delta A_N$, $y\in\delta A_N\Rightarrow x-y\in N$). There exists a continuous, linear one-to-one mapping, from $H_N(\xi_1)$ to R, say S_N, such that

$$S_N\delta A_N=S_A(A_0,\sigma_0)\delta A. \tag{2.51}$$

Then the inverse mapping theorem tells us that S_N has a continuous inverse, S_N^{-1}, as a linear mapping from R to $H_N(\xi_1)$. Let Π_N and Π_R be the orthogonal projection operators from $H(\xi_1)$ onto N and R, respectively. Then the pseudoinverse of $S_A(A_0,\sigma_0)$ is defined, as a bounded linear mapping from $H(\xi_1)$ to $N^\perp$, the subspace of $H(\xi_1)$ orthogonal to N, by

$$\tilde{S}_A^{-1}=(I-\Pi_N)_N S_N^{-1}\Pi_R, \tag{2.52}$$

where $(I-\Pi_N)_N$ is the linear mapping from $H_N(\xi_1)$ to $N^\perp$ defined by

$$(I-\Pi_N)_N\delta A_N=(I-\Pi_N)\delta A. \tag{2.53}$$

Clearly $(I-\Pi_N)_N$ is an isometry.

The pseudoinverse, $\tilde{S}_A^{-1}$, will now serve to transform Eq. (2.48), but only on condition that $U(\delta A,\delta\sigma)$ belongs to R. Consider in fact the equation

$$\delta A=-\tilde{S}_A^{-1}U(\delta A,\delta\sigma)+u, \tag{2.54}$$

where $u\in N$. We may write

$$u=\sum_{m=1}^{n}\lambda_m u_m \tag{2.55}$$

where $\{u_m\}$ is a real basis for N, and $\{\lambda_m\}$ is a set of real numbers. We shall show presently that, if $\|\delta\sigma\|_{\xi_0}$ and $\|u\|_{\xi_1}$ are small enough, Eq. (2.54) defines a contraction mapping, so that then a locally unique solution, say $\delta A(\delta\sigma,u)$, exists. Now from (2.52) we have that

$$S_A(A_0,\sigma_0)\tilde{S}_A^{-1}=\Pi_R \tag{2.56}$$

so that (2.54) implies

$$S_A(A_0,\sigma_0)\delta A=-\Pi_R U(\delta A,\delta\sigma), \tag{2.57}$$

and this reduces to (2.48) only if

$$(1-\Pi_R)U(\delta A(\delta\sigma,u),\delta\sigma)=0, \tag{2.58}$$

as expected.

The system (2.58) is in fact of dimension n, since $(1-\Pi_R)$ is the projection operator onto the nullspace of the adjoint operator $S_A^\dagger(A_0,\sigma_0)$. Since u depends on the n real numbers $\lambda_1,\lambda_2,\ldots,\lambda_n$ [Eq. (2.55)], we may regard (2.58) as a system of n nonlinear algebraic equations for the n variables λ_m, with $\delta\sigma$ as an infinite-dimensional parameter. This system is called the bifurcation equation, and in general there will be more than one solution for the λ_m. Clearly only real solutions are of interest: complex ones are simply to be ignored. For each real solution for the λ_m, there corresponds a solution $u(\delta\sigma)$ of the bifurcation equation (2.58), and for this solution, the function

$$\delta A(\delta\sigma,u(\delta\sigma)) \tag{2.59}$$

solves not only (2.54) [with $u=u(\delta\sigma)$], but also the original equation (2.48).

It remains to supply the contraction mapping proof. Define the nonlinear mapping F on $H(\xi_1)$:

$$F(\delta A)=-\tilde{S}_A^{-1}U(\delta A,\delta\sigma)+u. \tag{2.60}$$

Now according to (2.46) and (2.18),

$$U(\delta A,\delta\sigma)=S(A_0+\delta A,\sigma_0+\delta\sigma)-S(A_0,\sigma_0)-S_A(A_0,\sigma_0)\delta A \tag{2.61}$$

and hence we infer that

$$\begin{aligned}\|U(\delta A,\delta\sigma)\|_{\xi_1}\leq{}&\|S(A_0+\delta A,\sigma_0+\delta\sigma)-S(A_0+\delta A,\sigma_0)\|_{\xi_1}\\&+\|S(A_0+\delta A,\sigma_0)-S(A_0,\sigma_0)\\&-S_A(A_0,\sigma_0)\delta A\|_{\xi_1}.\end{aligned} \tag{2.62}$$

To bound the first term on the right-hand side of (2.62), we use the Banach space version of the mean-value theorem:

$$\|S(A,\sigma_0+\delta\sigma)-S(A,\sigma_0)\|_{\xi_1}\leq\sup_{0\leq x\leq 1}\|S_\sigma(A,\sigma_0+x\delta\sigma\|\cdot\|\delta\sigma\|_{\xi_0^\sigma}, \tag{2.63}$$

where $S_\sigma(A,\sigma)$ is the partial Fréchet derivative of $S(A,\sigma)$ with respect to σ. This is defined by

$$S_\sigma(A,\sigma)\delta\sigma=\sum_{l=0}^{\infty}(2l+1)P_l(z)\psi_l, \tag{2.64a}$$

in which

$$\psi_l=\frac{\overline{D}_l}{2i\pi}\oint_{\partial\epsilon(\xi_0^\sigma)}dtQ_l(t)\frac{\delta\sigma(t)}{[\sigma(t)-A^2(t)]^{1/2}}, \tag{2.64b}$$

and where $\delta\sigma \in \mathcal{H}(\zeta_0'')$. It is easy to show that $S_\sigma(A,\sigma)$ is a bounded, and in fact a compact linear operator from $\mathcal{H}(\zeta_0'')$ to $\mathcal{H}(\zeta_1)$, if $(A,\sigma)\in\Xi$. The method is precisely similar to the demonstration that $M_A(A,\sigma)$ is compact, and we leave the details to the reader [see Eq. (2.38) *et seq.*]. Hence there is a constant, C_1, such that the right-hand side of (2.63) is bounded by $C_1\|\delta\sigma\|_{\zeta_0''}$, so long as $(A,\sigma)\in\Xi$.

We turn now to the second term on the right-hand side of (2.62). Here we shall use the Banach space version of the second mean-value theorem, viz.,

$$\|S(A,\sigma_0)-S(A_0,\sigma_0)-S_A(A_0,\sigma_0)\delta A\| \le \tfrac{1}{2}\sup_{0\le x\le 1}\|S_{AA}(A_0+x\delta A,\sigma_0)\|\cdot\|\delta A\|^2 \quad (2.65)$$

where all norms refer to $\mathcal{H}(\zeta_1)$. Here the second partial Fréchet derivative with respect to A, $S_{AA}(A,\sigma)$, may be shown to be a bounded bilinear operator from $\mathcal{H}(\zeta_1)\times\mathcal{H}(\zeta_1)$ to $\mathcal{H}(\zeta_1)$, if $(A,\sigma)\in\Xi$, by methods similar to those used to show that $M_A(A,\sigma)$ is bounded. Hence there exists a constant C_2, such that the right-hand side of (2.65) is bounded by $C_2\|\delta A\|_{\zeta_1}^2$ (see Ref. 13 for a discussion of the second Fréchet derivative in a mathematically similar problem).

From the definition (2.60), we may therefore write the inequality

$$\|F(\delta A)\|_{\zeta_1} \le \|\tilde{S}_A^{-1}\|\{C_1\|\delta\sigma\|_{\zeta_0''}+C_2\|\delta A\|_{\zeta_1}^2\}+\|u\|_{\zeta_1}. \quad (2.66)$$

We have already shown that the pseudoinverse, $\tilde{S}_A^{-1}$, is a bounded linear operator, so it suffices to take

$$\|\delta A\|_{\zeta_1} \le b, \quad (2.67a)$$

$$\|\delta\sigma\|_{\zeta_0''} \le b[3\|\tilde{S}_A^{-1}\|C_1]^{-1}, \quad (2.67b)$$

$$\|u\|_{\zeta_1} \le b/3, \quad (2.67c)$$

where b is a number that satisfies

$$b \le [3\|\tilde{S}_A^{-1}\|C_2]^{-1}, \quad (2.68)$$

and is small enough to ensure that (2.67a, b) implies $(A,\sigma)\in\Xi$. The above conditions are sufficient to give

$$\|F(\delta A)\|_{\zeta_1} \le b, \quad (2.69)$$

so F is an injective mapping of the ball (2.67a) into itself.

To show that F is contractive, and not merely injective on the ball (2.67a), we consider

$$F(\delta A_1)-F(\delta A_2) = -\tilde{S}_A^{-1}\{U(\delta A_1,\delta\sigma)-U(\delta A_2,\delta\sigma)\} \quad (2.70)$$

for any δA_1 and δA_2 in the ball (2.67a). So

$$\|F(\delta A_1)-F(\delta A_2)\|_{\zeta_1} \le \|\tilde{S}_A^{-1}\|\{\|S(A_1,\sigma)-S(A_1,\sigma_0)-S(A_2,\sigma)+S(A_2,\sigma_0)\|_{\zeta_1} + \|S(A_1,\sigma_0)-S(A_2,\sigma_0)-S_A(A_0,\sigma_0)(A_1-A_2)\|_{\zeta_1}\}. \quad (2.71)$$

The first term within the parentheses may be bounded by

$$\sup_{0\le x\le 1}\sup_{0\le y\le 1}\|S_{A\sigma}(A_1+x(A_2-A_1),\sigma_0+y\delta\sigma)\|\cdot\|\delta\sigma\|_{\zeta_0''}\|A_1-A_2\|_{\zeta_1} \quad (2.72)$$

where $S_{A\sigma}$ is the mixed second-order Fréchet derivative of $S(A,\sigma)$ with respect to A and σ. It may be shown to be bounded. The second term within the parentheses is bounded by

$$\tfrac{1}{2}\sup_{0\le x\le 1}\|S_{AA}(A_1+x(A_2-A_1),\sigma_0)\|\cdot\|A_1-A_2\|_{\zeta_1}^2. \quad (2.73)$$

Hence there are constants, C_3 and C_4, such that

$$\|F(\delta A_1)-F(\delta A_2)\|_{\zeta_1} \le \kappa\|A_1-A_2\|_{\zeta_1} \quad (2.74)$$

with

$$\kappa = C_3\|\delta\sigma\|_{\zeta_0''}+C_4 b. \quad (2.75)$$

Clearly it is possible to choose b so small that simultaneously (2.67b) and (2.68) are satisfied, and $\kappa<1$. This is the condition for a contraction, and with it we have ended the proof.

3. ZEROS OF THE DISPERSIVE PART

In this section we consider how to ensure that

$$\bar{D}_l(\sigma) = D_l(\sigma), \quad (3.1)$$

so that elastic unitarity is satisfied by the implicit function $D(\sigma;z)+iA(\sigma;z)$, the existence of which we demonstrated in Sec. 2. We have shown that, if $\|\sigma-\sigma_0\|_{\zeta_0''}$ is small enough, the algebraic number of zeros of

$$R(A,\sigma;z) = \sigma(z)-A^2(z) \quad (3.2)$$

within $\epsilon(\zeta_0')$ is constant, where we understand that $A(z)$ in (3.2) is the implicit function defined by

$$S(A,\sigma;z) = 0. \quad (3.3)$$

Suppose that $R(A_0,\sigma_0;z)$ has N zeros within $\epsilon(\zeta_0')$, at the positions $z=p_{01},p_{02},\ldots,p_{0N}$, and that the orders of the zeros are respectively $2q_1,2q_2,\ldots,2q_N$ [the orders must be even, since $D_0(z)=R^{1/2}(A_0,\sigma_0;z)$ is analytic in $\epsilon(\zeta_0')$]. Then we know that

$$R^{(m)}(A_0,\sigma_0;p_{0n}) = 0 \quad (3.4)$$

where $m=0,1,\ldots,2q_n-1$, $n=1,2,\ldots,N$, and where

$$R^{(m)}(A,\sigma;z) = \left(\frac{\partial}{\partial z}\right)^m R(A,\sigma;z) \quad (3.5)$$

(with the understanding of course that $R^{(m)}$ just reduces to R for $m=0$). We shall show that σ can be so constrained that also

$$R^{(m)}(A,\sigma;p_n) = 0 \quad (3.6)$$

for the same values of m and n. In other words, the zeros of $R(A,\sigma;z)$ have moved from the old positions, p_{0n}, to new positions p_n, and are of the same (even) order as before. Thus $D(z)$ is still analytic and (3.1) is guaranteed.

To make this quite precise, we shall ensure that all the p_n, $n=1,2,\ldots,N$, remain distinct, so that then the zero at p_n is precisely of order $2q_n$ [for if it were of even higher order, the algebraic number of zeros of $R(A,\sigma;z)$ within $\epsilon(\zeta_0')$ would be greater than $2(q_1+q_2+\cdots+q_N)$, which is impossible].

We simply need to apply the implicit-function theorem to the finite-dimensional system

$$R^{(m)}(A(\sigma),\sigma;p_n) = 0 \quad (3.7)$$

for $m=0,1,\ldots,2q_n-1$, $n=1,2,\ldots,N$, where $A(\sigma)$ is

the implicit function defined by (3.3). There are in fact $2(q_1+q_2+\cdots+q_N)$ complex equations, and so we cannot hope to use (3.7) to define the N p's as implicit functions of an unrestricted σ. We shall in fact write

$$\sigma(z)=\sigma_f(z)+\sigma_c(z), \tag{3.8}$$

where we define the "constrained part" of the cross section by

$$\sigma_c(z)=\sum_{k=1}^{Q}(2l_k+1)\sigma_{l_k}P_{l_k}(z), \tag{3.9a}$$

where $l_1, l_2, \ldots, l_Q$, is an arbitrary sequence of integers (we shall define Q presently), and where the "free part" of the cross section is

$$\sigma_f(z)=\sum_{l\neq l_k}(2l+1)\sigma_l P_l(z), \quad k=1,2,\ldots,Q \tag{3.9b}$$

We may then write (3.7) as

$$R^{(m)}(A(\sigma_f+\sigma_c),\sigma_f+\sigma_c;p_n)=0. \tag{3.10}$$

Although there are $4(q_1+\cdots+q_N)$ real equations here, only half this number are independent, since complex p's must come in complex conjugate pairs, and for real p's, the corresponding equation is manifestly real. Accordingly, it is sufficient to consider only zeros on the real axis, or in the upper half-plane [and inside $\epsilon(\zeta_0'')$], and to define

$$Q=2(q_1+\cdots+p_N)-N. \tag{3.11}$$

Then (3.10) is a system of $Q+N$ real scalar equations for $Q+N$ real unknowns (namely the σ_{l_k} and the real and imaginary parts of the p's in the upper half-plane). The equations are to be solved for these unknowns, in terms of σ_f, which may be chosen freely.

The question of the existence of solutions of (3.10), for σ_f sufficiently close to σ_{0f}, can be answered by another application of the implicit function theorem.

The derivatives of $R^{(m)}(A(\sigma_f+\sigma_c),\sigma_f+\sigma_c;p_n)$, with respect to σ_c and p_n, are easy to calculate, and may be shown to be bounded, and continuous with respect to σ_f, σ_c, and p_n by methods following closely those of Sec. 2. The ordinary implicit function theorem is applicable if the derivative system has an inverse; if it does not, we can treat the bifurcation equation, as in Sec. 2.

The shifts in the positions of the zeros, $|p_n-p_{0n}|$, are proportional to $\|\sigma_f-\sigma_{0f}\|$, and so by making the latter quantity small enough, we can ensure that none of the zeros move by more than (say), one-third of the distance between the closest pair of zeros. In this way we can be sure that all zeros remain distinct, and that the orders, $2q_n$, do not change.

4. PRACTICAL IMPLEMENTATION OF THE METHOD

In practice, we set up a modified Newton-Kantorovich iteration for the numerical calculation of the new amplitudes that correspond to the changed cross-sections. We shall simply write down the equations and refer the reader to Ref. 14 for a detailed discussion of the method.

$$S_l(A^{(j)},\sigma_c^{(j)}+\sigma_{0f}+\delta\sigma_f)+\sum_{r=0}^{\infty}\frac{\partial S_l(A^{(0)},\sigma_c^{(0)}+\sigma_{0f}+\delta\sigma_f)}{\partial A_r}\delta A_r^{(j+1)}$$
$$+\sum_{k=1}^{Q}\frac{\partial S_l(A^{(0)},\sigma_c^{(0)}+\sigma_{0f}+\delta\sigma_f)}{\partial\sigma_{l_k}}\delta\sigma_{l_k}^{(j+1)}=0, \tag{4.1a}$$

$$R^{(m)}(A^{(j)},\sigma_c^{(j)}+\sigma_{0f}+\delta\sigma_f;p_n^{(j)})$$
$$+\sum_{r=0}^{\infty}\frac{\partial R^{(m)}(A^{(0)},\sigma_c^{(0)}+\sigma_{0f}+\delta\sigma_f,p_n^{(0)})}{\partial A_r}\delta A_r^{(j+1)}$$
$$+\sum_{k=1}^{Q}(2l_k+1)P_{l_k}^{(m)}(p_n^{(0)})\delta\sigma_{l_k}^{(j+1)}+\delta\sigma_f^{(m+1)}(p_n^{(0)})\delta p_n^{(j+1)}$$
$$+\delta_{m,2q_n-1}R^{(m+1)}(A^{(0)},\sigma_c^{(0)}+\sigma_{0f};p_n^{(0)})\delta p_n^{(j+1)}=0. \tag{4.1b}$$

Here S_l is the partial-wave projection of S, i.e.,

$$S_l(A,\sigma_c+\sigma_f)=A_l-A_l^2-\bar{D}_l^2(A,\sigma_c+\sigma_f). \tag{4.2}$$

For numerical convenience, we work in Eq. (4.1) directly with the partial waves A_l and σ_l, rather than with the functions $A(z)$ and $\sigma(z)$. The partial-wave index l runs from 0 to ∞, although in practice this means 0 to some sufficiently large $L_{\max}$, at which point the r-series in (4.1) are also cut off. In (4.1b), m runs over $0,2,\ldots,2q_n-1$, and n over the subset of $1,2,\ldots,N$ that corresponds to the zeros in the upper half-plane, or on the real axis, and within the ellipse $\epsilon(\zeta_0'')$. We have used the notation

$$P_l^{(m)}(z)=\left(\frac{d}{dz}\right)^m P_l(z), \tag{4.3}$$

$$\delta\sigma_f^{(m+1)}(z)=\left(\frac{d}{dz}\right)^{m+1}\delta\sigma_f(z)$$
$$=\sum_{l\neq l_k}(2l+1)\delta\sigma_{fl}P_l^{(m+1)}(z), \quad k=1,2,\ldots,Q, \tag{4.4}$$

and we have taken account of the fact that

$$R^{(m)}(A^{(0)},\sigma_c^{(0)}+\sigma_{0f};p_n^{(0)})=0 \tag{4.5}$$

for $m=0,1,\ldots,2q_n-1$, $n=1,2,\ldots,N$, in order to simplify the p_n-derivative term in (4.1b). Finally, j labels the iteration step, and we define

$$\begin{aligned}\delta A_r^{(j+1)}&=A_r^{(j+1)}-A_r^{(j)},\\ \delta\sigma_{l_k}^{(j+1)}&=\sigma_{l_k}^{(j+1)}-\sigma_{l_k}^{(j)},\\ \delta p_n^{(j+1)}&=p_n^{(j+1)}-p_n^{(j)}.\end{aligned} \tag{4.6}$$

The Kantorovich theorem[33] guarantees the convergence of the iteration (4.1), if the corresponding inverses exist,[14] since it may be shown that S and $R^{(m)}$ are twice Fréchet differentiable with respect to A and σ_c. In the event that (4.1) cannot be inverted to give the quantities (4.6), one may approximate the bifurcation equation by extending the Newton expansion to second order. We refer to Refs. 11 and 36 for further details.

5. EXTENSION TO INELASTIC UNITARITY

In Secs. 3 and 4 we discussed at length the construction of new amplitudes corresponding to changed cross sections. The continuum ambiguity resulting from changes in the inelastic contributions to the amplitude has been treated in Refs. 11 and 14. In this section we extend these methods is such a way as to allow us to change the cross sections and the inelasticities simultaneously.

At energies above the first inelastic threshold we write the unitarity condition

$$A_l = A_l^2 + D_l^2 + I_l, \tag{5.1}$$

where the inelasticities I_l have to satisfy the inequality

$$0 \leq I_l \leq \tfrac{1}{4}. \tag{5.2}$$

Following the technique of Sec. 2, we define an operator S, which will now also depend upon the I_l's,

$$S(A, \sigma, I; z) = A(z) - M(A, \sigma; z) - I(z) \tag{5.3}$$

where

$$I(z) = \sum_l (2l+1) I_l P_l(z). \tag{5.4}$$

Because of (5.1) and the equivalence (2.14) we know that

$$S(A_0, \sigma_0, I_0; z) = 0, \tag{5.5}$$

where $I_0(z)$ is the inelastic contribution to the amplitude $F_0(z)$. We now change the differential cross section $\sigma_0(z)$ and the inelastic part $I_0(z)$ by small amounts $\delta\sigma(z)$ and $\delta I(z)$, and we want to construct a new absorptive part $A(z)$ such that

$$S(A, \sigma_0 + \delta\sigma, I_0 + \delta I) = 0 \tag{5.6}$$

where we have suppressed the variable z. The proof that such an $A(z)$ exists is essentially the same as that given in Sec. 2. Again we have the problem of the zeros of the dispersive part. To prevent the zeros from parasitizing, we have to ensure, as in Sec. 3, that (3.6) is satisfied. However, we now have the choice of constraining either part of $\sigma(z)$, or part of $I(z)$, or both. We therefore write the following system of equations

$$S(A, \sigma_c + \sigma_f, I_c + I_f) = 0, \tag{5.7}$$

$$R^{(m)}(A(\sigma_f + \sigma_c, I_f + I_c), \sigma_f + \sigma_c; p_n) = 0 \tag{5.8}$$

and apply a modified Newton–Kantorovich iteration in order to solve them. The final equations are then similar to Eqs. (4.1) except for a term

$$-\sum_{n=1}^{R} \delta_{l,n} \delta I_{l_n}^{(j+1)} \tag{5.9}$$

in Eq. (4.1a) where R is the number of constrained I_l's and the index k in (4.1a) and (4.1b) runs from 1 to $Q - R$.

6. NEIGHBORHOODS OF THE CRICHTON AMBIGUITY

In this section, we shall first discuss in more detail the nature of the singularities of $\partial S/\partial A$. Then we shall illustrate the foregoing ideas by considering the case of a polynomial amplitude, in particular, certain aspects of the Crichton ambiguity will be elucidated.

As in the previous section, we set

$$S_l = A_l - A_l^2 - D_l^2 - I_l \tag{6.1}$$

where I_l is zero if the energy is below the first inelastic threshold, and is otherwise bounded between 0 and $\frac{1}{4}$. Then we may write the partial Fréchet derivative

$$\frac{\partial S_l}{\partial A_m} = [1 - 2A_l]\delta_{lm} - 2D_l \frac{\partial D_l}{\partial A_m} \tag{6.2}$$

with

$$\frac{\partial D_l}{\partial A_m} = -\frac{2m+1}{2\pi i} \oint_{\partial\epsilon(\zeta_0')} dz Q_l(z) P_m(z) \frac{A(z)}{D(z)}. \tag{6.3}$$

We know that $\partial S_l/\partial A_m - \delta_{lm}$ is a compact linear operator on the Hilbert space $\mathcal{H}(\zeta_1)$ of Sec. 2, and therefore $\partial S_l/\partial A_m$ will fail to have an inverse precisely when there exists a nonzero sequence $\{\alpha_l\}$, belonging to $\mathcal{H}(\zeta_1)$, for which

$$\sum_{m=0}^{\infty} \frac{\partial S_l}{\partial A_m} \alpha_m = 0. \tag{6.4}$$

If we consider only first order changes in A and σ, we may write for (2.19)

$$\frac{\partial S}{\partial A}\delta A + \frac{\partial S}{\partial \sigma}\delta\sigma = 0 \tag{6.5}$$

where we have not made the distinction between $\delta\sigma_c$ and $\delta\sigma_f$ explicit, and where the partial wave subscripts and summations are also implicit. If

$$\frac{\partial S}{\partial A}\alpha = 0 \tag{6.6}$$

which is (6.4) written implicitly, and if the normalized null function α is unique, then we impose the following linear constraint on $\delta\sigma$:

$$\left(\alpha, \frac{\partial S}{\partial \sigma}\delta\sigma\right)_{\zeta_1} = 0 \tag{6.7}$$

and then solve (6.5) as

$$\delta A = -\tilde{S}_A^{-1} \frac{\partial S}{\partial \sigma}\delta\sigma + \lambda\alpha \tag{6.8}$$

where $\tilde{S}_A^{-1}$ is the pseudoinverse that was introduced in Sec. 2, and (6.8) is the first-order version of (2.54). The number λ has to be determined from the bifurcation equation (2.58), which may be approximated by extending (6.5) to second order in δA, and by contracting this against α. It is easy to see that, as $\delta\sigma \to 0$, λ is generally of a lower order (apart from exceptional cases, λ is of order $\delta\sigma^{1/2}$). Hence, to order λ only, $\delta A = \lambda\alpha$, and since

$$\delta D = (\delta\sigma - 2A\delta A)/2D, \tag{6.9}$$

it follows that

$$\delta D = -\lambda A\alpha/D, \tag{6.10}$$

to order λ. If we have a bifurcation point of the complete system (3.3) and (3.7), then δD must be analytic within the ellipse of integration $\partial\epsilon(\zeta_0')$. Therefore any zeros of D within $\partial\epsilon(\zeta_0')$ which are not cancelled by zeros of A must be cancelled by zeros of α.

One interesting property of α immediately follows from the analyticity of δD within $\partial\epsilon(\zeta_0')$. Using (6.2) and (6.3), we write for (6.4)

$$(1 - 2A_l)\alpha_l + \frac{D_l}{\pi i} \oint_{\partial\epsilon(\zeta_0')} dz Q_l(z) \frac{A(z)\alpha(z)}{D(z)} = 0 \tag{6.11}$$

where

$$\alpha(z) = \sum_{m=0}^{\infty} (2m+1)\alpha_m P_m(z). \tag{6.12}$$

Because of (6.10) and the analyticity of δD, we can distort the contour $\partial\epsilon(\zeta_0')$ and squeeze it around the cut $(-1, +1)$ to obtain

$$(1-2A_l)\alpha_l + D_l \int_{-1}^{+1} dx P_l(x) \frac{A(x)\alpha(x)}{D(x)} = 0.$$

If we now multiply this by $(2l+1)$ and sum over l, we find

$$\alpha(1) = 0 \tag{6.13}$$

so that α vanishes in the forward direction.

Let us conclude this general discussion by listing sufficient conditions such that $F = D + iA$ is a bifurcation point of the complete system.

(a) there is a nontrivial solution α of (6.4);

(b) $A(z)\alpha(z)/D(z)$ is analytic within $\epsilon(\zeta_0')$;

(c) $\partial^2 S(A,\sigma)/\partial A^2 \cdot \alpha \cdot \alpha \neq 0$;

(d) F satisfies unitarity and $|F|^2 = \sigma$.

Now we shall consider the case that both $A(z)$ and $D(z)$ are polynomials of degree L, and that all zeros of $D(z)$ are simple and lie within the ellipse $\partial\epsilon(\zeta_0')$. We may write

$$\frac{A(z)}{D(z)} = \gamma_0 + \sum_{s=1}^{L} \frac{\gamma_s}{z-\beta_s} \tag{6.14}$$

where the β's are the zeros of $D(z)$. We may identify γ_0 by considering the limit $z \to \infty$ in (6.14):

$$\gamma_0 = A_L/D_L. \tag{6.15}$$

We now evaluate the integral (6.3) as follows:

$$\frac{\partial D_l}{\partial A_m} = -\frac{A_L}{D_L}\delta_{lm} - \theta(m-l-1)(2m+1) \times \sum_{s=1}^{L} \gamma_s [Q_l(\beta_s)P_m(\beta_s) - P_l(\beta_s)Q_m(\beta_s)] \tag{6.16}$$

and express the condition (6.4) in the form

$$\left[1 - 2A_l + 2\frac{A_L}{D_L}D_l\right]\alpha_l = -2D_l \sum_{m=l+1}^{\infty} (2m+1)\alpha_m \times \sum_{s=1}^{L} \gamma_s [Q_l(\beta_s)P_m(\beta_s) - P_l(\beta_s)Q_m(\beta_s)]. \tag{6.17}$$

For $l > L$ we have $D_l = 0 = A_l$, and therefore $\alpha_l = 0$. Hence we deduce from (6.17) in the case $l = L$ that $\alpha_L = 0$. The sum (6.4) is thus automatically truncated at $l = L-1$ or lower. For $l = L-1$ one finds

$$\alpha_{L-1} = 0 \quad \text{or} \quad 1 - 2A_{L-1} + 2A_L D_{L-1}/D_L = 0. \tag{6.18}$$

In the first case one then has

$$\alpha_{L-2} = 0 \quad \text{or} \quad 1 - 2A_{L-2} + 2A_L D_{L-2}/D_L = 0 \tag{6.19}$$

and so on. If

$$1 - 2A_l + 2A_L D_l/D_L \neq 0 \tag{6.20}$$

for $l = 0, 1, 2, \ldots, L-1$, then $\alpha_l = 0$, all l, which means that there is no nontrivial null sequence, and hence that $\partial S_l/\partial A_m$ is nonsingular and has an inverse. If, on the other hand,

$$1 - 2A_l + 2A_L D_l/D_L = 0 \tag{6.21}$$

with $l = n$, for one and only one integer n between 0 and $L-1$, then there is just one independent null function, which one may obtain from (6.17) by setting $\alpha_n = 1$, and then by solving successively for $\alpha_{n-1}, \alpha_{n-2}, \ldots, \alpha_0$. In the case that (6.21) is satisfied for more than one value of l, there may in general be more than one independent null function; but we shall not examine this case further.

For purely elastic amplitudes, the condition (6.21) for a singularity of $\partial S/\partial A$ can be reduced to:

$$2\delta_l = [(2N+1)/2]\pi + \delta_L \tag{6.22}$$

where the δ_l's are the real phase-shifts and N is an integer. There are many polynomial amplitudes that have one or more partial waves satisfying (6.22). However, the subsidiary condition that $\alpha A/D$ be analytic is met only in a few cases. Explicit examples of these are given by the endpoints of the SPD[26] and SPDF[28] Crichton-like ambiguities. Crichton-like ambiguities exist whenever there are two polynomial amplitudes F and F', with the same fixed inelasticities, each of degree L, that have the same modulus. It has been shown in the $L = 2$ and $L = 3$ cases, that the amplitudes F and F' are on closed curves in the space spanned by $A_0, A_1, \ldots, A_L$. These curves can be parametrized by the change in the differential cross section σ. The endpoints of the ranges of σ for these curves correspond precisely to bifurcation points of the complete system. In the SPD Crichton case there are in fact two singular points, in addition to the bifurcation points (which occur at $\delta_2 = 12.5°$ and $\delta_2 = 24.2°$). They correspond to the satisfaction of Eq. (6.22) for the S wave: for $\delta_2 = 13.5°$, $\partial S/\partial A$ is singular at F, and for $\delta_2 = 23.0°$, it is singular at F'.

Given F and F' with the same σ it is generally possible to construct two new amplitudes $F + \delta F$ and $F' + \delta F'$ corresponding to the same slightly changed cross section $\sigma + \delta\sigma$ by a simple modification of the method of Sec. 4. In particular, it is possible to follow the Crichton curves mentioned above, and we shall outline the method for the case $L = 2$. In this case D and D' each have two real simple zeros, and therefore two of the $\delta\sigma_l$ must be constrained in order to prevent the zeros from parasitizing. These constraints are different for D and D', and therefore in general we would expect $\delta\sigma_c \neq \delta\sigma_c'$. Nevertheless, we now show that it is possible to ensure that $\delta\sigma_c = \delta\sigma_c'$, and thus to ensure that $|F + \delta F| = |F' + \delta F'|$. Indeed the cross section $\sigma(z)$ is a fourth-order polynomial, so there are five Legendre coefficients, $\sigma_0, \sigma_1, \ldots, \sigma_4$; so that it suffices to take four of the σ_l, instead of two, as members of the constrained set σ_c. If we exclude the singular points of $\partial S/\partial A$ (which are the two bifurcation points, and the points $\delta_2 = 13.5°$ and $\delta_2 = 23.0°$ to which we alluded above), we may multiply Eq. (4.1a) by $(\partial S/\partial A)^{-1}$ and substitute the resulting expression for $\delta A_r^{(j+1)}$ into Eq. (4.1b). This gives four real inhomogeneous equations for the *six* unknowns, $\delta p_1^{(j+1)}$, $\delta p_2^{(j+1)}$ and the four $\delta\sigma_{l_k}^{(j+1)}$. Now we write the corresponding equations for the alternative amplitude F' and obtain four more equations for the six unknowns $\delta p_1'^{(j+1)}$, $\delta p_2'^{(j+1)}$, and the same four $\delta\sigma_{l_k}^{(j+1)}$. Evidently we have in all eight equations for eight unknowns, and in general we can find a solution. Hence we generate new amplitudes that satisfy the Crichton requirement $|F + \delta F| = |F' + \delta F'|$. Evidently, since $\delta\sigma_f$ contains only one Legendre coefficient, the one-dimensional degree of freedom corresponds precisely to following the SPD Crichton curve.

It is possible with the same method to obtain nontrivial continuations away from the Crichton SPD cross section by including some new components $\delta\sigma_l$, $l > 4$, in $\delta\sigma_f$. If the number of the new $\delta\sigma_l$ is finite then $\sigma + \delta\sigma$ will still be a polynomial, but $F + \delta F$ and $F' + \delta F'$ will in general possess parasitic branch cuts which can be kept out of the ellipse of integration by choosing $\delta\sigma_f$ small enough. It is possible that, by a sequence of Newton-steps, one could get rid of the branch cuts and finish with new polynomial amplitudes $F + \Delta F$ and $F' + \Delta F'$, of a higher degree than F and F'. For example, there may well exist a continuous connection between the SPD ambiguities and some, or all, of the SPDF cases that have been studied by Berends and Ruijsenaars.

The above demonstrations have been based on the Newton method; but a more satisfactory existence proof may easily be constructed by using the Hildebrandt–Graves theorem, as in Sec. 2; and one could also consider then nonpolynomial changes in σ.

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Percolation on a Cayley tree with second nearest neighbor bonds

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We derive the critical concentration for site percolation on a Cayley tree "decorated" with second nearest neighbor bonds. For a tree with connectivity K the result is $c_{crit} = <1+K-[(1+K)^2-4]^{1/2}>/2K$.

The percolation problem[1-6] deals with a lattice composed of sites and bonds. It is assumed that a finite fraction c of the sites are marked or "open," the remaining ones being unmarked or "closed." Clusters of open sites interconnected by bonds will be formed, and one wants to study the distribution of cluster sizes as a function of c. Of particular importance for several applications (e.g., magnetism) is the appearance of the first infinite cluster, which occurs at some critical concentration c_{crit} called the percolation threshold.

Let us pick at random one of the open sites and declare it "wet" (suggesting that some kind of fluid is poured into the lattice at this site). We will refer to this site as "the origin" or site 0, but it should be remembered that it could be any open site. We will define any other site j to be wet if and only if it is open and there exists a path on the lattice going from 0 to j and avoiding all closed sites. (To give some physical interpretation to this definition, imagine that the fluid poured into 0 flows along the bonds but is stopped by closed sites.) We shall say that a site j is at distance n if there exists an n-step path but no $(n-1)$ step path from 0 to j.

Let $P_n(c)$ be the probability that *at least one* site at distance larger than n is wet. $P_n(c)$ is a decreasing function of n, and the following limit exists,

$$\lim_{n\to\infty} P_n(c) = P(c), \tag{1}$$

and is called the *percolation probability*. The critical concentration or percolation threshold is defined as

$$c_{crit} = \sup\{c \mid P(c) = 0\}. \tag{2}$$

This quantity depends, of course, on the lattice under consideration. We study here the problem of a Cayley tree "decorated" with second nearest neighbor bonds. A Cayley tree[7] is a pseudolattice containing no closed loops, and on which each site has the same number $\gamma \equiv K+1$ of nearest neighbors. K is called the connectivity of the tree. Figure 1 shows in full lines a portion of a Cayley tree of connectivity $K=2$. The percolation problem can be solved exactly on a Cayley tree[7]; the percolation threshold turns out to be $c_{crit} = 1/K$. The persent work differs from that of Ref. 7 in that we will include second nearest neighbor bonds (dotted lines in Fig. 1), thus increasing the number of paths along which the fluid can flow. For simplicity we still define distances on the lattice in terms of the original bonds (full lines).

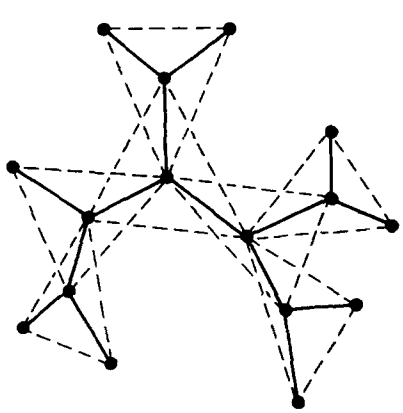

FIG. 1. Portion of a Cayley tree with $K=2$ and bonds between second nearest neighbors (dotted lines).

Since our bonds are not oriented (liquids can flow either way) the following alternative but equivalent definition of $P_n(c)$ is possible: Let us pick one of the open sites at random and call it the origin 0. Imagine liquid poured into all open sites at distances larger than n, and define $P_n(c)$ as the probability that the liquid, now flowing inwards, will reach the origin 0. It is this second definition of $P_n(c)$ that will be most convenient for our purposes.

We also introduce the idea of an *n-branch*, we define this term in the following way: take one site and call it the the zeroth generation or vertex; connect it to K other sites and call these the first generation sites; connect each first generation site to K others and call these the second generation sites, etc. Stop the process when nth generation has been added. The resulting graph is an n-branch. Figure 2 shows a 3-branch of connectivity $K=2$. Since an infinite Cayley tree is obtained by attaching $\gamma = K+1$ ∞-branches to any of its sites, we expect some relation between percolation on trees and branches. We will make this relation explicit later, and work only with branches for the time being.

Let α_n be the probability that the vertex of an n-branch is dry if all open sites on both the nth and $(n-1)$th generation are wet. Let β_n be the probability that the vertex and all its nearest neighbors are simultaneously dry under the same conditions. It is clear from our definitions that

$$\alpha_1 = 1 - c, \tag{3}$$

$$\beta_1 = (1-c)^{K+1}. \tag{4}$$

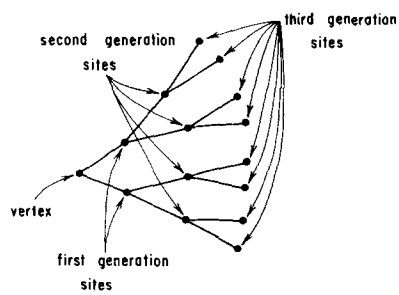

FIG. 2. A 3-branch for $K=2$

An $(n+1)$-branch is formed by attaching K n-branches to its vertex. We use this fact to write down recurrence relations for the quantities α_n, β_n. The vertex of the $(n+1)$-branch will be dry if (a) it is closed or (b) it is open and all its first and second nearest neighbors are dry:

$$\alpha_{n+1} = 1 - c + c\beta_n^K \tag{5}$$

For β_{n+1} we need the vertex of the $(n+1)$-branch and all its nearest neighbors to be dry. Situation (b) above meets this requirement, but (a) does not. We must impose in addition to (a) that all first generation sites, which are themselves vertices of attached n-branches, should be dry. We therefore get

$$\beta_{n+1} = (1-c)\alpha_n^K + c\beta_n^K. \tag{6}$$

It is not difficult to find the behavior of the sequences $\{\alpha_n\}$, $\{\beta_n\}$ for $n \to \infty$. From (3)—(6) we have $\alpha_1 \leq \alpha_2$, $\beta_1 \leq \beta_2$. Moreover, since the right-hand sides of (5) and (6) are increasing functions of both α_n and β_n, the two sequences $\{\alpha_n\}$ and $\{\beta_n\}$ are nondecreasing.

Consider next the equations obtained by requiring that a point (α, β) be a fixed point of the transformation (5), (6):

$$\alpha = 1 - c + c\beta^K, \tag{7}$$

$$\beta = (1-c)(1-c+c\beta^K)^K + c\beta^K \equiv f(\beta, c). \tag{8}$$

Let $\bar{\beta}$ be the smallest root of (8) in the interval $[0,1]$ and $\bar{\alpha} = 1 - c + c\bar{\beta}^K$ the corresponding α. We have $\bar{\beta} = f(\bar{\beta}, c) \geq f(0, c) = \beta_1$ and $\bar{\alpha} = 1 - c + c\beta^K \geq 1 - c = \alpha_1$. One can now use the monotonicity of the right-hand sides of (5) and (6) to prove by induction that $\beta_n \leq \bar{\beta}$ and $\alpha_n \leq \bar{\alpha}$ for all n. Thus the sequences $\{\alpha_n\}$ and $\{\beta_n\}$ have finite limits $\bar{\bar{\alpha}}$ and $\bar{\bar{\beta}}$ respectively, with $\bar{\bar{\alpha}} \leq \bar{\alpha}$, $\bar{\bar{\beta}} \leq \bar{\beta}$. But $\bar{\bar{\beta}} < \bar{\beta}$ is impossible since β is the smallest root of (8) in $[0,1]$. We conclude that

$$\lim_{n\to\infty} \alpha_n = \bar{\alpha} = \bar{\alpha}(c), \tag{9}$$

$$\lim_{n\to\infty} \beta_n = \bar{\beta} = \bar{\beta}(c). \tag{10}$$

The function $f(\beta, c)$ is convex in $[0,1]$ as a function of β (it is polynomial of degree $2K$ with positive coefficients), and $f(0,c) < 1$, $f(1,c) = 1$. There will be a solution $\bar{\beta} < 1$ if and only if $df(\beta, c)/d\beta|_{\beta=1} > 1$; otherwise $\bar{\beta} = 1$. The function $f(\beta, c)$ is explicitly known [Eq. (8)], and after some elementary algebra we can express this as

$$\bar{\beta} < 1 \quad \text{iff} \quad c > \{1 + K - [(1+K)^2 - 4]^{1/2}\}/2K. \tag{11}$$

Let us now return to the infinite Cayley tree. We assume that we have picked one open site as the origin, and ask for the probability $P_n(c)$ that it will be wet when every open site $n+1$ or more steps away is wet. There are only first and second neighbor bonds in the problem; we can therefore eliminate all sites at distances larger than $n+2$ without modifying $P_n(c)$. Once this elimination is done, what remains of the tree looks very much like an $(n+2)$-branch, with the only slight modification that the vertex has $K+1$ neighbors instead of K, and is open by definition.

The probability $\tilde{\alpha}_{n+2}$ that this vertex will be dry is consequently

$$\tilde{\alpha}_{n+2} = \beta_{n+1}^{K+1}, \tag{12}$$

obtained from (6) by letting $c \to 1$ (it is open) and $K \to K+1$. But $\tilde{\alpha}_{n+2} = 1 - P_n(c)$ so that

$$P(c) = \lim_{n\to\infty} P_n(c) = \lim_{n\to\infty} 1 - \beta_{n+1}^{K+1} = 1 - \bar{\beta}^{K+1}. \tag{13}$$

We conclude that the critical concentration is the highest one that makes $\bar{\beta} = 1$, and from (11)

$$c_{\text{crit}} = \{1 + K - [(1+K)^2 - 4]^{1/2}\}/2K. \tag{14}$$

We also find from our discussion the behavior of $P(c)$ for $c \to c_{\text{crit}}^+$. Close to c_{crit} we can expand Eq. (8) in the form

$$0 = \frac{\partial^2 f(1, c_{\text{crit}})}{\partial\beta\partial c}(c - c_{\text{crit}}) + \frac{1}{2}\frac{\partial^2 f(1, c_{\text{crit}})}{\partial\beta^2}(\beta - 1) + \cdots. \tag{15}$$

It is readily checked that $\partial^2 f(1, c_{\text{crit}})/\partial\beta\partial c > 0$ and $\partial^2 f(1, c_{\text{crit}})/\partial\beta^2 > 0$, which implies a linear increase of $1 - \bar{\beta}$ with $c - c_{\text{crit}}$ for $c \to c_{\text{crit}}^+$. From (13)

$$P(c) \propto (c - c_{\text{crit}}), \quad c \to c_{\text{crit}}^+. \tag{16}$$

We conclude this work with a few remarks. First, the procedure can be generalized to include bonds of any finite range. For third neighbor bonds, for example, one would define in addition to α_n, β_n a third quantity γ_n equal to the probability that the vertex of a branch and the two adjacent layers are all dry, and set up an equation for γ in analogy with (8). And second, one can study properties other than the threshold, for instance the mean cluster size at $c < c_{\text{crit}}$, by investigating the behavior of α_n and β_n as functions of n, not just their limits.

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Conserved vectors of the Komar type and compatability identities in Lagrangian field theories

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Given a Lagrangian which is an invariant density and a concomitant of a set of independent geometrical objects, it is shown that there is a unique conserved vector associated with the Lagrangian. For cases of interest the vector is constructed and is seen to be identical with Komar's conserved vector for general relativity. For a general Lagrangian we also construct the "compatability identity" relating the Euler–Lagrange tensors. The connection between these identities, the invariance identities of Rund, and Lie derivatives of invariant densities is found.

INTRODUCTION

In theoretical physics it is well known that there are numerous symmetry and differential identities associated with the Lagrangian formulation of multiple integral field theories. For example, in relativity theory, one often considers invariant densities of the form $\mathcal{L}(g_{ij}, g_{ij,l}, g_{ij,kl})$ where g_{ij} is a metric tensor. Taking $\mathcal{L}$ as a Lagrangian and performing a variation with respect to the metric tensor one obtains

$$E^{ij} \equiv \frac{\delta \mathcal{L}}{\delta g_{ij}} \equiv \frac{\partial \mathcal{L}}{\partial g_{ij}} - \frac{\partial}{\partial x^k}\frac{\partial \mathcal{L}}{\partial g_{ij,k}} + \frac{\partial^2}{\partial x^k \partial x^l}\frac{\partial \mathcal{L}}{\partial g_{ij,kl}}$$

as the result of the action principle. Alternately, it has been shown[1] that

$$E^{ij} \equiv \tfrac{1}{2} g^{ij} \mathcal{L} - \tfrac{2}{3} R^i{}_{stu} Z^{jstu} + Z^{ijkl}{}_{|kl}$$

is an equivalent definition for E^{ij} and clearly, of more use than the usual definition.[2] This tensorial identity is one example of a symmetry property derived from the fact that $\mathcal{L}$ is an invariant density. In addition, $E^{ij}{}_{|j} \equiv 0$ for any choice of $\mathcal{L}$ where the slash denotes covariant differentiation. This type of differential identity which we call the "compatability identity" is also a consequence of the transformation property of $\mathcal{L}$. In general relativity, for $\mathcal{L} = R\sqrt{g}$ where R is the scalar curvature, one has Komar's conserved vector $(\xi^{i|j} - \xi^{j|i})_{|j}$, where ξ^i is an arbitrary vector field.[3] Recently a conserved vector of the Komar-type has been constructed by us for the Brans–Dicke Lagrangian.[4,5] This kind of conserved vector also arises from the invariance of $\mathcal{L}$.

Below we show that the three types of identities described above are closely related and may be derived for arbitrary scalar densities constructed from arbitrary tensor fields. Some applications of interest are considered.

In the past there have been numerous discussions on identities and conservation laws arising from Lagrangians which are scalar densities.[6] However, these papers seem to be restricted to Lagrangians constructed from objects and their first derivatives. This is done to allow a Hamiltonian formulation at a later stage, but is a severe restriction on the Lagrangian itself. For example, it is well known that a scalar density cannot be constructed from the metric tensor and its first derivative alone. The argument that the Lagrangian of general relativity is equivalent to a first order Lagrangian which differs from the scalar curvature by an ordinary divergence is valid but irrelevant since more complicated invariant densities, e.g., $R^2\sqrt{g}$, will never possess this decomposition property.[7] Restricting Lagrangians in this manner allows the simple formulation of nontensorial conserved complexes such as the Landau–Lifshitz energy–momentum pseudotensors, and the superpotentials of von Freud. However, our desire is to obtain tensorial identities and ultimately a conserved vector which is the generalization of Komar's vector. In a forthcoming paper[8] it will be shown that our conserved vector, for many Lagrangians, may be used to establish connections between quantum fields and current algebra.

A question which arises is the relation (if any) between the Komar-type vector and the conserved quantities from Noether's theorem.[9] The answer is not clear for the following reasons: In a recent paper Hart[10] derives conserved vectors for Lagrangians which are concomitants of the metric tensor and its derivatives and a scalar field and its derivatives. Employing Noether's theorem and methods of Bergmann,[11] Hart constructs vectors which he claims to be analogs of the Komar vector applied to scalar–tensor theories. However, if one applies his results to the Brans–Dicke Lagrangian it is found that his conserved vector is quite different from the one we derived[5] using methods similar to those below. Also, Noether's theorem gives the so-called weak conservation laws which are satisfied as a consequence of the field equations. The vectors we construct below are conserved independently of the field equations. On the other hand, many people believe that every conservation law results from an invariance property of the system. This converse of Noether's theorem, which has been proved for restricted cases,[12] nonetheless clouds the picture and raises the posed question. We are considering this at the present time.

The section on invariance identities is somewhat related to work by duPlessis.[13] We present it below for its relation to the remainder of the paper and the fact that duPlessis' notation is not readily applicable to the analysis we consider.

1. CHAIN RULE FOR LIE DIFFERENTIATION

Consider an n-dimensional manifold and a function of the coordinates $\Omega(x^i)$, $1 < i \leq n$ of class C^∞. We shall restrict Ω to be a relative tensor with arbitrary rank and weight (with indices suppressed for notation) or the

components of an affine connection. This will insure that the Lie derivative of Ω in the direction of an arbitrary vector field will be tensorial,[15] and this property is essential in the theorem below.

Consider now a relative tensorial concomitant constructed from Ω and its derivatives with respect to the coordinates to arbitrary order m. We express the relative tensor in functional form as

$$T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}(\Omega, \Omega_{,k_1}, \Omega_{,k_1 k_2}, \ldots, \Omega_{,k_1 k_2 \cdots k_m}) \tag{1.1}$$

where $\Omega_{,k_1 k_2 \cdots k_m} = \partial^m \Omega / \partial x^{k_1} \partial x^{k_2} \cdots \partial x^{k_m}$ and assign the weight W to (1.1). We then have the chain rule for Lie differentiation:

Theorem 1: For a relative tensor of the type (1.1) the identity

$$\underset{\xi}{L}\, T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j} = \sum_{l=0}^{m} \frac{\partial T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}}{\partial \Omega_{,k_1 k_2 \cdots k_l}} (\underset{\xi}{L}\, \Omega)_{,k_1 k_2 \cdots k_l} \tag{1.2}$$

is satisfied where L_ξ is the appropriate Lie derivative in the direction of an arbitrary vector field ξ^a.

Proof: See Appendix 1.

2. TENSORIAL IDENTITIES

There are three types of tensorial identities associated with the chain rule for Lie differentiation. To obtain them we consider a relative tensor T (with suppressed indices) of arbitrary rank and weight which is constructed from "p" independent objects $\underset{1}{\Omega}, \underset{2}{\Omega}, \ldots, \underset{p}{\Omega}$ and their derivatives to any required order. Thus T has the functional dependence

$$T(\underset{1}{\Omega}, \underset{1}{\Omega}_{,k_1}, \underset{1}{\Omega}_{,k_1 k_2 \cdots k_{m_1}}, \ldots, \underset{p}{\Omega}, \underset{p}{\Omega}_{,k_1}, \ldots, \underset{p}{\Omega}_{,k_1 k_2 \cdots k_{m_p}}). \tag{2.1}$$

For this tensor the chain rule (1.2) may easily be generalized and yields

$$\underset{\xi}{L}\, T = \sum_{j=1}^{p} \left(\frac{\partial T}{\partial \underset{j}{\Omega}}\, \underset{\xi}{L}\, \underset{j}{\Omega} + \cdots + \frac{\partial T}{\partial \underset{j}{\Omega}_{,k_1 k_2 \cdots k_{m_j}}} (\underset{\xi}{L}\, \underset{j}{\Omega})_{,k_1 k_2 \cdots k_{m_j}} \right) \tag{2.2}$$

We write this as

$$\underset{\xi}{L}\, T = \underset{j}{\epsilon}\, \underset{\xi}{L}\, \underset{j}{\Omega} + \cdots + \underset{j}{\epsilon}^{(k_1 k_2 \cdots k_{m_j})} (\underset{\xi}{L}\, \underset{j}{\Omega})_{,k_1 k_2 \cdots k_{m_j}} \tag{2.3}$$

where, for the remainder of this section, the repeated index "j" runs from 1 to p while all other repeated indices run from 1 to n (dimension number). We also adopt the notation that round brackets surrounding tensorial indices denote the complete symmetrization of the enclosed indices,[17] and employ the summation convention. We shall have occasion to symmetrize expressions in which contravariant indices are not completely symmetric. We adopt the notation whereby /s/ following an expression means that this operation has been performed. The left-hand side of (2.3) is tensorial. However, the right-hand side is not yet in manifest tensor form. Let us therefore replace each partial derivative $(\underset{\xi}{L}\, \underset{j}{\Omega})_{,k_1 k_2 \cdots k_{m_j}}$ with the corresponding covariant derivative $(\underset{\xi}{L}\, \underset{j}{\Omega})_{|k_1 k_2 \cdots k_{m_j}}$ in addition to the appropriate connection coefficients and their derivatives as required by the definition of covariant differentiation. We may then write (2.3) in the equivalent form

$$\underset{\xi}{L}\, T = \underset{j}{\lambda}\, \underset{\xi}{L}\, \underset{j}{\Omega} + \underset{j}{\lambda}^{k_1} (\underset{\xi}{L}\, \underset{j}{\Omega})_{|k_1} + \cdots + \underset{j}{\lambda}^{(k_1 k_2 \cdots k_{m_j})} (\underset{\xi}{L}\, \underset{j}{\Omega})_{|k_1 k_2 \cdots k_{m_j}} /s/. \tag{2.4}$$

This procedure insures that each term on the right in (2.4) is tensorial.[18] Owing to the symmetrization of the contravariant indices, one finds that each element of the set $\underset{j}{\lambda}, \underset{j}{\lambda}^{k_1}, \ldots, \underset{j}{\lambda}^{(k_1 k_2 \cdots k_{m_j})}$ is also linearly independent.[13] This set of tensors is identical to the "tensorial derivatives" found by Rund by a different method.[1] From (2.4) we are in a position to extract three types of tensorial identities in general form:

A. Invariance identities

Invariance identities found by Rund follow from the invariance of scalars under arbitrary coordinate transformation. They may be used, for example, to find the explicit tensorial form of the variational derivative of scalar densities. The notion of invariance identities will now be generalized to the identities which follow from the form invariance of all tensors as in the proof of Theorem 1.

To obtain these identities we examine (2.4) in more detail. This identity contains $\underset{\xi}{L}\, \underset{j}{\Omega}$. We may make some definite statements about this Lie derivative without a knowledge of the actual fields it operates upon. We are specifically interested in the dependence of $\underset{\xi}{L}\, \underset{j}{\Omega}$ upon the vector field ξ^i (Lie vector). For example, if $\underset{j}{\Omega}$ are relative tensors then the Lie derivative involves the vector field and its first covariant derivative.[15] On the other hand, if $\underset{j}{\Omega}$ contain the components of an affine connection, then the Lie derivative contains the vector field ξ^i and its second symmetrized covariant derivative. Thus, for the class of $\underset{j}{\Omega}$ under consideration we may state quite generally

$$\underset{\xi}{L}\, \underset{j}{\Omega} = \underset{j}{\theta}_a\, \xi^a + \underset{j}{\theta}^b_a\, \xi^a{}_{|b} + \underset{j}{\theta}^{(bc)}_a\, \xi^a{}_{|bc} \tag{2.5}$$

where $\underset{j}{\theta}_a$, $\underset{j}{\theta}^b_a$, and $\underset{j}{\theta}^{(bc)}_a$ are tensorial concomitants constructed from $\underset{j}{\Omega}$ and its covariant derivatives in addition, possibly, to the curvature tensor.

We are primarily concerned with the occurrence of the Lie vector and its covariant derivatives when (2.5) is substituted into (2.4). This gives

$$\underset{\xi}{L}\, T \equiv \underset{j}{\lambda} (\underset{j}{\theta}_a\, \xi^a + \underset{j}{\theta}^b_a \xi^a{}_{|b} + \underset{j}{\theta}^{(bc)}_a\, \xi^a{}_{|bc}) + \cdots + \underset{j}{\lambda}^{(k_1 k_2 \cdots k_{m_j})} (\underset{j}{\theta}_a \xi^a + \underset{j}{\theta}^b_a \xi^a{}_{|b} + \underset{j}{\theta}^{(bc)}_a \xi^a{}_{|bc})_{|k_1 k_2 \cdots k_{m_j}} \tag{2.6}$$

We write this as

$$\underset{\xi}{L}\, T \equiv \underset{j}{\phi}_a \xi^a + \underset{j}{\phi}^b_a \xi^a{}_{|b} + \cdots + \underset{j}{\phi}^{bck_1 k_2 \cdots k_{m_j}}_a \xi^a{}_{|bck_1 k_2 \cdots k_{m_j}} \tag{2.7}$$

by collecting terms containing the same covariant derivatives of the Lie vector. In (2.7), however, not all of the terms are independent because the indices under covariant differentiation are not completely symmetrized.

Following duPlessis[13] we write

$$\xi^a{}_{|bck_1k_2\cdots k_{m_p}} \equiv \xi^a{}_{|(bck_1k_2\cdots k_{m_p})} + \cdots, \tag{2.8}$$

where the dots denote tensors which always involve lower order covariant derivatives of the Lie vector and the curvature tensor, in addition to their covariant derivatives.[19] While (2.8) is quite complicated for only small values of "m_p", it nonetheless enables us to write (2.7) in the general form

$$\underset{\xi}{L}T \equiv \underset{j}{\psi}_a \xi^a + \underset{j}{\psi}{}^b_a \xi^a{}_{|b} + \cdots + \underset{j}{\psi}{}^{(bck_1k_2\cdots k_{m_j})}_a \xi^a{}_{|bck_1k_2\cdots k_{m_j}} \quad /s/. \tag{2.9}$$

Here all terms on the right-hand side are independent. But on the left we have the Lie derivative of a tensor which may be written in the general form

$$\underset{\xi}{L}T \equiv B_a \xi^a + D^b_a \xi^a{}_{|b}. \tag{2.10}$$

Thus in view of the independence of the various tensors, by equating (2.9) and (2.10) we obtain the invariance identities in the form

$$B_a \equiv \sum_{j=1}^{p} \underset{j}{\psi}_a, \qquad D^b_a \equiv \sum_{j=1}^{p} \underset{j}{\psi}{}^b_a,$$

$$\sum_{j=1}^{p} \underset{j}{\psi}{}^{(bc)}_a \equiv \sum_{j=1}^{p} \underset{j}{\psi}{}^{(bck_1)}_a \equiv \cdots \equiv \sum_{j=1}^{p} \underset{j}{\psi}{}^{(bck_1k_2\cdots k_{m_j})}_a \equiv 0. \tag{2.11}$$

Here we have reintroduced the summation over "j" to illustrate that there is an additive coupling between the tensors corresponding to the various Ω. By proper choice of the set $\underset{j}{\Omega}$ the identities (2.11) will reduce to the identities found for particular cases of interest.[1]

For all but the most simple choices of $\underset{j}{\Omega}$ and a restriction upon the order of derivatives of $\underset{j}{\Omega}$ which occur in (2.1), the identities (2.11) are extremely complicated. They are required, however, if one wishes to write Euler–Lagrange equations in tensorial form or find the Komar-type conserved vectors which will be discussed below.

B. "Compatibility identity"

While invariance identities are associated with relative tensors of arbitrary rank and weight the "compatability identity," which is a differential identity relating the Euler–Lagrange tensors, is defined only for scalar densities. Also, whereas invariance identities are normally complicated, the compatability identities are relatively simple in form.

In (2.4) let us choose $T = \mathcal{L}$, a scalar density. We then have

$$\underset{\xi}{L}\mathcal{L} \equiv (\mathcal{L}\,\xi^a)_{,a}. \tag{2.12}$$

From (2.4) and (2.12) we have

$$(\mathcal{L}\,\xi^a)_{,a} \equiv \underset{j}{\lambda}\underset{\xi}{L}\underset{j}{\Omega} + \underset{j}{\lambda}{}^{k_1}(\underset{\xi}{L}\underset{j}{\Omega})_{|k_1} + \cdots + \underset{j}{\lambda}{}^{(k_1k_2\cdots k_{m_j})}(\underset{\xi}{L}\underset{j}{\Omega})_{|k_1k_2\cdots k_{m_j}}. \tag{2.13}$$

Integrating by parts, the right side becomes

$$(\mathcal{L}\,\xi^a)_{,a} \equiv \Big[\underset{j}{\lambda} - \underset{j}{\lambda}{}^{k_1}{}_{|k_1} + \cdots + (-1)^{m_j}\underset{j}{\lambda}{}^{(k_1k_2\cdots k_{m_j})}{}_{|k_1k_2\cdots k_{m_j}}\Big]\underset{\xi}{L}\underset{j}{\Omega} + V^a{}_{|a} \tag{2.14}$$

where V^a is the vector density

$$V^a \equiv (\underset{j}{\lambda}{}^a - \underset{j}{\lambda}{}^{ak_2}{}_{|k_2} + \underset{j}{\lambda}{}^{a(k_2k_3)}{}_{|k_2k_3} + \cdots)\underset{\xi}{L}\underset{j}{\Omega} + (\underset{j}{\lambda}{}^{ak_2} - \underset{j}{\lambda}{}^{a(k_2k_3)}{}_{|k_3} + \underset{j}{\lambda}{}^{a(k_2k_3k_4)}{}_{|k_3k_4} + \cdots)(\underset{\xi}{L}\underset{j}{\Omega})_{|k_2} + \cdots. \tag{2.15}$$

The coefficient of $\underset{\xi}{L}\underset{j}{\Omega}$ in (2.14) is the set of Euler–Lagrange expressions[20] which we now write as

$$\underset{j}{E} \equiv \frac{\delta \mathcal{L}}{\delta \underset{j}{\Omega}} \equiv \underset{j}{\lambda} - \underset{j}{\lambda}{}^{k_1}{}_{|k_1} + \cdots + (-1)^{m_j}\underset{j}{\lambda}{}^{(k_1k_2\cdots k_{m_j})}{}_{|k_1k_2\cdots k_{m_j}}. \tag{2.16}$$

The tensorial nature of these expressions is now obvious. The vector density appearing in (2.15) is the term which is normally discarded in variational problems because it contributes only boundary terms upon integration over a volume of the manifold. However, this term has importance as it is fundamental in the construction of tensorial conservation laws.

From (2.5) and (2.16) we find (2.14) becomes

$$(\mathcal{L}\,\xi^a)_{,a} \equiv \underset{j}{E}\cdot(\underset{j}{\theta}_a\,\xi^a + \underset{j}{\theta}{}^b_a\,\xi^a{}_{|b} + \underset{j}{\theta}{}^{(bc)}_a\,\xi^a{}_{|bc}) + V^a{}_{,a}. \tag{2.17}$$

We now integrate by parts once more to write this as

$$(\mathcal{L}\,\xi^a)_{,a} \equiv (\underset{j}{E}\underset{j}{\theta}_a - \underset{j}{E}_{|b}\underset{j}{\theta}{}^b_a + \underset{j}{E}_{|bc}\underset{j}{\theta}{}^{(bc)}_a)\xi^a + [\underset{j}{E}\underset{j}{\theta}{}^a_b\,\xi^b + \underset{j}{E}\underset{j}{\theta}{}^{(ab)}_c\,\xi^c{}_{|b} - (\underset{j}{E}\underset{j}{\theta}{}^{(ab)}_c)_{|b}\,\xi^c + V^a]_{|a}. \tag{2.18}$$

The final term on the right is the covariant divergence of a vector density and we may therefore replace the covariant derivative with an ordinary derivative. Our objective is now to show that the coefficient of ξ^a in (2.18) vanishes identically. The standard method of integrating (2.18) over a fixed volume of the manifold and choosing the vector ξ^a and its ordinary derivatives to vanish on the boundary is not obviously valid. On the one hand, it is not clear that this condition can be satisfied. In addition, we wish to place no restriction upon ξ^a as we shall have occasion to choose them to take specific forms in the Komar vector. We shall therefore prove our claim with an algebraic theorem which leaves the Lie vectors arbitrary.

In (2.18) we replace covariant derivatives by ordinary derivatives in addition to the appropriate connection coefficients required by covariant differentiation. Then from (2.5) and (2.15) we see that (2.18) may be written in the general form

$$\epsilon_i \xi^i \equiv \sum_{s=0}^{r} (A^{ij_1j_2\cdots j_s}_a\,\xi^a{}_{,j_1j_2\cdots j_s})_{,i} \tag{2.19}$$

where "r" is a positive integer. We then have

Theorem 2: Given an arbitrary vector field ξ^a and its derivatives to any required order and a set of functions $A^{ij_1j_2\cdots j_s}_a$, $1 \le s \le r$, which are independent of ξ^a and its derivatives, then if (2.19) is an identity for all possible choices of ξ^a it follows that $\epsilon_i \equiv 0$.

Proof: See Appendix 2.

In view of (2.18) and Theorem 2 we find

$$\underset{j}{E}\underset{j}{\theta}{}^{i}_{a} - \underset{j}{E}{}^{i}_{|b}\,\underset{j}{\theta}{}^{b}_{a} + \underset{j}{E}{}^{i}_{|bc}\,\underset{j}{\theta}{}^{(bc)}_{a} \equiv 0. \tag{2.20}$$

This is the tensorial compatability identity relating the Euler–Lagrange tensors.

There are two immediate features one notices in this identity. We need not know the Euler–Lagrange tensors $\underset{j}{E}$ explicitly nor do we need know the dependence of the Lagrangian upon the derivatives of $\underset{j}{\Omega}$. Secondly, (2.20) implies an additive rather than multiplicative coupling for various E. Therefore, to employ (2.20) we need only define a set of quantities $\underset{j}{\Omega}$, define their corresponding Euler–Lagrange tensors and then determine the appropriate $\underset{j}{\theta}{}^{i}_{a}$, $\underset{j}{\theta}{}^{b}_{a}$, $\underset{j}{\theta}{}^{(bc)}_{a}$ from the definitions of the corresponding Lie derivatives.

We now choose the set $\underset{j}{\Omega}$ to correspond to Lagrangians of interest and compute the compatability identities (2.20). We assume that a symmetric metric field g_{ij} is imposed upon the manifold.[26]

(1) $\mathcal{L} = \mathcal{L}(g_{ij}, g_{ij,k_1}, \cdots, g_{ij,k_1 k_2 \cdots k_p}), \quad p \geq 2,$

$$E^{b}_{a|b} \equiv 0. \tag{2.21}$$

This is the most familiar identity of this type and corresponds to the well-known fact that the Euler–Lagrange tensor of a Riemannian invariant density possesses an identically vanishing covariant divergence.

(2) $\mathcal{L} = \mathcal{L}(g_{ij}, g_{ij,k}, \ldots, \phi, \phi_{,a}, \ldots),$

$$2E^{b}_{a|b} \equiv E\,\phi_{|a}. \tag{2.22}$$

Here we consider a Lagrangian which is a concomitant of the metric tensor and its derivatives and a scalar field and its derivatives. This identity may be applied to the Brans–Dicke[4] theory (in which the identity is not mentioned) or the original Yilmaz theory[21] (where it is employed). Note that the vanishing of E^{ij} implies the vanishing of E. One thus obtains the solution of $E = 0$ automatically by solving the equation $E^{ij} = 0$.

(3) $\mathcal{L} = \mathcal{L}(g_{ij}, g_{ij,k}, \ldots, A_i, A_{i,j}, \ldots),$

$$2E^{b}_{a|b} \equiv E^{i}A_{i|a} - (E^{i}A_{a})_{|i}. \tag{2.23}$$

Here we consider a combined metric-vector Lagrangian where the fields are coupled arbitrarily. The identity may be applied to the Einstein–Maxwell Lagrangian which is an obvious choice. This identity has been given elsewhere.[14]

(4) $\mathcal{L} = \mathcal{L}(g_{ij}, g_{ij,k}, \ldots, \Gamma^{r}_{st}, \Gamma^{r}_{st,r}, \ldots)$

$$2E^{b}_{a|b} \equiv E^{(st)}_{a\ |st} + R_{ast}{}^{i}E^{(st)}_{i}. \tag{2.24}$$

Owing to the recent return of interest in the Cartan–Einstein theory,[22] we consider the Lagrangian constructed from the metric tensor and its derivatives in addition to a symmetric affine connection and its derivatives. The covariant derivative on the left is defined with respect to the Christoffel connection while the right-hand side has covariant derivatives with respect to a symmetric affine connection.

(5) $\mathcal{L} = \mathcal{L}(g_{ij}, g_{ij,k}, \ldots, \phi^{i}_{\cdot j}, \phi^{i}_{\cdot j,k}, \ldots),$

$$2E^{b}_{a|b} \equiv \epsilon^{\cdot j}_{i}\,\phi^{i}_{\cdot j|a} + \epsilon^{\cdot j}_{a|i}\phi^{i}_{\cdot j} - \epsilon^{\cdot j}_{i|j}\phi^{i}_{\cdot a}. \tag{2.25}$$

Lagrangians which are concomitants of the metric tensor and its derivatives and a mixed tensor and its derivatives are currently being considered. All covariant derivatives in 2.25 are defined for the Christoffel connection.

An examination of (2.21)–(2.25) shows that if the Euler–Lagrange tensors on the right-hand side are set to zero then it follows as a consequence that $E^{b}_{a|b} = 0$. This is a useful feature of coupled metrical theories for it allows the association of E^{ij} with the energy–momentum tensor. It is easily seen from (2.20) that this property occurs whenever the Lagrangian contains the metric tensor as one of the fields.

C. Conserved vector densities of Komar-type

Let us substitute (2.20) into (2.18). We find (2.15)

$$W^{i}{}_{,i} \equiv (\underset{j}{E}\underset{j}{\theta}{}^{i}_{b}\xi^{b} + \underset{j}{E}\underset{j}{\theta}{}^{(ib)}_{c}\,\xi^{c}{}_{|b} - (\underset{j}{E}\underset{j}{\theta}{}^{(ib)}_{c})_{|b}\,\xi^{c} + V^{i} - \mathcal{L}\,\xi^{i})_{,i} \equiv 0. \tag{2.26}$$

The term in brackets is a vector density whose covariant (and hence) ordinary divergence vanishes identically. It is apparent that each Lagrangian has a conserved vector associated with it.[23] As we shall see these vectors, for particular Lagrangians, are identical to the conservation laws of Komar.

Given a vector density whose ordinary divergence vanishes identically it is well known that locally there exists a two index skew object whose divergence is identically equal to the vector density.[24] Thus we should be able to write (2.26), locally, in the form

$$W^{i} = (T^{ij} - T^{ji})_{,j}. \tag{2.27}$$

If it turns out that the T^{ij} is tensorial then, of course, (2.27) is a global result. For the cases we consider below we shall find global expressions for the conserved vectors in the form (2.27).

We now consider a general Lagrangian which is constructed from fields of physical interest. We take our Lagrange density to be

$$\mathcal{L} = \mathcal{L}(g_{ij}, g_{ij,k}, g_{ij,kl}, \phi, \phi_{,i}, A_i, A_{i,j}) \tag{2.28}$$

where g_{ij} is the metric tensor, ϕ is a scalar field, and A_i is a vector field. We shall now find (2.26) for this Lagrangian and write it in the form of (2.27). Then we may choose ϕ or A_i to vanish and apply the identity to cases of more immediate interest.

For the Lagrangian (2.28) it is not difficult to show that (2.26) becomes

$$W^{i} \equiv 2E^{ri}\,\xi_{r} + 2Y^{rsi}\,\xi_{r|s} + 2Z^{rsti}\,\xi_{r|st} - 2Z^{rsti}{}_{|t}\xi_{r|s} + \psi^{i}\phi_{,j}\,\xi^{j} + \Omega^{ai}(\xi^{j}A_{a|j} + A_{j}\xi^{j}{}_{|a}) + E^{i}A_{j}\xi^{j} \tag{2.29}$$

where the various tensors are defined by

$$E^{ri} \equiv \frac{\delta \mathcal{L}}{\delta g_{ri}}, \tag{2.30a}$$

$$y^{rsi} \equiv \text{Tensorial derivative of } \frac{\partial \mathcal{L}}{\partial g_{rs,i}},^{1} \tag{2.30b}$$

$$Z^{rsti} \equiv \frac{\partial \mathcal{L}}{\partial g_{rs,ti}}, \tag{2.30c}$$

$$\psi^{i} \equiv \frac{\partial \mathcal{L}}{\partial \phi_{,i}}, \tag{2.30d}$$

$$\Omega^{ai} \equiv \frac{\partial \mathcal{L}}{\partial A_{a,i}}, \tag{2.30e}$$

$$E^{i} \equiv \frac{\delta \mathcal{L}}{\delta A_{i}}. \tag{2.30f}$$

To write (2.29) in the form (2.27) one needs the explicit form of the tensorial derivatives as in (2.11). It is found that one has the following identities:

$$E^{ij} \equiv \tfrac{1}{2} g^{ij} \mathcal{L} - \tfrac{2}{3} Z^{istu} R^{j}{}_{stu} - \tfrac{1}{4}(\lambda^{ij} + 3\lambda^{ji}) - \lambda^{ijt}{}_{|t} + Z^{ijkl}{}_{|kl} \tag{2.31a}$$

where

$$\lambda^{ij} \equiv \tfrac{1}{2}(\psi^{j}\phi^{,i} + \Omega^{j}A^{i} + \Omega^{aj}A_{a}{}^{|i} + \Omega^{ja}A^{i}{}_{|a}). \tag{2.31b}$$

Also,

$$y^{rsi} \equiv -\tfrac{1}{4}(\Omega^{(ir)}A^{s} + \Omega^{(si)}A^{r} - \Omega^{(rs)}A^{i}) \equiv y^{sri} \tag{2.31c}$$

and

$$E^{i} \equiv \Omega^{i} - \Omega^{ij}{}_{|j}. \tag{2.31d}$$

where Ω^{i} is the tensorial derivative for $\partial \mathcal{L}/\partial A_{i}$.[25] We also find that the tensor Z^{rsti} defined in (2.30c) satisfies the identities

$$Z^{abci} \equiv Z^{baci} \equiv Z^{baic}, \tag{2.31e}$$

$$Z^{abci} + Z^{bcai} + Z^{cabi} \equiv 0.$$

By employing the identities (2.31e) and the commutation relations to the third term on the right in (2.29) and from the other identities in (2.31) it can be shown that all terms in (2.29) containing ξ^{r} explicitly vanish. The resultant expression can, with some difficulty, be written in the form

$$W_{i} \equiv \{\tfrac{4}{3}(Z^{a[ji]k}\xi_{a|k} - 2Z^{a[ji]k}{}_{|k}\xi_{a}) + (A^{i}\Omega^{(aj)} - A^{j}\Omega^{(ai)})\xi_{a} + A^{a}\xi_{a}(\Omega^{ji} - \Omega^{ij})\}_{,j}. \tag{2.32}$$

Note that this is the expression for the divergence of the curl[17] of a vector density and as such the divergence index symbol may be an ordinary or covariant derivative.

We shall now consider (2.32) for cases of immediate interest in which we choose Lagrangians which are more simple than (2.28).

$\mathcal{L}(g_{ab}, g_{ab,c}, g_{ab,cd})$: To obtain the vector conservation identity for this case we set $A_{i} = 0$ in (2.32). Noting that there is no explicit dependence upon ϕ in (2.32), we obtain

$$W^{i} \equiv \tfrac{4}{3}(Z^{a[ji]k}\xi_{a|k} - 2Z^{a[ji]k}{}_{|k}\xi_{a})_{,j} \tag{2.33}$$

as the conserved vector for Riemannian invariant densities constructed from the metric tensor and its first two derivatives. Let us now apply this to the case of the scalar curvature density. For $\mathcal{L} = R(g)^{1/2}$ it is easily found that[2]

$$Z^{ajik} \equiv (g)^{1/2}(g^{aj}g^{ik} - \tfrac{1}{2}g^{ai}g^{jk} - \tfrac{1}{2}g^{ak}g^{ji}). \tag{2.34}$$

Hence, (2.33) becomes

$$W^{i} \propto \xi^{[i|j]}{}_{|j} \tag{2.35}$$

and this is precisely Komar's tensorial vector conservation law for general relativity.[3] By integrating (2.35) over an asymptotically Schwarzchild universe for a particular choice of ξ^{i} Komar shows that the total energy of a particle is mc^{2}.

$\mathcal{L} = \mathcal{L}(g_{ij}, g_{ij,k}, g_{ij,kl}, \phi, \phi_{,i})$: By eliminating the vector field A_{i} in (2.32), we obtain the conserved vector for the coupled metric and scalar field as

$$W^{i} \propto (Z^{a[ji]k}\xi_{a|k} - 2Z^{a[ji]k}{}_{|k}\xi_{a})_{|j}. \tag{2.36}$$

We may apply this to the Brans–Dicke Lagrangian by choosing $\mathcal{L} = g^{1/2}\phi R$. We find

$$W^{i} \propto (\phi\xi^{[i|j]} + 2\phi^{[|i}\xi^{j]})_{|j} \tag{2.37}$$

which is the expression we have obtained elsewhere by a different method.[5]

$\mathcal{L} = \mathcal{L}(g_{ij}, A_{i}, A_{i,j})$: This type of Lagrangian will include the Maxwell equations as a special case. To obtain the conserved vector we eliminate first and second derivatives of the metric tensor from (2.32) with the result

$$W^{i} \propto [(A^{i}\Omega^{(aj)} - A^{j}\Omega^{(ai)})\xi_{a} + A^{a}\xi_{a}(\Omega^{ji} - \Omega^{ij})]_{|j}. \tag{2.38}$$

Now it is not difficult to show that for this type of Lagrangian (in which first derivatives of the metric tensor are absent) $\Omega^{ij} = -\Omega^{ji}$.[1] Hence the first two terms on the right in (2.38) vanish and the conserved vector may be written as

$$W^{i} \propto (A^{a}\xi_{a}\Omega^{ij})_{|j}. \tag{2.39}$$

If we choose $\mathcal{L}$ to be the Maxwell invariant density and choose $\xi_{a} = A_{a}/(A_{r}A^{r})$, then one could interpret W^{i} as the current and the conservation law is the statement of charge conservation. The significance of the Komar-type vector for Lagrangians of physical interest will be discussed in a forthcoming paper.[8]

APPENDIX A

Proof: The transformation law for the tensor (1.1) is

$$\bar{T}^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}(\bar{x}^{d}) = B^{w}B^{b_1}_{s_1}B^{b_2}_{s_2} \cdots B^{b_j}_{s_j}A^{r_1}_{c_1}A^{r_2}_{c_2} \cdots A^{r_i}_{c_i}T^{c_1 c_2 \cdots c_i}_{b_1 b_2 \cdots b_i} \tag{A1}$$

where we write

$$B^{b}_{s} = \frac{\partial x^{b}}{\partial \bar{x}^{s}}, \quad B = \det(B^{b}_{s}), \quad \text{and} \quad A^{r}_{c} = \frac{\partial \bar{x}^{r}}{\partial x^{c}}.$$

We now specify a coordinate transformation given by

$$\bar{x}^{d} = x^{d} - \lambda\xi^{d}(x^{l}) \tag{A2}$$

where λ is a constant and ξ^{d} is an arbitrary nonnull ($\xi^{d}\xi_{d} \neq 0$) vector field. We do not require λ to be small and (A2) need not be considered an infinitesimal coordinate transformation. From (A2) the components of

the transformation become

$$B^b_s = \delta^b_s + \lambda \xi^b{}_{,s} + O(\lambda^2), \quad B = 1 + \lambda \xi^a{}_{,a} + O(\lambda^2),$$

$$A^r_c = \delta^r_c - \lambda \xi^r{}_{,c}, \tag{A3}$$

where here and in the following $O(\lambda^2)$ collectively denotes all terms containing λ^2 and higher order terms as explicit multiplicative factors. In (A3) and the following all derivatives are taken with respect to unbarred coordinates unless stated to the contrary. We now substitute (A3) into (A1) to find

$$\begin{aligned}\overline{T}^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}(\bar{x}^d) = T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}(x^d) + \lambda[& W\xi^a{}_{,a}\, T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}(x^d) \\ & + \xi^a{}_{,s_1}\, T^{r_1 r_2 \cdots r_i}_{a s_2 \cdots s_j}(x^d) + \cdots \\ & + \xi^a{}_{,s_j}\, T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j a}(x^d) - \xi^{r_1}{}_{,a}\, T^{a r_2 r_3 \cdots r_i}_{s_1 s_2 \cdots s_j}(x^d) \\ & - \cdots - \xi^{r_i}{}_{,a}\, T^{r_1 r_2 \cdots r_{i-1} a}_{s_1 s_2 \cdots s_j}(x^d)] + O(\lambda^2). \end{aligned} \tag{A4}$$

At this point we compare the coefficient of λ in (A4) to the Lie derivative of $T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}$ which is, by definition.[15]

$$\begin{aligned} L_\xi T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j} = {} & \xi^a T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j, a} + W\xi^a{}_{,a}\, T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j} \\ & + \xi^a{}_{,s_1}\, T^{r_1 r_2 \cdots r_i}_{a s_2 \cdots s_j} + \cdots \\ & + \xi^a{}_{,s_j}\, T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_{j-1} a} - \xi^{r_1}{}_{,a}\, T^{a r_2 \cdots r_i}_{s_1 s_2 \cdots s_j} \\ & - \cdots - \xi^{r_i}{}_{,a}\, T^{r_1 r_2 \cdots r_{i-1} a}_{s_1 s_2 \cdots s_j}. \end{aligned} \tag{A5}$$

Note that these functionals differ only by the first term on the right-hand side of (A5).

We now examine the functional dependence of (1.1) and to simplify the notation we suppress the indices on this relative tensor. From (1.1) it is clear that (A1) means

$$\overline{T}(\bar{x}^d) = \overline{T}(\overline{\Omega}(\bar{x}^d),\ \overline{\Omega}(\bar{x}^d)_{,\bar{k}_1}, \overline{\Omega}(\bar{x}^d)_{,\bar{k}_1\bar{k}_2}, \cdots, \overline{\Omega}(\bar{x}^d)_{,\bar{k}_1\bar{k}_2\cdots\bar{k}_m}) \tag{A6}$$

where

$$\overline{\Omega}(\bar{x}^d)_{,\bar{k}_1\bar{k}_2\cdots\bar{k}_m} \equiv \frac{\partial^m \overline{\Omega}(\bar{x}^d)}{\partial \bar{x}^{k_1}\, \partial \bar{x}^{k_2} \cdots \partial \bar{x}^{k_m}}. \tag{A7}$$

From (A2) and (A6) we have

$$\overline{T}(\bar{x}^d) = \overline{T}(x^d - \lambda \xi^d) = \overline{T}(x^d) - \lambda \overline{T}_{,a}\, \xi^a + O(\lambda^2) \tag{A8}$$

where now $\overline{T}(x^d)$ represents

$$\overline{T}(x^d) = \overline{T}(\overline{\Omega}(x^d), \overline{\Omega}(x^d)_{,\bar{k}_1}, \cdots, \overline{\Omega}(x^d)_{,\bar{k}_1\bar{k}_2\cdots\bar{k}_m}). \tag{A9}$$

In view of (A1) and (A3) we may write (A9) in terms of derivatives with respect to unbarred coordinates as

$$\overline{T}(x^d) = \overline{T}(\overline{\Omega}(x^d), \overline{\Omega}(x^d)_{,k_1} + O(\lambda), \cdots, \overline{\Omega}(x^d)_{,k_1 k_2 \cdots k_m} + O(\lambda)) \tag{A10}$$

We may examine (A9) or (A10) from "Form invariance"[16] of tensors. We state the result that form invariance allows us to drop the bar over T (only) on the right-hand side of (A10). Thus (A10) becomes

$$\overline{T}(x^d) = T(\overline{\Omega}(x^d), \overline{\Omega}(x^d)_{,k_1} + O(\lambda), \cdots, \overline{\Omega}(x^d)_{,k_1 k_2 \cdots k_m} + O(\lambda)). \tag{A11}$$

We now eliminate the function dependence from $\overline{\Omega}(x^d)$ on the right-hand side of (A11) by considering the transformation (A2), and expanding $\overline{\Omega}(x^d) - \Omega(x^d)$ in powers of λ. The coefficient of λ in the resultant series is defined to be the Lie derivative of Ω in the direction ξ^r and is tensorial if Ω is a relative tensor or the component of an affine connection. That is

$$\overline{\Omega}(x^d) = \Omega(x^d) + \lambda L_\xi \Omega + O(\lambda^2). \tag{A12}$$

We now substitute (A12) into (A11) and expand the resulting functional in powers of λ. It is easily seen that

$$\begin{aligned}\overline{T}(x^d) = {} & T(\Omega(x^d), \Omega_{,k_1}, \cdots, \Omega_{,k_1 k_2 \cdots k_m}) \\ & + \lambda \sum_{l=0}^{m} \frac{\partial T}{\partial \Omega_{,k_1 k_2 \cdots k_l}} (L_\xi \Omega)_{,k_1 k_2 \cdots k_l} + O(\lambda^2). \end{aligned} \tag{A13}$$

From this it is clear that $\overline{T}(x^d) - T(x^d) = 0\ (\lambda)$ and we may therefore replace $\overline{T}(x^d)$ in the second term on the right-hand side of (A8) by $T(x^d)$ and affect only the term $O(\lambda^2)$. Thus, from (A13) we find (A8) becomes

$$\begin{aligned}\overline{T}(\bar{x}^d) = {} & T(x^d) - \lambda T_{,a}\, \xi^a \\ & - \lambda \sum_{l=0}^{m} \frac{\partial T}{\partial \Omega_{,k_1 k_2 \cdots k_l}} (L_\xi \Omega)_{,k_1 k_2 \cdots k_l} + O(\lambda^2). \end{aligned} \tag{A14}$$

At this point we exhibit the tensor indices explicitly and (A14) becomes

$$\begin{aligned}\overline{T}^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}(\bar{x}^d) = {} & T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}(x^d) - \lambda \xi^a T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j, a} \\ & + \lambda \sum_{l=0}^{m} \frac{\partial T}{\partial \Omega_{,k_1 k_2 \cdots k_l}} (L_\xi \Omega)_{,k_1 k_2 \cdots k_l} + O(\lambda^2). \end{aligned} \tag{A15}$$

We equate (A4) to (A15) and divide by λ to obtain

$$\begin{aligned} & \xi^a T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j, a} + W\xi^a{}_{,a}\, T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j} + \xi^a{}_{,s_1}\, T^{r_1 r_2 \cdots r_i}_{a s_2 \cdots s_j} + \cdots \\ & + \xi^a{}_{,s_j}\, T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_{j-1} a} - \xi^{r_1}{}_{,a}\, T^{a r_2 \cdots r_i}_{s_1 s_2 \cdots s_j} - \cdots - \xi^{r_i}{}_{,a}\, T^{r_1 r_2 \cdots r_{i-1} a}_{s_1 s_2 \cdots s_j} \\ & = \sum_{l=0}^{m} \frac{\partial T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}}{\partial \Omega_{,k_1 k_2 \cdots k_l}} (L_\xi \Omega)_{,k_1 k_2 \cdots k_l}. \end{aligned} \tag{A16}$$

From (A5) we identify the left-hand side of (A16) with the Lie derivative of $T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}$. Thus (A16) is

$$L_\xi T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j} - \sum_{l=0}^{m} \frac{\partial T^{r_1 r_2 \cdots r_i}_{s_1 s_2 \cdots s_j}}{\partial \Omega_{,k_1 k_2 \cdots k_l}} (L_\xi \Omega)_{,k_1 k_2 \cdots k_l} = O(\lambda). \tag{A17}$$

Now the left-hand side is independent of λ while the right-hand side contains λ explicitly. Since λ is arbitrary the left-hand side vanishes identically and this is the statement of our theorem.

APPENDIX B

Differentiating in the sum we write (2.19) as

$$\epsilon_a \xi^a - A^i_{a,i}\, \xi^a \equiv \sum_{s=1}^{r} (A^{j_1 j_2 \cdots j_s}_a + A^{i j_1 j_2 \cdots j_s}_a{}_{,i}) \xi^a{}_{,j_1 j_2 \cdots j_s}$$

$$+A_a^{ij_1j_2\cdots j_r}\xi^a{}_{,ij_1j_2\cdots j_r}. \tag{B1}$$

The left-hand side is independent of derivatives of ξ^i. Hence we may differentiate (B1) with respect to the various derivatives of ξ^i to obtain the identities

$$\epsilon_a \equiv A^i_{a,i}, \tag{B2}$$

$$A_a^{(j_1j_2\cdots j_s)}+A_a^{i(j_1j_2\cdots j_s)}{}_{,i}\equiv 0, \quad s=1,2,\ldots,r, \tag{B3}$$

$$A_a^{(ij_1j_2\cdots j_r)}\equiv 0 \tag{B4}$$

where the round brackets again denote complete symmetrization of the enclosed indices. Let us now differentiation (B3) with respect to $\partial/\partial x^{j_1}$ for $s=1$. Then

$$A^i_{a,i}\equiv -A_a^{(ij_1)}{}_{,ij_1}. \tag{B5}$$

which together with (B2) implies

$$\epsilon_a \equiv -A_a^{(ij_1)}{}_{ij_1}. \tag{B6}$$

Similarly, by differentiating (2.20b) with respect to $\partial/\partial x^{j_2}$, $\partial/\partial x^{j_3}$, $\cdots$ for $s=2,3,\cdots$, it is easily seen that (B2) becomes

$$\epsilon_a \equiv (-1)^s A_a^{(ij_1j_2\cdots j_s)}{}_{,ij_1j_2\cdots j_s}, \quad s=1,2,\cdots,r. \tag{B7}$$

In particular, for $s=r$, (B7) gives

$$\epsilon_a \equiv (-1)^r A_a^{(ij_1j_2\cdots j_r)}{}_{,ij_1j_2\cdots j_r} \tag{B8}$$

and this vanishes identically from (B4) which proves the theorem.

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$$Z^{ijkl}=\frac{\partial \mathcal{L}}{\partial g_{ij,kl}}$$

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[16]This is simply a statement of the fact that tensorial concomitants are the same functions of their arguments in all coordinate systems.
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[20]Equation (2.14) can be looked at in the following way: For an arbitrary variation of the Ω_j, say $\Delta\Omega_j$, it is clear that $\Delta\mathcal{L}\equiv\delta\mathcal{L}/\delta\Omega_j\cdot\Delta\Omega_j+V^i{}_{,i}$ is the standard action principle result. For the particular choice of Δ corresponding to $\Delta\Omega_j=L\Omega_j$ one obtains, after some manipulation, (2.14). Hence (2.16) follows.
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[24]This is the converse of Poincare's lemma. See, for example, H. Flanders, *Differential Forms with Applications to the Physical Sciences* (Academic, New York, 1963), p. 27.
[25]Identity (2.4) above or Ref. 1, Sec. 4.
[26]In each of the following identities, the left hand side corresponds to the Euler—Lagrange tensor for the metric field.

Renormalization group solution of the one-dimensional Ising model

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A renormalization group approach is applied to the one-dimensional Ising model to obtain a rapidly convergent infinite series expansion for the free energy. This series can be summed and yields the well-known analytic solution.

The renormalization group ideas of Kadanoff[1] and Wilson[2] have given us considerable insight into the nature of critical phenomena. The application of renormalization group methods to calculate the critical exponents and the critical temperature for Ising spin models in two and higher dimensions have been quite successful.[3,4] However, these calculations are mathematically very complex and many approximations have to be made which obscure the underlying mathematical ideas. Accurate values for the fixed points and the corresponding eigenvalues in the renormalization transformation for planar Ising models can be obtained in general only with the aid of a large computer.[4,5] Recently it has been shown[5] that the renormalization group approach is actually more powerful than had been originally envisaged, and that it can be applied to obtain not just the singular part, but a complete solution for the free energy of general Ising spin systems. Calculations for a square Ising spin lattice in a four cell cluster approximation have given excellent agreement with previously known analytical and numerical results. In order to understand the basic ideas involved it is worthwhile to consider the simpler case of a one-dimensional Ising model with nearest neighbor interactions which leads to a much simpler renormalization transformation. It is well known that this model, which is readily solved by the transfer matrix technique of Kramers and Wannier,[6] does not exhibit a phase transition, and thus it appears unsuited to discuss a renormalization group method developed specifically to consider critical phenomena. It will be shown, however, that this is not the case and that our approach can also be applied here to obtain a rapidly convergent infinite series for the free energy. We sum explicitly the infinite series for the free energy with the aid of a nonlinear transformation and obtain the well-known analytic solution of the one-dimensional Ising model.

We start with the familiar Hamiltonian $H_N(K)$ for the one-dimensional Ising spin model for N spins, $S_i = \pm 1$, $i = 1, 2 \cdots N$, with nearest neighbor interaction coupling constant K,

$$H_N(K) = -K \sum_{i=1}^{N} S_i S_{i+1} \tag{1}$$

where $S_{N+1} = S_1$. Following Kramers and Wannier,[6] we introduce the 2×2 transfer matrix $\mathbb{P}_{S_1 S_2} = \exp(K S_1 S_2)$ which enables us to write the Boltzmann probability function $\exp(-H_N(K))$ $(kT = 1)$ in the form

$$\exp[-H_N(K)] = \mathbb{P}_{S_1 S_2}\, \mathbb{P}_{S_2 S_3} \cdots \mathbb{P}_{S_N S_1}. \tag{2}$$

Instead of computing the usual partition sum, $\sum_{\{S\}} \exp[-H_N(K)] = \operatorname{tr} \mathbb{P}^N$, we consider here only the partial sum of $\exp[-H_N(K)]$ over all possible values of the even spins, $s_i = \pm 1$, $i = 2, 4 \cdots$ and obtain for N even

$$\sum_{\{S_2 S_4 \cdots S_N\}} \exp[-H_N(K)] = \mathbb{P}^2_{S_1 S_3}\, \mathbb{P}^2_{S_3 S_5} \cdots \mathbb{P}^2_{S_{N-1} S_1}. \tag{3}$$

The idea behind this partial summation is to find a renormalization transformation $K \to K'$ such that

$$\mathbb{P}^2(K) = \exp[2g(K)]\, \mathbb{P}(K'), \tag{4}$$

where $g(K)$ is a scalar of function K. Then K' can be interpreted as an effective Ising coupling constant for the remaining odd spins S_i, $i = 1, 3, 5 \cdots N-1$ and Eq. (3) takes the form

$$\sum_{\{S_2 S_4 \cdots S_N\}} \exp[-H_N(K)] = \exp[-H_{N/2}(K) + Ng(K)]. \tag{5}$$

This is the basic equation of the renormalization group approach. The matrix condition Eq. (4) is readily satisfied by

$$K' = \tfrac{1}{2} \ln \cosh 2K \tag{6}$$

and

$$g(K) = \tfrac{1}{2} K' + \tfrac{1}{2} \ln 2. \tag{7}$$

The nonlinear renormalization transformation Eq. (6) has fixed points at $K^* = 0$ and $K^* = \infty$ with associated eigenvalues $\lambda = 0$ and $\lambda = 1$, respectively, where $\lambda = dK'/dK$ evaluated at $K = K^*$. Since a necessary condition for a critical transition is the existence of an eigenvalue $\lambda > 1$, this establishes the well-known result that there is no phase transition for the one-dimensional Ising model. After applying the renormalization transformation n times, the mapping $K \to K^{(n)}$ can be obtained from the recurrence relation

$$K^{(n)} = \tfrac{1}{2} \ln \{\cosh 2K^{(n-1)}\} \tag{8}$$

where $K^{(0)} = K$. It can be readily shown that $\lim_{n \to \infty} K^{(n)} = 0$, i.e., every finite point K is mapped towards the fixed point at the origin $K^* = 0$. In order to solve Eq. (8) we introduce a new variable ζ related to K by a nonlinear transformation in such a way that the renormalization transformation in the ζ variable becomes simpler. For $\lambda \neq 0, 1$ this transformation is defined by the condition[5,7] $\zeta' = \lambda \zeta$, but this is not possible in the present case. Instead, we require

$$\zeta' = \zeta^2 \tag{9}$$

and find the solution

$$\zeta = \tanh K \tag{10}$$

and

$$K^{(n)} = \tfrac{1}{2} \ln\left(\frac{1+\zeta^{2^n}}{1+\zeta^{2^n}}\right), \quad -1 < \zeta < 1. \tag{11}$$

Introducing the free energy per spin for N spins

$$f_N(K) = \frac{1}{N} \ln \sum_{\{S\}} \exp[H_N(K)]. \tag{12}$$

we obtain from Eq. (5) the functional relation

$$f_{N/2}(K') = 2\{f_N(K) - g(K)\}. \tag{13}$$

In the thermodynamic limit, Eq. (13) then leads to the scaling equation for $f(K) = \lim_{N\to\infty} f_N(K)$,

$$f(K') = 2\{f(K) - g(K)\}. \tag{14}$$

To obtain a unique solution of Eq. (14), we must impose a boundary condition on $f(K)$, e.g., for $K = 0$, absence of spin interactions, $f(0) = \ln 2$. To prove uniqueness suppose there are two solutions $f_1(K)$ and $f_2(K)$ of Eq. (14) which satisfy this boundary condition. Then the difference $f_-(K) = f_1(K) - f_2(K)$ satisfies the homogeneous scaling equation

$$f_-(K') = 2f_-(K) \tag{15}$$

and applying the renormalization mapping n-times leads to the relation

$$f_-(K) = (1/2^n) f_-(K^{(n)}). \tag{16}$$

Since $\lim_{n\to\infty} K^{(n)} = 0$, and $f_-(0) = 0$, Eq. (16) implies $f_-(K) = 0$. QED

Actually, this proof shows that we need to demand only the weaker boundary condition that $f(K)$ be finite at $K = 0$, because the solution of Eq. (14) determines the value of $f(0)$.

We now solve the scaling equation by considering the effect of repeated applications of the renormalization transformation Eq. (6) on Eq. (14). After the nth mapping we obtain the relation

$$f(K) = \frac{f(K^{(n)})}{2^n} + \sum_{m=0}^{m=n-1} \frac{g(K^{(m)})}{2^m} \tag{17}$$

which is valid for each integer $n \geq 1$. Taking the limit $n \to \infty$, we obtain[5]

$$f(K) = h(K) + \sum_{n=0}^{\infty} \frac{g(K^{(n)})}{2^n}, \tag{18}$$

where

$$h(K) = \lim_{n\to\infty} \frac{f(K^{(n)})}{2^n} \tag{19}$$

If we require $f(0)$ to be finite, we have $h(K) = 0$ and substituting Eq. (6) in Eq. (19), we obtain

$$f(K) = \ln 2 + \sum_{n=1}^{\infty} \frac{K^{(n)}}{2^n}. \tag{20}$$

This series converges very rapidly and can be readily used to evaluate $f(K)$. For example, for $K = 1$, the sum of the first four terms of this series gives an accuracy of 10^{-4}. We can also sum this series by substituting Eq. (11) in Eq. (20) to obtain

$$f(K) = \ln 2 + \ln \prod_{n=1}^{\infty} \left(\frac{1+\zeta^{2^n}}{1+\zeta^{2^n}}\right)^{1/2^{n+1}}. \tag{21}$$

Applying the easily proven identity

$$\frac{1}{1-x} = \prod_{n=0}^{\infty} \left(\frac{1+x^{2^n}}{1-x^{2^n}}\right)^{1/2^{n+1}}, \quad -1 < x < 1, \tag{22}$$

we find

$$f(K) = \ln(2/\sqrt{1-\zeta^2}) \tag{23}$$

and from Eq. (10), we obtain

$$f(K) = \ln(2\cosh K) \tag{24}$$

which is the well-known solution of the one-dimensional Ising model. We can verify that this solution satisfies the scaling equation by substituting Eq. (24) together with Eq. (7) into Eq. (14). A second solution of the scaling equation is $\tilde{f}(K) = \ln(2\sinh K)$, for which $h(K) = \ln(\tanh K)$. This second solution does not correspond to the free energy because it does not satisfy the correct boundary condition $f(0) = \ln 2$, but it is also of physical interest because it can be shown that the spin correlation function $C_{|i-j|}(K) = \langle s_i s_j \rangle$ is given by

$$C_{|i-j|}(K) = \exp(-|i-j|/l(K), \tag{25}$$

where the correlation length $l(K) = |f(K) - \tilde{f}(K)|^{-1}$. Hence $l(K)$ satisfies the expected homogeneous scaling relation

$$l(K') = \tfrac{1}{2} l(K). \tag{26}$$

These results can be readily extended to include a magnetic field, and to higher spins. The main point that we want to emphasize is that the infinite series expansion Eq. (18) can be applied directly to evaluate the free energy. This is important for general Ising models in two dimensions and higher, including symmetry breaking fields, because the renormalization transformations are much more complicated and it has not been possible to obtain analytic solutions by any methods except for very special cases. After completion of this paper, related work of Kadanoff, [8] M. E. Fisher and R. Nelson, [9] R. E. Prange, [10] S. Krinsky and D. Furman, [11] and R. Priest[12] have been brought to my attention.

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A new approach to the stability of matter problem. II*

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The main stability of matter result of Dyson and Lenard is proven by an alternate method.

INTRODUCTION

In a previous paper[1] stability of matter was shown for matter in a (periodic) cube. The methods used had the flavor of constructive quantum field theory as distinct to the original proof.[2,3] Here we continue the work of Ref. 1, to obtain the Dyson—Lenard result that the lower bound in the infinite volume may be picked proportional to N.

The essential physics of stability we feel is revealed in Ref. 1, what takes place in a cube. It is typical in constructive quantum field theory to first bound the energy in a finite volume and then obtain the infinite volume result as a sum of local contributions. This is not simply a sum of the isolated local bounds; there are interactions between local regions, and the important ingredients in controlling these interactions are the local nature of the kinetic energy and the falloff of the interaction with distance. Both of these effects are present in our problem. The long range nature of the Coulomb forces is not dangerous (as distinct from the situation in scattering say), the treatment of H_4 in Ref. 1 shows that forces can be given an exponential falloff trivially without affecting a linear lower bound in N. Another localization must be shown, the localization of positivity of the Coulomb energy. This is possibly the most interesting new physics in the infinite volume.

Basically space is cut into a union of unit cubes, with interactions smoothed over the edges. The kinetic energy is localized not with local N_τ operators as in field theory, but by writing the free kinetic energy as a sum of local kinetic energies in cubes with Neumann boundary conditions. The change in boundary conditions is an inessential change from Ref. 1. The most difficult problem is the interaction of neighboring cubes when the cutoffs (introduced in Ref. 1) are different in the different cubes. Finally, however, everything reduces to the local problem already treated.

It is hoped that some of the techniques herein employed will have applications in other situations. The degree of simplification over the Dyson—Lenard development is arguable, but, most significant, the present treatment fits the stability result into a framework of greater flexibility. We feel a good next step is the development of a cluster expansion for the matter problem and thence the infinite volume correlation functions.

1. NOTATION

We proceed to establish the notation. There are N bosons of charge $+q$, and N fermions of charge $-q$, and mass m. The boson mass is not relevant. The fermions are described by fields $\bar{\psi}$ and ψ, the bosons by $\bar{\phi}$ and ϕ. The two point distribution function for the bosons is given by

$$\rho(x,y)=\langle :\bar{\phi}(x)\phi(x)\bar{\phi}(y)\phi(y):\rangle. \tag{1.1}$$

Expectation values are always taken with respect to a given wavefunction. We also want the one point distribution function for the bosons,

$$\rho_1(x)=\langle\bar{\phi}(x)\phi(x)\rangle. \tag{1.2}$$

Space is filled with disjoint unit cubes, Δ_i, labeled by i. We introduce approximate characteristic functions χ_i, for the Δ_i, satisfying

$$\begin{aligned}&\sum\chi_i=1,\quad \chi_i\geq 0,\\ &\chi_i(x)=0 \text{ if } d(x,\Delta_i)>\tfrac{1}{10},\end{aligned} \tag{1.3}$$

and χ_i having two continuous derivatives. We want a uniform bound on the derivatives of all the χ_i, easily obtained by making the χ_i translates of each other. We also introduce the extended ith cube $\hat{\Delta}_i$, consisting of the union of the 125 unit cubes comprising a $5\times5\times5$ cube centered at Δ_i. This is extravagant, but it is convenient for $\hat{\Delta}_i$ to contain the region where χ_i and the χ_j's of all 26 Δ_j's touching Δ_i are nonzero. We define

$$N_i=\int\rho_1\chi_i, \tag{1.4}$$

$$\hat{N}_i=\int_{\hat{\Delta}_i}\rho_1, \tag{1.5}$$

and similarly $N_i^{(-)}$ and $\hat{N}_i^{(-)}$ for the negative charges. We let $\tilde{N}_i=N_i+N_i^{(-)}$.

Later a cutoff n_i will be assigned to Δ_i; we take it as already given. We define $\mu_0=0$ and $\mu_1,\mu_2,\cdots$ to be the values of $\{n_i\}$ arranged in increasing order. V_j is the interaction with cutoff μ_j,

$$V_j=q^2\exp(-\mu_j r)/r, \tag{1.6}$$

P_j is the approximate characteristic function of the union of Δ_i with $n_i\leq\mu_j$,

$$P_j=\sum_{\{i\,|\,n_i\leq\mu_j\}}\chi_i, \tag{1.7}$$

W_i is the interaction with cutoff n_i,

$$W_i=q^2\exp(-n_i r)/r, \tag{1.8}$$

and $W_{i,k}$ is the interaction with cutoff equal $\min(n_i,n_k)$.

Finally we define F_i to be the rescaled fermion kinetic energy form on $\hat{\Delta}_i$ with Neumann boundary conditions. We note in expectations between nice states

$$F=N+H_{0F}=\tfrac{1}{125}\sum_i F_i \tag{1.9}$$

Constants c_α all satisfy

$$0 < c_\alpha < \infty.$$

2. RESULTS

We summerize the results of the present paper in four facts, to continue the three in Ref. 1. The first is a variation of Fact 1, and the final is the main result.

Fact 1′: Suppose Supp $\chi_j \subset \hat{\Delta}_k$ and supp $\chi_i \subset \hat{\Delta}_k$, then for given $c_1 > 0$ and $\epsilon > 0$ there is a $c(\epsilon)$ such that

$$c_1 F_k - \int : \bar{\psi}\psi \chi_j W \chi_i \bar{\phi}\phi : \geq -c(\epsilon)[\int \bar{\phi}\phi \chi_i W \chi_j^2 W \chi_i \bar{\phi}\phi]^{2+\epsilon}. \tag{2.1}$$

Fact 4: There is c_4 such that

$$\langle F_i \rangle \geq + c_4 (\hat{N}_i^{(-)})^{5/3}. \tag{2.2}$$

Fact 5: Let $\{\chi_i\}$ be translates over a lattice of a C^2 function of compact support; then there is a c_5 (dependent on χ_i) such that

$$1/r - e^{-r}/r \geq c_5 \sum \bar{\chi}_i \chi_i. \tag{2.3}$$

Fact 6: There is a B such that

$$\tilde{H} = H + BN \geq 0. \tag{2.4}$$

It is understood that B must be independent of N.

Fact 4 is proven in Sec. 3 and Fact 5 is proven in Sec. 4. Fact 6 is shown in the remaining sections. Fact 1′ is a slightly modified form of (5.23) and (5.24) in Ref. 1. The only interesting difference is the use of Neumann instead of periodic boundary conditions. But the eigenfunctions are as explicit for these boundary conditions and the computation as easily performed.

3. LOCALIZATION OF FERMI SEA ENERGY

We expand

$$\langle F_i \rangle = \sum_l \langle l | F_i | l \rangle, \tag{3.1}$$

where $|\rangle = \sum_l |l\rangle$ is decomposition of $|\ \rangle$ into states satisfying

$$\hat{N}_i^{(-)} |l\rangle = l |l\rangle.$$

We get

$$\langle F_i \rangle \geq \sum_l \langle l | l \rangle c l^{5/3} \tag{3.2}$$

by the distribution of eigenvalues of F_i, and

$$\langle F_i \rangle \geq c(\sum \langle l | l \rangle l)^{5/3} \tag{3.3}$$

by convexity of $x^{5/3}$. And thus

$$\langle F_i \rangle \geq c \langle \hat{N}_i^{(-)} \rangle^{5/3}. \tag{3.4}$$

4. LOCALIZATION OF PART OF COULOMB ENERGY

Using notation of Fact 5, define $g_i = \tilde{\chi}_i$. We get the following chain of implications:

$$\frac{1}{r} - \frac{\exp(-r)}{r} \geq c \sum \bar{\chi}_i \chi_i \tag{4.1}$$

$$\Leftrightarrow \frac{1}{k^2} - \frac{1}{k^2+1} \geq \sum c \bar{g}_i g_i \tag{4.2}$$

$$\Leftarrow \left(\frac{1}{k^2+1}\right)^2 \geq c \sum \bar{g}_i g_i \tag{4.3}$$

$$\Leftrightarrow 1 \geq c \sum (k^2+1) \bar{g}_i g_i (k^2+1) \tag{4.4}$$

$$\Leftrightarrow 1 \geq c \sum (1-\Delta) \bar{\chi}_i (1-\Delta) \chi_i. \tag{4.5}$$

But if $\{f_i\}$ is an orthonormal set of vectors,

$$1 \geq \sum \bar{f}_i f_i, \tag{4.6}$$

and, if $\{f_i\}$ is a bounded set of orthogonal vectors,

$$1 \geq c \sum \bar{f}_i f_i, \tag{4.7}$$

but $\sum (1-\Delta)\bar{\chi}_i (1-\Delta)\chi_i$ can be written as a finite number of sums of disjoint and therefore orthogonal (and bounded) $(1-\Delta)\chi_i$.

Fact 5 leads to a number of questions of mathematical generalizations. In particular to N_τ operators for τ negative. Does N_τ then dominate a sum of local N_ν operators? Fact 5 and variations may be used to derive results on thermodynamic charge density fluctuations. This is not pursued here.

5. THE BASIC PROBLEM

We split $\tilde{H}$ into seven pieces patterned after Ref. 1:

$$\tilde{H} = H_1 + H_2 + \cdots + H_6 + (B-1)N, \tag{5.1}$$

$$H_1 = H_{0B}, \tag{5.2}$$

$$H_2 = \tfrac{1}{2} F, \tag{5.3}$$

$$H_3 = \tfrac{1}{2} \sum_j \int : \bar{\psi}\psi [(V_j - V_{j+1}) - P_{j+1}(V_j - V_{j+1})P_{j+1}] \bar{\psi}\psi :, \tag{5.4}$$

$$H_4 = \tfrac{1}{2} \sum_j \int : (\bar{\psi}\psi - \bar{\phi}\phi)[P_{j+1}(V_j - V_{j+1})P_{j+1}]P_{j+1}](\bar{\psi}\psi - \bar{\phi}\phi) :, \tag{5.5}$$

$$H_5 = \tfrac{1}{2} F - \sum_j \int : \bar{\psi}\psi [(V_j - V_{j+1}) - P_{j+1}(V_j - V_{j+1})P_{j+1}] \bar{\phi}\phi :, \tag{5.6}$$

$$H_6 = \tfrac{1}{2} \sum_j \int : \bar{\phi}\phi [(V_j - V_{j+1}) - P_{j+1}(V_j - V_{j+1})P_{j+1}] \bar{\phi}\phi :. \tag{5.7}$$

As in Ref. 1, the boson field is in a fixed classical distribution, and we neglect H_{0B}. The terms are written in the above forms mainly to exhibit certain positivity properties.

Considering the terms in order, we have

$$H_2 = F/2 = \sum_i \tfrac{1}{2} \cdot \tfrac{1}{125} F_i \tag{5.8}$$

$$\geq c \sum_i (\hat{N}_i^{(-)})^{5/3} \tag{5.9}$$

by Fact 4. H_3 may be treated as in Ref. 1:

$$H_3 \geq 0. \tag{5.10}$$

We break H_4 into two parts:

$$H_{41} = \tfrac{1}{2}\sum_j \int (\bar\psi\psi - \bar\phi\phi)P_{j+1}(V_j - V_{j+1})P_{j+1}(\bar\psi\psi - \bar\phi\phi), \tag{5.11}$$

$$H_{42} = \tfrac{1}{2}\sum_j \int [:(\bar\psi\psi - \bar\phi\phi)P_{j+1}(V_j - V_{j+1})P_{j+1}(\bar\psi\psi - \bar\phi\phi):$$

$$-(\bar\psi\psi - \bar\phi\phi)P_{j+1}(V_j - V_{j+1})P_{j+1}(\bar\psi\psi - \bar\phi\phi)]. \tag{5.12}$$

Similar to Ref. 1,

$$H_{42} \geq -\tfrac{1}{2}\sum_j q^2(N_j + N_j^{(-)})n_j. \tag{5.13}$$

H_{41} is positive as before, but now we need more. We first note that

$$H_{41} \geq \tfrac{1}{2}\int (\bar\psi\psi - \bar\phi\phi)(q^2/r - q^2 e^{-r}/r)(\bar\psi\psi - \bar\phi\phi) \tag{5.14}$$

since we will require

$$n_i \geq 1. \tag{5.15}$$

Fact 5 now gives

$$H_{41} \geq c\sum_i (N_i - N_i^{(-)})^2. \tag{5.16}$$

In Ref. 1 there was guaranteed to N plus charges a fermion kinetic energy $\sim N^{5/3}$. Here locally there may be many plus charges and few negative charges. But the contribution to the sum of H_2 and H_{41} here is large when there are many positive charges locally.

H_5 and H_6 are now rewritten in a different form:

$$H_5 = \tfrac{1}{2}F - \sum_i :\bar\psi\psi\chi_i W_i\chi_i\bar\phi\phi: - \sum_{i\neq k}\int :\bar\psi\psi\chi_i W_{i,k}\chi_k\bar\phi\phi:, \tag{5.17}$$

$$H_6 = \tfrac{1}{2}\sum_i \int :\bar\phi\phi\chi_i W_i\chi_i\bar\phi\phi: + \tfrac{1}{2}\sum_{i\neq k}\int :\bar\phi\phi\chi_i W_{i,k}\chi_k\bar\phi\phi:. \tag{5.18}$$

We will ignore the second (positive) sum in (5.18) in obtaining our bounds.

In (5.17) let D denote those terms in the second sum where k is not one of i's 26 neighbors. We require n_i to satisfy in addition to $n_i \geq 1$ that there is some α such that

$$n_i \geq \alpha \tilde N_i^{2/3}. \tag{5.19}$$

We define

$$D_k = \max(1, \alpha \tilde N_k^{2/3}), \tag{5.20}$$

$$d_{i,k} = \mathrm{dist}(\Delta_i, \Delta_k) - \tfrac{2}{10}; \tag{5.21}$$

we then get

$$D \geq \sum_i (-q^2)N_i^{(-)}\left(\sum_k \frac{\exp(-d_{i,k}D_k)}{d_{i,k}}N_k\right) + \sum_i (-q^2)N_i\left(\sum_k \frac{\exp(-d_{i,k}D_k)}{d_{i,k}}N_k^{(-)}\right) \tag{5.22}$$

(with k restricted as described). Maximizing the expression in braces over N_k and $N_k^{(-)}$, we get

$$D \geq -c\sum_i (N_i^{(-)} + N_i). \tag{5.23}$$

6. WITHIN WHICH PROBLEMS WITH NEIGHBORS ARE RESOLVED

We write $k\mathrm{R}i$ to mean k is one i's 26 neighbors. Those terms in (5.17) not included in D we call L:

$$H_5 = L + D, \tag{6.1}$$

$$L = \sum_i L_{ii} + \sum_{i\,\mathrm{R}\,k} L_{ik}, \tag{6.2}$$

$$L_{ii} = \frac{1}{2\cdot 125\cdot 27}F_i - \int :\bar\psi\psi\chi_i W_i\chi_i\bar\phi\phi:, \tag{6.3}$$

$$L_{ik} = \frac{1}{2\cdot 125\cdot 27}F_i - \int :\bar\psi\psi\chi_i W_{i,k}\chi_k\bar\phi\phi:. \tag{6.4}$$

By Fact 1′ we get

$$L_{ii} \geq -c(\epsilon)\left(\int \bar\phi\phi\chi_i W_i\chi_i^2 W_i\chi_i\bar\phi\phi\right)^{2+\epsilon} \tag{6.5}$$

$$\geq -c(\epsilon)\left(\int \bar\phi\phi\chi_i W_i W_i\chi_i\bar\phi\phi\right)^{2+\epsilon} \tag{6.6}$$

$$\geq -c'(\epsilon)\left(\int \bar\phi\phi\chi_i \frac{\exp(-n_i r)}{n_i}\chi_i\bar\phi\phi\right)^{2+\epsilon}. \tag{6.7}$$

Defining

$$\rho_i = \chi_i\rho\chi_i,$$

we have

$$L_{ii} \geq -c''(\epsilon)\left(\int \rho_i \exp(-n_i r)/n_i\right)^{2+\epsilon} - c''(\epsilon)(N_i/n_i)^{2+\epsilon}. \tag{6.8}$$

We now turn to L_{ik}, $k\neq i$, and assume, as Case 1, $n_i \geq n_k$. Applying Fact 1′ again, we have

$$L_{ik} \geq -c(\epsilon)\left(\int \bar\phi\phi\chi_k W_{i,k}\chi_i^2 W_{i,k}\chi_k\bar\phi\phi\right)^{2+\epsilon} \tag{6.9}$$

$$\geq -c''(\epsilon)\left[\int \rho_k \exp(-n_k r)/n_k\right]^{2+\epsilon} - c''(\epsilon)(N_k/n_k)^{2+\epsilon}. \tag{6.10}$$

In Case 2, when $n_i < n_k$, we have the most difficulty. We define

$$c_{i,k} = \chi_k W_{i,k} - W_{i,k}\chi_k; \tag{6.11}$$

we get

$$L_{ik} \geq -c(\epsilon)\left(\int \bar\phi\phi\chi_k W_{i,k}\chi_i^2 W_{i,k}\chi_k\bar\phi\phi\right)^{2+\epsilon} \tag{6.12}$$

$$\geq -\tilde c(\epsilon)\left(\int \bar\phi\phi\chi_k\chi_i W_{i,k} W_{i,k}\chi_i\chi_k\bar\phi\phi\right)^{2+\epsilon} - \tilde c(\epsilon)\left(\int \bar\phi\phi\chi_k c_{i,k} c_{i,k}\chi_k\bar\phi\phi\right)^{2+\epsilon}. \tag{6.13}$$

The first term on right side of (6.13) satisfies

$$\left(\int \bar\phi\phi\chi_k\chi_i W_{i,k}W_{i,k}\chi_i\chi_k\bar\phi\phi\right)^{2+\epsilon} \leq c\left(\int \bar\phi\phi\chi_i W_{i,k}W_{i,k}\chi_i\bar\phi\phi\right)^{2+\epsilon} \leq c'\left(\int \rho_i \frac{\exp(-n_i r)}{n_i}\right)^{2+\epsilon} + c'\left(\frac{N_i}{n_i}\right)^{2+\epsilon}. \tag{6.14}$$

Looking at the second term, we need some properties of $c_{i,k}$:

$$\chi_k W_{i,k} - W_{i,k}\chi_k = c\chi_k(x) - \frac{\exp(-n|x-y|)}{|x-y|} - c\frac{\exp(-n|x-y|)}{|x-y|}\chi_k(y). \tag{6.15}$$

Here n has the obvious definition:

$$c_{i,k} = c[\chi_k(x) - \chi_k(y)]\exp(-n|x-y|)/|x-y|. \tag{6.16}$$

By the uniform bound on derivatives of the $\{\chi_k\}$,

$$|c_{i,k}| \leq c\exp(-n|x-y|) \tag{6.17}$$

and

$$|c_{i,k}c_{i,k}| \leq c/n^3. \tag{6.18}$$

The last estimate is a crude estimate of the convolution of $c_{i,k}$ with itself. The second term on the right side of (6.13) satisfies

$$(\int \bar{\phi}\phi\chi_k c_{i,k}c_{i,k}\chi_k\bar{\phi}\phi)^{2+\epsilon} \leq c(\int \rho_k/n_i^3)^{2+\epsilon} + c(N_k/n_i^3)^{2+\epsilon}. \tag{6.19}$$

7. FINAL ESTIMATES

We first pick the value of ϵ and two new parameters γ and γ' equal to the values of ϵ', γ, and γ' of Ref. 1. We now collect contributions to $\tilde{H}$.

We begin with H_1 and $(B-1)N$

$$H_1 + (B-1)N \geq (B-1)N. \tag{7.1}$$

From (5.9)

$$H_2 \geq c\sum_i (\hat{N}_i^{(-)})^{5/3} \geq c\sum_i (N_i^{(-)})^{5/3} \geq c\sum_i \Big((N_i^{(-)})^{5/3} + \sum_{\substack{k \\ kRi}} (N_k^{(-)})^{5/3}\Big). \tag{7.2}$$

We have averaged the contributions over neighboring cubes. As in (5.10),

$$H_3 \geq 0. \tag{7.3}$$

From (5.13) and (5.16)

$$H_4 = H_{41} + H_{42},$$

$$H_{41} \geq c\sum_i \Big((N_i - N_i^{(-)})^2 + \sum_{\substack{k \\ kRi}} (N_k - N_k^{(-)})^2\Big), \tag{7.4}$$

$$H_{42} \geq -c\sum_i (N_i + N_i^{(-)})n_i. \tag{7.5}$$

From (5.23), (6.8), (6.10), (6.14), and (6.19)

$$H_5 = L + D, \quad D \geq -c\sum_i (N_i + N_i^{(-)}), \tag{7.6}$$

$$L \geq -c\sum_i \Big((\int \rho_i \exp(-n_i r)/n_i)^{2+\epsilon} + (N_i/n_i)^{2+\epsilon} + \sum_{\substack{k \\ kRi}} [(\int \rho_i/n_k^3)^{2+\epsilon} + (N_i/n_k^3)^{2+\epsilon}]\Big). \tag{7.7}$$

From (5.18)

$$H_6 \geq \sum_i \int \rho_i \exp(-n_i r)/r. \tag{7.8}$$

We observe that for $x \geq 0$, $y \geq 0$, there is a $c > 0$ such that

$$x + (x-y)^2 + y^{5/3} \geq cx^{5/3}. \tag{7.9}$$

We can collect (7.1)—(7.8), using (7.9), to obtain

$$\begin{aligned}\tilde{H} \geq \sum_i & (C_I BN_i + C_{II}BN_i^{(-)} - C_{III}N_i - C_{IV}N_i^{(-)} \\ & + C_V N_i^{5/3} + C_{VI}(N_i^{(-)})^{5/3} - C_{VII}N_i n_i - C_{VIII}N_i^{(-)}n_i \\ & + C_{IX}\int \rho_i \exp(-n_i r)/r - C_X(\int \rho_i \exp(-n_i r)/n_i)^{2+\epsilon} \\ & - C_{XI}(N_i/n_i)^{2+\epsilon} + \sum_{\substack{k \\ kRi}} [-C_{XII}(\int \rho_i/n_k^3)^{2+\epsilon} \\ & - C_{XIII}(N_i/n_k^3)^{2+\epsilon} + C_{XIV}N_k^{5/3} + C_{XV}(N_k^{(-)})^{5/3}]).\end{aligned} \tag{7.10}$$

With the proper choice for B and n_i we claim that each term in the sum over i is positive.

Two cases are considered for each i as in Ref. 1:

Case I:

$$\int_{|x-y|<N^{-2/3+\gamma}} \rho_i < N_i \cdot N_i^{1-\gamma'}, \tag{7.11}$$

$$n_i = \max(1, \lambda(\bar{N}_i)^{2/3}). \tag{7.12}$$

Case II:

$$\int_{|x-y|<N^{-2/3+\gamma}} \rho_i \geq N_i \cdot N_i^{1-\gamma'}, \tag{7.13}$$

$$n_i = \max(1, \lambda(\bar{N}_i)^{2/3}, N_i^{2/3+\gamma}). \tag{7.14}$$

We have defined $\bar{N}_i$ as the maximum over $\tilde{N}_i$ and the $\tilde{N}_k$ with k neighboring i. λ is greater than zero and satisfies

$$\lambda < \min(C_V, C_{VI}, C_{VIV}, C_{XV})/C_{VII} + C_{VIII}. \tag{7.15}$$

When $\tilde{N}_i$ is large enough for any value of $B \geq 0$, the contribution of the ith summand is positive by arguments similar to that in Ref. 1. For smaller values of $\tilde{N}_i$, B may be picked large enough to dominate the summand.

The value of B Dyson and Lenard achieve is roughly 14 orders of magnitude larger than a realistic bound. To extract good bounds from the present procedure, we would have to experiment on values of the parameters and cube size, as well as trace all the numerical factors and find a good value for c_2. If done, this would provide an objective basis for comparison of the effectiveness of the lower bounds. We do not expect a realistic lower bound of the present procedure either.

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A definition of quantum detection point processes

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A definition of quantum particle detection point processes is given for normal and locally normal systems. This is realized by building coincidence measurement operators, describing in a thoroughly quantum formalism the coincidence experiments that have been actually performed (photon) or that might be performed (electron, neutron). The quantum mean values of these coincidence operators are shown to be the coincidence probabilities of a mathematically well-defined regular process. Some applications of the latter result are given, in particular in the case of fermion point processes.

INTRODUCTION

The starting point of the present work is to be found in the great number of experimental[1-3] as well as theoretical[4] results obtained in studying the statistical properties of light beams. Among the different types of experiment performed, we shall focus on the low intensity ones, such as counting[2] or coincidence[3] experiments. In fact, with such experiments, the photon detection point process consisting of the electronic pulses getting out of the detector may be attained.

In the present paper, we would like to give a general definition of the quantum particle detection point process[5] which can be reached by coincidence or counting experiments performed on a quantum particle system. We shall consider any particle, boson or fermion, and give a thoroughly quantum description of the system they constitute. Since we want our definition to apply to actually performed experiments (or experiments that could be performed) we shall give a quantum description of coincidence experiments in conditions which are generally realized, considering the performances of the present particle detectors that might be used. Our quantum description of these coincidence measurements will consist of the definition of a coincidence operator wide enough for not taking into account the particular mechanism of the considered detector.

These quantum descriptions of both the particle system and the measurements will allow the definition of probabilistic magnitudes which are the stochastic events "detection of a particle at a point a_i at a time instant t_i" and the point processes[6] $\rho_t(V)$ and $\rho_a(t)$ they constitute in the volume V of the system and in the observation time interval T respectively.

To understand what we are speaking about, let us show, in a very intuitive way, how these detection point processes may be introduced (our subsequent work, which is the aim of this paper, will be, on the contrary, to introduce the detection point processes in a rigorous way!). Let us set a detector of volume ΔV in a particle beam, localized itself in a volume V. Without describing the detection mechanism, let us assume that the following output is obtained: At time t, n particles (n is an integer) have been detected in ΔV. We know, from quantum mechanics, that n is stochastic, depending of the presence probability of the particles in ΔV. Thus, we can introduce the stochastic variable $N(\Delta V, t)$, the number of particles detected in ΔV at time t. If we now imagine an infinite number of detectors occupying the whole volume V, the particle detection point process $\rho_t(V)$ at time t in the volume V may be introduced. Indeed a point process is a stochastic distribution of points in a given space, and it is known if the probability $p(n_1, n_2, \ldots, n_q)$ that n_i points be in q disconnected volumes ΔV_i, for any q and any ΔV_i, is known. From the experimental viewpoint, it may be interesting to introduce another point process $\rho_a(T)$, more closely connected with the experiment: Let us consider an absorbing detector (such as a photomultiplier for photons) acting on a small volume around a point a; its output consists of a time distribution of stochastic pulses connected with the absorption time instants t_i of the particles; this random time distribution is the time point process $\rho_a(T)$.

In the first section, we will give the mathematical definition of a regular point process (I. 1). The fact that such a point process (p. p.) is entirely defined by its coincidence probability densities (c. p. d.) is underlined.[7,8] The c. p. d. of $\rho_t(V)$ are the probability densities that p distinct particles will be detected in p points a_i of V, at a given time t, $P_p[\{a_i\}, t]$; the c. p. d. of $\rho_a(T)$ are the probability densities that p distinct particles will be detected at p time instants t_i in T, at a given point a, $I_p[a, \{t_i\}]$. In the same section, the conditions[9,10] for a coincidence measurement to give these c. p. d. are studied [(I. 2)] in a thoroughly probabilistic approach.

In the second section, the c. p. d. measured in such an experiment are expressed in terms of the density matrix describing the observed system and of a coincidence operator describing the measurement. The problem of the localization[11,12] of quantum particles is set in Sec. IIA, a definition of a coincidence operator is proposed in Sec. IIB and the validity of such a definition is established in Sec. IIC. Finally, in Sec. IID, some properties of the coincidence operator are studied.

In Sec. III, some applications of our preceding results are given. The fermion detection process[5,13,14] is shown to be mathematically well-defined [(III. 1)]. And a simple physical interpretation of the results of Frisch and Bourret[15] is given, (III. 2).

I. DETECTION POINT PROCESSES

Let us consider a volume V of a given particle system, at a time t. For the point process $\rho_t(V)$ constituted by the stochastic events "presence of a particle in the small volume Δ_1 ($\Delta_1 \subset V$) at time t," "presence of another particle in Δ_2 ($\Delta_2 \subset V$) at time t," and so on, to be mathematically well-defined, its coincidence probabili-

ties (c. p.) $Q_p[\{\Delta_i\}, t]$, the probabilities that p particles will be in p small volumes Δ_i ($\Delta_i \subset V$) at time t, must fulfill given conditions.[7,8] (By saying that a quantity is small we mean that, from the mathematical standpoint, this quantity will be considered as infinitely small.) These conditions are complicated to express. And it is simpler to give them for another set of probabilities, the exclusive probabilities (e. p.) which can be easily be related to the c. p. d. and, as the latter, entirely define the point process.[7,8]

The properties which are given below can be applied to the spatial c. p. $Q_p[\{\Delta_i\}, t]$ defining $\rho_t(V)$ or to the time c. p. $Q_p[a, \{\Delta t_i\}]$ defining $\rho_a(T)$. But we must be careful to notice that the set of stochastic events "presence of a particle in Δ_i at t_i" does not constitute a point process. Indeed two such events may be the same one in fact.

A. Regular point processes

1. Probability densities

In the Introduction, we speak of coincidence probability *density* (d. p. c.) $P_p[\{a_i\}, t]$, $I_p[a, \{t_i\}]$. Such quantities do exist only if the following mathematical limits exist:

$$P_p[\{a_i\}, t] = \lim_{\{\Delta_i\} \to \{0\}} \left(Q_p[\{\Delta_i\}, t] \Big/ \prod_{i=1}^{p} \Delta_i \right) \tag{I. 1}$$

$$I_p[a, \{t_i\}] = \lim_{\{\Delta t_i\} \to \{0\}} \left(Q_p[a, \{\Delta t_i\}] \Big/ \prod_{i=1}^{p} \Delta t_i \right) \tag{I. 2}$$

The existence of such limits implies that the probability for an event to take place in a small domain Δ_i or Δt_i is of the same order of magnitude as Δ_i or Δt_i. The probability for more than one event to occur in Δ_i or Δt_i is negligible. The point processes such that these limits exist are said to be regular.[8] In the following, we will consider only regular processes, because they are much easier to handle.

It is necessary, but not sufficient, for a p. p. to be well-defined, that its c. p. d. verify the two following properties:

Property α: The c. p. d. are nonnegative;

Property β: they are symmetrical with respect to their arguments ($\{a_i\}$ or $\{t_i\}$).

We will also admit the existence of the following densities:

$$P_p[\{a_i\}, \{t_i\}] = \lim_{\{\Delta_i\} \to \{0\}} \left(Q_p[\{\Delta_i\}, \{t_i\}] \prod_{i=1}^{p} \Delta_i \right), \tag{I. 3}$$

$$I_p[\{a_i\}, \{t_i\}] = \lim_{\{\Delta t_i\} \to \{0\}} \left(Q_p[\{a_i\}, \{\Delta t_i\}] \prod_{i=1}^{p} \Delta t_i \right). \tag{I. 4}$$

They will be called coincidence probabilities, although they do not define a p. p.

If the particles are assumed to be quasimonochromatic, that is to say, if the velocity v is nearly the same for every particle, then

$$I_p[\{a_i\}, \{t_i\}] = v^p P_p[\{a_i\}, \{t_i\}]. \tag{I. 5}$$

Let us notice that $P_1[a, t]$ is nothing but the mean number of detected particles in a unit volume. $P_2[a_1 a_2, t]$ is the double density in a_1 and a_2.[16] Similarly, $I_1[a, t]$ is the beam intensity at point a at time t. For $p = 1$, Eq. (I. 5) reduces to the relation

$$I_1[a, t] = v P_1[a, t]. \tag{I. 5'}$$

2. Definition of a point process by its exclusive probabilities

The exclusive probability $H_p^{\,D}[\{D_i\}]$ is the probability that an event occurs in a small domain D_1, another in $D_2, \ldots,$ another in D_p, and *not any other* occurs in the whole domain D where the events necessarily take place. For the p. p. $\rho_t(V)$ and $\rho_a(T)$, the e. p. will be called $H_p^{\,V}[\{\Delta_i\}, t]$ and $H_p^{\,T}[a, \{\Delta t_i\}]$ respectively.

A regular process is such that an e. p. d. exists:

$$G_p^{\,D}[\{x_i\}] = \lim_{\{\|D_i\|\} \to \{0\}} \left(H_p^{\,D}[\{D_i\}] \Big/ \prod_{i=1}^{p} \|D_i\| \right), \tag{I. 6}$$

where x_i is a point of D_i and $\|D_i\|$ the measure of D_i.

For $\rho_t(V)$ and $\rho_a(T)$ we have

$$G_p^{\,V}[\{a_i\}, t] = \lim_{\{\Delta_i\} \to \{0\}} \left(H_p^{\,V}[\{\Delta_i\}, t] \Big/ \prod_{i=1}^{p} \Delta_i \right) \tag{I. 6'}$$

and

$$G_p^{\,T}[a, \{t_i\}] = \lim_{\{\Delta t_i\} \to \{0\}} \left(H_p^{\,T}[a, \{\Delta t_i\}] \Big/ \prod_{i=1}^{p} \Delta t_i \right). \tag{I. 6''}$$

For a regular point process to be well-defined, the e. p. d. must verify properties α and β and the following one, that we called Property γ:

Property γ:

$$\sum_{p=0}^{+\infty} \frac{1}{p!} \int_{D^p} G_p^{\,D}[\{x_i\}]\, dx_1 \cdots dx_p = 1. \tag{I. 7}$$

Indeed if P_p is the probability for p events to occur in D, then

$$P_p = \frac{1}{p!} \int_{D^p} G_p^{\,D}[\{x_i\}]\, dx_1 \cdots dx_p, \tag{I. 8}$$

where $1/p!$ comes from the symmetry of $G_p^{\,D}$. Relation (I. 7) follows from (I. 8) and

$$\sum_{p=0}^{+\infty} P_p = 1. \tag{I. 9}$$

e. p. d. and c. p. d. are related in the following way

$$P_p[\{x_i\}] = \sum_{k=0}^{+\infty} \frac{1}{k!} \int_{D^k} G_{p+k}^{\,D}[\{x_1, x_2, \ldots, x_{p+k}\}]\, dx_{p+1} \cdots dx_{p+k} \tag{I. 10}$$

or

$$G_p^{\,D}[\{x_i\}] = \sum_{k=0}^{+\infty} \frac{(-1)^k}{k!} \int_{D^k} G_{p+k}[\{x_1, \ldots, x_{p+k}\}]\, dx_{p+1} \cdots dx_{p+k}, \tag{I. 11}$$

relations which are equivalent, as shown by Macchi.[8] From these two relations, it follows that knowing either the e. p. d. or the c. p. d. is equivalent and sufficient. Moreover, a set of functions defines a p. p. and is its set of e. p. d. if and only if the functions verify α, β, and γ.

B. Coincidence measurements

Without getting into the description of detectors nor tickling the question of the localization of quantum particles but using only the notion of presence probability

of a particle, we study the conditions that must be fulfilled for actually realized coincidence experiments to give c. p. d. We define two ideal types of coincidence measurement. The first one is based on the usual instantaneous reduction of the state of a measured system[17] and gives instantaneous presence probabilities. The second one schematically describes the action of a detector such as a photomultiplier.[9] It is shown that, providing given hypotheses, these two ideal types of measurement can be identified and considered as good descriptions of actually performed measurements.

1. Ideal coincidence measurements of type 1

p detectors are set in the volume V of the system. Each one is of *volume* Δ around a point a_i ($\Delta_i = \{a_i, \Delta\}$) and acts *instantaneously* at time t_i. Every detector is able to localize a particle in Δ_i at time t_i: Used alone, it gives the spatial presence probability of the particles in Δ_i at time t_i. This implies that Δ is small enough for the probability of detecting more than one particle in Δ to be negligible. For a p-order coincidence measurement, the p detectors are connected with one another in such a way that an output is obtained every time the event $C_p[\{\Delta_i\}, \{t_i\}]$, that, for every i from 1 to p, a particle is localized in Δ_i at time t_i, is realized. The ensemble average gives the probability $Q_p[\{\Delta_i\}, \{t_i\}]$ to occur.

2. Ideal coincidence measurements of type 2

p points detectors are at distinct points a_i in V. They act during *time interval* $\Delta t_i = \{t_i, \Delta t\}$. Every detector may absorb a particle at a_i during Δt_i: Δt is weak enough for the probability that more than one particle will be detected to be negligible. Used alone, such a detector gives the time presence probability of the particles in Δt_i at point a_i. For a p-order coincidence measurement, the detectors are connected with one another in such a way that an output is obtained every time the event $C_p[\{a_i\}, \{\Delta t_i\}]$, that, for every i from 1 to p, a particle is localized at point a_i during Δt_i, is realized. The probability $Q_p[\{a_i\}, \{\Delta t_i\}]$ that $C_p[\{a_i\}, \{\Delta t_i\}]$ will occur is obtained by ensemble average.

Generally, the two events $C_p[\{\Delta_i\}, \{t_i\}]$ and $C_p[\{a_i\}, \{\Delta t_i\}]$ cannot be linked easily. The two foregoing ideal measurements provide different probabilities $Q_p[\{a_i\}, \{\Delta t_i\}]$ and $Q_p[\{\Delta_i\}, \{t_i\}]$. Nevertheless, if V is assumed to be one-dimensional, say L, as it can be done for a parallel beam the section of which is small compared with the coherence area, and if the particle velocity v is nearly the same for every particle (which is always true for photons but implies quasimonochromaticity for nonzero mass particles), Δ and Δt can be chosen in such a way that

$$\Delta = v\Delta t.$$

With these conditions, $C_p[\{a_i\}, \{\Delta t_i\}]$ is still the event "for every i from 1 to p, a particle is localized in Δt_i at point a_i," but $C_p[\{\Delta_i\}, \{t_i\}]$ can be considered as the event "for every i from 1 to p, a particle is localized at t_i in $\Delta_i = \{a_i, v\Delta t_i\}$." Thus these two events are identical and

$$Q_p[\{a_i\}, \{\Delta t_i\}] = Q_p[\{\Delta_i\}, \{t_i\}].$$

Simple geometrical considerations would allow us the extend this identity to nonparallel quasimonochromatic beams. Thus, to identify type 1 and 2 experiments we need only the quasimonochromaticity hypothesis, which we call Hypothesis 1:

Hypothesis 1: If ΔE is the energy width of the wave-packets describing the particles, and E_0 the mean energy of the particles, the following relation is verified:

$$\Delta E \ll E_0.$$

This inequality defines quasimonochromaticity.

3. Actually performed coincidence measurements

What conditions must be fulfilled by the actual detectors for them to be described by the type 2 ideal model?

Let us consider the experiments actually performed on photon beams.[3] The detectors are photomultiplier (P. M.) interacting with the electromagnetic field during a time Δt in an active volume Δ. For the equivalence between P. M. and type 2 detectors to be set, two questions must be solved:

(1) What are the conditions for a P. M., which appreciates the square modulus of the electric field to behave as a particle detector? This problem is left for Sec. II. Let us assume here that the conditions are realized.

(2) What are the conditions for a detector of finite volume Δ, acting during a time Δt (such as a P. M.) to behave as a *point* detector that may absorb one particle during Δt. These conditions are given in Hypothesis 2:

Hypothesis 2: The dimensions of Δ and Δt, on one hand, and the measured field intensity, on the other hand, are weak enough for the probability that the detector will absorb more than one particle to be negligible. In particular, more-than-one-particle interactions are not considered.

Thus, from a mathematical standpoint:

(1) Δ and Δt may be considered as infinitely small. The linear dimensions of Δ and $v\Delta t$, where v is the particle mean velocity, are of the same order.

(2) The probability that a particle is localized in Δ at a given time or that a particle is localized during Δt at a given point are infinitely small of the order of Δ or Δt. And the probability for localizing more than one particle in Δ on Δt is infinitely small of upper order.

Hypothesis 2 is actually realized in coincidence measurements.[3] The only consequence of the finite volumes of detection is that a mean value of $Q_p[\{a_i\}, \{\Delta t_i\}]$ is performed on Δ in the measurements.

To conclude, we see that, providing Hypothesis 2, type 2 experiments and actual experiments can be identified. Moreover, the quasimonochromaticity hypothesis allows the identification of type 1 and type 2 experiments. Finally, providing these two hypotheses, type 1 and actual experiments can be identified. Thus our problem is reduced to a correct quantum description of type 1 experiments, which will be done in Sec. II.

II. QUANTUM DEFINITION OF A COINCIDENCE OPERATOR

We consider a free system of particles any finite part of which, of volume V, can be defined by a density operator ρ_V. And we look for a coincidence operator $\mathcal{N}_p[\{\Delta_i\},\{t_i\}]$ describing type 1 p-order coincidence measurements in V, when Hypotheses 1 and 2 are realized. $\mathcal{N}_p[\{\Delta_i\},\{t_i\}]$ must be such that

$$\mathrm{Tr}\{\rho\mathcal{N}_p[\{\Delta_i\},\{t_i\}]\} = Q_p[\{\Delta_i\},\{t_i\}], \tag{II. 1}$$

where $Q_p[\{\Delta_i\},t]$ defines a regular p. p. $\rho_V(t)$.

We first justify the reason why we consider only free normal or locally normal[18] systems. Then a position operator $\mathcal{N}_1[\Delta,t]$ is defined. This definition is not original and entirely based on the papers of Newton and Wigner,[11] Jauch and Piron,[19] and the thesis of Amrein.[12] The merits of our choice, from the experimental standpoint, is emphasized. Finally $\mathcal{N}_p$ is deduced from $\mathcal{N}_1$ and shown to verify (II. 1), in a theorem which is the main result of the present section.

A. Localization of quantum particles

1. Considered systems

A normal system is finite such that it can be described by a density operator ρ (positive operator with trace I).[18] A locally normal system reduces to a normal system on any finite part V of its total volume. For normal and locally normal systems, a number operator N_V exists on any finite volume V of the system.[18] As a consequence, the number of particles on any finite volume V of the system is finite. This is characteristic of normal and locally normal systems. On the other hand, regular processes and, more generally, ordinary processes[8] have the property that the number of points in a finite volume is finite. This property explains why, wanting to have regular detection processes, we shall *a priori* limit ourselves to normal or locally normal systems.

Moreover, concerning the observed system, the following hypothesis will be used that will appear necessary in defining the position operator later on:

Hypothesis 3: The particles of the volume V where the measurements are performed do not interact with the source(s), that is to say, the field associated with the particles in volume V is a free field.

Practically this means that the volume where the measurements are performed is far enough from the source(s) for the interaction between the system and the source(s) to be negligible.

2. Nonrelativistic position operator

Let us first define the position operator $\mathcal{N}_1^1[\Delta]$ on the one-particle-state space H. H is invariant by Euclidean motion. We have

$$\mathcal{N}_1^1[\Delta] = \int_\Delta \chi(a)\,da, \tag{II. 2}$$

where $\chi(a)$ is the position operator at point a. It has the properties of a *projection operator*[20] and can be written

$$\chi(a) = |a)(a|, \tag{II. 3}$$

where $|a)$ is the state of H that describes the particle in point a. If we introduce the time t, we shall write

$$\mathcal{N}_1^1[\Delta,t] = \int_\Delta \chi(a(t))\,da(t) = \int_\Delta |a(t))(a(t)|\,da(t). \tag{II. 4}$$

The mean value $(\phi|\chi(a)|\phi) = |\phi(a)|^2$ is the particle presence probability density for the state $|\phi)$ of H.

Let us now define the position operator $\mathcal{N}_1^n[\Delta]$ on the symmetrized or antisymmetrized n-particle-state space ${}_A^S H^{\otimes n}$.[21] ${}_A^S H^{\otimes n}$ is obtained by symmetrization (S) or antisymmetrization (A) of $H^{\otimes n}$, the latter being the tensorial product of n spaces H_i, identical to H.[22] We have

$$\mathcal{N}_1^n[\Delta] = \sum_{i=1}^n \int_\Delta \chi_i(a)\,da, \tag{II. 5}$$

where $\chi_i(a)$ is the position operator on H_i.

$\mathcal{N}_1^n[\Delta]$ can be rewritten in the configuration space representation.[23] In this representation the operators act on the space ${}_A^S\tilde{H}^{\otimes n}$ built from $\tilde{H}$ in the same way as ${}_A^S H^{\otimes n}$ from H. $\tilde{H}$ is the space of the linear forms $(x|\phi) = \phi(x)$, where $|\phi)$ belongs to H and $(x|$ to its dual H^*. The ket $|x)$ describes a particle in point x. In the configuration space representation the action of any operator W, diagonal on the states ${}_A^S|x_1)\,|x_2)\cdots|x_n) = |\{x\})$ of ${}_A^S H^{\otimes n}$, can be described with the help of its diagonal elements $W(\{x\})$[24]:

$$(\{x\}|(W|\phi)) = W(\{x\})\phi(\{x\}). \tag{II. 6}$$

Thus, in the configuration space representation, $\mathcal{N}_1^n[\Delta]$ is written

$$\mathcal{N}_1^n[\Delta] = \sum_{i=1}^n \int_\Delta \delta(a - x_i)\,da. \tag{II. 5'}$$

This expression (II. 5′) allows us to write $\mathcal{N}_1[\Delta]$ acting on the Fock space (union of all ${}_A^S H^{\otimes n}$ for the integer $n \in [0, +\infty[$), in the second quantization formalism.

Let $\{|\psi_k)\}$ be an orthonormal basis of H [in the following, $|\psi_k)$ will describe a particle of wave vector k] and a_k^+ and a_k be the creation and annihilation operators of $|\psi_k)$ respectively. They are normalized in such a way that

$$\begin{aligned} &[a_k, a_{k'}^+]_\pm = \delta_{kk'} && (V \text{ finite}),\\ &[a_k, a_{k'}^+] = \delta^3(k-k') && (V \text{ infinite})\\ &[a_k, a_{k'}]_\pm = [a_k^+, a_{k'}^+]_\pm = 0. \end{aligned} \tag{II. 7}$$

The sign − (+) indicates a commutator (anticommutator).

For a one-particle operator, we know how to go from the configuration space representation to the Fock representation[25]:

Theorem: Let a one-particle operator W be

$$W = \sum_{k_1 k_2} (\psi_{k_1}|w|\psi_{k_2}) a_{k_1}^+ a_{k_2} \tag{II. 8}$$

in the Fock representation. The operator w acts on H. Let, on the other hand, $\mathcal{W}$ be an operator the restriction $\mathcal{W}^n$ of which is

$$\mathcal{W}^n = \sum_{i=1}^n w(x_i) \tag{II. 9}$$

on ${}_A^S\tilde{H}^{\otimes n}$. By definition

$$w(x_i) = (x_i|w|x_i). \tag{II. 10}$$

The operators W and $\mathcal{W}$ are identical.

This theorem allows us to write $\mathcal{N}_1[\Delta]$ in the Fock representation

$$\mathcal{N}_1[\Delta] = \int_\Delta \mathcal{Y}(a)\, da, \tag{II. 11}$$

or introducing the time t

$$\mathcal{N}_1[\Delta, t] = \int_\Delta \mathcal{Y}(a, t)\, da, \tag{II. 11'}$$

where

$$\mathcal{Y}(a, t) = \mathcal{A}^+(a, t)\mathcal{A}(a, t), \tag{II. 12}$$

with

$$\mathcal{A}(a, t) = V^{-1/2} \sum_k \exp[2i\pi k \cdot a - 2i\pi \nu(k)t] a_k \tag{II. 13}$$

if the considered system is of finite volume V, or

$$\mathcal{A}(a, t) = \int \exp[2i\pi k \cdot a - 2i\pi \nu(k)t] a_k\, dk, \tag{II. 13'}$$

if the system is infinite. $\nu(k)$ is the frequency associated with the wave vector k. $\mathcal{N}_1[\Delta]$ is deduced from $\mathcal{N}_1[\Delta, t]$ by putting $t = 0$ in the foregoing formulas.

$\mathcal{A}(a, t)$ and $\mathcal{A}^+(a, t)$ verify the following commutation relations, which are easily deduced from (II. 7) and (II. 13):

$$\begin{aligned} &[\mathcal{A}(a, t)\mathcal{A}(a', t')]_\pm = [\mathcal{A}^+(a, t)\mathcal{A}(a', t')]_\pm = 0, \\ &[\mathcal{A}(a, t)\mathcal{A}^+(a', t)]_\pm = \delta(a - a'). \end{aligned} \tag{II. 14}$$

Let us underline the fact that in the nonrelativistic case a density is introduced without mathematical difficulties as proved by formulas (II. 2), (II. 5), (II. 5'), or (II. 11).

3. Difficulties in building a position operator for nonzero mass relativistic particles

The position operator $\mathcal{N}_1^1[\Delta]$ is now defined as a projection operator acting on the one particle-state space $\mathcal{H}$, which is invariant by Lorentz transformation.[11,12,19] A main property of $\mathcal{N}_1^1[\Delta]$ is that the representation $\mathcal{T}$ on $\mathcal{H}$ of any translation T in the Euclidean space that transforms Δ into Δ' such that $\Delta \cap \Delta' = 0$ transforms the eigenfunction $|\phi)$ of $\mathcal{N}_1^1[\Delta]$ into the eigenfunction $\mathcal{T}|\phi)$ of $\mathcal{N}_1^1[\Delta']$ which is orthogonal to $|\phi)$:

$$(\phi, \mathcal{T}\phi) = 0, \tag{II. 15}$$

where $(\cdots, \cdots)$ indicates a Lorentz invariant scalar product. This scalar product is written[26]

$$(\chi, \psi) \int \frac{d^3k}{k_0} (\chi|k)(k|\psi), \tag{II. 16}$$

where $|k)$ is of square modulus k_0^2 and describes a particle of wave vector k and where $k_0 = (k^2 + m^2)^{1/2}$, m being the mass of the considered particle. $\hbar$ is taken equal to one. The spin is not introduced, for simplification.

From (II. 15) and (II. 16), Newton and Wigner show that the function $|\phi_a)$ of $\mathcal{H}$ describing a particle localized at point a is

$$|\phi_a) = \int \frac{d^3k}{k_0} \sqrt{k_0} \exp(-2i\pi k a)|k), \tag{II. 17}$$

or, in the configuration space representation,

$$\phi_a(x) = (x|\phi_a) = \int \frac{d^3k}{k_0} \sqrt{k_0} \exp(-2i\pi k a)(x|k)$$

$$= \int \frac{d^3k}{k_0} \sqrt{k_0} \exp[-2i\pi k(a - x)]. \tag{II. 17'}$$

We see that, because of the Lorentz invariant definition of the scalar product and contrary to the nonrelativistic case, this function is not the Dirac function $\delta^3(a - x)$. As a consequence, contrary to the nonrelativistic case, the eigenfunction $\phi(x) = (x|\phi)$ of $\mathcal{N}_1^1[\Delta]$ is nonzero out of Δ. From this follows that, although the particle is localized in Δ, its energy in nonzero out of Δ: *there is a nonlocal relation between the position and the energy of a particle.*[12]

It appears, as a consequence of the foregoing result that our description of detection should have to tell between particle detection and energy detection. Let us see that in more detail. To begin with, let us express $\mathcal{N}_1[\Delta]$ in the Fock representation. The Fock space is now built from $\mathcal{H}$ and the creation and annihilation b_k and b_k^+ of state $|k)$ are normalized in such a way that

$$[b_k, b_{k'}^+]_\mp = k_0 \delta^3(k - k'). \tag{II. 18}$$

Thus, a state $|\phi)$ of $\mathcal{H}$ is written

$$|\phi) = \int \frac{d^3k}{k_0} \phi(k)|k) = \int \frac{d^3k}{k_0} \phi(k) b_k^+ |0), \tag{II. 19}$$

where $|0)$ is the vacuum state.

Then, it can be easily shown that

$$\mathcal{N}_1[\Delta] = \int_\Delta \mathcal{Y}(a)\, da, \tag{II. 20}$$

where

$$\mathcal{Y}(a) = \mathcal{B}^+(a)\mathcal{B}(a), \tag{II. 21}$$

with

$$\mathcal{B}(a) = \int \frac{d^3k}{k_0} \sqrt{k_0} \exp(+2i\pi k a) b_k, \tag{II. 22}$$

such that, according to (II. 17) and (II. 19), the eigenfunction $|\phi_a)$ of $\mathcal{Y}(a)$ is

$$|\phi_a) = \mathcal{B}^+(a)|0). \tag{II. 23}$$

From (II. 17) and (II. 18), we see that we can go from the relativistic formulation to the nonrelativistic one by setting

$$b_k = \sqrt{k_0} a_k, \tag{II. 24}$$

and, thus, it follows from (II. 13) and (II. 22) that

$$\mathcal{B}(a) = \mathcal{A}(a). \tag{II. 25}$$

Consequently, $\mathcal{Y}(a)$ is the same operator in both relativistic and nonrelativistic cases, for nonzero mass particles.

Let us now compare $\mathcal{Y}(a)$ with what should be an energy localization operator $\mathcal{E}(a)$[9]:

$$\mathcal{E}(a) = E^+(x)E(x), \tag{II. 26}$$

where $E(x)$ is the positive frequency part of the field operator

$$E(x) = iV^{1/2} \sum_k [\tfrac{1}{2}h\nu(k)]^{1/2} \exp(2i\pi k \cdot x) a_k \quad (V \text{ finite}) \tag{II. 27}$$

or

$$E(x) = i \int [\tfrac{1}{2}h\nu(k)]^{1/2} \exp(2i\pi k \cdot x) a_k \quad (V \text{ infinite}). \tag{II. 27'}$$

Hypothesis 1 allows us to write

$$[\nu(k)-\nu(K)]\ll\nu(K), \quad \text{where } K \text{ is the mean wave vector,} \tag{II. 28}$$

and to rewrite $E(x)$ as

$$E(x)=iV^{1/2}[\tfrac{1}{2}h\nu(K)]^{1/2}\sum_k \exp(2i\pi k\cdot x)a_k, \tag{II. 29}$$

or

$$E(x)=i[\tfrac{1}{2}h\nu(K)]^{1/2}\int \exp(2i\pi k\cdot x)a_k\,dk. \tag{II. 29'}$$

Thus, $\mathcal{Y}(a)$ and $\mathcal{E}(a)$ may be identified, up to a constant factor. Hypothesis 1 reduces particle detection and energy detection essentially to the same operation.

4. Position operator for zero-mass particles

We are now left with an ultimate question, the detection of zero-mass particles.

It has been known for a long time that a zero-mass particle position operator cannot be defined as a *projection* operator.[27] Jauch and Piron[19] have established the existence of a position operator $\mathcal{N}_1[\Delta]$ that does not possess the characteristic additive property of projection operators; for two disjoined volumes Δ and Δ', instead of having

$$\mathcal{N}_1[\Delta]+\mathcal{N}_1[\Delta']=\mathcal{N}_1[\Delta\cup\Delta'] \quad \text{(additive property)}, \tag{II. 30}$$

we have

$$\mathcal{N}_1[\Delta]+\mathcal{N}_1[\Delta']<\mathcal{N}_1[\Delta\cup\Delta']. \tag{II. 31}$$

From this, Amrein[12] deduces that

$$\mathcal{N}_1[\Delta]=\int_\Delta da\int_\Delta da' K_\Delta(a,a')\mathcal{A}^+(a)\mathcal{A}(a'). \tag{II. 32}$$

This operator differs from the nonzero mass one by the kernel $K_\Delta(a,a')$, and it would be reduced to the nonzero mass operator if $K_\Delta(a,a')$ were equal to $\delta^3(a-a')$. Equation (II. 32) shows the nonexistence of a density operator $\mathcal{Y}(a)$. From this, the impossibility of defining a probability *density* by a quantum mean value $\mathrm{Tr}\{\rho\mathcal{Y}(a)\}$ follows. Thus a *regular* detection p. p. cannot be defined.

Fortunately, Amrein has shown[12] that if Hypotheses 1 and 3 plus a third hypothesis, that we shall call Hypothesis 4, are fulfilled, $\mathcal{N}_1[\Delta]$ can be written, for zero mass particles, in the same way as for nonzero mass particles:

$$\mathcal{N}_1[\Delta]=\int_\Delta \mathcal{A}^+(a)\mathcal{A}(a)\,da. \tag{II. 11'}$$

Then a density can be defined. The third hypothesis, allowing the use of (II. 11), is

Hypothesis 4: The linear dimensions of the localization volume Δ are much larger than the mean wavelength λ of the observed field.

Finally, we are left with the following result: If hypotheses 1—4 are realized, the particle detection may be described with operator (II. 11).

It is interesting to emphasize that Hypothesis 4 characterizes the detectors that may be used. Indeed the active area of a P. M. is of the order of 0. 1 to 1 mm^2 and its resolution time is about 10^{-9} sec, which corresponds to a position incertainty of about 30 cm. These magnitudes are much larger than the mean wavelength of the observed visible light. The condition $\Delta\gg\lambda^3$ is *a fortiori* fulfilled for electrons: The experiments should be performed on electrons whose wavelength is of the order of one angström with detectors the dimensions of which are of a few microns at least.[5] Let us notice that our condition $\Delta\gg\lambda^3$ necessary to define a presence probability density in the photon case appears under the form $\Delta t\gg\nu(K)^{-1}$ to define a counting rate, that is to say, a time density, in the study of P. M. done by Glauber.[9]

Let us also underline that, for the usual detectors, Hypotheses 2 and 4 are noncontradictory.

All these remarks lead us to the conclusion that our four hypotheses well describe the usual experimental conditions (and even the potential ones, in the electron case) and provide us with a rather simple operator describing the action of the detectors.

B. Coincidence operator

1. Instantaneous coincidence operator

The operator $\mathcal{N}_p[\{\Delta_i\}]$ describing the instantaneous action, in p different volumes of space, of p type 1 detectors verifying Hypotheses 1—4, is defined.

From the property β of the c. p. d. and from Eq. (II. 1), $\mathcal{N}_p[\{\Delta_i\}]$ is deduced to be symmetrical with respect to its arguments. From Hypothesis 2, we deduce that if the field is an n-particle field, the ith detector $(1\leq i\leq p)$ will act on a $(n-i+1)$-particle field.

These two remarks suggest the following form of $\mathcal{N}_p[\{\Delta_i\}]$:

$$\mathcal{N}_p[\{\Delta_i\}]=\int_{\{\Delta_i\}}\cdots\int \mathcal{Y}_p\{a_i\}\,da_1\cdots da_p, \tag{II. 33}$$

where

$$\mathcal{Y}_p\{a_i\}=\mathcal{A}^+(a_1)\mathcal{A}^+(a_2)\cdots\mathcal{A}^+(a_p)\mathcal{A}(a_p)\cdots\mathcal{A}(a_1). \tag{II. 34}$$

Introducing the time t, we have

$$\mathcal{N}_p[\{\Delta_i\},t]=\int_{\{\Delta_i\}}\cdots\int \mathcal{Y}_p\{a_i,t\}\,da_1\cdots da_p, \tag{II. 33'}$$

where

$$\mathcal{Y}_p\{a_i,t\}=\mathcal{A}^+(a_1,t)\cdots\mathcal{A}^+(a_p,t)\mathcal{A}(a_p,t)\cdots\mathcal{A}(a_1,t). \tag{II. 34'}$$

Remark 1: Let us notice that expression (II. 34) is very similar to the one obtained by Glauber[28] in calculating the p-order intensity correlation function in the photon case, $\Gamma_p(a_1,a_2,\ldots,a_p)$. Indeed, he sets

$$\Gamma_p(a_1,a_2,\ldots,a_p)=\mathrm{Tr}(\rho\mathcal{G}_p\{a_i\})$$

with

$$\mathcal{G}_p\{a_i\}=E^+(a_1)\cdots E^+(a_p)E(a_p)\cdots E(a_1). \tag{II. 35}$$

According to our Hypotheses 1—4, $\mathcal{Y}_p\{a_i\}$ and $\mathcal{G}_p\{a_i\}$ are proportional. This result is quite satisfactory: Indeed the photon detection p. p. is known to be a compound Poisson process,[29] and the proportionality between $\mathcal{Y}_p\{a_i\}$ and $\mathcal{G}_p\{a_i\}$ expresses nothing but a well-known property of compound Poisson process, the identity between the process density correlation functions and its c. p. d.

Remark 2: From (II. 14) and (II. 33), we deduce that if

the volumes Δ_i are disjoined, every $\mathcal{A}(a_i)$ commutes with every $\mathcal{A}^+(a_j)$ as long as a_i and a_j belong to two different volumes and that

$$\mathcal{N}_p[\{\Delta_i\}] = \prod_{i=1}^{p} \mathcal{A}^+(a_i)\mathcal{A}(a_i)\,da_i = \prod_{i=1}^{p} \mathcal{N}_1[\Delta_i] \tag{II. 36}$$

This result has already been formulated in other ways, by Schweber, for instance,[30] and in the photon case by Mandel.[31] If the volumes Δ_i are not disjoined, (II. 36) does not hold.

To compare the expression (II. 34) of $\mathcal{Y}_p\{a_i\}$ with non-quantum results, let us establish the reduction of $\mathcal{Y}_p\{a_i\}$ on ${}_A^S\tilde{H}^{\otimes n}$. To do so, we shall use the following theorem:

Theorem: Let W_p be a p-particle operator, in the Fock representation, such that

$$W_p = \sum_{\{k_i\}\{k'_i\}} (\psi^p_{\{k_i\}} | w | \psi^p_{\{k'_i\}}) \prod_{i=1}^{p} a^+_{k_i} a_{k'_i} \tag{II. 37}$$

where

$$\sum_{\{k_i\}\{k'_i\}} = \left(\prod_{i=1}^{p} \sum_{k_i}\right)\left(\prod_{i=1}^{p} \sum_{k'_i}\right) \tag{II. 38}$$

$$|\psi^p_{\{k_i\}}) = {}_A^S(|\psi_{k_1}) \cdots |\psi_{k_p})), \tag{II. 39}$$

and w is an operator on ${}_A^S H^{\otimes p}$.

Let, on the other hand, W_p be defined by its restriction $\tilde{W}_p^n$ on ${}_A^S\tilde{H}^{\otimes n}$:

$$\tilde{W}_p^n = \sum_{i\neq} w\,(x_{i1}, x_{i2}, \ldots, x_{ip}) \tag{II. 40}$$

where

$$w\,(x_1, x_2, \ldots, x_p) = (\{x\}|w|\{x\}) \tag{II. 41}$$

and $\sum_{i\neq}$ indicates a sum such that i_1 may take any value from 1 to n, i_2 any value from 1 to n different from $i_1, \ldots, i_p$ any value from 1 to n different from $i_1, i_2, \ldots, i_{p-1}$. It can be shown that

$$W_p \equiv W_p. \tag{II. 42}$$

This theorem is established in Ref. 25 for $p = 2$, and in Ref. 5 for any p.

Thus, the restriction $\tilde{\mathcal{Y}}^n_p\{a_i\}$ of $\mathcal{Y}_p\{a_i\}$ on ${}_A^S\tilde{H}^{\otimes n}$ is

$$\tilde{\mathcal{Y}}^n_p\{a_i\} = \sum_{i\neq} \delta(a_1 - x_{i_1}) \cdots \delta(a_p - x_{i_p}) \tag{II. 43}$$

and the restriction $\tilde{\mathcal{N}}^n_p[\{\Delta_i\}]$ of $\mathcal{N}_p\{\Delta_i\}$ on ${}_A^S\tilde{H}^{\otimes n}$ is

$$\tilde{\mathcal{N}}^n_p[\{\Delta_i\}] \int_{\{\Delta_i\}} \cdots \sum_{i\neq} \delta(a_1 - x_{i_1}) \cdots \delta(a_p - x_{i_p})\,da_1 \cdots da_p. \tag{II. 44}$$

From (II. 1) and (II. 43), we deduce that

$$P_p[\{a_i\}, t] = \mathrm{Tr}[\rho(t)\mathcal{Y}_p\{a_i\}] = \sum_{n=0}^{+\infty} \int \rho_n(x_1, x_2, \ldots, x_n; t) \times \sum_{i\neq} \delta(a_1 - x_{i_1}) \cdots \delta(a_p - x_{i_p}) \prod_{j=1}^{n} dx_j, \tag{II. 45}$$

where

$$\rho_n(x_1, x_2, \ldots, x_n; t) = (\{x\}|\rho(t)|\{x\}). \tag{II. 46}$$

Relation (II. 45) is similar to the one that can be established in classical statistical mechanics. Indeed, if a classical particle system is characterized by its configuration space probability density $D_c(x_1, x_2, \ldots, x_n; t)$ and if the result obtained by Yvon[16] for two particles is extended to p particles, the classical p-order c. p. d. (that Yvon would call p-order particle density) is given by

$$P_p[\{a_i\}, t] = \int D_c(x_1, \ldots, x_n; t) \sum_{i\neq} \delta(a_1 - x_{i_1}) \cdots \delta(a_p - x_{i_p}) \times \prod_{j=1}^{n} dx_j, \tag{II. 47}$$

the classical equivalent of (II. 45).

2. Multitime coincidence operator

The multitime operator $\mathcal{Y}_p\{a_i, t_i\}$ such that

$$\mathcal{N}_p[\{\Delta_i\}, \{t_i\}] = \int_{\{\Delta_i\}} \int \mathcal{Y}_p\{a_i, t_i\} \prod_{i=1}^{p} da_i \tag{II. 48}$$

is now defined.

The measurement described by $\mathcal{Y}_p\{a_i, t_i\}$ is a sequence of measurements at successive time instants $t_1, t_2, \ldots, t_p$, such that if the system is in a given state $|\psi)$ (or in a given mixture of states) before the measurement, and if its time evolution can be described by the evolution operator $U(t)$, at time t, the state $|\psi)$ is reduced to a nonnormalized time-dependent state,[10]

$$\mathcal{A}(a_1)U(t_1)|\psi),$$

which in its turn is reduced to a nonnormalized time-dependent state, at time t_2,

$$\mathcal{A}(a_2)U(t_2, t_1)\mathcal{A}(a_1)U(t_1)|\psi) = \mathcal{A}(a_2)U(t_2)\mathcal{A}(a_1, t_1)|\psi),$$

and so on until time t_p when the following nonnormalized time independent state is obtained:

$$U^+(t_p)\mathcal{A}(a_p)U(t_p)\mathcal{A}(a_{p-1}, t_{p-1}) \cdots \mathcal{A}(a_1, t_1)|\psi) = \mathcal{A}(a_p, t_p) \cdots \mathcal{A}(a_1, t_1)|\psi). \tag{II. 49}$$

The only difference between an instantaneous coincidence measurement lies in the fact that the reductions of the initial state which are done in a chronological order in the second case are performed in any logical order in the first case. Thus, whereas in the first case every reduction is described by the action of $\mathcal{A}(a_i, t)$, in the second case it is described by the action of $\mathcal{A}(a_i, t_i)$. $\mathcal{Y}_p\{a_i, t_i\}$ is deduced from $\mathcal{Y}_p\{a_i, t\}$ by putting $\mathcal{A}_p(a_i, t_i)$ in the place of $\mathcal{A}_p(a_i, t)$:

$$\mathcal{Y}_p\{a_i, t_i\} = T\{\mathcal{A}^+(a_1, t_1) \cdots \mathcal{A}^+(a_p, t_p)\mathcal{A}(a_p, t_p) \cdots \mathcal{A}(a_1, t_1)\}, \tag{II. 50}$$

where the time ordering operator T orders the operators $\mathcal{A}^+$ in the opposite way.

Expression (II. 50) can be simplified. In fact, with our Hypotheses 1–4, we have been able to describe the particle detection with free field creation and annihilation and annihilation operators $\mathcal{A}^+(a, t)$ and $\mathcal{A}(a, t)$ which verify the communication relations (II. 14). This entails that the product $\{\mathcal{A}^+(a_1, t_1) \cdots \mathcal{A}^+(a_p, t_p)\mathcal{A}(a_p, t_p) \cdots \mathcal{A}(a_1, t_1)\}$ does not vary if two pairs $\mathcal{A}(a_j, t_j)\mathcal{A}(a_i, t_i)$ and $\mathcal{A}^+(a_i, t_i)$ $\mathcal{A}^+(a_j, t_j)$ are permuted respectively. Thus, we can write

$$\mathcal{Y}_p\{a_i, t_i\} = \mathcal{A}^+(a_1, t_1) \cdots \mathcal{A}^+(a_p, t_p)\mathcal{A}(a_p, t_p) \cdots \mathcal{A}(a_1, t_1) \tag{II. 50'}$$

without time ordering operator, the creation and annihilation operators being written in two opposite orders.

And

$$P_p[\{a_i\}, \{t_i\}] = \mathrm{Tr}(\rho\mathcal{Y}_p\{a_i, t_i\}). \tag{II. 51}$$

Remark: In the photon field case, if the beam is parallel, we have

$$\mathcal{A}(x,t) \equiv \mathcal{A}(x-ct), \tag{II. 52}$$

and thus

$$\mathcal{Y}_p\{a_i,t_i\} \equiv \mathcal{Y}_p\{a_i - ct_i\}. \tag{II. 53}$$

C. Validity theorem

The quantity $P_p[\{a_i\},t]$ defined by

$$P_p[\{a_i\},t] = \mathrm{Tr}[\rho(t)\mathcal{Y}_p\{a_i\}], \tag{II. 54}$$

where $\mathcal{Y}_p\{a_i\}$ is given by (II. 12) in its nonrelativistic form and (II. 21) in its relativistic form, is shown to be a well-defined c. p. d. : The corresponding p. p. is regular p. p.

This result will be formulated as a theorem:

Validity Theorem: Let a particle system be normal (locally normal) and Hypotheses 1—4 be verified, then the detection p. p. $\mathcal{P}_t(V)$ defined on the volume V of the system (on a any finite part V of the system) by its c. p. d.

$$P_p[\{a_i\},t] = \mathrm{Tr}[\rho(t)\mathcal{Y}_p\{a_i\}] \tag{II. 54}$$

where $\mathcal{Y}_p\{a_i\}$ is given by (II. 12) or (II. 21), is a regular p. p.

Demonstration: To establish that the p. p. is regular, we first show that the c. p. d. verify properties α and β and that the e. p. d., moreover, verify property γ.

Property α: We must establish that

$$\mathrm{Tr}[\rho(t)\mathcal{Y}_p\{a_i\}] \geq 0. \tag{II. 55}$$

Indeed, $\rho(t)$ is a bounded Hermitian positive operator; thus the form W defined on the operator space $\mathcal{U}$ by

$$W(A) = \mathrm{Tr}[\rho(t)A] \quad \forall A \in \mathcal{U} \tag{II. 56}$$

is positive definite. This means that if

$$A = Z^+Z \quad \text{where } Z \in \mathcal{U}, \tag{II. 57}$$

$$W(A) = W(Z^+Z) \geq 0, \tag{II. 58}$$

now

$$\mathcal{Y}_p\{a_i\} = \mathcal{A}^+(a_1)\cdots\mathcal{A}^+(a_p)\mathcal{A}(a_p)\cdots\mathcal{A}(a_1) = Z_p^+Z_p,$$

then (II. 55) is verified.

Property β: It is obviously verified from the very form chosen for $\mathcal{Y}_p\{a_i\}$.

Property γ: The e. p. d. $G^V_p[\{a_i\},t]$ is obtained by detecting p particles in a volume V knowing that only p particles are present in this volume. Thus it is given by

$$G^V_p[\{a_i\},t] = \mathrm{Tr}[\rho^p(t)\tilde{\mathcal{Y}}^p_p\{a_i\}], \tag{II. 59}$$

where the restriction $\tilde{\mathcal{Y}}^p_p\{a_i\}$ on ${}^S_A\tilde{H}^{\otimes p}$ is given by (II. 43) and where $\rho^p(t)$ is the projection of $\rho(t)$ on ${}^S_A\tilde{H}^{\otimes p}$.

It follows from (II. 43) that

$$\int\cdots\int \tilde{\mathcal{Y}}^p_p\{a_i\} \prod_{i=1}^{p} da_i = p!\,I, \tag{II. 60}$$

where I is the unity operator. Then, using (II. 59) and (II. 60), we may write

$$\begin{aligned} 1 = \mathrm{Tr}[\rho(t)] &= \mathrm{Tr}\left(\sum_{p=0}^{+\infty}\rho^p(t)\right) \\ &= \mathrm{Tr}\left[\sum_{p=0}^{+\infty}\left(\rho^p(t)\frac{1}{p!}\int\cdots\int \tilde{\mathcal{Y}}^p_p\{a_i\}\prod_{i=1}^{p}da_i\right)\right] \\ &= \sum_{p=0}^{+\infty}\frac{1}{p!}\int\cdots\int \mathrm{Tr}[\rho^p(t)\mathcal{Y}^p_p\{a_i\}]\prod_{i=1}^{p}da_i \\ &= \sum_{p=0}^{+\infty}\frac{1}{p!}\int\cdots\int G^V_p[\{a_i\},t]. \end{aligned} \tag{II. 61}$$

The equality between the first and the last terms expresses Property γ. This achieves the demonstration of the validity theorem.

D. Properties of a regular point processes and properties of the coincidence operator

Let us consider different probabilities that may be defined for regular p. p. We show how their properties correspond to similar properties of the coincidence operator that may be associated with the p. p. according to the preceding method.

Let $\xi^n_p[\{a_i\},t]$ be the probability density that a *given* particle is at point a_1, another given particle at point $a_2\ldots$, a pth particle at point a_p, the total number of particles in V being n $(n \geq p)$. Let $P^n_p[\{a_i\},t]$ be the probability that any p particles are in $a_1,\ldots,a_p$, knowing that the total number of particles in V is n,

$$P^n_p[\{a_i\},t] = n^{[p]}\xi^n_p[\{a_i\},t]. \tag{II. 62}$$

From the quantum standpoint this will be written

$$P^n_p[\{a_i\},t] = \mathrm{Tr}[\rho^n(t)\tilde{\mathcal{Y}}^n_p\{a_i\}] \tag{II. 63}$$

or, introducing

$$\rho^n(\{x\},t) = (\{x\}|\rho^n(t)|\{x\}) \quad (|\{x\}\in {}^S_AH^{\otimes n}) \tag{II. 64}$$

and using (II. 43),

$$P^n_p[\{a_i\},t] = \int\cdots\int n^{[p]}\rho^n(\{x\},t)\prod_{j=p+1}^{n}dx_j. \tag{II. 65}$$

Thus

$$\xi^n_p[\{a_i\},t] = \int\cdots\int \rho^n(\{x\},t)\prod_{j=p+1}^{n}dx_j. \tag{II. 66}$$

In particular

$$\xi^p_p[\{a_i\},t] = G^V_p[\{a_i\},t], \tag{II. 67}$$

and

$$G^V_p[\{a_i\},t] = \rho^p(\{a_i\},t). \tag{II. 66'}$$

We have

$$\int\cdots\int \xi^n_p[\{a_i\},t]\prod_{i=1}^{p}da_i = 1, \tag{II. 68}$$

which entails,

$$\int\cdots\int P^n_p[\{a_i\},t]\prod_{i=1}^{p}da_i = n^{[p]} \tag{II. 69}$$

and, since

$$P_p[\{a_i\},t] = \sum_{n=p}^{+\infty}P^n_p[\{a_i\},t], \tag{II. 70}$$

$$\int\cdots\int P_p[\{a_i\},t] = \langle N^{[p]}\rangle, \tag{II. 71}$$

where N is a stochastic variable, the total number of particles in the considered system.

From the quantum standpoint, let us introduce the operator

$$\mathcal{Y}_p(V) = \int \cdots \int \mathcal{Y}_p\{a_i\} \prod_{i=1}^{p} da_i, \tag{II. 72}$$

the p order coincidence operator on the whole volume V of the system. Introducing the quantum operator

$$N = \sum_k a_k^+ a_k, \tag{II. 73}$$

the total number of particles in V, and using Eq. (II. 7), we may write (II. 72) as

$$\mathcal{Y}_p(V) = N(N-1)\cdots(N-p-1), \tag{II. 74}$$

the quantum mean of which gives (II. 71).

Let us notice that

$$\xi^n_p[\{a_i\}, t] = \int \xi^n_{p+1}[\{\{a_i\}, a_{p+1}\}, t]\, da_{p+1}, \tag{II. 75}$$

which implies

$$P^n_p[\{a_i\}, t] = \frac{1}{n-p} \int P^n_{p+1}[\{\{a_i\}, a_{p+1}\}, t]\, da_{p+1}. \tag{II. 76}$$

From (II. 67), (II. 70), and (II. 76), the relation (I. 10) between c. p. d. and e. p. d. follows.

From the quantum standpoint, (II. 63) and (II. 76) lead to

$$\tilde{\mathcal{Y}}^n_p\{a_i\} = \frac{1}{n-p} \int \tilde{\mathcal{Y}}^n_{p+1}\{\{a_i\}, a_{p+1}\}\, da_{p+1}, \tag{II. 77}$$

which in its turn confirms that the e. p. d. and c. p. d., given by (II. 59) and (II. 45) respectively, verify (I. 10).

III. APPLICATIONS

A. Fermion detection processes

According to the validity theorem of Sec. II, if Hypotheses 1–4 are verified, the detection point process measured on any normal or locally normal fermion system is regular. Let us apply this result to the particular case of fermion chaotic system.[5,13,14,32] Such systems can be characterized by their density operator[33]

$$\rho = \prod_k \rho_k \tag{III. 1}$$

with

$$\rho_k = (1 - \langle n_k \rangle)\,|0)(0| + \langle n_k \rangle\,|\phi_k)(\phi_k|, \tag{III. 2}$$

where the ket $|\phi_k)$ describes a fermion in mode k. $\langle n_k \rangle$ is the mean number of fermions in mode k,

$$\langle n_k \rangle \leq 1. \tag{III. 3}$$

(Once more, the spin has been removed, for simplifications.) In the second quantization formalism, ρ_k would be[32]

$$\rho_k = (1 - \langle n_k \rangle) \exp(-\beta_k a_k^+ a_k) \tag{III. 4}$$

with

$$\exp(-\beta_k) = \langle n_k \rangle / (1 - \langle n_k \rangle). \tag{III. 5}$$

With such a density operator, the c. p. d. obtained by using Eq. (II. 45) are[5,14]

$$P_p[\{a_i\}] = \sum P_\alpha(-1) \prod_{i=1}^{p} C(a_i - a_{\alpha i}), \tag{III. 6}$$

where the positive definite function $C(a_i - a_{\alpha i})$ verifies

$$C(a_i - a_{\alpha i}) = (1/V) \sum_k \langle n_k \rangle \exp[2i\pi k(a_i - a_{\alpha i})]$$

$$= \mathrm{Tr}[\rho \mathcal{A}^+(a_{\alpha i}) \mathcal{A}(a_i)]. \tag{III. 7}$$

It is the correlation function of the field operator, up to a constant factor (according to the quasimonochromaticity hypothesis). It can be any covariance function in the limits where (III. 3) is verified. The symbol $\sum P_\alpha(-1)$ indicates a sum over every permutation of $\{1, 2, \ldots, p\}$, each term in the sum being multiplied by $(-1)^r$, where r is the order of the permutation in the considered term.

The validity theorem proves that the functions given by (III. 6), (III. 7), and (III. 3) are the actual c. p. d. of a mathematically well-defined regular point process.

B. Probabilistic interpretation of vacuum mean values

Let us here comment the following result of Frisch and Bourret (F. B.)[15,34]:

They consider vacuum mean values such as

$$(0|\, M(a_1)\cdots M(a_p)\,|0), \tag{III. 8}$$

where

$$M(a_i) = B(a_i) + B^+(a_i). \tag{III. 9}$$

$B(a_i)$ and $B^+(a_i)$ are annihilation and creation operators in a nonnormalized state $|\chi_i)$ defined by

$$|\chi_i) = \sum_k (\langle n_k \rangle / V)^{1/2} \exp(-2i\pi k a_i) a_k^+ |0). \tag{III. 10}$$

For boson, $\langle n_k \rangle$ may take any nonnegative value; for fermion (III. 3) must be verified.

We have

$$(\chi_j|\,\chi_l) = \sum_k (\langle n_k \rangle / V) \exp[2i\pi k(a_j - a_l)] = C(a_j - a_l), \tag{III. 11}$$

which entails

$$[B(a_j)B^+(a_l)]_+ = (0|\, B(a_j)B^+(a_l)\,|0) = C(a_j - a_l). \tag{III. 12}$$

$C(a_j - a_l)$ is a positive-definite function and thus a covariance.

The problem of F. B. is to associate with $M(a_i)$ a stochastic function $\mathcal{M}(a_i)$ the p-order momentum of which $\langle \mathcal{M}(a_i) \cdots \mathcal{M}(a_p) \rangle$ is identical to (III. 8). In the boson case, they show that a stochastic *Gaussian* function $\mathcal{M}(a_i)$ can be defined in this manner, the correlation function of which is $C(a_j - a_l)$. In the fermion case, they know how to define $\mathcal{M}(a_i)$ if $C(a_j - a_l)$, which will be its covariance, is an *exponential* function. In these conditions, $\mathcal{M}(a_i)$ is shown to be a *dichotomic Markov* function: It is a Markov[35] function that may be $+1$ or -1 only.

Our foregoing results allow a physical interpretation of these facts. Indeed, it has been established[5,13,14] that, for any chaotic system, the density operator of which is by definition[32]

$$\rho = \prod_k \rho_k,$$

$$\rho_k = (1 + \epsilon\langle n_k \rangle)^{-\epsilon} \exp(-\beta_k a_k^+ a_k) \tag{III. 13}$$

with

$$\exp(-\beta_k) = \langle n_k \rangle / (1 + \epsilon\langle n_k \rangle), \tag{III. 14}$$

[$\epsilon = +1$ (-1) for boson (fermion)], the detection c. p. d. are

$$P_p[\{a_i\}] = \mathrm{Tr}[\rho \mathcal{A}^+(a_1)\cdots\mathcal{A}^+(a_p)\mathcal{A}(a_p)\cdots\mathcal{A}(a_1)]$$
$$= \sum P_\alpha(\epsilon) \prod_{i=1}^{n} \mathrm{Tr}[\rho \mathcal{A}^+(a_i)\mathcal{A}(a_{\alpha i})]$$
$$= \sum P_\alpha(\epsilon) \prod_{i=1}^{n} C(a_i - a_{\alpha i}). \qquad \text{(III. 15)}$$

[The definition of $\sum P_\alpha(\epsilon)$ is deduced from the one of $P_\alpha(-1)$ by setting ϵ everywhere instead of -1.]

From (III. 15) and (III. 12), it follows that

$$P_p[\{a_i\}] = \sum P_\alpha(\epsilon) \prod_{i=1}^{n} (0 \,|\, B(a_i)B^+(a_{\alpha i}) \,|\, 0)$$

or, by using Wick theorem,[36]

$$P_p[\{a_i\}] = (0 \,|\, B(a_1)\cdots B(a_p)B^+(a_p)\cdots B^+(a_1) \,|\, 0).$$

Thus, the vacuum mean values $(0 \,|\, B(a_1)\cdots B(a_p) \times B^+(a_p)\cdots B^+(a_1) \,|\, 0)$ are nothing but the c. p. d. of the chaotic detection p. p. characterized by covariance (III. 11).

As a consequence the result of F. B. concerning bosons is nothing but the affirmation that a chaotic boson field can be described by a Gaussian stochastic function[9,29]: The moments of the intensity (square modulus of the field) are equal to the c. p. d. of the corresponding point process. This property characterizes compound Poisson processes and thus in particular boson detection processes, which are necessarily compound Poisson processes.[29] For exponential chaotic fermion fields, the p. p. defined by (III. 15) has been shown[5,13,14] to be a renewal[6] process. Thus it can be well understood that a Markov dichotomic variable be associated with the process.[5]

IV. CONCLUSION

As a conclusion, we would like to underline that our definition of a coincidence operator fulfills all the present experimental requirements and nevertheless is built in a mathematically rigourous formalism. From a theoretical point of view, other coincidence operators could be thought of, and it would be interesting to check whether they become equivalent to our coincidence operator when Hypotheses1—4 are fulfilled. From the experimental point of view our results allow the formulation of potential measurement results such as fermion coincidence measurements.[5]

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Path-integral evaluation of a nonstationary Calogero model

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The path integral for a three-body problem in one dimension described by the Lagrangian $L=(1/2)\left(\xi_1^2+\xi_2^2+\xi_3^2\right)-\left[(1/4)\omega^2(t)\ (\xi_1-\xi_2)^2+(\xi_2-\xi_3)^2+(\xi_3-\xi_1)^2\right]-g(\xi_1-\xi_2)^{-2}$ is examined, where ξ_1, ξ_2, and ξ_3 are the coordinates of the three particles and $\omega(t)$ is the time-dependent angular frequency indicating the coupling strength of the harmonic potentials.

I. INTRODUCTION

In Ref. 1 Khandekar and Lawande examined the path integral for a three-body problem described by the Lagrangian

$$L=\tfrac{1}{2}\{\dot{\xi}_1^2+\dot{\xi}_2^2+\dot{\xi}_3^2\}-\tfrac{1}{4}\omega^2\{(\xi_1-\xi_2)^2+(\xi_2-\xi_3)^2+(\xi_3-\xi_1)^2\}-g(\xi_1-\xi_2)^{-2}, \tag{1}$$

where ξ_1, ξ_2, and ξ_3 are the coordinates of the three particles, ω the constant angular frequency arising from the strength of the harmonic potentials, and g is the strength of the inverse square potential acting between particles 1 and 2. In Ref. 1 the method for evaluating the corresponding path integral is mainly based on the important results obtained by Peak and Inomata (Ref. 2.) They have been able to evaluate some central force path integrals. Also, some general expressions for the Feynman propagator in the central force problem have been derived. In the present paper the Lagrangian under consideration is

$$L(\dot{\bar{\xi}},\bar{\xi},t)=\tfrac{1}{2}\{\dot{\xi}_1^2+\dot{\xi}_2^2+\dot{\xi}_3^2\}-\tfrac{1}{4}\omega^2(t)\{(\xi_1-\xi_2)^2+(\xi_2-\xi_3)^2+(\xi_3-\xi_1)^2\}-g(\xi_1-\xi_2)^{-2}, \tag{2}$$

where now the angular frequency $\omega(t)$ is time dependent and where $\bar{\xi}$ stands for (ξ_1,ξ_2,ξ_3). The present situation also arises in connection with a three-body problem considered by Calogero in Ref. 3. Let us first transform the Lagrangian (1) by introducing the center of mass and Jacobi coordinates, defined by

$$\begin{aligned}&\xi_1+\xi_2+\xi_3=3R,\\&\xi_1-\xi_2=\sqrt{2}x,\\&\xi_1+\xi_2-2\xi_3=\sqrt{6}y.\end{aligned} \tag{3}$$

These transformation formulas make it possible to separate L as follows:

$$L=\tfrac{3}{2}\dot{R}^2+\tfrac{1}{2}(\dot{x}^2+\dot{y}^2)-\tfrac{3}{4}\omega^2(t)(x^2+y^2)-g/2x^2. \tag{4}$$

Introducing (4) into the definition formula of a path integral (see, e.g., Ref. 4),

$$K(\bar{\xi}_t,t;\bar{\xi}_0,0)=\int_{0,\bar{\xi}_0}^{t,\bar{\xi}_t}D\bar{\xi}_t\exp[i\int_0^t L(\dot{\bar{\xi}},\bar{\xi},t)\,dt], \tag{5}$$

results in

$$K(\bar{\xi}_t,t,\bar{\xi}_0,0)=K_0(R_t,t;R_0,0)\bar{K}(x_t,y_t,t;x_0,y_0,0). \tag{6}$$

K_0 denotes a free particle propagator corresponding to the centre of mass. $\bar{K}$ represents the relative motion and is given by

$$\bar{K}(x_t,y_t,t;x_0,y_0,0)=\int_{0,x_0,y_0}^{t,x_t,y_t}Dx(t)\,Dy(t)\exp\left(\frac{1}{2}i\int_0^t(\dot{x}^2+\dot{y}^2)\,dt-\tfrac{3}{4}i\int_0^t dt\omega^2(t)(x^2+y^2)-i\int_0^t\frac{1}{2}\frac{g}{x^2}\,dt\right). \tag{7}$$

In fact, the problem of evaluating the right-hand side of (7) can be reduced to calculating the following integrals:

$$\bar{K}_0(y_t,t;y_0,0)=\int_{0,y_0}^{t,y_t}Dy(t)\exp\left(\frac{i}{2}\int_0^t\dot{y}^2\,dt-\frac{3}{4}\int_0^t\omega^2(t)y^2\,dt\right) \tag{8}$$

and

$$\bar{K}(x_t,t;x_0,0)=\int_{0,x_0}^{t,x_t}Dx(t)\exp\left(\frac{i}{2}\int_0^t\dot{x}^2\,dt-\frac{3}{4}i\int_0^t\omega^2(t)y^2\,dt-ig\int_0^t\frac{dt}{2x^2}\right). \tag{9}$$

The path integral of (8) is a simple Gaussian one and can be evaluated by following Feynman's theorem (see, e.g., Refs. 4–6). In fact, (9) is the path integral of the quantal problem of a particle interacting in one dimension with an external time-dependent quadratic potential and a constant inverse square potential. This problem was solved completely by Camiz *et al.* in Ref. 7 in the Schrödinger formalism. In turn, the path integral evaluation of (9) is obtained here as a by-product of our calculation of (7). Indeed, one has

$$\bar{K}(x_t,t;x_0,0)=\frac{\bar{K}(x_t,y_t,t;x_0,y_0,0)}{\bar{K}_0(y_t,t;y_0,0)}. \tag{10}$$

Let us concentrate next to the evaluation of (7) which is the main concern of the present paper. From now on the bar on K is dropped.

II. EVALUATION OF $K(x_t,y_t,t;x_0,y_0,0)$

Frist of all "plane polar" coordinates are introduced:

$$\begin{aligned}&r=(x^2+y^2)^{1/2}\quad(0\leq x<\infty)\\&x=r\sin\theta,\qquad y=r\cos\theta\\&\theta=\mathrm{Arctan}x/y\quad(0\leq\theta<2\pi).\end{aligned} \tag{11}$$

The Langrangian

$$L(\dot{x},\dot{y},x,y,t)=\tfrac{1}{2}\dot{x}^2+\tfrac{1}{2}\dot{y}^2-\tfrac{3}{4}\omega^2(t)(x^2+y^2)-g/2x^2 \tag{12}$$

occurring in the argument of the exponential function in the integrand of (7) is transformed into

$$L=\tfrac{1}{2}(\dot r^2+r^2\dot\theta^2)-\tfrac{3}{4}\omega^2(t)r^2-g/2r^2\sin^2\theta. \tag{13}$$

For the action S corresponding to this Lagrangian, one has

$$S=\sum_{j=1}^{N}\left(\frac{1}{2\epsilon}(r_j^2+r_{j-1}^2-2r_jr_{j-1}\cos(\theta_j-\theta_{j-1})-\epsilon\tfrac{3}{4}\omega^2(j\epsilon)r_j^2 - \frac{\epsilon(a^2-\frac{1}{4})}{2r_j^2\sin^2\theta_j}\right)+O(\epsilon^2N), \tag{14}$$

where

$$a=\tfrac{1}{2}(1+4g)^{1/2} \tag{15}$$

Of course, S can be cast into the form

$$S=\sum_{j=1}^{N}\left(\frac{1}{2\epsilon}(r_j^2+r_{j-1}^2-2r_jr_{j-1}\cos(\theta_j-\theta_{j-1})-\tfrac{3}{4}\epsilon\omega^2(j\epsilon)r_j^2 - \frac{\epsilon(a^2-\frac{1}{4})}{2r_jr_{j-1}\sin\theta_j\sin\theta_{j-1}}\right)+O(\epsilon^2N), \tag{16}$$

whence

$$\exp(iS)=\prod_{j=1}^{N}\left[\exp\left(\frac{i}{2\epsilon}(r_j^2+r_{j-1}^2)-i\epsilon\tfrac{3}{4}\omega^2(j\epsilon)r_j^2\right)\times\exp\left(\frac{r_jr_{j-1}}{i\epsilon}\cos\theta_j\cos\theta_{j-1}\right)\exp\left(\frac{r_jr_{j-1}}{i\epsilon}\sin\theta_j\sin\theta_{j-1} - \frac{i\epsilon(a^2-\frac{1}{4})}{2r_jr_{j-1}\sin\theta_j\sin\theta_{j-1}}\right)\exp[O(\epsilon^2)]\right]. \tag{17}$$

Noting that the asymptotic form of $I_a(u/\epsilon)$, the modified Bessel function, for small ϵ, is given by

$$I_a\left(\frac{u}{\epsilon}\right)\sim\left(\frac{\epsilon}{2\pi u}\right)^{1/2}\left[\exp\frac{u}{\epsilon}-\frac{1}{2}\left(a^2-\frac{1}{4}\right)\frac{\epsilon}{u}+\left(O\ \frac{\epsilon^2}{u^2}\right)\right], \tag{18}$$

one gets

$$\exp(iS)=\prod_{j=1}^{N}\left[\exp\left(\frac{i}{2\epsilon}(r_j^2+r_{j-1}^2)-i\epsilon\frac{3}{4}\omega^2(j\epsilon)r_j^2\right)\times\exp\left(\frac{r_jr_{j-1}}{i\epsilon}\cos\theta_j\cos\theta_{j-1}\right)\times\left(\frac{2\pi r_jr_{j-1}\sin\theta_j\sin\theta_{j-1}}{i\epsilon}\right)^{1/2}I_a\left(\frac{r_jr_{j-1}\sin\theta_j\sin\theta_{j-1}}{i\epsilon}\right)\right]. \tag{19}$$

It has to be remarked first that the factor

$$\prod_{j=1}^{N}\exp\left[O\left(\frac{\epsilon^2}{(r_jr_{j-1}\sin\theta_j\sin\theta_{j-1})^2}\right)+O(\epsilon^2)\right]$$

can be omitted because the argument of the exponential function doesn't contribute to S in the limit for $\epsilon\to 0$. Making use of the expansion formula,

$$(\sin\alpha\sin\beta)^{1/2-\lambda}I_{\lambda-1/2}(z\sin\alpha\sin\beta)\exp(z\cos\alpha\cos\beta) =2^{2\lambda}(2\pi z)^{-1/2}(\Gamma(\lambda))^2\sum_{l=0}^{\infty}\frac{l!(\lambda+1)}{\Gamma(2\lambda+1)}I_{l+\lambda}(z)C_l^{\lambda}(\cos\alpha)C_l^{\lambda}(\cos\beta) \tag{20}$$

in $\exp(iS)$ of (19) gives

$$\exp(iS)=\sum_{l_1l_2\ldots l_N}\left(\prod_{j=1}^{N}N_{l_j}^2(\sin\theta_j\sin\theta_{j-1})^{a+1/2}C_{l_j}^{a+1/2}(\cos\theta_j)C_{l_j}^{a+1/2}(\cos\theta_{j-1})R_{l_j}(r_jr_{j-1})\right), \tag{21}$$

where N_l is the normalizing factor of the Gegenbauer polynomial $C_l^{a+1/2}(\cos\theta)$, and $R_{l_j}(r_j,r_{j-1})$ is defined as

$$R_l(r_j,r_{j-1})=(2\pi)\exp\frac{i}{2\epsilon}(r_j^2+r_{j-1}^2)-i\epsilon\frac{3}{4}\omega^2(j\epsilon)r_j^2 \times I_{l+a+}\frac{1}{2}\left(\frac{r_jr_{j-1}}{i\epsilon}\right). \tag{22}$$

Expressing $\bar K(x_t,y_t,t;x_0,y_0,0)$ of (7) in polar coordinates and replacing the exponential function of (7) by (21), we find

$$K(r_t,\theta_t;r_0,\theta_0)=\lim_{N\to\infty}B_N\sum_{l_1\ldots l_N}\int\prod_{j=1}^{N}N_{l_j}^2(\sin\theta_j\sin\theta_{j-1})^{a+1/2} \times C_{l_j}^{a+1/2}(\cos\theta_j)C_{l_j}^{a+1/2}(\cos\theta_{j-1})R_{l_j}(r_j,r_{j-1})\prod_{j=1}^{N-1}r_j\,dr_j\,d\theta_j \tag{23}$$

with

$$B_N=(1/2\pi i\epsilon)^N. \tag{24}$$

The integrations over the angular variables can be performed by taking into account the normalization and orthogonality condition for the Gegenbauer polynomials. Therefore, we have

$$K(r_t,\theta_t;r_0,\theta_0) =\sum_{l=0}^{\infty}K_l(r_t,r_0)N_l^2(\sin\theta_t\sin\theta_0)^{a+1/2} \times C_l^{a+1/2}(\cos\theta_t)C_l^{a+1/2}(\cos\theta_0), \tag{25}$$

where

$$K_l(r_t,r_0)=\lim_{N\to\infty}B_N\int\prod_{j=1}^{N}R_{l_j}(r_j,r_{j-1})\prod_{j=1}^{N-1}r_j\,dr_j. \tag{26}$$

III. EVALUATION OF THE RADIAL PROPAGATOR

To obtain an analytical expression for (26) we still have to carry out the radial integrations of

$$K_l(r_t,r_0)=\lim_{N\to\infty}(-i\alpha)^N\exp\left(\frac{i\alpha}{2}(r_t^2+r_0^2)\right) \times\int\exp\{i(\beta_1r_1^2+\beta_2r_2^2+\cdots+\beta_{N-1}r_{N-1})\} \times I_\mu(-i\alpha r_0r_1)\cdots I_\mu(-i\alpha r_{N-1}r_N)\prod_{j=1}^{N-1}r_j\,dr_j, \tag{27}$$

where

$$\alpha=\epsilon^{-1},\quad \beta_j=\alpha\left(1-\frac{\epsilon^2}{2}\omega^2(j\epsilon)\right) \tag{28}$$

and

$$\mu=l+a+\tfrac{1}{2}$$

The intergrations in (27) may be performed by repeated use of the formula of Peak and Inomata deduced in Ref. 2:

$$\int_0^{\infty}\exp(i\alpha r^2)I_\nu(-ibr)I_\nu(-icr)r\,dr =\frac{i}{2\alpha}\exp\left(-i\frac{(b^2+c^2)}{4\alpha}\right)I_\mu\left(-i\frac{bc}{2\alpha}\right), \tag{29}$$

valid for $\mathrm{Re}(\mu) > -1$ and $\mathrm{Re}(\alpha) > 0$. The result is given by

$$K_1(r_t, r_0) = \lim_{N\to\infty} (1/i)\alpha_N \exp(ip_N r_0^2 + iq_N r_t^2) I_\mu(-\alpha_N i r_t r_0), \quad (30)$$

where

$$\begin{aligned} \alpha_N &= \alpha \sum_{k=1}^{N-1} \left(\frac{\alpha}{2\gamma_k}\right), \\ p_N &= \frac{\alpha}{2} - \sum_{k=1}^{N-1} \frac{\alpha_k^2}{4\gamma_k}, \\ q_N &= \alpha/2 - \alpha^2/4\gamma_{N-1}, \\ \alpha_1 &= \alpha, \quad \alpha_{k+1} = \alpha \prod_{j=1}^{k} \left(\frac{\alpha}{2\gamma_j}\right) \quad (k \geq 1), \\ \gamma_1 &= \beta_1, \quad \gamma_{k+1} = \beta_{k+1} - \alpha^2/4\gamma_k. \end{aligned} \quad (31)$$

The main point in getting an analytical expression for $K_1(r_t, r_0)$ turns out to be the evaluation of α_N, p_N, and q_N. Let us first aim our attention to the evaluation of γ_k. Putting

$$2\gamma_{k+1}/\alpha = y_{k+1}/y_k, \quad (32)$$

we rewrite the difference equation for γ_K in (31) as

$$y_{k+1} - 2y_k + y_{k-1} + \omega^2(k\epsilon)\epsilon^2 y_k = 0. \quad (33)$$

To solve this equation, let us consider the differential equation

$$\ddot{y} + \omega^2(t)y = 0. \quad (34)$$

Let us denote the solution of this equation satisfying the boundary conditions

$$y(0) = 0 \quad \text{and} \quad \dot{y}(0) = 1 \quad (35)$$

by $y(t) = \eta(t)$. Substituting $y_k = \eta(k+1)\epsilon) + O(\epsilon^3)$ into (34), we observe that the equation,

$$(y_{k+1} - 2y_k + y_{k-1}) + \omega^2(k\epsilon)y_k\epsilon^2 = 0, \quad (36)$$

is satisfied up to the second order in ϵ. Let us consider next the initial condition $\gamma_1 = \beta_1$, or

$$\frac{1}{2}\frac{\eta(2\epsilon)}{\eta(\epsilon)} = \left(1 - \frac{\epsilon^2}{2}\omega^2(0)\right) + O(\epsilon^3). \quad (37)$$

It is readily shown that this equation is also satisfied up to the second order in ϵ.

So one gets for (32)

$$\gamma_{k+1} = \frac{1}{2} \cdot \frac{\eta((k+2)\epsilon) + O(\epsilon^3)}{\eta((k+1)\epsilon) + O(\epsilon^3)}. \quad (38)$$

Let us now calculate α_{k+1} of (31) in a similar manner;

$$\begin{aligned} \alpha_{k+1} &= \frac{1}{\epsilon} \prod_{j=1}^{k} \frac{\eta(j\epsilon) + O(\epsilon^3)}{\eta((j+1)\epsilon) + O(\epsilon^3)} \\ &= \frac{1}{\epsilon} \frac{\eta(\epsilon) + O(\epsilon^3)}{\eta((k+1)\epsilon) + O(\epsilon^3)}. \end{aligned} \quad (39)$$

Thus we obtain

$$\lim_{N\to\infty} \alpha_N = 1/\eta(t) \quad \text{with } N\epsilon = t. \quad (40)$$

Next the limit of q_N is evaluated;

$$\begin{aligned} \lim_{N\to\infty} q_N &= \lim_{N\to\infty} \left(\frac{1}{2\epsilon} - \frac{1}{2\epsilon} \frac{\eta((N-1)\epsilon) + O(\epsilon^3)}{\eta(N\epsilon) + O(\epsilon^3)}\right) \\ &= \frac{1}{2} \cdot \frac{1}{\eta(t)} \cdot \lim_{N\to\infty} \frac{\eta(N\epsilon) - \eta((N-1)\epsilon)}{\epsilon}, \end{aligned}$$

or

$$\lim_{N\to\infty} q_N = \dot{\eta}(t)/2\eta(t) \quad (41)$$

The most difficult step turns out to be the evaluation of $\lim_{N\to\infty} p_N$:

$$\begin{aligned} \lim_{N\to\infty} p_N &= \lim_{N\to\infty} \left(\frac{1}{2\epsilon} - \frac{1}{2}\sum_{k=1}^{N-1} \frac{\epsilon}{(\eta(k+1)\epsilon) + O(\epsilon^3))^2}\right) \\ &= \lim_{N\to\infty} \left(\frac{1}{2\epsilon} - \frac{1}{2}\int_\epsilon^t \frac{dt}{\eta^2(t)}\right). \end{aligned} \quad (42)$$

It is readily seen that this limit exists in the form

$$\lim_{N\to\infty} p_N = \frac{1}{2\eta(t)} \lim_{N\to\infty} \left(\frac{1}{\epsilon}\eta(t) - \eta(t)\int_\epsilon^t \frac{dt}{\eta^2(t)}\right). \quad (43)$$

For every $\epsilon \neq 0$,

$$\xi(t) = \frac{1}{\epsilon}\eta(t) - \eta(t)\int_\epsilon^t \frac{dt}{\eta^2(t)} \quad (44)$$

is a solution of (29) which is linearly independent of the solution $y(t) = \eta(t)$. Evidently, $\xi(\epsilon) = \eta(\epsilon)/\epsilon$, so that $\lim_{\epsilon\to 0}\xi(\epsilon) = 1$. Furthermore,

$$\dot{\xi}(t) = \frac{\dot{\eta}(t)}{\epsilon} - \dot{\eta}(t)\int_\epsilon^t \frac{dt}{\eta^2(t)} - \eta(t)\frac{1}{\eta^2(t)}$$

and hence

$$\dot{\xi}(\epsilon) = \frac{\dot{\eta}(\epsilon)}{\epsilon} - \frac{1}{\eta(\epsilon)} = \frac{\dot{\eta}(\epsilon)\eta(\epsilon) - \epsilon}{\epsilon\eta(\epsilon)}$$

from which follows

$$\lim_{\epsilon\to 0} \dot{\xi}(\epsilon) = 0.$$

So $\xi(t)$ is a solution of $\ddot{x} + \omega^2(t)x = 0$ satisfying the boundary conditions $\xi(0) = 1$ and $\dot{\xi}(0) = 0$. So we obtain

$$\lim_{N\to\infty} p_N = \frac{1}{2}\frac{\xi(t)}{\eta(t)}. \quad (45)$$

As a result, the radial propagator is given by

$$K_1(r_t, r_0) = \frac{1}{i\eta(t)} \exp\left(i\frac{\xi(t)}{2\eta(t)}r_0^2 + i\frac{\dot{\eta}(t)}{2\eta(t)}r_t^2\right) I_\mu\left(-i\frac{r_t r_0}{\eta(t)}\right). \quad (46)$$

IV. CONCLUSIONS

Our expression (25) for $K(r_t, \theta_t; r_0, \theta_0)$ becomes

$$\begin{aligned} K(r_t, \theta_t; r_0, \theta_0) = \sum_{l=0}^{\infty} N_l^2 (\sin\theta_t \sin\theta_0)^{\mu+1/2} C_l^{\alpha+1/2}(\cos\theta_t) C_l^{\alpha+1/2} \\ \times (\cos\theta_0) \frac{1}{i\eta(t)} \exp\left(i\frac{\xi(t)}{2\eta(t)}r_0^2 + i\frac{\dot{\eta}(t)}{2\eta(t)}r_t^2\right) I_\mu\left(-i\frac{r_t r_0}{\eta(t)}\right). \end{aligned} \quad (47)$$

So the path integral for a nonstationary Calogero model described by the Lagrangian (2) is achieved. As a by-product of our calculations an analytical expression for the propagator of a time-dependent quantal harmonic oscillator with a singular perturbation can be obtained from (10). The result so obtained is equivalent with that of Camiz *et al.* in Ref. 3. In their paper the solutions are found both in the Schrödinger representation, by using a generating function or a time-dependent raising

operator, and in the Heisenberg picture. In the Appendix it is shown how starting from the Feynman propagator (47) and making use of formula (10) one can deduce the wavefunctions obtained by Camiz *et al.*

APPENDIX

It will be shown how the wavefunctions of the time-dependent quantal harmonic oscillator with a singular perturbation described by the path integral (9) can be obtained.

Formula (10) is valid for $y_t = y_0 = 0$, so that

$$\bar{K}(x_t, t; x_0, 0) = \frac{K(x_t, 0, t; x_0, 0, 0)}{\bar{K}_0(0, t; 0, 0)}.$$

Using the formula (20) in (47), one finds

$$K(r_t, \theta_t; r_0, \theta_0) = \frac{1}{\sqrt{2\pi} i\eta(t)} \left(\frac{r_t \sin\theta_t r_0 \sin\theta_0}{i\eta(t)}\right)^{1/2}$$
$$\times \exp\left(\frac{i\xi(t)}{2\eta(t)} r_0^2 + i\frac{\dot{\eta}(t)}{2\eta(t)} r_t^2\right) I_a\left(\frac{r_t r_0}{i\eta(t)} \sin\theta_t \sin\theta_0\right)$$
$$\times \exp\left(\frac{r_t r_0}{i\eta(t)} \cos\theta_t \cdot \cos\theta_0\right).$$

Again introducing the variables x_t, x_0, y_t, and y_0 by (11) and setting $y_0 = y_t = 0$, one obtains

$$\bar{K}(x_t, t; x_0, 0) = \varphi(t) \left(\frac{x_t x_0}{i\eta(t)}\right)^{1/2} \exp\left(i\frac{\xi(t)}{2\eta(t)} x_0^2 + i\frac{\dot{\eta}(t)}{\eta(t)} x_t^2\right)$$
$$\times I_a\left(\frac{x_t x_0}{i\eta(t)}\right),$$

where $\varphi(t)$ is a function of t alone.

Let us define next two functions $p(t)$ and $\gamma(t)$ by

$$\eta(t) = p(t)\sin\gamma(t),$$
$$\xi(t) = p(t)\cos\gamma(t).$$

It is clear that $y(t) = p(t)\exp[i\gamma(t)]$ is a solution of the differential equation

$$\ddot{y} + \omega^2(t) y = 0,$$

which satisfies

$$y(0) = 1 \quad \text{and} \quad \dot{y}(0) = 1$$

provided that

$$p(0) = 1, \quad \gamma(0) = 0, \quad \dot{\gamma}(0) = 1$$

and

$$p^2(t)\dot{\gamma}(t) = 1.$$

So $\bar{K}(x_t, t; x_0, 0)$ is transformed into

$$\bar{K}(x_t, t; x_0, 0) = \varphi(t) \left(\frac{x_t}{p(t)} \frac{x_0}{i\sin(t)}\right)^{1/2} \exp[i\tfrac{1}{2}\cot\gamma(t) x_0^2 + i x_t^2]$$
$$\times \tfrac{1}{2}\frac{\dot{p}(t)\sin\gamma(t) + p(t)\dot{\gamma}(t)\cos\gamma(t)}{p(t)\sin\gamma(t)} I_a\left(\frac{x_t}{p(t)} \frac{x_0}{i\sin\gamma(t)}\right).$$

From the well-known Hille–Hardy formula (Erdélyi 1953), one can deduce

$$\frac{1}{i\sin t} I_{a+1/2}\left(\frac{r' r''}{i\sin t}\right) \exp\left(\frac{i}{2}(x_0^2\cot t) + \frac{i}{2}(x_t^2\cot t)\right)$$
$$= \sum_{n=0}^{\infty} \frac{n!\,2}{\Gamma(n+a+\frac{3}{2})} \exp[-i(2n+a+\tfrac{3}{2})t](r' r'')^{a+1/2}$$
$$\times \exp[-\tfrac{1}{2}(r''^2 + r'^2)] L_n^{a+1/2}(r''^2) L_n^{a+1/2}(r'^2).$$

Therefore, use of this formula leads to

$$\bar{K}(x_t, t; x_0, 0) = \varphi(t) \cdot \exp\left(\frac{i}{2} x_t^2 \frac{\dot{p}(t)}{p(t)}\right)$$
$$\times \sum_{n=0}^{\infty} \frac{n!\,2}{\Gamma(n+a+1)} \exp[-i(2n+a+1)\gamma(t)]$$
$$\times \left(\frac{x_t}{p(t)} \cdot \frac{x_0}{p(0)}\right)^{a+1/2}$$
$$\times \exp\left[-\frac{1}{2}\left(\frac{x_t^2}{p^2(t)} + x_0^2\right) \cdot L_n^a\left(\frac{x_t^2}{p^2(t)}\right)\right.$$
$$\left. \times L_n^a\left(\frac{x_0^2}{p^2(0)}\right)\right),$$

which can still be cast into the form

$$\bar{K}(x_t, t; x_0, 0) = \varphi_0(t) \sum_{n=0}^{\infty} \left(\frac{2\Gamma(n+1)}{\Gamma(n+a+1)}\right)^{1/2} x_t^{(2a+1)/2}$$
$$\times \exp[2i\gamma(t)(a+n+1)]$$
$$\times \exp\left[\frac{x_t^2}{2}\left(i\frac{\dot{p}(t)}{p(t)} - \dot{\gamma}(t)\right)\right] L_n^a(x_t^2\dot{\gamma}(t))$$
$$\times \left(\frac{2\Gamma(n+1)}{\Gamma(n+a+1)}\right)^{1/2} x_0^{(2a+1)/2}$$
$$\times \exp[-2i\gamma(0)(a+n+1)] \exp\left[\frac{x_0^2}{2}\left(-i\frac{\dot{p}(0)}{p(0)} - \dot{\gamma}(0)\right)\right]$$
$$\times L_n^a(x_0^2\dot{\gamma}(0)).$$

Here $\varphi_0(t)$ is an unimportant time-dependent factor which can be determined by the normalizing condition. Apparently, the wavefunction appropriate for our propagator is

$$\Psi_n(x, t) = \left(\frac{2\Gamma(n+1)}{\Gamma(n+a+1)}\right)^{1/2} x_t^{(2a+1)/2} \exp[2i\gamma(t)(a+n+1)]$$
$$\times \exp\left[\frac{x_t^2}{2}\left(i\frac{\dot{p}(t)}{p(t)} - \dot{\gamma}(t)\right)\right] L_n^a(x_t^2\dot{\gamma}(t))$$

which is exactly the same result as obtained in Ref. 3.

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An expansion theorem for the twisted product with applications

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A mathematically rigorous asymptotic formula in powers of the index c is obtained for the twisted product associated with the Weyl form of CCR for n degrees of freedom. When c is identified with the Planck constant, the asymptotic formula is used to give a precise meaning to the usual notion of "classical limit."

I. INTRODUCTION

The "twisted convolution" and the "twisted product" associated with the Weyl form of canonical commutation relations for n degrees of freedom are used by many authors[1,2,3] in constructing C^*-algebras of quantum observables. In Ref. 3, special attention is given to the noncommutative Banach $*$-algebra $L^2(R^{2n}, c)$, consisting of the square-integrable functions on the phase space R^{2n}, with multiplication given by the twisted product of index $c>0$. The main concern in Ref. 3 is the relationship between the phase space formulation of quantum mechanics and the theory of pseudodifferential operators. While our expansion theorem is suggested by the heuristic formula in Ref. 3, our interests lie in the asymptotic behavior of the twisted product as the index $c \downarrow 0$. After some preliminaries and definitions in Sec. II, the main results are stated in Sec. III, whose proofs are found in Sec. V. Section IV contains a number of applications. When the index c is identified with the Planck constant, results in this section can be viewed as a mathematically controlled version of the theory of quantum corrections to the particle-distribution functions.[4]

II. PRELIMINARIES

Let $\alpha=(\alpha_1, \alpha_2, \ldots, \alpha_k)$ be a k-tuple index of nonnegative integers. We shall write

$$\alpha! = \alpha_1!\alpha_2!\cdots\alpha_k!,$$

$$|\alpha| = \sum_{j=1}^{k}\alpha_j.$$

For $x=(x_1, x_2, \ldots, x_k)\in R^k$,

$$x^\alpha = x_1^{\alpha_1}x_2^{\alpha_2}\ldots x_k^{\alpha_k},$$

$$D^\alpha = (-i)^{|\alpha|}\left(\frac{\partial}{\partial x_1}\right)^{\alpha_1}\left(\frac{\partial}{\partial x_2}\right)^{\alpha_2}\cdots\left(\frac{\partial}{\partial x_k}\right)^{\alpha_k}.$$

When $k=2n$,

$$\partial^\alpha = (-i)^{|\alpha|}\left(\frac{\partial}{\partial x_{n+1}}\right)^{\alpha_1}\left(\frac{\partial}{\partial x_{n+2}}\right)^{\alpha_2}\cdots\left(\frac{\partial}{\partial x_{2n}}\right)^{\alpha_n} \times\left(-\frac{\partial}{\partial x_1}\right)^{\alpha_{n+1}}\left(-\frac{\partial}{\partial x_2}\right)^{\alpha_{n+2}}\cdots\left(-\frac{\partial}{\partial x_n}\right)^{\alpha_{2n}}.$$

Let $S(R^k)$ denote the space of complex functions on R^k, rapidly decreasing at ∞. For $\varphi\in S(R^k)$, define its Fourier transform $F\varphi$ by

$$(F\varphi)(\xi) = (2\pi)^{-k/2}\int \exp(i\xi\cdot x)\varphi(x)\,dx$$

where $\cdot$ is the inner product in R^k. The inverse Fourier transform $F^{-1}\Psi$ of $\Psi\in S(R^k)$ is given by

$$(F^{-1}\Psi)(x) = (2\pi)^{-k/2}\int \exp(-ix\cdot\xi)\Psi(\xi)\,d\xi.$$

Unless otherwise indicated, our integrals are over R^k with $d\xi$ denoting the Lebesque measure.

Definition 2.1: Let $\varphi, \Psi\in S(R^{2n})$. The twisted convolution and the twisted product of φ and Ψ (of index c, c real) are given respectively by,

$$(\varphi *_c \Psi)(\eta) = \int \exp(-ic/2(\eta\times u))\varphi(u)\Psi(\eta-u)\,du \qquad \text{(II.1)}$$

and

$$(\varphi\circ_c\Psi)(\xi) = (2\pi)^{-n}F^{-1}(F\varphi *_c F\Psi)(\xi) \qquad \text{(II.2)}$$

where $\eta=(l,m)$, $u=(s,t)$ are elements of R^{2n} and $\eta\times u = l\cdot t - m\cdot s$.

Remark 2.1:

1. One can verify readily that $\varphi *_c\Psi$ is again rapidly decreasing at ∞, so that (2) is well defined and $\varphi\circ_c\Psi$ is in $S(R^{2n})$.

2. If we set $c=0$ in (II.1) and (II.2), the twisted convolution becomes the usual convolution $*$ and the twisted product is the pointwise product of φ and Ψ. For $c\neq 0$, $\varphi *_c\Psi$ and $\varphi\circ_c\Psi$ are not commutative in general.

Let H be an infinite-dimensional separable Hilbert space with inner product $\langle\cdot,\cdot\rangle$ and norm $\|\cdot\|$. $\beta(H)$ will denote the algebra of bounded linear operators on H, and $\beta_1(H)$, $\beta_2(H)$ are the subalgebras of $\beta(H)$, of trace and Hilbert–Schmidt class, respectively. Also $U(H)$ will denote the group of unitary operators in $\beta(H)$.

Definition 2.2: Let $c>0$ and $\pi(c)$ be a map from R^{2n} to $U(H)$. $\pi(c)$ is said to be a Weyl system on H if the following are satisfied:

(i) $(\pi(c))(0)=I$, the identity operator on H,

(ii) $\xi\to\langle\pi(c)(\xi)x, y\rangle$ is continuous for each pair $x, y\in H$,

(iii) for each pair ξ, $\eta\in R^{2n}$,

$$(\pi(c))(\xi)(\pi(c))(\eta) = \exp(-ic/2(\eta\times\xi))(\pi(c))(\xi+\eta).$$

$\pi(c)$ is said to be irreducible if whenever $M\neq 0$ is a closed subspace of H, then $(\pi(c))(\xi)M\subset M$ for all $\xi\in R^{2n}$ implies $M=H$. (Whenever the context is clear, we will drop the c dependence and write π.)

If π is an irreducible Weyl system on H and $f\in S(R^{2n})$, we denote

$$B(f)[(x,y)]=\int \langle \pi(\xi)x,y\rangle (Ff)(\xi)\,d\xi$$

for each pair $x,y\in H$. $B(f)$ is a bounded sesquilinear functional on H since $|\langle \pi(\xi)x,y\rangle| \leq \|x\|\,\|y\|$. By a theorem on the general form of a bounded sesquilinear functional, there exists a bounded linear operator $W(f)$ in H, uniquely determined by $B(f)$ and

$$\langle W(f)x,y\rangle = B(f)[(x,y)].$$

Definition 2.3: The operator $W(f)$ associated with f is called the Weyl operator and the map W: $S(R^{2n})\to \beta(H)$ given by $f\to W(f)$ is called the Weyl mapping (correspondence).

Remarks 2.2:

1. A well known example of an irreducible Weyl system is given by the Weyl canonical commutation relations in the "Schrödinger representation" (Ref. 5, p. 119). In fact, all irreducible Weyl systems are unitarily equivalent, a theorem due to J. von Neumann.

2. The operator $W(f)$ was suggested by H. Weyl[6] as a recipe to obtain quantum observable from its classical counterpart f. If one considers $S(R^{2n})$ as a dense subspace of $L^2(R^{2n},c)$, all our definitions can be extended to ones involving functions in $L^2(R^{2n},c)$. The Weyl mapping W has been shown to be a faithful *-representation of the B^*-algebra $L^2(R^{2n},c)$ on the Hilbert space H. Furthermore, the range of W is $\beta_2(H)$ and the Weyl mapping is isometric up to a factor $\lambda(c)$ with respect to the Hilbert–Schmidt norm. For the above results, see Ref. 3, Proposition 1 and the references cited there.

III. MAIN RESULTS

Theorem 3.1: Let f,g be elements of $S(R^{2n})$ and $F(c,\xi)=(f\circ cg)(\xi)$ is their twisted product. Then for $c>0$ and a positive integer N,

$$F(c,\xi)=\sum_{k=0}^{N}(b_k[f,g])(\xi)c^k+\circ(c^N)$$

as $c\downarrow 0$ uniformly in the parameter ξ, where

$$(b_k[f,g])(\xi)=(i/2)^k\sum 1/\alpha!\,(D^\alpha f)(\partial^\alpha g)(\xi) \qquad \text{(III.1)}$$

and the summation is over all distinct $2n$-tuples α with $|\alpha|=k$.

Corollary 3.1: Let h be a measurable function on R^{2n}. Denote

$$G(c)=\int h(\xi)F(c,\xi)\,d\xi$$

and

$$B_k=\int h(\xi)(b_k[f,g])(\xi)\,d\xi,\quad k\geq 0.$$

Then

$$G(c)=\sum_{k=0}^{N}B_k c^k+\circ(c^N)\ \text{ as } c\downarrow 0$$

if one of the following conditions is satisfied:

(i) h is absolutely integrable,

(ii) h is bounded,

(iii) h is a polynomial in ξ.

The proofs for these results will be given in Sec. V.

IV. APPLICATIONS

Definition 4.1: Let $f\in S(R^{2n})$ and $\bar f$ be its complex conjugate. Set $(P[f])(c,\xi)=(f\circ c\bar f)(\xi)$. $P[f]$ is called the phase space distribution function determined by f.

Remark 4.1: From the definition of $P[f]$ and Remark 2.2.2, we see that if π is an irreducible Weyl system and W is the corresponding Weyl mapping, then $W(P[f])=W(f)W(f)^*$. The Weyl operator associated with $P[f]$ is positive and of trace class. $W(P[f])$ has properties expected of a density operator for a quantum statistical system of n particles in equilibrium.

Let $g\in L^2(R^{2n},c)$ and $g=\bar g$. For a given $f\in S(R^{2n})$, $W(g)W(P[f])$ is of trace class since $\beta_1(H)$ is a two-sided ideal in $\beta(H)$. Consider $S(R^{2n})$ as a dense subspace of $L^2(R^{2n})$ and let $\langle f,f\rangle=1$; we denote

$$\langle g(P[f])\rangle=\frac{\operatorname{tr}(W(g)W(P[f]))}{\operatorname{tr}(W(P[f]))}$$

where tr $(\cdot)$ is the trace of any operator in $\beta_1(H)$.

Theorem 4.1: For $c>0$ and $b_k[f,\bar f]$ given by Eq. (III.1),

$$\langle g(P[f])\rangle=\sum_{k=0}^{N}G_k c^k+\circ(c^N)\ \text{ as } c\downarrow 0$$

where

$$G_k=\int_k (b_k[f,\bar f])(\xi)g(\xi)\,d\xi,$$

if one of the following conditions on g is satisfied:

(i) g is absolutely integrable,

(ii) g is bounded.

Proof: From the almost isometric isomorphic properties of the Weyl mapping (see 2 in Remark 2.2), we have

$$\operatorname{tr}(W(g)W(P[f]),\ W(g))=\langle W(g)\rangle=\lambda(c)\langle P[f],g\rangle,$$

where $(\cdot,\cdot)$ is the inner product in $\beta_2(H)$.

Similarly,

$$\operatorname{tr}(W(P[f]))=\operatorname{tr}(W(f)W(\bar f))=\lambda(c)\langle f,f\rangle.$$

Thus, since $\langle f,f\rangle=1$,

$$\langle g(P[f])\rangle=\langle P[f],g\rangle=\int g(\xi)P[f](\xi)\,d\xi\ \text{ since } g=\bar g.$$

Then

$$\langle g(P[f])\rangle=\sum_{k=0}^{N}G_k c^k+\circ(c^N)\ \text{ as } c\downarrow 0$$

follows from (i) and (ii) of Corollary 3.1 by letting $g=h$.

Let f,g be elements of $S(R^{2n})$ and $W(f\circ cg)$ be the Weyl operator corresponding to $f\circ cg$. Then for each φ,Ψ in the representing Hilbert space H of the irreducible Weyl system π,

$$\langle W(f\circ cg)\varphi,\Psi\rangle=\int\langle\pi(\xi)\varphi,\Psi\rangle F(f\circ cg)(\xi)\,d\xi.$$

Since $F(f\circ cg)=(2\pi)^{-n}(Ff*cFg)$ and $|\langle\pi(\xi)\varphi,\Psi\rangle|\leq\|\varphi\|\ \|\Psi\|$ is bounded, we have

$$\langle W(f\circ cg)\varphi,\Psi\rangle=\sum_{k=0}^{N}\langle W(b_k[f,g])\varphi,\Psi\rangle c^k+\circ(c^N)\quad\text{as } c\downarrow 0$$

by Corollary 3.1, (ii).

The above discussion suggests the following definition:

Definition 4.2 We say the Weyl operator $W(f\circ cg)$ has an asymptotic power series in c to N terms whenever, for each φ,Ψ in H,

$$\langle W(f\circ cg)\varphi,\Psi\rangle=\sum_{k=0}^{N}\langle W(b_k[f,g])\varphi,\Psi\rangle c^k+\circ(c^N)\quad\text{as } c\downarrow 0,$$

where $b_k[f,g]$ is given by (III.1). For notation we shall write

$$W(f\circ cg)=\sum_{k=0}^{N}W(b_k[f,g])c^k+\circ(c^N)\quad\text{as } c\downarrow 0.$$

If $[W(f),W(g)]=W(f)W(g)-W(g)W(f)=W(f\circ cg)-W(g\circ cf)$ is the commutator of $W(f)$, $W(g)$ and

$$\{f,g\}=\sum_{j=1}^{N}\left(\frac{\partial f}{\partial q_j}\frac{\partial g}{\partial p_j}-\frac{\partial f}{\partial p_j}\frac{\partial g}{\partial q_j}\right)$$

where $\xi\in R^{2n}$ and

$$\xi=(q_1,q_2,\ldots,q_n,\ p_1,p_2,\ldots,p_n)$$

is the Poisson bracket of f and g, the following theorem can be interpreted as saying that the commutator of quantum observables goes over to the Poisson bracket $\{f,g\}$ of the classical observables f,g in the "classical limt" as $c\downarrow 0$. Here c plays the role of the Planck constant.

Theorem 4.2: For $c>0$,

$$\frac{1}{ic}[W(f),W(g)]=\sum_{k=1}^{N}W(d_k)c^{k-1}+\circ(c^N)\quad\text{as } c\downarrow 0,$$

where

$$d_k=\frac{1}{i}(b_k[f,g]-b_k[g,f])$$

and $b_k[f,g]$, $b_k[g,f]$ are coefficients of expansion for $f\circ cg$ and $g\circ cf$ given by Theorem 3.1.

Proof: By Theorem 3.1,

$$(f\circ cg)-(g\circ cf)(\xi)=\sum_{k=0}^{N}(b_k[f,g]-b_k[g,f])(\xi)c^k$$
$$+\circ(c^N)\quad\text{as } c\downarrow 0\text{ uniformly in }\xi.$$

Since $b_0[f,g]=b_0[g,f]$, we have

$$\frac{1}{ic}((f\circ cg)-(g\circ cf))=\sum_{k=1}^{N}d_k(\xi)c^{k-1}+\circ(c^N)$$
$$\text{as } c\downarrow 0\text{ uniformly in }\xi.$$

Then the discussion leading to Definition 4.2 can be used to complete the proof.

It is to be noted that $d_1=\{f,g\}$.

V. PROOFS FOR THEOREM 3.1 AND ITS COROLLARIES

To prove Theorem 3.1, we begin with a lemma:

Let $u=(s,t)$ and $\eta=(l,m)$ with s,t,l,m in R^n so that u,η are elements of R^{2n}. Denote $u'=(t,-s)$, $\eta'=(m,-l)$, and $u\times\eta=s\cdot m-t\cdot l$.

Lemma 5.1:

$$(u\times\eta)^k=\sum\frac{k!}{\alpha!}u^\alpha(\eta'-u')^\alpha\tag{V.1}$$

where the summation is over all distinct $2n$-tuple α with $|\alpha|=k$.

Proof: Since $\eta\times u=-u\times\eta$ and $u\times(\eta-u)=u\times\eta$, it follows then

$$(u\times\eta)^k=[u\times(\eta-u)]^k=[s\cdot(m-t)+t\cdot(s-l)]^k$$
$$=\sum\frac{k!}{\alpha!}u^\alpha(\eta'-u')^\alpha$$

by multinomial expansion.

Lemma 5.2: For each $\xi\in R^{2n}$, $F(c,\xi)=(f\circ cg)(\xi)$ is infinitely differentiable for all real numbers c.

Proof: Let k be a positive integer and $\xi\in R^{2n}$,

$$F^{(k)}(c,\xi)=\frac{\partial^k}{\partial c^k}F(c,\xi)$$
$$=(2\pi)^{-2n}\int\exp(-i\xi\cdot\eta)\int(-i/2)^k(\eta\times u)^k$$
$$\times\exp(-ic/2(\eta\times u))(Ff)(u)(Fg)(\eta-u)\,du\,d\eta.\tag{V.2}$$

The above differentiation under the integral sign is legitimate since the integral given by (V.2) is uniformly convergent in c. This can be seen by using (V.1) and rewriting

$$[-(\eta\times u)]^k=\sum\frac{k!}{\alpha!}u^\alpha(\eta'-u')^\alpha,$$

then substituting into (V.2). The integral becomes

$$(2\pi)^{-2n}(i/2)^k\sum\frac{k!}{\alpha!}\int\exp(-i\xi\cdot\eta)\int\exp(-ic/2(\eta\times u))u^\alpha(Ff)$$
$$\times(u)(\eta'-u')^\alpha Fg(\eta-u)\,du\,d\eta.\tag{V.3}$$

Thus,

$$|F^{(k)}(c,\xi)|\leq(2\pi)^{-2n}(1/2)^k\sum\frac{k!}{\alpha!}\int h_\alpha(\eta)\,d\eta<\infty\tag{V.4}$$

uniformly in c since

$$h_\alpha(\eta)=\int|u^\alpha(Ff)(u)|\,|(\eta'-u')^\alpha(Fg)(\eta-u)|\,du$$

is the convolution of absolutely integrable functions $|u^\alpha Ff|$ and $|(u')^\alpha Fg|$.

Lemma 5.3

$$F^{(k)}(0,\xi)/k!=(b_k[f,g])(\xi),\quad k\geq 0.$$

Proof: From (V.3),

$$F^{(k)}(0,\xi)/k!$$
$$=(2\pi)^{-n}(i/2)^k\sum\frac{1}{\alpha!}F^{-1}(u^\alpha Ff*(u')^\alpha Fg)$$

$$= (i/2)^k \sum \frac{1}{\alpha!} (D^\alpha f)(\partial^\alpha g)(\xi). \tag{V.5}$$

In the above we have made use of the fact that

$$F^{-1}(u^\alpha F f) = D^\alpha f$$

and

$$F^{-1}(u'^\alpha F g) = \partial^\alpha g,$$

so that from the properties of convolution

$$F^{-1}[u^\alpha F f * (u')^\alpha F g] = F^{-1}[F D^\alpha f * F \partial^\alpha g] = (2\pi)^n (D^\alpha f)(\partial^\alpha g).$$

Comparing (v.5) with (III.1),

$$(b_k[f,g])(\xi) = F^{(k)}(0,\xi)/k! \quad \text{for } k > 0.$$

When $k = 0$, $F^{(0)}(0,\xi) = F(0,\xi) = b_0[f,g]$.

Proof of Theorem 3.1

By Lemma 5.2 and considering ξ as a parameter, $F(c,\xi)$ is infinitely differentiable for all real numbers c. Using Taylor's theorem with a remainder and expanding $F(c,\xi)$ to N terms about 0 in powers of $c > 0$, we have

$$F(c,\xi) = \sum_{k=0}^{N} F^{(k)}(0,\xi)/k! + R_N(c,\xi,\tau(\xi)),$$

where

$$R_N(c,\xi,\tau(\xi)) = \frac{F^{(N+1)}(\xi,\tau(\xi))}{(N+1)!} c^{N+1} \tag{V.6}$$

and $\tau(\xi)$ is a number depending on ξ such that $0 < \tau(\xi) < c$. From (V.4),

$$|F^{(N+1)}(\xi,\tau(\xi))/(N+1)!| \le B < \infty \tag{V.7}$$

uniformly in $\tau(\xi)$ and ξ, where

$$B = (2\pi)^{-2n} (1/2)^{N+1} \sum \frac{1}{\alpha!} \int h_\alpha(\eta)\, d\eta.$$

Thus,

$$c^{-N} |R_N(c,\xi,\tau(\xi))| \le cB \to 0 \quad \text{as } c \downarrow 0,$$

uniformly in ξ.

The next two lemmas are needed to prove Corollary 3.1.

Lemma 5.4: Let α, β be multi-indices and $f, g \in S(R^{2n})$. Then for $0 < c \le 1$ and $0 < \tau(\xi) < c$,

$$|F^{-1}(D^\beta(u^\alpha F f_* \tau(\xi)(u')^\alpha F g))| \le L(\alpha,\beta) \tag{V.8}$$

where $L(\alpha,\beta)$ is a constant independent of $\tau(\xi)$ and ξ.

Proof: To show (V.8) is true for each $\tau(\xi)$ is readily done. Since $D^\beta(u^\alpha F f_* \tau(\xi)(u')^\alpha F g)$ is rapidly decreasing, so is its inverse Fourier transform. Then let

$$B(\tau(\xi)) = \int |D^\beta(u^\alpha F f_* \tau(\xi)(u')^\alpha F g)(\eta)|\, d\eta < \infty$$

and we have (V.8). Tof ruther show that (V.8) is true for $L(\alpha,\beta)$ independent of $\tau(\xi)$, we need to show

$$|D^\beta(u^\alpha F f_* \tau(\xi)(u')^\alpha F g)(\eta)| \le h_{\alpha,\beta}(\eta),$$

where $h_{\alpha,\beta}$ is absolutely integrable and independent of $\tau(\xi)$. This is done by the following reasoning:

Using Definition 2.1 and differentiating formally under the integral sign, one can show that

$$|D^\beta(u^\alpha F f_* \tau(\xi)(u')^\alpha F g)(\eta)|$$

is dominated by a finite sum of convolution integrals of the form

$$(1/2)^{|\gamma_1|}(|u^{\gamma_1} u^\alpha F f| * |D^{\gamma_2}(u')^\alpha F g|)(\eta),$$

where γ_1, γ_2 are muti-indices with $|\gamma_1| \le |\beta|$ and $|\gamma_2| \le |\beta|$. In the above, we made use of the fact that $0 < \tau(\xi) < c \le 1$. If we denote the sum by $h_{\alpha,\beta}(\eta)$ which is absolutely integrable and independent of $\tau(\xi)$, we have

$$|F^{-1}(D^\beta(u^\alpha F f_* \tau(\xi)(u')^\alpha F g))(\xi)| \le (2\pi)^{-n} \times \int |h_{\alpha,\beta}(\eta)|\, d\eta = L(\alpha,\beta) < \infty$$

independent of $\tau(\xi)$ and ξ.

Lemma 5.5: Let β be a multi-index. Then for $0 < c \le 1$,

$$\left|\xi^\beta\left((f \circ cg)(\xi) - \sum_{k=0}^{N} (b_k[f,g])(\xi) c^k\right)\right| \le c^{N+1} L(\beta)$$

where $L(\beta)$ is a constant independent of $\tau(\xi)$ and ξ.

Proof: For each $0 < \tau(\xi) < c \le 1$ and using (V.6) and (V.7), we have

$$\begin{aligned}
&\left|\xi^\beta\left((f \circ cg)(\xi) - \sum_{k=0}^{N} (b_k[f,g])(\xi) c^k\right)\right| \\
&= |\xi^\beta R_N(c,\xi,\tau(\xi))| \\
&= c^{N+1}(2\pi)^{-n}(1/2)^{N+1} \left|\sum \frac{1}{\alpha!} \xi^\beta F^{-1}(u^\alpha F f * \tau(\xi)(u')^\alpha F g)(\xi)\right| \\
&\le c^{N+1}(2\pi)^{-n}(1/2)^{N+1} \sum \frac{1}{\alpha!} |F^{-1}(D^\beta(u^\alpha F f_* \tau(\xi)(u')^\alpha F g))| \\
&\le c^{N+1} L(\beta) < \infty
\end{aligned}$$

uniformly in ξ and $\tau(\xi)$ by Lemma 5.4, where

$$L(\beta) = (2\pi)^{-n}(1/2)^{N+1} \sum \frac{1}{\alpha!} L(\alpha,\beta).$$

Proof of Corollary 3.1

In all cases, $G(c)$ and B_k exist for each c and $k \ge 0$ since $f \circ cg$ and $b_k[f,g]$ are $S(R^{2n})$ functions.

To prove (i), we note that

$$\begin{aligned}
&c^{-N}\left|G(c) - \sum_{k=0}^{N} B_k c^k\right| \\
&= c^{-N}\left|\int h(\xi)\left((f \circ cg)(\xi) - \sum_{k=0}^{N} b_k(\xi) c^k\right) d\xi\right| \\
&\le c^{-N} \int |h(\xi)| \left|(f \circ cg)(\xi) - \sum_{k=0}^{N} b_k(\xi) c^k\right| d\xi \qquad \text{(V.9)} \\
&\le cB \int |h(\xi)|\, d\xi
\end{aligned}$$

by (v.6) and (v.7). Hence

$$\lim_{c \downarrow 0} c^{-N}\left|G(c) - \sum_{k=0}^{N} B_k c^k\right| = 0$$

since h is absolutely integrable by assumption.

To prove (ii), let $M > 0$ be a bound for h. From (V.9), we have

$$c^{-N}\left|G(c)-\sum_{k=0}^{N}B_k c^k\right| \le c^{-N}M\left|\int_{R^{2n}}\left((f\circ cg)(\xi)-\sum_{k=0}^{N}b_k(\xi)c^k\right)d\xi\right|.$$

Let K be the closed unit ball in R^{2n} centered at the origin and $R^{2n}-K$ is the complimentary set of K. Then for $c>0$,

$$\int_{R^{2n}}\left((f\circ cg)(\xi)-\sum_{k=0}^{N}b_k(\xi)c^k\right)d\xi$$
$$=\int_{K}\left((f\circ cg)(\xi)-\sum_{k=0}^{N}b_k(\xi)c^k\right)d\xi$$
$$+\int_{R^{2n}-K}\frac{1}{\xi^\beta}\xi^\beta\left((f\circ cg)(\xi)-\sum_{k=0}^{N}b_k(\xi)c^k\right)d\xi$$

for any multi-index β.

By (V.6) and (V.7), the absolute value of the first integral is bounded by $c^{N+1}Bm(K)<\infty$ uniformly in $\tau(\xi)$ and ξ since $m(K)$ is the Lebesque measure of a compact set. By Lemma 5.5, the absolute value of the second integral is bounded uniformly in $\tau(\xi)$ by (for $c\le 1$)

$$c^{N+1}L(\beta)\int_{R^{2n}-K}\left|\frac{1}{\xi^\beta}\right|d\xi<\infty$$

if β is chosen so that $1/\xi^\beta$ is integrable on $R^{2n}-K$. Combining these results, we have

$$c^{-N}M\left|\int_{R^{2n}}\left((f\circ cg)(\xi)-\sum_{k=0}^{N}b_k(\xi)c^k\right)d\xi\right|$$
$$\le cM\left(Bm(k)+L(\beta)\int_{R^{2n}-K}\left|\frac{1}{\xi^\beta}\right|d\xi\right)\to 0 \quad \text{as } c\to 0.$$

To prove (iii), we note that

$$c^{-N}\left|G(c)-\sum_{k=0}^{N}B_k c^k\right|$$
$$=c^{-N}\left|\int_{K}h(\xi)\left((f\circ cg)(\xi)-\sum_{k=0}^{N}b_k(\xi)c^k\right)d\xi\right.$$
$$\left.+\int_{R^{2n}-K}\frac{h(\xi)}{\xi^\beta}\xi^\beta\left((f\circ cg)(\xi)-\sum_{k=0}^{N}b_k(\xi)c^k\right)d\xi\right|$$
$$\le c\left(B\int_{K}|h(\xi)|\,d\xi+L(\beta)\int_{R^{2n}-K}\left|\frac{h(\xi)}{\xi^\beta}\right|d\xi\right),$$

as in the previous proof. The bound is finite and uniform in ξ and $\tau(\xi)$ since h is continuous and K is compact so that

$$\int_{K}|h(\xi)|\,d\xi<\infty.$$

If β is chosen so that $h(\xi)/\xi^\beta$ is integrable on $R^{2n}-K$, then

$$\int_{R^{2n}-K}\left|\frac{h(\xi)}{\xi^\beta}\right|d\xi<\infty.$$

This can be done since h is a polynomial in ξ by assumption.

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A model of quantum field theory treated in the Fock–Cook formalism. II

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The Fock–Cook formalism for quantum field theory is further generalized, and the methods developed are used to remove all cutoffs from a variety of Yukawa-type interactions in one and two space dimensions. We conclude that the usual operator-valued distribution approach to quantum field theory is not always necessary.

I. INTRODUCTION

In a previous paper,[1] henceforth referred to as Paper I, we generalized the Cook formalism for Fock space[2] by giving a Hilbert space discussion of second-quantized forms of n-body operators. (In this formalism the fields are bona fide operators in Fock space creating or annihilating "particles" with wavefunctions in the proper one-particle Hilbert space. In this way the difficulties inherent with multiplying operator-valued distributions[3] are circumvented.) We showed that many of the mathematical properties of a second-quantized n-body operator (self-adjointness, etc.) are inherited from the corresponding first-quantized operator.

In a subsequent paper,[4] henceforth referred to as Paper II, we developed additional results for the Fock–Cook formalism (therein denoted "lemmas") and commenced a discussion of a generalization of the scalar field model[5] (denoted "assertions") which includes the Nelson model[6] and other similar persistent models[7] as well. Thus the singularities in the model are of the usual types, but we are attempting to analyze them in a nonstandard but rigorous formalism. {For example, in the case where spins and charges are neglected, the model reduces to precisely the scalar field model in which the potential is written[5] formally, in the usual formalism, $V=\lambda\int d\rho\, dk\omega(k)^{-1/2}[a(k)+a^*(-k)]\psi^*(p+k)\times\psi(p)$.} In the present work, we continue generalizing the Fock–Cook formalism, illustrating the results with the model. The designations "lemma" and "assertion" will again be used to distinguish general results from properties of the particular model.

In Paper II, the potential for the model is written as a sum of products of second-quantized forms of one-particle operators with fields whose wavefunctions are chosen from an arbitrary basis for the single-particle Hilbert space. In order to establish the self-adjointness of the Hamiltonian, these sums over the basis were restricted (the so-called "mode cutoffs"), and momentum-space cutoffs were introduced.

In Sec. II of this paper we review some of the results of Papers I and II, and present several new lemmas. In Sec. III we discuss the removal of the mode cutoffs, treating the removal of the remaining cutoffs in Sec. IV.

II. NOTATION AND OTHER PRELIMINARIES

The model introduced in Paper II treats two types of particle, designated here as "a particles" and "ψ particles":

The a particles are taken to be bosons of mass $\mu>0$ with n_a spin/charge states. We let $p=(p_1,\ldots,p_s)\in\mathbb{R}^s$, $p^2=p_1^2+\cdots+p_s^2$, $\omega(p)=(p^2+\mu^2)^{1/2}$, s henceforth denoting the dimension of configuration space. The single particle quantum-mechanical Hilbert space for the a particles, $\mathcal{H}_a^{(1)}$, is taken to be the direct sum of n_a copies of $\mathcal{L}_a^2(\mathbb{R}^s)$, the space of functions square-integrable with respect to the measure $\omega(p)^{-1}d^sp$. The variables for functions in $\mathcal{L}_a^2(\mathbb{R}^s)$ are interpreted as momentum. The hat $\hat{}$ will denote Fourier transform and the wedge $\check{}$ inverse Fourier transform. The transformed variables correspond to position in configuration space. Check $\check{}$ denotes second Fourier transform [thus $\check{f}(x)=f(-x)$]. Elements of $\mathcal{H}_a^{(1)}$ will be distinguished from elements of $\mathcal{L}_a^2(\mathbb{R}^s)$ by a vector bar $\rightarrow$ [thus $\vec{f}=\{f_\alpha\}$, $f_\alpha\in\mathcal{L}_a^2(\mathbb{R}^s)$]. Henceforth the subscript α will be understood to run over the n_a spin/charge labels. We define natural injections from $\mathcal{L}_a^2(\mathbb{R}^s)$ to $\mathcal{H}_a^{(1)}$ by

$$f\in\mathcal{L}_a^2(\mathbb{R}^s)\to\vec{f}_{,\alpha}\in\mathcal{H}_a^{(1)}\quad\text{where}\quad(\vec{f}_{,\alpha})_{\alpha'}=\delta_{\alpha,\alpha'}f.$$

The n-particle spaces and the Fock space for the a particles are denoted $\mathcal{H}_a^{(n)}$ and $\mathcal{F}_a$ respectively. The space of finitely many a particles, denoted $\mathcal{F}_a^0$, is defined as $\{\phi\in\mathcal{F}$ such that ϕ has nonvanishing components in at most a finite number of the $\mathcal{H}_a^{(n)}\}$. Scalar product in any of these spaces is denoted $(\cdot,\cdot)_a$ with no chance of confusion. The creation and annihilation operators for an a particle corresponding to the wavefunction $\vec{f}$ are denoted $a^\dagger(\vec{f})$ and $a(\vec{f})$ respectively, and obey the canonical equal-time commutation relations $[a(\vec{f}),a^\dagger(\vec{g})]^\sim=(\vec{f},\vec{g})_a\mathbb{1}_a$, etc., where $\mathbb{1}_a$ is the identity operator on $\mathcal{F}_a$, and $\sim$ denotes the smallest closed extension. Ω_a denotes the second-quantizer defined in Paper I. In particular, if $\mathbb{1}$ is the identity operator in $\mathcal{H}_a^{(1)}$ and N_a is the number operator for the a particles, then $N_a=\Omega_a(\mathbb{1})$. The kinetic energy operator is multiplication by $\omega(p)$ in $\mathcal{L}_a^2(\mathbb{R}^s)$ and is denoted h_a there. In $\mathcal{H}_a^{(1)}$ it is denoted by $H_{0a}^{(1)}$ and satisfies $(H_{0a}^{(1)}\vec{f})_\alpha=h_af_\alpha$. In $\mathcal{F}_a$ we have $H_{0a}\equiv\Omega_a(H_{0a}^{(1)})$, which from Paper I is easily seen to be self-adjoint and positive.

The ψ particles are of mass $m>0$ with n_ψ spin/charge states (henceforth indexed by the subscript β). The single particle quantum mechanical Hilbert space for the ψ particles, $\mathcal{H}_\psi^{(1)}$, is taken to be the direct sum of n_ψ copies of $\mathcal{L}^2(\mathbb{R}^s)$ (Lebesgue measure). The overarrow will here also be used to distinguish vectors in $\mathcal{H}_\psi^{(1)}$ from those in $\mathcal{L}^2(\mathbb{R}^s)$, and we define $\vec{f}_{,\beta}$ as in the previous case. $\mathcal{H}_\psi^{(n)}$ and $\mathcal{F}_\psi$ denote the n-particle space and Fock space for the ψ particles, and scalar product in either of these, or in $\mathcal{L}^2(\mathbb{R}^s)$, is denoted $(\cdot,\cdot)$. We

shall not employ the ψ particle fields singly here (see Papers I and II) since only the second-quantized forms, $\Omega_\psi(A;r)$ (see Paper I) for first-quantized r-particle operators A appear in the model. (Thus the particular statistics chosen for the ψ particles is immaterial; some authors choose boson statistics,[7] others Fermi statistics,[5] but parastatistics will do as well.) The number operator N_ψ is given by $\Omega_\psi(\mathbb{1})$, etc. We shall treat three cases for the kinetic energy: $\epsilon(p)=m$ (recoilless), $\epsilon(p)=m+p^2/2m$ (Galilean recoil), and $\epsilon(p)=(p^2+m^2)^{1/2}$ (relativistic recoil). The kinetic energy operators are multiplication by $\epsilon(p)$ in $\mathcal{L}^2(\mathbb{R}^s)$ and $\mathcal{H}_\psi^{(1)}$ and are denoted h_ψ and $H_{0\psi}^{(1)}$ respectively. $H_{0\psi}\equiv\Omega_\psi(H_{0\psi}^{(1)})$. We remark that the relativistic recoil choice does not make the model relativistic since the measure on $\mathcal{H}_\psi^{(1)}$ is not relativistic, there are no antiparticles, and even $\mathcal{H}_a^{(1)}$ has the wrong measure if the a particles are not of spin zero (see Paper II).

The Hilbert space accommodating the model is taken to be $\mathcal{J}_a\otimes\mathcal{J}_\psi$. Thanks to the ample a, ψ, α, and β subscripts, the $\otimes$ notation is superfluous and will be dropped. For example the positive, self-adjoint free Hamiltonian, H_0, is written $H_0=[H_{0a}+H_{0\psi}]^\sim$ rather than $H_0=[H_{0a}\otimes\mathbb{1}_\psi+\mathbb{1}_a\otimes H_{0\psi}]^\sim$.

Having established the definitions of the spaces in which we work, we next introduce some of the operators which appear in the model.

For $\rho\in\mathcal{L}^\infty(\mathbb{R}^s)$, define the bounded linear operator J_ρ on $\mathcal{L}_a^2(\mathbb{R}^s)$ by $(J_\rho f)(p)=\rho(p)f(p)$, $f\in\mathcal{L}_a^2(\mathbb{R}^s)$. The definition of J_ρ is extended to $\mathcal{H}_a^{(1)}$ by $(J_\rho\vec{f})_\alpha=J_\rho f_\alpha$ for $\vec{f}=\{f_\alpha\}\in\mathcal{H}_a^{(1)}$. The regularized (smeared) fields are accordingly defined by $a_\rho(\vec{f})\equiv a(J_\rho\vec{f})$, $a_\rho^\dagger(\vec{f})\equiv a^\dagger(J_\rho\vec{f})$.

We emphasize that J_ρ is multiplication in momentum space. For configuration space we let $\hat{f}\in\mathcal{L}^\infty(\mathbb{R}^s)$ and define the bounded linear operator $O(f)$ by $O(f)g=\hat{f}\hat{g}$, $g\in\mathcal{L}^2(\mathbb{R}^s)$ [or $\mathcal{L}_a^2(\mathbb{R}^s)$]. Then $O(f)O(h)=O(h)O(f)$, $\hat{h}\in\mathcal{L}^\infty(\mathbb{R}^s)$. For this definition it is not necessary that $\hat{f}$ be the Fourier transform of any function, in which case the caret is purely notational; however, if $f,h\in\mathcal{L}^1(\mathbb{R}^s)\cap\mathcal{L}^2(\mathbb{R}^s)$, then $O(f)g=f\star g$, where $\star$ denotes $(2\pi)^{-s/2}$ times the usual convolution, and $O(g)O(h)=O(g\star h)$. Now let C be an $n_\psi\times n_\psi$ complex matrix and define the bounded operator $M(f,C)$ on $\mathcal{H}_\psi^{(1)}$ by

$$(M(f,C)\vec{g})_\beta=\sum_{\beta'=1}^{n_\psi}C_{\beta\beta'}O(f)g_{\beta'},$$

where $\vec{g}=\{g_\beta\}\in\mathcal{H}_\psi^{(1)}$.

We remark that J_ρ and $O(f)$ could have been defined for any $\rho,\hat{f}$ that are Lebesgue measurable with only the loss of the bounded operator property. The unbounded operators of primary interest here are the momentum and kinetic energy operators and are given special notations.

Lemma 1: Let $\hat{f},\hat{g}\in\mathcal{L}^\infty(\mathbb{R}^s)$, and let C,C_1 be $n_\psi\times n_\psi$ complex matrices with $\|C\|$ the matrix bound on C. Then

(i) $\|M(f,C)\|\le\|\hat{f}\|_\infty\|C\|$;

(ii) $M(f,C)^\dagger=M(\hat{f}^*,C^\dagger)$;

(iii) $M(f,C)M(g,C_1)=M(f\star g,CC_1)$;

(iv) for $[C,C_1]=0$, $[M(f,C),M(g,C_1)]=0$.

The proofs follow from the definitions and $\hat{f}^*=\widehat{f^*}$.

Since the $M(f,C)$ are bounded operators, applying Theorem 2 of Paper I, we immediately obtain

Lemma 2: Let $\hat{f},\hat{g}\in\mathcal{L}^\infty(\mathbb{R}^s)$ and let C,C_1 be $n_\psi\times n_\psi$ complex matrices. Then

(i) $\Omega_\psi(M(f,C))^\dagger=\Omega_\psi(M(\hat{f}^*,C^\dagger))$;

(ii) $[\Omega_\psi(M(f,C))\Omega_\psi(M(g,C_1))]^\sim$
$=[\Omega_\psi(M(f,C)\otimes M(g,C_1);2)+\Omega_\psi(M(f\star g,CC_1))]^\sim$;

(iii) for $[C,C_1]=0$, $[\Omega_\psi(M(f,C)),\Omega_\psi(M(g,C_1))]^\sim=0$.

The momentum operators are defined in the canonical fashion: Let P_i denote the momentum operator for the ith spatial dimension. Then $D(P_i)=\{f\in\mathcal{L}^2(\mathbb{R}^s)\,|\,\int k_i^2|f(k)|^2\times d^sk<\infty\}$, and for $f\in D(P_i)$, $(P_if)(k)\equiv k_if(k)$. Furthermore, for $\vec{f}=\{f_\beta\}\in\mathcal{H}_\psi^{(1)}$, $f_\beta\in D(P_i)$, define $(P_i\vec{f})_\beta=P_if_\beta$.

The momentum operators and the M operators are related by

Lemma 3: Let g,h be such that $\widehat{P_i^ng},\widehat{P_i^nh}\in\mathcal{L}^\infty(\mathbb{R}^s)$ for $n=0,1,2$, and let C,C_1 be $n_\psi\times n_\psi$ complex matrices. Then

(i) $[P_i,O(g)]^\sim=O(P_ig)$;

(ii) $[P_i,M(g,C)]^\sim=M(P_ig,C)$;

(iii) $[P_i^2,M(g,C)]^\sim=M(P_i^2g,C)+2M(P_ig,C)P_i$;

(iv) If $[C,C_1]=0$, $[M(h,C_1),[M(g,C),P_i^2]]^\sim$
$=2M(P_ig,C)M(P_ih,C_1)=2M((P_ig)\star P_ih,CC_1)$;

(v) Multiple commutators of P_1^2 with more than two M operators vanish.

Proof: (i) holds since Fourier transform preserves the derivation property of the derivative. The rest follow from application to $\vec{f}=\{f_\beta\}\in\mathcal{H}_\psi^{(1)}$, such that $f_\beta\in D(P_i^2)$.

In the Galilean recoil case we have $\epsilon(k)=m+k^2/2m$; i.e., $H_{0\psi}^{(1)}=m\mathbb{1}+\sum_{i=1}^s P_i^2/2m$. Thus we have

Corollary 1: If $H_{0\psi}^{(1)}$ denotes the Galilean kinetic energy operator and g,h,C,C_1 are as before, then

(i) $[M(g,C),H_{0\psi}^{(1)}]^\sim$
$=-(2m)^{-1}M\left(\sum_{i=1}^s P_i^2g,C\right)-m^{-1}\sum_{i=1}^s M(P_ig,C)P_i$;

(ii) $[\Omega_\psi(M(g,C)),H_{0\psi}]^\sim$
$=\left\{-(2m)^{-1}\Omega_\psi\left(M\left(\sum_{i=1}^s P_i^2g,C\right)\right)-m^{-1}\times\sum_{i=1}^s\Omega_\psi(M(P_ig,C)P_i)\right\}^\sim$;

(iii) $[M(g,C),[M(h,C_1),H_{0\psi}^{(1)}]]^\sim$
$=m^{-1}\sum_{i=1}^s M([P_ig]\star P_ih,CC_1)$;

(iv) $[\Omega_\psi(M(g,C)),[\Omega_\psi(M(h,C_1)),H_{0\psi}]]^\sim$
$=m^{-1}\Omega_\psi\left(\sum_{i=1}^s M([P_ig]\star P_ih,CC_1)\right)$.

Finally we consider the potential for the model. We

introduce and discuss a family of operators which includes the potential as a special case, the more general operators being useful for defining the dressing transformations.

Assertion 1: Let $\{g_n\}_{n=0}^{\infty}$ be an orthonormal basis for $\mathcal{L}^2(\mathbb{R}^s)$ such that $\{g_n\} \subseteq \mathcal{S}(\mathbb{R}^s)$. Let $\rho \in \mathcal{L}^\infty(\mathbb{R}^s)$ and let $\sigma \in C^\infty(\mathbb{R}^s)$ be polynomially bounded in absolute value. Let L be a fixed extended real number. Let $\{K_n\}$ be a sequence of real numbers such that the sums

$$F(p,q) \equiv \sum_{n=0}^{\infty} |K_n| \, \| h_a^p J_\rho g_n \|_a \| h_\psi^q \sigma g_n \|_1$$

converge for all positive integers p, q such that $p+q < L$. Let

$$V^N_{\rho,\sigma,K} \equiv \sum_{\alpha=1}^{n_a} \sum_{n=0}^{N} K_n a_\rho(\overrightarrow{g_{n,\alpha}}) \Omega_\psi(M(\sigma g_n, C_\alpha)) + \sum_{\alpha=1}^{n_a} \sum_{n=0}^{N} K_n a^\dagger_\rho(\overrightarrow{g_{n,\alpha}}) \Omega^\dagger_\psi(M(\sigma g_n, C_\alpha)).$$

Then the sequence $\{V^N_{\rho,\sigma,K}\}_{N=0}^{\infty}$ converges strongly on each $D(N_a^{1/2}) \otimes \mathcal{H}_\psi^{(\nu)}$, $\nu = 0, 1, \cdots$, to a self-adjoint operator $V^{(\nu)}_{\rho,\sigma,K}$; i. e., $\{V^N_{\rho,\sigma,K}\}$ converges strongly on $D(N_a^{1/2}) \otimes \mathcal{J}_\psi$ to the self-adjoint operator $V_{\rho,\sigma,K} \equiv \sum_{\nu=0}^{\infty} \oplus V^{(\nu)}_{\rho,\sigma,K}$. Furthermore, $H_0 + V_{\rho,\sigma,K}$ is self-adjoint and $D([H_0 + V_{\rho,\sigma,K}]^p) = D(H_0^p)$ for all integers $p < L$. Also, defining the remainders $R(p)$ by $R(p) = [H_0 + V_{\rho,\sigma,K}]^p - H_0^p$, there exist constants θ, δ, γ_i, $i = 1, 2, 3, 4$ (depending on ν, p, ρ, σ, K, which labels will be omitted below) such that $H_0 + V + \delta \mathbb{1}$ is positive in $\mathcal{J}_a \otimes \mathcal{H}_\psi^{(\nu)}$, and for all χ in $D(H_0^p) \cap \mathcal{J}_a \otimes \mathcal{H}_\psi^{(\nu)}$,

$$\| R\chi \| \leq \gamma_1 \| (H_0 + V + \delta \mathbb{1})^p \chi \|,$$

$$\| (R + \delta \mathbb{1})\chi \| \leq \gamma_2 \| (H_0 + V + \delta \mathbb{1})^p \chi \|,$$

$$\| H_0^p \chi \| \leq \| (H_0 + \theta \mathbb{1})^p \chi \| \leq \gamma_3 \| (H_0 + V + \delta \mathbb{1})^p \chi \|,$$

and

$$\| (H_0 + V + \delta \mathbb{1})^p \chi \| \leq \gamma_4 \| (H_0 + \theta \mathbb{1})^p \chi \|.$$

Furthermore, $\mathcal{J}_a^0 \otimes \mathcal{H}_\psi^{(\nu)}$ is an analytic domain for $V^{(\nu)}_{\rho,\sigma,K}$.

Proof: The case $\sigma \equiv 1$ is the potential for the model and a proof for that case accompanies Assertion II and Corollary 3 of Paper II.[8] We remark here that if we include the antiparticles for the ψ fields and disregard the terms in $:\psi^\dagger\psi:$ which doubly create or doubly annihilate to obtain a so-called "persistent interaction",[7] we still have a model of the present form if we introduce another dimension to the charge label, namely one to distinguish particles from antiparticles. In both of the assertions the restriction $\{g_n\} \subseteq \mathcal{S}(\mathbb{R}^s)$ is made to insure in a simple manner that the arguments of the M and $\mathcal{O}$ operators remain in $\mathcal{S}(\mathbb{R}^s) \subseteq \mathcal{L}^\infty(\mathbb{R}^s)$, as well as possessing other nice properties.

To treat the case $\sigma \neq 1$, the proof for the $\sigma \equiv 1$ case is altered as follows: Lines 8—14 of the proof of Assertion II of Paper II are changed to read:

"Since $P_i(g \star f) = (P_i g) \star f + g \star P_i f$, then $g, f \in D(P_i^p)$ implies $g \star f \in D(P_i^p)$. Furthermore,

$$D(h_\psi^p) = \bigcap_{i=1}^{s} D(P_i^{\theta p}) \supseteq \mathcal{S}(\mathbb{R}^s),$$

where

$$\theta = \begin{cases} 0 & \text{in the recoilless case} \\ 1 & \text{in the relativistic recoil case} \\ 2 & \text{in the Galilean recoil case.} \end{cases}$$

Since $g_n \in \mathcal{S}(\mathbb{R}^s)$ and $\sigma \in C^\infty(\mathbb{R}^s)$ is polynomially bounded, then $\sigma g_n \in \mathcal{S}(\mathbb{R}^s) \subseteq C^\infty(h_\psi)$. Now let $\vec{f} = \{f_\beta\} \in D(H_{0\psi}^p)$. Then

$$[M(\sigma g_n, C_\alpha)\vec{f}]_\beta = \sum_{\beta'} C_{\alpha\beta\beta'}(\sigma g_n) \star f_{\beta'},$$

so that $M(\sigma g_n, C_\alpha) D(H_0^p) \subseteq D(H_0^p)$."

From here the proof is the same with the exception of the substitution $g_n \to \sigma g_n$ in the appropriate places, and with the printing correction $(m/\theta)^{q-p} \to (m/\theta)^{p-q}$ in two places.

The physical derivation of the interaction is contained in Paper II, from which we recall that $C_{\alpha\beta\beta'}$ is the coupling constant for the process of annihilating a ψ particle in spin/charge state β', creating one in spin/charge state β, and annihilating an a particle in spin/charge state α. Since these C_α are real matrices, $C_\alpha^T = C_\alpha^\dagger$. Let $\alpha^\dagger$ represent the a particle spin/charge state of opposite spin/charge as α. Then $(C_{\alpha^\dagger})_{\beta'\beta}$ is the coupling constant for annihilating a ψ particle in state β, creating one in state β', and creating an a particle in state $\alpha^\dagger$. Since the changes in spin/charge in the processes described by $C_{\alpha^\dagger\beta'\beta}$ and $C_{\alpha\beta\beta'}$ differ only in sign, it seems physically reasonable to require them to be equal; i. e., $C_{\alpha^\dagger} = C_\alpha^T = C_\alpha^\dagger$. In the sequel we shall use the weaker condition that the adjoint operation rearranges the set of C_α's.

Under the following conditions the C_α's commute:

(a) the ψ particles are scalar particles ($C_\alpha \in \mathbb{R}$),

(b) the a particles are scalar particles (one value for α),

(c) a particle spin/charge independence (all C_α's are equal).

To simplify the otherwise cumbersome calculations in the model, we shall assume that the C_α's commute. We shall say that the set of matrices $\{C_\alpha\}$ satisfies "condition C" if the adjoint rearranges the set, and all C_α's commute.

Assertion 2: Let $\{C_\alpha\}$ satisfy condition C, let $\rho, \rho', \rho'' \in \mathcal{L}^\infty(\mathbb{R}^s)$, and let $\sigma, \sigma', \sigma''$ be $C^\infty(\mathbb{R}^s)$ polynomially bounded functions. Let $\{g_n\}$ be an orthonormal basis for $\mathcal{L}^2(\mathbb{R}^s)$ such that $\{g_n\} \subseteq \mathcal{S}(\mathbb{R}^s)$. Let $K = \{K_n\}$, $K' = \{K'_n\}$, $K'' = \{K''_n\}$ be sequences of real numbers such that the corresponding $F(0,0)$ of Assertion 1 converge. Then

(a) $[V_{\rho,\sigma,K}, V_{\rho',\sigma',K'}]^\sim$

$$= \text{closure of} \sum_{\alpha} \sum_{n,n'} K_n K'_{n'} (\rho g_n, \rho' g_{n'})_a \times \Omega_\psi(M(\overset{\nearrow * \nearrow *}{\sigma' g_{n'}}, C_\alpha^\dagger)) \Omega_\psi(M(\sigma g_n, C_\alpha)) - \sum_{\alpha} \sum_{n,n'} K_n K'_{n'} (\rho' g_{n'}, \rho g_n)_a \Omega_\psi(M(\sigma' g_{n'}, C_\alpha)) \times \Omega_\psi(M(\overset{\nearrow * \nearrow *}{\sigma g_n}, C_\alpha^\dagger));$$

(b) if in particular $\sigma = \sigma'$, then

$$[V_{\rho,\sigma,K}, V_{\rho',\sigma',K'}]^{\sim}$$
$$= \text{closure of}$$
$$\sum_{\alpha}\sum_{n,n'}[-K_nK'_{n'}(\rho' g_{n'}, \rho g_n)_a + K_{n'}K'_n(\rho g_{n'}, \rho' g_n)_a]$$
$$\times[\Omega_\psi(M(\sigma^{\wedge *}g_n, C_\alpha^\dagger)\otimes M(\sigma g_{n'}, C_\alpha);2)$$
$$+\Omega_\psi(M([\sigma g_n]^{\wedge *}\star(\sigma g_{n'}), C_\alpha^\dagger C_\alpha))];$$

(c) if $\sigma=\sigma'$, $K=K'$, and $\rho\rho'^*=\rho^*\rho'$, then
$[V_{\rho,\sigma,K}, V_{\rho',\sigma,K}]^{\sim}=0$;

(d) if $(\sigma g_n)^{\wedge *}=\theta_n\sigma g_n$, $(\sigma' g_n)^{\wedge *}=\theta_n\sigma' g_n$, where $\theta_n=\pm 1$, and if $(\rho^*\rho')^{\wedge}=\rho'^*\rho$, then
$[V_{\rho,\sigma,K}, V_{\rho',\sigma',K'}]^{\sim}=0$;

(e) $[V_{\rho,\sigma,K}, [V_{\rho',\sigma',K'}, V_{\rho'',\sigma'',K''}]]^{\sim}=0$.

Proof: Since $\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}$, $\nu=0,1,2,\cdots$, are dense invariant analytic domains for the V's, it suffices to establish the commutation relations here. [The commutation relations here imply corresponding commutation relations for the exponentiated operators $\exp(iVt)$, for t real, on this domain, which are then uniquely extended to the entire space. The general commutation relations are then those of the generators of these exponentiated forms.] Since, on $\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}$, the series defining the V's converge absolutely, we may evaluate the commutators term by term. From Condition C and Lemma 2(iii), the Ω_ψ factors in the summands commute giving result (a). Interchanging dummy indices n, n' gives (b) and (c), and the fact that the adjoint rearranges the C_α's gives (d), terms cancelling in pairs. (e) follows from (a) and another application of Lemma 2(iii).

III. REMOVAL OF THE MODE CUTOFF

Up to the present it has not been necessary to specify any particular basis for $\mathcal{L}^2(\mathbb{R}^s)$, although it was convenient to require $\{g_n\}\subseteq\mathcal{S}(\mathbb{R}^s)$. Once a basis is chosen, however, the cutoff $\{K_n\}$ must be chosen to insure convergence of $F(0,0)$. The removal of the mode cutoff then corresponds to having all K_n's converge to 1 in some limit. We shall parametrize $K=K(t)=\{K_n(t)\}$ so that, as the parameter approaches some limit, each of the $K_n(t)$ converges to 1. As we shall see shortly, it is most convenient if one can choose $K(t)$ such that the sums

$$B(x,y,t)\equiv\sum_{n=0}^{\infty}K_n(t)g_n(x)g_n(y),\quad x,y\in\mathbb{R}^s,$$

may be explicitly evaluated and correspond to the canonical form used in the demonstration of the completeness of the basis. This choice is not rigid, however, since one could choose any cutoff $K'(t)$ for which (a) $F(0,0)$ also converges and such that (b) $K_n(t)-K'_n(t)$ converges (as a function of t) to zero nicely enough so that $V_{\rho,\sigma,K-K'}$ converges strongly to the zero operator. [For example, $K_n(t)$ and $K'_n(t)$ could differ for a finite number of n's and have this property.] (b) defines an equivalence relation, and (a) specifies the equivalence classes of cutoffs which make mathematical sense in the model. It is also necessary that (c) as the parameter t approaches its limit, $V_{\rho,\sigma,K(t)}$ converges strongly to some (symmetric) operator $V_{\rho,\sigma}$. It is not known if (a), (b), (c) determine a unique class of cutoff. If the uniqueness fails, there is no unique limit operator for the potential. We will show that in the case of the harmonic oscillator basis, the class of the canonical choice of cutoff satisfies (a) (Assertion 3) and (c) (Assertion 4).

We choose to work with the harmonic oscillator basis since it is familiar to a wide audience. We list the harmonic oscillator properties that we shall use[9–11]:

(i) Let $k\in\mathbb{R}$, $n\in\mathbb{Z}_+\equiv\{0,1,2,\cdots\}$. Let $H_n(k)$ denote the nth Hermite polynomial. The harmonic oscillator (h. o.) basis $\{g_n\}$ for $\mathcal{L}^2(\mathbb{R})$ is given by

$$g_n(k)=(2^n n!\pi^{1/2})^{-1/2}H_n(k)\exp(-k^2/2).$$

Furthermore $\{g_n\}\subseteq\mathcal{S}(\mathbb{R})$.

(ii) There is a constant, herein denoted d, such that $\|g_n\|_\infty\le d$, for all $n\in\mathbb{Z}_+$, $(d\approx 1.09)$.

(iii) $kg_n(k)=[(n+1)/2]^{1/2}g_{n+1}(k)+(n/2)^{1/2}g_{n-1}(k)$.

(iv) $\hat{g}_n=(-i)^n g_n$; $g_n^*=g_n$; $\check{g}_n=(-1)^n g_n$.

(v) Mehler's formula: Let $t\in\mathbb{C}$, $|t|<1$. Then

$$B(k,p,t)=\sum_{n=0}^{\infty}t^n g_n(k)g_n(p)$$
$$=[\pi(1-t^2)]^{-1/2}\exp\left(\frac{4kpt-(k^2+p^2)(1+t^2)}{2(1-t^2)}\right)$$

and, for all $f\in\mathcal{L}^2(\mathbb{R})$,

$$f(k)=\text{l. i. m.}_{t\to 1^-}\int_{-\infty}^{\infty}f(p)B(k,p,t)\,dp$$
$$=\text{l. i. m.}_{t\to 1^-}\sum_{n=0}^{\infty}t^n g_n(k)\int_{-\infty}^{\infty}f(p)g_n(p)\,dp.$$

(vi) In s dimensions, the h. o. basis is given by $g_n(k)=g_{n_1}(k)\cdots g_{n_s}(k_s)$; $n=(n_1,\ldots,n_s)$, $n_j\in\mathbb{Z}_+$; $k=(k_1,\ldots,k_s)\in\mathbb{R}^s$. Then $g_n\in\mathcal{S}(\mathbb{R}^s)$. Set $|n|=n_1+\cdots+n_s$ and $k^n=k_1^{n_1}\cdots k_s^{n_s}$.

(vii) From (iii) we deduce the existence of constants $b(l), c(l), l=(l_1,\ldots,l_s)$, $l_i\in\mathbb{Z}_+$ such that

$$\|k^l g_n(k)\|_\infty\le b(l)\prod_{j=1}^{s}(1+n_j)^{l_j},$$

$$\|k^l g_n(k)\|_2\le c(l)\prod_{j=1}^{s}(1+n_j)^{l_j},$$

$$\|k^l g_n(k)\|_1$$
$$=\left\|k^l\prod_{j=1}^{s}(1+k_j^2)\prod_{i=1}^{s}(1+k_i^2)^{-1}g_n(k)\right\|_1$$
$$\le\left\|\prod_{j=1}^{s}k_j^{l_j}(1+k_j^2)g_n(k)\right\|_\infty[\int(1+x^2)^{-1}dx]^s$$
$$\le e(l)\prod_{j=1}^{s}(1+n_j)^{l_j+2}$$

where $e(l)=[b(l)+b(l+2)][\int(1+x^2)^{-1}dx]^s$.

(viii) Let

$$B(p,k,t)\equiv B(p_1,k_1,t_1)B(p_2,k_2,t_2)\cdots B(p_s,k_s,t_s);$$

then

$$\text{l. i. m.}_{\text{all } t_i\to 1^-}\int f(p)B(k,p,t)\,d^sp=f(k),\quad f\in\mathcal{L}^2(\mathbb{R}^s).$$

Let

$$F(k,t) \equiv \int f(p) B(k,p,t)\, d^s p = \sum_{n=0}^{\infty} t^n g_n(k) \int f(p) g_n(p)\, d^s p.$$

Then $\|F\|_2 \leq \|f\|_2$, which in turn implies that the l. i. m. property holds for $t_1 = t_2 = \cdots = t_s$ with a single limit being taken.

In view of properties (v) and (viii) we see that the canonical choice for the mode cutoff is $K_n(t) = t^{|n|}$, $t \in (-1, 1)$.

Assertion 3: Let $\{g_n\}$ denote the harmonic oscillator basis, let $\rho \in \mathcal{L}^\infty(\mathbb{R}^s)$, let $\sigma \in C^\infty(\mathbb{R}^s)$ be a function polynomially bounded in absolute value, and let $K_n(t) = t^{|n|}$. Then $V_{\rho,\sigma,K(t)}$ satisfies Assertion 1 with $F(p,q)$ converging for all $p, q \in \mathbb{Z}_+$.

Proof: Since h_a^{2p} is a polynomial of order $2p$, by property (vii) of the h. o. functions, $\|h_a^p J_\rho g_n\|_a \leq \|\rho\|_\infty \mu^{-1/2} \times \|h_a^p g_n\|$ which in turn is bounded by a sum of terms of the form $c(l) \prod_{j=1}^s (1+n_j)^{l_j}$ with $|l| \leq p$; i. e., $\|h_a^p J_\rho g_n\|_a$ is bounded by a multinomial in the components of n of order $\leq p$. Similarly, for $\epsilon(k)$ one of m, $m + |k|^2/2m$, $[m^2 + |k|^2]^{1/2} \leq m + |k|$, h_ψ^q is polynomially bounded by a polynomial of order θq, where $\theta = 0, 2, 1$ in the respective recoil cases. Let σ' be a polynomial bounding σ and let r be the order of σ'. Then $\|h_\psi^q \sigma g_n\|_1$ is bounded by a multinomial in the components of n of order $\theta q + 2s + r$. Thus $F(p,q) \leq \sum_n$ (multinomial in the components of n of order $p + \theta q + 2s + r) t^{|n|}$, which converges for all p, q whenever $|t| < 1$.

For removal of the mode cutoff we have

Assertion 4: Let $\rho \in \mathcal{L}_a^2(\mathbb{R}^s)$, $\hat{\sigma} \in \mathcal{L}^1(\mathbb{R}^s)$ or $\sigma \equiv 1$, $K_n(t) = t^{|n|}$, $-1 < t < 1$, and $\{g_n\}$ denote the h. o. basis. Then $V_{\rho,\sigma,K(t)}$ converges strongly on $\mathcal{F}_a^0 \otimes \mathcal{H}_\psi^{(\nu)}$ for each $\nu \in \mathbb{Z}_+$, to a self-adjoint operator $V_{\rho\sigma}$ which is reduced by N_ψ and for which the vectors in $\mathcal{F}_a^0 \otimes \mathcal{H}_\psi^{(\nu)}$ are analytic.

Proof: Since $\mathcal{S}(\mathbb{R}^s)$ is dense in $\mathcal{L}^1(\mathbb{R}^s)$ and invariant under Fourier transform, we may consider a sequence of functions $\{\sigma_r\}$ such that $\sigma_r \in \mathcal{S}(\mathbb{R}^s)$ and $\hat{\sigma}_r$ converges to $\hat{\sigma}$ in $\mathcal{L}^1(\mathbb{R}^s)$ norm. For such σ_r, Assertions 1, 2 apply so that the sum defining $V_{\rho,\sigma_r,K(t)}$ converges strongly on any $\chi \in \mathcal{H}_a^{(\eta)} \otimes \mathcal{H}_\psi^{(\nu)}$. Thus in computing $\|V_{\rho,\sigma_r,K(t)}\chi\|$ we may interchange summation with the scalar products involved in taking the norm. Furthermore, since χ has a fixed number, η, of a particles, the "$a^\dagger a^\dagger$" and "aa" terms in $\|V_{\rho,\sigma_r,K(t)}\chi\|^2$ vanish. Using Lemma 2(i), (ii), and

$$[a_\rho(\overrightarrow{g_{n,\alpha}}), a_\rho^\dagger(\overrightarrow{g_{n',\alpha'}})]^\sim = (J_\rho \overrightarrow{g_{n,\alpha}}, J_\rho \overrightarrow{g_{n',\alpha'}})_a \mathbb{1} = \delta_{\alpha,\alpha'}(\rho g_n, \rho g_{n'})_a \mathbb{1},$$

and interchanging dummy indices $(n,\alpha) \rightleftharpoons (n',\alpha')$ in one place, we obtain

$$\|V_{\rho,\sigma_r,K(t)}\chi\|^2 = \sum_{l=1}^5 I_l(t),$$

where

$$I_1(t) = \sum_\alpha \sum_{n,n'} t^{|n+n'|} (\rho g_n, \rho g_{n'})_a \times (\chi, \Omega_\psi(M(\sigma_r g_n \star [\sigma_r g_{n'}]^{\checkmark *}, C_\alpha C_\alpha^\dagger))\chi),$$

$$I_2(t) = \sum_\alpha \sum_{n,n'} t^{|n+n'|} (\rho g_n, \rho g_{n'})_a \times (\chi, \Omega_\psi(M(\sigma_r g_n, C_\alpha) \otimes M([\sigma_r g_{n'}]^{\checkmark *}, C_\alpha^\dagger); 2)\chi),$$

$$I_3(t) = 2 \sum_{\alpha,\alpha'} \sum_{n,n'} t^{|n+n'|} (\chi, a_\rho^\dagger(\overrightarrow{g_{n',\alpha'}}) a_\rho(\overrightarrow{g_{n,\alpha}}) \times \Omega_\psi(M(\sigma_r g_n, C_\alpha) \otimes M([\sigma_r g_{n'}]^{\checkmark *}, C_{\alpha'}^\dagger); 2)\chi),$$

$$I_4(t) = \sum_{\alpha,\alpha'} \sum_{n,n'} t^{|n+n'|} \times (\chi, a_\rho^\dagger(\overrightarrow{g_{n',\alpha'}}) a_\rho(\overrightarrow{g_{n,\alpha}}) \Omega_\psi(M(\sigma_r g_n \star [\sigma_r g_{n'}]^{\checkmark *}, C_\alpha C_{\alpha'}^\dagger))\chi)$$

and $I_5(t)$ is as in $I_4(t)$ but with (n,α) interchanged with (n',α') in the $a^\dagger a$ factors only.

Now $\chi \in \mathcal{H}_a^{(\eta)} \otimes \mathcal{H}_\psi^{(\nu)}$ may be written $\chi = \sum_{\otimes\alpha,\otimes\beta} \chi_{\otimes\alpha,\otimes\beta}$, where $\otimes\alpha$ runs over the η-tuples $(\alpha_1, \alpha_2, \ldots, \alpha_\eta)$, $\otimes\beta$ runs over the ν-tuples $(\beta_1, \ldots, \beta_\nu)$, and $\chi_{\otimes\alpha,\otimes\beta}$ is an element of the product space of η copies of $\mathcal{L}_a^2(\mathbb{R}^s)$ and ν copies of $\mathcal{L}^2(\mathbb{R}^s)$. For the present calculations we Fourier-transform the ν $\mathcal{L}^2(\mathbb{R}^s)$ variables and write $\hat{\chi}_{\otimes\alpha,\otimes\beta}(k_1, \ldots, k_\eta; y_1, \ldots, y_\nu)$. Subsequent calculations are simplified by recalling from Paper I that $[a^\dagger(f)a(g)]^\sim = \Omega_a(fg^*)$, where $(fg^*)(h) = (g,h)_a f$ for all $f, g, h \in \mathcal{H}_a^{(1)}$. Writing the indicated integrals in the $I_i(t)$, we see that the Fourier transformation of the ψ variables leads to sums in n of the form

$$\sum_n t^{|n|} g_n(k) \hat{g}_n(v) = B(k, v, -it).$$

Since $|B(k, v, \pm it)| \leq (2\pi)^{-s/2}$, from the conditions on σ_r, ρ, and χ we may then bound each term, the σ_r occurring only in the form $\|\widehat{\sigma_r}\|_1$. We first take the limit $\sigma_r \to \sigma$ and then apply Lebesque's dominated convergence theorem to take the limit $t \to 1^-$, obtaining

$$I_1(t) \to (2\pi)^{-s} \|\sigma\rho\|_a^2 \left(\chi, \Omega_\psi\left(\sum_\alpha C_\alpha C_\alpha^\dagger\right)\chi\right),$$

$$I_2(t) \to \sum_\alpha \sum_{\substack{\otimes\alpha' \\ \otimes\beta'}} \sum_{\substack{\otimes\alpha'' \\ \otimes\beta''}} \sum_{\substack{i,j=1 \\ i\neq j}}^{\eta} (C_\alpha)_{\beta_j' \beta_j''} (C_\alpha^\dagger)_{\beta_i' \beta_i''} \times (2\pi)^{-s/2} \int \frac{d^s k_1}{\omega(k_1)} \cdots \frac{d^s k_\eta}{\omega(k_\eta)}\, d^s y_1 \cdots d^s y_\nu \times \widehat{\omega^{-1}|\rho\sigma|^2}(y_j - y_i) \times \hat{\chi}^*_{\otimes\alpha',\otimes\beta'}(k_1, \ldots, k_\eta; y_1, \ldots, y_\nu) \times \hat{\chi}_{\otimes\alpha'',\otimes\beta''}(k_1, \ldots, k_\eta; y_1, \ldots, y_\nu),$$

$$I_3(t) \to 2 \sum_{\substack{\otimes\alpha \\ \otimes\beta}} \sum_{\substack{\otimes\alpha' \\ \otimes\beta'}} \sum_{i=1}^{\eta} \sum_{\substack{j,l=1 \\ j\neq l}}^{\nu} (C_{\alpha_i'})_{\beta_j \beta_j'} (C_{\alpha_i}^\dagger)_{\beta_l \beta_l'} \times (2\pi)^{-s} \int \frac{d^s k_0}{\omega(k_0)} \cdots \frac{d^s k_\eta}{\omega(k_\eta)}\, d^s y_1 \cdots d^s y_\nu \times \exp(-ik_0 y_j + ik_i y_l)(\sigma\rho^*)(k_0)(\sigma^*\rho)(k_i) \times \chi^*_{\otimes\alpha,\otimes\beta}(k_1, \ldots, k_\eta; y_1, \ldots, y_\nu) \times \hat{\chi}_{\otimes\alpha',\otimes\beta'}(k_1, \ldots, k_i \to k_0, \ldots, k_\eta; y_1, \ldots, y_\nu),$$

$$I_4(t) \to \sum_{\substack{\otimes\alpha \\ \otimes\beta}} \sum_{\substack{\otimes\alpha' \\ \otimes\beta'}} \sum_{i=1}^{\eta} \sum_{j=1}^{\nu} (C_{\alpha_i'} C_{\alpha_i}^\dagger)_{\beta_i \beta_i'} \times (2\pi)^{-s} \int \frac{d^s k_0}{\omega(k_0)} \cdots \frac{d^s k_\eta}{\omega(k_\eta)}\, d^s y_1 \cdots d^s y_\nu \times \exp[-iy_j(k_0 - k_i)](\sigma\rho^*)(k_0)(\sigma^*\rho)(k_i)$$

$$\times \hat{\chi}^*_{\otimes\alpha,\otimes\beta}(k_1,\ldots,k_\eta;y_1,\ldots,y_\nu)$$
$$\times \hat{\chi}_{\otimes\alpha',\otimes\beta'}(k_1,\ldots,k_i\to k_0,\ldots,k_\eta;y_1,\ldots,y_\nu),$$

and I_5 is similar to I_4.

We shall call the limit operator $V_{\rho\sigma}$. For $\chi\in\mathcal{H}_a^{(\eta)}\otimes\mathcal{H}_\psi^{(\nu)}$ the bound used in the dominated convergence proof reads $\|V_{\rho\sigma}\chi\|^2\le(A+B\eta)\|\chi\|^2$, where A,B are constants depending on $\|\sigma\rho\|_a\le\|\sigma\|_\infty\|\rho\|_a$ and on the C_α, are polynomials of order two in the number, ν, of ψ particles in χ, and are otherwise independent of χ. A proof similar to that of Corollary 2 of Paper II then establishes that $\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}$ is a dense analytic domain for $V_{\rho\sigma}$ as a self-adjoint operator on $\mathcal{J}_a\otimes\mathcal{H}_\psi^{(\nu)}$. Since N_ψ reduces $V_{\rho,\sigma,K(t)}$ and hence $V_{\rho\sigma}$, it follows that $V_{\rho\sigma}$ is self-adjoint. This bound on $V_{\rho\sigma}$ also indicates that it is inconsequential whether the $\sigma_a\to\sigma$ limit is taken before or after the $t\to1^-$ limit.

Corollary: $H_{0a}+V_{\rho\sigma}$, $H_0+V_{\rho\sigma}$ are self-adjoint with domains $D(H_{0a})$, $D(H_0)$ respectively.

Proof: From the estimate[8]: For any $\epsilon>0$, there exists b such that

$$\eta^{1/2}\|\chi\| = \|N_a^{1/2}\chi\| \le \mu^{-1/2}\|H_{0a}^{1/2}\chi\|$$
$$\le \epsilon\|H_{0a}\chi\| + b\|\chi\| \le \epsilon\|H_0\chi\| + b\|\chi\|$$

and Kato's perturbation theorem,[12] the corollary follows from the bound on $V_{\rho\sigma}$.

We conclude the discussion of $V_{\rho\sigma}$ with

Assertion 5: Let the $\{C_\alpha\}$ satisfy condition C, and let $\rho,\rho',\sigma,\sigma'$ satisfy the conditions of Assertions 4 and 2(c) or 2(d). Then

$$[V_{\rho\sigma},V_{\rho',\sigma',K(t)}]^\sim=0,\quad [V_{\rho\sigma},V_{\rho'\sigma'}]^\sim=0,$$

and for all $\chi\in\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}$, $\nu\in\mathbb{Z}_+$, and $s\in\mathbb{R}$,

$$\exp(isV_{\rho,\sigma,K(t)})\chi \underset{t\to1^-}{\to} \exp(isV_{\rho\sigma})\chi.$$

Proof: Since our Hilbert space is separable and the $V_{\rho,\sigma,K(t)}$ form a commuting set of self-adjoint operators, there is a spectral family $\{E_\lambda\}$ independent of ρ,σ,t such that

$$V_{\rho,\sigma,K(t)}=\int \vartheta(\rho,\sigma,t,\lambda)\,dE_\lambda,$$

where the ϑ are measurable functions.[13] Since the strong limits as $t\to1^-$ exist on a (dense) core, $\lim_{t\to1^-}\vartheta(\rho,\sigma,t,\lambda)\equiv\vartheta(\rho,\sigma,\lambda)$ exists a. e., and $V_{\rho\sigma}=\int\vartheta(\rho,\sigma,\lambda)\,dE_\lambda$. Thus $V_{\rho\sigma}$ commutes with $V_{\rho',\sigma',K(t)}$ and with $V_{\rho'\sigma'}$ as well. Furthermore, for χ in $\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}\subseteq D(V_{\rho,\sigma,K(t)})\cap D(V_{\rho\sigma})$,

$$\|(\exp(isV_{\rho,\sigma,K(t)})-\exp(isV_{\rho\sigma}))\chi\|$$
$$=\|\int_0^s d\tau\exp[i\tau(V_{\rho,\sigma,K(t)}-V_{\rho\sigma})]i(V_{\rho,\sigma,K(t)}-V_{\rho\sigma})\chi\|$$
$$\le s\|(V_{\rho,\sigma,K(t)}-V_{\rho\sigma})\chi\|,$$

providing the convergence of the exponentials.

IV. REMOVAL OF THE REMAINING CUTOFFS

In order to exhibit the self-adjointness of the full Hamiltonian with all cutoffs removed, we shall employ the method of "dressing operators"[14] which we understand as follows: If the Hamiltonian H is self-adjoint, a dressing operator is a unitary operator U such that UHU^{-1} is manifestly self-adjoint. If the Hamiltonian requires an infinite mass renormalization, a dressing operator is a family of unitary operators $\{U_K\}$ depending on the cutoff for the Hamiltonian such that (a) U_K converges strongly to a unitary operator as the cutoff is removed, (b) a diverging term δE_K is isolated in $U_KH_KU_K^{-1}$, δE_K commutes with U_K, and deletion of δE_K does not change the dynamics of the system other than to alter the mass, (c) $U_KH_KU_K^{-1}-\delta E_K$ converges strongly to a manifestly self-adjoint operator. (a) Prohibits the occurrence of the so-called wavefunction renormalization which would require a change from Fock space to another Hilbert space for a mathematical interpretation.[15] The requirement of strong convergence in (a), (c), rather than weak convergence, is to prohibit a vehicle for nonuniqueness of the limit operator.[16]

In the present model we shall exponentiate $V_{\rho,\sigma,K(t)}$ and $V_{\rho\sigma}$ to obtain the dressing operators. We consider $\exp(iV_{\rho,\sigma,K(t)})(H_0+V_{\rho',\sigma',K(t)})\exp(-iV_{\rho,\sigma,K(t)})$ and remove the cutoffs in the following order: First let $t\to1^-$; then substract δE if necessary; finally let $\rho',\sigma'\to1$. The recipe is carried out in detail in the recoilless and Galilean recoil cases while in the relativistic recoil case we only prove that the limit operator is symmetric.

Analysis of UHU^{-1} is simplified by employing

Lemma 4: Let A be a self-adjoint operator and let

$$D_1=\left\{\chi\in C^\infty(A)\,\middle|\,\sum_{n=0}^\infty\frac{1}{n!}\|A^n\chi\|<\infty\right\}.$$

Let $\chi\in D_1$ and let B be a closed linear operator such that

$$(\mathrm{ad}A)^{(k)}(B)\chi\in D_1,\quad k=0,1,\ldots,K,$$
$$(\mathrm{ad}A)^{(k)}(B)\chi=0,\quad k>K.$$

Then $\exp(iA)\chi\in D(B)$ and

$$\exp(-iA)B\exp(iA)\chi=\sum_{k=0}^K\frac{(-1)^k}{k!}(\mathrm{ad}iA)^{(k)}(B)\chi.$$

Proof: For $\chi\in D_1$, the series $\sum_{n=0}^\infty(1/n!)(iA)^n\chi$ converges to $\exp(iA)\chi$. By induction

$$B(iA)^n\chi=\sum_{k=1}^n(-1)^k\binom{n}{k}(iA)^{n-k}(\mathrm{ad}iA)^{(k)}(B)\chi.$$

Thus

$$\sum_{n=0}^N B\frac{(iA)^n}{n!}\chi$$
$$=\sum_{n=0}^N\sum_{k=1}^n\frac{(-1)^k}{n!}\binom{n}{k}(iA)^{n-k}(\mathrm{ad}iA)^{(k)}(B)\chi$$
$$=\sum_{k=1}^K\frac{(-1)^k}{k!}\sum_{n=0}^N\frac{1}{(n-k)!}(iA)^{n-k}(\mathrm{ad}iA)^{(k)}(B)\chi.$$

Taking the limit $N\to\infty$ and invoking the fact that B is closed implies the result.

We recall that $V_{\rho,\sigma,K(t)}D(H_0^n)\subseteq D(H_0^{n-1})$ and $V_{\rho,\sigma,K(t)}\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}\subseteq\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}$ for $|t|<1$. Thus we may choose $A=V_{\rho,\sigma,K(t)}$, $B=$ either $H_{0\psi}$ or H_{0a} or $V_{\rho',\sigma',K(t)}$, and $\chi\in C^\infty(H_0)\cap\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}\subseteq D_1$. We will show that the multiple commutators vanish for $k>2$ under the assumptions (a) Galilean recoil or recoilless ψ particles and (b) the C_α obey condition C.

In the following calculations all operators will be understood to be applied to vectors in $C^\infty(H_0)\cap \mathcal{J}_a^0\otimes \mathcal{H}_\psi^{(\nu)}$, $\nu\in \mathbf{Z}_+$.

In Assertion 2 and its corollary $(\mathrm{ad}V_{\rho,\sigma,K(t)})^{(k)}$ on $V_{\rho',\sigma',K(t')}$ is computed, vanishing for $k\geq 2$. Since $[iV_{\rho,\sigma,K(t)}, H_{0a}] = V_{-i\omega\rho,\sigma,K(t)}$, it follows that $(\mathrm{ad}V_{\rho,\sigma,K(t)})^{(k)}$ on (H_{0a}) is also computed and vanishes for $k>2$. For the recoilless case $H_{0\psi}=mN_\psi$ which commutes with $V_{\rho,\sigma,K(t)}$. For the Galilean recoil case we apply the corollary to Lemma 3 to give $(\mathrm{ad}V_{\rho,\sigma,K(t)})^{(k)}(H_{0\psi})=0$ for $k>2$. Collecting these results we have Eq. E:

$$
\begin{aligned}
&\exp\{iV_{\rho,\sigma,K(t)}\}(H_{0a}+H_{0\psi}+V_{\rho',\sigma',K(t)})\exp\{-iV_{\rho,\sigma,K(t)}\}\\
&\quad = H_{0a}+H_{0\psi}+V_{\rho',\sigma',K(t)}+V_{-i\omega\rho,\sigma,K(t)}\\
&\qquad +\tfrac{1}{2}i[V_{\rho,\sigma,K(t)}, V_{-i\omega\rho,\sigma,K(t)}]+i[V_{\rho,\sigma,K(t)}, V_{\rho',\sigma',K(t)}]\\
&\qquad +\Big\{V_{\rho,-iP^2\sigma/2m,K(t)}-im^{-1}\sum_\alpha\sum_n t^{|n|}a_\rho(\overrightarrow{g_n,\alpha})\\
&\qquad \times\Omega_\psi\Big(\sum_{j=1}^s M(P_j\sigma g_n, C_\alpha)P_j\Big)-im^{-1}\sum_\alpha\sum_n t^{|n|}a_\rho^\dagger(\overrightarrow{g_n,\alpha})\\
&\qquad \times\Omega_\psi\Big(\sum_{j=1}^s M(P_j\sigma'^*g_n'^*, C_\alpha^\dagger)P_j\Big)-(2m)^{-1}\\
&\qquad \times\sum_{\alpha,\alpha'}\sum_{n,n'} t^{|n+n'|}a_\rho(\overrightarrow{g_{n'},\alpha'})a_\rho(\overrightarrow{g_n,\alpha})\\
&\qquad \times\Omega_\psi\Big(\sum_{j=1}^s M([P_j\sigma g_n]\check{}^*\star[P_j\sigma g_{n'}]\check{}^*, C_\alpha C_{\alpha'}^\dagger)\Big)\\
&\qquad -(2m)^{-1}\sum_{\alpha,\alpha'}\sum_{n,n'} t^{|n-n'|}a_\rho^\dagger(\overrightarrow{g_{n'},\alpha'})a_\rho^\dagger(\overrightarrow{g_n,\alpha})\\
&\qquad \times\Omega_\psi\Big(\sum_{j=1}^s M([P_j\sigma g_n]\check{}^*\star[P_j\sigma g_{n'}]\check{}^*, C_\alpha^\dagger C_{\alpha'}^\dagger)\Big)\Big\}\\
&\qquad -(2m)^{-1}\sum_{\alpha,\alpha'}\sum_{n,n'} t^{|n+n'|}[a_\rho(\overrightarrow{g_{n'},\alpha'})a_\rho^\dagger(\overrightarrow{g_n,\alpha})\\
&\qquad +a_\rho^\dagger(\overrightarrow{g_n,\alpha})a_\rho(\overrightarrow{g_{n'},\alpha'})]\\
&\qquad \times\Omega_\psi\Big(\sum_{j=1}^s M([P_j\sigma g_n]\check{}^*\star[P_j\sigma g_{n'}], C_\alpha^\dagger C_{\alpha'})\Big)\Big\},
\end{aligned}
$$

where the terms in braces { } appear in the Galilean recoil case only. (We will treat the relativistic recoil case separately later.)

The recoilless case

For this case we may choose $\sigma=\sigma'=1$ and $\rho'=i\omega\rho$ to simplify the right-hand side of Eq. E which now reads

$$H_{0a}+H_{0\psi}+\tfrac{1}{2}i[V_{-i\omega^{-1}\rho',\sigma,K(t)}, V_{\rho',\sigma,K(t)}]$$

and which equals $H_{0a}+H_{0\psi}+Y(t)+\delta E_t$, where

$$
\begin{aligned}
&Y(t)=-\Omega_\psi(Y_t^{(2)};2),\quad \delta E_t=-\Omega_\psi(\delta E_t^{(1)}),\\
&Y_t^{(2)}=\sum_\alpha\sum_{n,n'} t^{|n+n'|}(g_n,\omega^{-2}|\rho'|^2 g_{n'})\\
&\qquad \times M(g_n, C_\alpha)\otimes M(g_{n'}\check{}^*, C_\alpha^\dagger),\\
&\delta E_t^{(1)}=\sum_\alpha\sum_{n,n'} t^{|n+n'|}(g_n,\omega^{-2}|\rho'|^2 g_{n'})M(g_n\star g_{n'}\check{}^*, C_\alpha C_\alpha^\dagger).
\end{aligned}
$$

To remove the remaining t,ρ' cutoffs, we follow the method of the proof of Assertion 4 first choosing $\rho'=\rho_L'$, where ρ_L' is a symmetric function in $\mathcal{S}(\mathbf{R}^s)$ such that $0\leq\rho_L'\leq 1$, $\rho_L'(k)=1$ for $k<L$, $\rho'(k)=0$ for $k>L+1$, and then letting $L\to\infty$. Thus the dressing operator converges to a unitary operator since $\rho=-i\omega^{-1}\rho_L'$ remains in $\mathcal{L}_a^2(\mathbf{R}^s)$ as $L\to\infty$ for $s=1,2$. For $s>2$, for this choice of recoil, and for this choice of dressing operator, wavefunction renormalization difficulties arise.

It remains to remove the t,ρ' cutoffs from $Y(t)$, δE_t. The analysis of these terms (as well as I_1, I_2 of Assertion 4) is simplified by the continuity property of the second quantizer:

Lemma 5: Let $\{A_\alpha\}$ be a family of symmetrized operators on $\mathcal{H}^{(n)}$ (see Paper I, Theorem 2). Then $\{A_\alpha\}$ converges weakly (resp. strongly, or uniformly) to operator A on $\mathcal{H}^{(n)}$ iff $\Omega(A_\alpha;n)$ converges weakly (resp. strongly, or uniformly on each $\mathcal{H}^{(m)}$, $m\geq n$) to $\Omega(A;n)$ as an operator on Fock space.

Proof: Convergence of the A_α implies the convergence of the $\Omega(A_\alpha;n)$, since N reduces Ω and on $\mathcal{H}^{(m)}$, $m\geq n$, $\Omega(A_\alpha;n)$ is a finite sum of operators of the form $UA_\alpha\otimes \mathbb{I}^{m-n}U^{-1}$, where U is a unitary permutation operator. (See Paper I.) The extra condition for uniform convergence is necessitated by Theorem 2f of Paper I. The converse follows from $\Omega(A;n)_{\mathcal{H}^{(n)}}=A$.

Furthermore, the operator $Y_t^{(2)}$ is a special case of the following considerations:

Let W be an operator on $\mathcal{L}^2(\mathbf{R}^{2s})$, and let $C_1\otimes C_2$ be the direct product of the two $n_\psi\times n_\psi$ complex matrices C_1, C_2. Let $\phi\in\mathcal{H}_\psi^{(2)}$. Then $\phi=\{\phi_{\beta,\gamma}\}_{\beta,\gamma=1}^{n_\psi}$, $\phi_{\beta,\gamma}\in\mathcal{L}^2(\mathbf{R}^{2s})$. If in addition $\phi_{\beta,\gamma}\in D(W)$ for each β,γ, we write "$\phi\in D(W)$." We define the operator $WC_1\otimes C_2$ by

$$(WC_1\otimes C_2\phi)_{\beta',\gamma'}=\sum_{\beta,\gamma=1}^{n_\psi} C_{1\beta'\beta}C_{2\gamma'\gamma}W\phi_{\beta,\gamma}$$

for $\phi\in D(W)$.

Lemma 6: Let $f\in\mathcal{L}^1(\mathbf{R}^s)$, σ,σ' either $\equiv 1$ or $\hat\sigma,\hat\sigma'$ in $\mathcal{L}^1(\mathbf{R}^s)$. Let $\{g_n\}$ be the h. o. basis, and let W_f be the operator defined by $D(W_f)=\{\phi\in\mathcal{L}^2(\mathbf{R}^{2s})\,|\,\int d^sp\,d^sq \times|\hat f(p-q)\hat\phi(p,q)|^2<\infty\}$ and, for $\phi\in D(W_f)$, $(\widehat{W_f\phi})(p,q)=(2\pi)^{-s/2}\hat f(p-q)\hat\phi(p,q)$. Furthermore, let

$$
\begin{aligned}
Y^{(2)}(t,f,\sigma,\sigma')\equiv\sum_\alpha\sum_{n,n'} t^{|n+n'|}(g_n, fg_{n'})M(\sigma' g_n, C_\alpha)\\
\otimes M(\check{\sigma}^*g_{n'}\check{}^*, C_\alpha^\dagger).
\end{aligned}
$$

Then the strong limit of $Y^{(2)}(t,f,\sigma,\sigma')$ as $t\to 1^-$ exists on a core for the limit operator, which equals $\sum_\alpha W_{\sigma'\sigma^*f}C_\alpha\otimes C_\alpha^\dagger$ and which is self-adjoint if $\widehat{\sigma'\sigma^*f}$, and the C_α are real.

Proof: From the definition of $Y^{(2)}(t,f,\sigma,\sigma')$ we obtain the bound

$$
\begin{aligned}
\|Y^{(2)}(t,f,\sigma,\sigma')\|\leq\sum_\alpha\sum_{n,n'} t^{|n+n'|}\|f\|_1\|g_n\|_\infty\|g_{n'}\|_\infty\\
\times\|C_\alpha\|^2\|\sigma' g_n\|_1\|\sigma g_{n'}\|_1,
\end{aligned}
$$

which is seen to converge for $-1<t<1$ by estimates similar to those in Assertion 3. Thus $D(Y^{(2)}(t,f,\sigma,\sigma'))=\mathcal{H}_\psi^{(2)}$.

Since $\sigma'\sigma^*f\in\mathcal{L}^1(\mathbf{R}^s)$, $D(W_f)=\mathcal{L}^2(\mathbf{R}^{2s})$ so that any dense linear set is a core for the limit operator.

Let $\phi=\{\phi_{\beta\gamma}\}\in\mathcal{H}_\psi^{(2)}$. Then

$$\|Y^{(2)}(t,f,\sigma,\sigma')\phi\|^2$$

$$= \sum_{\alpha,\alpha'} \sum_{\substack{\beta,\beta',\gamma \\ \gamma',\rho,\rho'}} C_{\alpha\rho'\beta} C^\dagger_{\alpha\rho\gamma} C^\dagger_{\alpha'\rho'\beta'} C_{\alpha'\rho\gamma'}$$

$$\times \int d^s x\, d^s y\, d^s p\, d^s q\, f(x) f^*(y) \hat{\phi}^*_{\beta',\gamma'}(p,q)$$

$$\times \hat{\phi}_{\beta,\gamma}(p,q) \beta(x,y,p,q)$$

where

$$\beta(x,y,p,q) = \sum_{n,n',n'',n'''} t^{|n+n'+n''+n'''|} g^*_n(x) g_{n'}(x) g_{n''}(y) g^*_{n'''}(y)$$

$$\times \widehat{\sigma' g_n}(p) \widehat{\sigma g}^*_{n'}(q) \widehat{\sigma' g}^*_{n''}(p) \widehat{\sigma g}_{n'''}(q)$$

$$= \begin{cases} B(x,p,-it)B(x,q,it)B(y,p,it)B(y,q,-it), \\ \qquad \text{if } \sigma,\sigma' = 1, \\ (2\pi)^{-2s} \int d^s w\, d^s z\, d^s r\, d^s v\, \hat{\sigma}'(p-w) \hat{\sigma}^*(q-z) \\ \quad \times \hat{\sigma}'^*(p-r) \hat{\sigma}(q-v) B(x,w,-it) B(x,z,it) \\ \quad \times B(y,r,it) B(y,v,-it), \quad \text{if } \hat{\sigma}', \hat{\sigma} \in \mathcal{L}^1(\mathbb{R}^s). \end{cases}$$

In either case $\beta(x,y,p,q)$ is bounded, and so we may use Lebesgue's dominated convergence theorem to take the limit $t \to 1^-$, obtaining

$$\| Y^{(2)}(t,f,\sigma,\sigma')\phi \|^2$$

$$\to \sum_{\alpha,\alpha'} \sum_{\substack{\beta,\beta',\gamma \\ \gamma',\rho,\rho'}} C_{\alpha\rho'\beta} C^\dagger_{\alpha\rho\gamma} C^\dagger_{\alpha'\rho'\beta'} C_{\alpha'\rho\gamma'} (2\pi)^{-2s}$$

$$\times \int d^s p\, d^s q\, d^s x\, d^s y\, f(x) f^*(y) \hat{\phi}^*_{\beta',\gamma'}(p,q) \hat{\phi}_{\beta,\gamma}(p,q)$$

$$\times \exp[-i(x-y)(p-q)] (\sigma'\sigma^*)(x) (\sigma'\sigma^*)(y)$$

$$= \| \sum_\alpha W_{\sigma'\sigma^* f} C_\alpha \otimes C^\dagger_\alpha \phi \|^2.$$

For $\sigma'\sigma^* f$ real-valued and C_α real matrices, self-adjointness follows from the spectral theorem.

Corollary: The result of the previous lemma also holds whenever $\sigma'\sigma^* f \in \mathcal{L}^2(\mathbb{R}^s)$ and σ, σ', f are viewed as limits of a sequence of functions σ_j, σ'_j, f_j such that $\hat{\sigma}_j, \hat{\sigma}'_j, f_j \in \mathcal{L}^1(\mathbb{R}^s) \cap \mathcal{L}^2(\mathbb{R}^s)$ (or $\sigma = \sigma' = 1$).

Proof: Since $\mathcal{L}^1(\mathbb{R}^s) \cap \mathcal{L}^2(\mathbb{R}^s)$ is dense in $\mathcal{L}^2(\mathbb{R}^s)$, viewing $\sigma'\sigma^* f$ as the above limit is natural. Now for $\hat{\sigma}_j, \hat{\sigma}'_j, f_j \in \mathcal{L}^1(\mathbb{R}^s)$ or $\sigma_j, \sigma'_j \equiv 1$,

$$Y^{(2)}(t, f_j, \sigma_j, \sigma'_j) \underset{t \to 1^-}{\to} \sum_\alpha W_{\sigma'_j \sigma^*_j f_j} C_\alpha \otimes C^\dagger_\alpha.$$

Since $\sigma'\sigma^* f \in \mathcal{L}^2(\mathbb{R}^s)$, $\mathcal{S}(\mathbb{R}^{2s})$ is a core for $W_{\sigma'\sigma^* f}$ [17]; we choose $\phi = \{\phi_{\beta,\gamma}\}$, $\phi_{\beta,\gamma} \in \mathcal{S}(\mathbb{R}^{2s})$. Thus

$$\| \sum_\alpha W_{\sigma'_j \sigma^*_j f_j} C_\alpha \otimes C^\dagger_\alpha \phi - \sum_\alpha W_{\sigma'_i \sigma^*_i f_i} C_\alpha \otimes C^\dagger_\alpha \phi \|^2$$

$$\leq \sum_{\alpha,\alpha'} \sum_{\substack{\beta,\beta',\gamma_i \\ \gamma',\rho,\sigma}} | C^\dagger_{\alpha'\beta'\rho} C_{\alpha'\gamma'\sigma} C_{\alpha\rho\beta} C^\dagger_{\alpha\sigma\gamma} |$$

$$\times \| \sigma'_j \sigma^*_j f_j - \sigma'_i \sigma^*_i f_i \|^2 (2\pi)^{-s} \int d^s q$$

$$\times \operatorname*{ess\,sup}_{p \in \mathbb{R}^s} | \hat{\phi}^*_{\beta',\gamma'}(p,q) \hat{\phi}_{\beta,\gamma}(p,q) |$$

from which convergence follows.

For the model, we have $f = |\rho'_L|^2 \omega^{-2} \to \omega^{-2}$ as $L \to \infty$, and $\sigma = \sigma' \equiv 1$. Furthermore, $\omega^{-2} \in \mathcal{L}^1(\mathbb{R}^s)$ for $s = 1$ and $\omega^{-2} \in \mathcal{L}^2(\mathbb{R}^s)$ for $s = 1, 2, 3$. We recall that we have obtained $Y^{(2)}_t$ on the domain $C^\infty(H_0) \cap \mathcal{F}^0_a \otimes \mathcal{H}^{(\nu)}_\psi$ which contains all of the ψ-particle wavefunctions of fast decrease, a core for the limit operator. [17]

Computing $\widehat{\omega^{-2}}$ (to understand the physics in the W_f operator), we obtain

$$\widehat{\omega^{-2}}(x-y) = \begin{cases} c_1 \exp(-\mu|x-y|), & s = 1, \\ c_2 K_0(\mu|x-y|), & s = 2, \\ c_3 |x-y|^{-1} \exp(-\mu|x-y|), & s = 3, \end{cases}$$

where c_1, c_2, c_3 are positive constants and K_0 is the modified Bessell function of the second kind. Therefore, the $s = 1$ and $s = 2$ cases are the one- and two-dimensional analogs of the Yukawa potential.

It remains to consider δE_t which is the potentially divergent mass renormalization term. In the words of Cook[2]: "Divergence cannot be properly coped with when convergence itself has never been rigorously defined."

Lemma 7: Let $f \in \mathcal{L}^1(\mathbb{R}^s)$ and $\sigma, \sigma' \equiv 1$ or $\hat{\sigma}, \hat{\sigma}' \in \mathcal{L}^1(\mathbb{R}^s)$. Let

$$\delta E^{(1)}(t,f,\sigma,\sigma') \equiv \sum_\alpha \sum_{n,n'} t^{|n+n'|} (g_n, f g_{n'})$$

$$\times M((\sigma' g_n) \star (\sigma g_{n'})^*, C_\alpha C^\dagger_\alpha).$$

Then as $t \to 1^-$,

$$\delta E^{(1)}(t,f,\sigma,\sigma') \to (2\pi)^{-s} \int d^s x\, f(x) \sigma'(x) \sigma^*(x) \sum_\alpha C_\alpha C^\dagger_\alpha.$$

Proof: We have

$$\| \delta E^{(1)}(t,f,\sigma,\sigma') \|$$

$$\leq \sum_\alpha \sum_{n,n'} t^{|n+n'|} \|f\|_1 \|g_n\|_\infty \|g_{n'}\|_\infty \|\sigma' g_n\|_1 \|\sigma g_{n'}\|_1 \|C_\alpha\|^2,$$

which is convergent for $-1 < t < 1$. For $\chi = \{\chi_\beta\} \in \mathcal{H}^{(1)}_\psi$ we then have

$$\| \delta E^{(1)}(t,f,\sigma,\sigma')\chi \|^2$$

$$= \sum_{\alpha,\alpha'} \sum_{\beta',\beta''} (C_\alpha C^\dagger_\alpha C_{\alpha'} C^\dagger_{\alpha'})_{\beta''\beta'} \int d^s p\, d^s x\, d^s y$$

$$\times f(x) f^*(y) \hat{\chi}^*_{\beta''}(p) \hat{\chi}_{\beta'}(p) \beta_2(x,y,p),$$

where $\beta_2(x,y,p) = \beta(x,y,p,p)$. Thus $\beta_2(x,y,p)$ is bounded, so that we may apply the dominated convergence theorem to obtain

$$\| \delta E^{(1)}(t,f,\sigma,\sigma')\chi \|$$

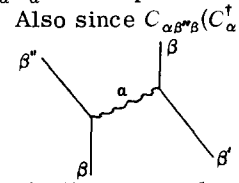
$$\underset{t \to 1^-}{\to} \| (2\pi)^{-s} \int d^s x\, f(x) \sigma'(x) \sigma^*(x) \sum_\alpha C_\alpha C^\dagger_\alpha \chi \|,$$

and the lemma follows.

Corollary: If $\{f_j\}, \{\hat{\sigma}_j\}, \{\hat{\sigma}'_j\}$ are sequences in $\mathcal{L}^1(\mathbb{R}^s)$ such that $f_j \sigma'_j \sigma^*_j \to g$ in $\mathcal{L}^1(\mathbb{R}^s)$ norm, then as $t \to 1^-$ followed by $j \to \infty$,

$$\delta E^{(1)}(t, f_j, \sigma_j, \sigma'_j) \to (2\pi)^{-s} \int d^s x\, g(x) \sum_\alpha C_\alpha C^\dagger_\alpha.$$

For the recoilless model we have $\sigma \equiv 1$, and $f_L = \omega^{-2} |\rho'_L|^2$ which remains in $\mathcal{L}^1(R^s)$ as $L \to \infty$ for $s = 1$ only. Since $\int \omega^{-2}(k)\, dk = \pi \mu^{-1}$, we have for $s = 1$, $\delta E^{(1)}_t \to (\pi/2)^{1/2} \mu^{-1} \sum_\alpha C_\alpha C^\dagger_\alpha$ which operates only on the spin/charge variables. Also since $C_{\alpha\beta''\beta}(C^\dagger_\alpha)_{\beta\beta'}$ corresponds to the diagram



which does not physically occur unless $\beta' = \beta''$, $C_\alpha C^\dagger_\alpha$ is diagonal, and $\delta E^{(1)}$ is a finite mass renormalization with values possibly depending on the spin/charge state.

δE may be analyzed further in the usual language of the $SU(n)$ analysis of particle physics.[18]

To treat the case $s=2$, we observe that, by Lemma 2, δE_t commutes with the dressing operator. We then perform a "mass renormalization"; i. e., we simply subtract δE_t and take the strong limit

$$\lim_{L\to\infty}\lim_{t\to 1^-}\exp(iV_{\rho_L,1,K(t)})(H_0+V_{\rho'_L,1,K(t)}-\delta E_t)\times\exp(-iV_{\rho_L,1,K(t)})=H_{0a}+H_{0\psi}-\Omega_\psi\Big(\sum_\alpha W_{\omega^{-2}}C_\alpha\otimes C_\alpha^\dagger;2\Big)$$

on $C^\infty(H_0)\cap\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}\cap D(W_{\omega^{-2}})$. Since $K_0(x)$ is singular only at $x=0$ (where it diverges like $-\ln|x|$), it is in $\mathcal{L}^2(\mathbb{R}^s)$. Alternatively $K_0=\widehat{\omega^{-2}}\in\mathcal{L}^2(\mathbb{R}^2)$ since $\omega^{-2}\in\mathcal{L}^2(\mathbb{R}^2)$. It follows[17] that finite linear combinations of the h. o. basis form a core for the self-adjoint operator $H_{0a}+H_{0\psi}-\Omega_\psi(\sum_\alpha W_{\omega^{-2}}C_\alpha\otimes C_\alpha;2)$ since that set is a subset of $C^\infty(H_0)\cap\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}\cap D(W_{\omega^{-2}})$, $\nu\in\mathbb{Z}_+$. Self-adjointness in the case $s=1$ is less difficult since the mass renormalization term as well as the Yukawa interaction term are bounded in each $\mathcal{H}_\psi^{(\nu)}$, $\nu\in\mathbb{Z}_+$, so that no subtraction of the mass renormalization term is needed.

We summarize these results in

Assertion 6: For this model with the recoilless approximation on the ψ particles and $s=1$, all cutoffs may be removed from the Hamiltonian in the strong topology. For $s=2$ the cutoffs may be removed after a well-defined mass-renormalization subtraction. In both cases the dressing operator converges to a unitary operator and the Hamiltonian to a self-adjoint operator.

We remark that the domains of the resulting Hamiltonians include the image of a subset of $\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}$ under the unitary dressing operator. For the case $s=1$, $\rho_L\to 1$ we see from term I_1 in Assertion 4 that the domain of V does not intersect $\mathcal{J}_a^0\otimes\mathcal{H}_\psi^{(\nu)}$. Thus the domain of the Hamiltonian without cutoffs (or finite mass renormalization), as an operator H_0+V, consists entirely of vectors with an infinite number of a particles, and cannot be characterized by its effect on finite numbers of particles. Nonetheless, we have not left Fock space, contrary to a common myth.

The Galilean recoil case

Again we choose ρ,σ so as to obtain the greatest simplification of Eq. E. We have $V_{\rho',\sigma',K(t)}+V_{-i\omega\rho,\sigma,K(t)}+V_{\rho,-iP^2\sigma/2m,K(t)}$ which by Assertion 4 converges as $t\to 1^-$ to $V_{\rho'\sigma'}+V_{-i\omega\rho\sigma}+V_{-i(\epsilon-m)\rho\sigma}=V_{\rho'\sigma'-i(\omega+\epsilon-m)\rho\sigma}$ subject to the requirements $\hat\sigma,\hat\sigma',\widehat{P^2\sigma}\in\mathcal{L}^1(\mathbb{R}^s)$ (or equal to 1), and $\rho',\omega\rho,\rho\in\mathcal{L}_a^2(\mathbb{R}^s)$. We choose $\sigma'=\sigma=\sigma_L\in\mathcal{S}(\mathbb{R}^s)$ such that $0\le\sigma_L\le 1$, $\sigma_L(k)=0$ for $|k|>L+1$, $\sigma_L(k)=1$ for $|k|<L$, L fixed. Then $P^2\sigma\in\mathcal{S}(\mathbb{R}^s)$ so that all conditions on σ,σ' are met. We choose $\rho'=\rho'_l=\sigma_l$ for some l chosen independently of L. We choose $\rho=\rho_l$ such that $\rho'-i(\omega+\epsilon-m)\rho=0$. Taking the limits $l\to\infty$, $L\to\infty$ will remove the remaining cutoffs from the interaction. Since $\rho_l\xrightarrow[l\to\infty]{}-i(\omega+\epsilon-m)^{-1}\in\mathcal{L}_a^2(\mathbb{R}^s)$ for $s=1,2,3,4$, we may apply Assertions 2(c), 4, and a minor generalization of Assertion 5 to obtain a unitary dressing operator in the limit $l\to\infty$, $L\to\infty$. We conclude that this recoil case is free of wavefunction renormalization difficulties for $s=1,2,3,4$.

Using Assertion 2(b) and Lemmas 5, 6, 7, we see that $i2^{-1}[V_{\rho,\sigma,K(t)},V_{-i\omega\rho,\sigma,K(t)}]+i[V_{\rho,\sigma,K(t)},V_{\rho',\sigma',K(t)}]$ converges as $t\to 1^-$ to $-\Omega_\psi(W_f\sum_\alpha C_\alpha\otimes C_\alpha^\dagger;2)-(2\pi)^{-s/2}\int f(k)\,d^sk\times\Omega_\psi(\sum_\alpha C_\alpha C_\alpha^\dagger)$, where $f=f_{l,L}=-(\omega+2\epsilon-2m)(\omega+\epsilon-m)^{-2}\times\omega^{-1}|\sigma_L|^2|\rho'_l|^2$. Since $\lim_{l,L\to\infty}f_{l,L}$ is in $\mathcal{L}^1(\mathbb{R}^s)$ for $s=1,2$, and in $\mathcal{L}^2(\mathbb{R}^s)$ for $s\le 5$, Lemmas 6, 7 imply that (a) for $s=1,2$ the mass renormalization is finite and W_f is a bounded operator and (b) for $s\le 5$, $\Omega_\psi(W_f\sum_\alpha C_\alpha\otimes C_\alpha^\dagger;2)$ is self-adjoint.

The remaining terms in Eq. E are different in form from any previously considered, so that we return to a direct calculation of them by methods similar to those used in Assertion 4. As before, we start with a vector $\chi\in\mathcal{H}_a^{(n)}\otimes\mathcal{H}_\psi^{(\nu)}$. Here, however, we only obtain convergence for $\chi\in D(H_{0\psi}^{1/2})$ as we take the limits $t\to 1^-$, $l,L\to\infty$. A further necessary condition for convergence turns out to be $P\rho\in\mathcal{L}_a^2(\mathbb{R}^s)$, which only occurs for $s=1,2$, and under these conditions we obtain bounds on the limit operators of the form of a linear combination of $\|H_{0\psi}^{1/2}\chi\|$, $\|N_a^{1/2}H_{0\psi}^{1/2}\chi\|$, and $\|N_a\chi\|$ (all of which may be overestimated by $\|H_0\chi\|$). The coefficients of these terms all contain a factor of either $\|C_\alpha\|$ or $\sum|C_{\alpha\beta\beta'}|$ so that for sufficiently small coupling constants these terms comprise a Kato perturbation[12] of H_0. Since for $s=1,2$, the W_f operator is a bounded operator and the mass renormalization is finite, we conclude that the limit dressed Hamiltonian is self-adjoint. Since the dressing operator is also unitary for $s=1,2$, we then conclude that

Assertion 7: For this model, with Galilean recoil on the ψ particles and $s=1,2$, all cutoffs may be removed from the Hamiltonian as strong limits and without mass renormalization. The dressing operator converges to a unitary operator and the Hamiltonian to a self-adjoint operator for $\|C\|$ small.

The failure of the method for the case $s=3$ may be overcome by allowing convergence in the weak topology as the cutoffs are removed. This has been accomplished by Nelson[6] using a slightly different dressing operator, arising as follows: If, in the first paragraph of this section, we had chosen $\rho'-i(\omega+\epsilon-m)\rho=\zeta$ for $\zeta\in\mathcal{L}_a^2(\mathbb{R}^s)$ rather than $=0$, then by Assertion 4 we still obtain a unitary dressing operator. (Nelson[6] takes ζ to be the characteristic function for a ball of radius K in momentum space, whereas Gross[19] chooses $\zeta=0$.) Now, in the limit $l\to\infty$, $\rho=i(\omega+\epsilon-m)^{-1}(\zeta-1)$ so that the asymptotic behavior of ρ is unchanged by inclusion of ζ. Thus none of the singularities throughout the analysis are altered.

Since the dressing operator, the dressed Hamiltonian, the mass renormalization, etc., all depend on ζ, we cannot justify attaching any physical interpretation to the dressed objects. This is doubly true since there is no physical justification for the form of the dressing transformation either. It follows that arguments for choosing the mass renormalization "so that the resulting one-*dressed*-particle spectrum is correct" are to be avoided. These arguments do not furnish sufficient information to fix ζ anyway, since they only determine $\int f(k)\,d^sk$ and not f in the mass renormalization term. In fact even $\int f(k)\,d^sk$ is determined from an argument based on mass splittings of the dressed particles and is

not determined from a single dressed mass, since the bare mass is unknown. f would better be determined by measuring the Yukawa type interaction (which is beyond present experimental capabilities). Rather than expanding on this argument, we turn to the relativistic recoil case.

The relativistic recoil case

In the previous cases the dressed Hamiltonian consisted of a finite number of terms each of which was susceptible to complete analysis. Furthermore, the fact that there were a finite number of terms was a reflection of the form of $h_{0\psi}$ (e.g., Lemma 3 and Corollary 1). If we choose the relativistic form for $h_{0\psi}$, then this termination of the series for the dressed Hamiltonian no longer occurs and we are faced with the problem of "resumming the Born series," or of finding alternative methods.[7,20] We present here a method which is perhaps a new approach and encouragingly simple.

Let us initially consider Q to be any function of momentum for which termination of the series for the dressed Hamiltonian occurs. Then consider $h_{0\psi} - Q$ as a perturbation of the resulting (self-adjoint) operator. For example, take Q to be $P_\Sigma = \sum_{i=1}^{s} P_i$, the sum of the momentum operators. Then Lemma 3 implies $[M(h, C), [P_\Sigma, M(g, C_1)]]^\sim = 0$ if $[C, C_1] = 0$ and similarly for the second-quantized forms. Now using $\Omega_\psi(P_\Sigma)$ for $H_{0\psi}$ in the left-hand side of Eq. E, the right-hand side becomes

$$H_{0a} + \Omega_\psi(P_\Sigma) + V_{\rho',\sigma',K(t)} + V_{-i\omega\rho,\sigma,K(t)} + V_{\rho,-iP_\Sigma\sigma,K(t)} + i[V_{\rho,\sigma,K(t)}, V_{\rho',\sigma',K(t)}] + \tfrac{1}{2} i[V_{\rho,\sigma,K(t)}, V_{-i\omega\rho,\sigma,K(t)}] + \tfrac{1}{2} i[V_{\rho,\sigma,K(t)}, V_{\rho,-iP_\Sigma\sigma,K(t)}].$$

Thus we may choose $\sigma = \sigma' = \sigma_L$ as before, $\rho' = \sigma_I$ as before, and ρ such that $\rho'\sigma' - i\omega\rho\sigma - i\rho P_\Sigma\sigma = 0$; i.e., $\rho = -i(\omega + P_\Sigma)^{-1}\rho'$, which is in $\mathcal{L}_a^2(\mathbb{R}^s)$ for $s = 1, 2$ in the limit $l \to \infty$. We therefore obtain a unitary dressing transformation, in the limit as all cutoffs are removed, for $s = 1, 2$. The commutations, by applying Lemmas 6, 7, yield a Yukawa type term and a mass renormalization:

$$-\Omega_\psi\left(W_f \sum_\alpha C_\alpha \otimes C_\alpha^\dagger; 2\right) - (2\pi)^{-s/2} \int f(k)\, d^s k\, \Omega_\psi\left(\sum_\alpha C_\alpha C_\alpha^\dagger\right),$$

where now

$$f(k) = \tfrac{1}{2}\omega(k)^{-1}\left(\omega(k) + \sum_{i=1}^{s} k_i\right)^{-1}.$$

Since $f \in \mathcal{L}^1(\mathbb{R}^s)$ for $s = 1$ and $f \in \mathcal{L}^2(\mathbb{R}^s)$ for $s = 1, 2, 3$, we obtain (a) finite mass renormalization and W_f a bounded operator for $s = 1$, (b) self-adjoint Yukawa-type interaction for $s = 1, 2, 3$. Furthermore, from Paper I, Theorem 2c, we have

$$\Omega_\psi(P_\Sigma \otimes \mathbb{1}; 2)\big|_{\mathcal{H}^{(n+m)}} = m\Omega_\psi(P_\Sigma)\big|_{\mathcal{H}^{(n+m)}}.$$

However,

$$(1/2m)(P_\Sigma \otimes \mathbb{1} + \mathbb{1} \otimes P_\Sigma) - W_f \sum_\alpha C_\alpha \otimes C_\alpha^\dagger$$

is self-adjoint by a standard classical argument. Thus $\Omega_\psi(P_\Sigma) + H_{0a} + V(-\delta E)$ is self-adjoint for $s = 1, 2$ with domain $= D(H_0)$, since $D(H_{0\psi}) = D(\Omega_\psi(P_\Sigma))$. (The dressed form of this is even self-adjoint for $s = 3$.) Thus (after subtraction of a mass renormalization for $s > 1$)

$$H_{0\psi} + H_{0a} + V(-\delta E) = [H_{0\psi} - \Omega_\psi(P_\Sigma)] + [\Omega_\psi(P_\Sigma) + H_{0a} + V(-\delta E)]$$

is a symmetric operator defined on $D(H_0)$. We summarize in

Assertion 8: For the model, with relativistic recoil on the ψ particles and $s = 1$, all cutoffs may be removed from the Hamiltonian in the strong topology. For $s = 2$, the cutoffs may be removed strongly after a mass renormalization. For $s = 3$ the present dressing operator causes wavefunction renormalization problems.

We may now compare the results of Assertions 6, 7, and 8 to emphasize that the singularities of the model depend on the choice of recoil, as has been previously noted in other models.[21] The behavior in the recoilless and relativistic recoil cases is the same but different from the Galilean recoil case, the differences arising from the contribution to the form of ρ in the dressing operator. [$\rho \sim (\omega + \epsilon)^{-1}$ so that until ϵ is of order higher than linear in momentum, $\rho \sim \omega^{-1}$.] For $s = 1$ all three recoil cases are well behaved. For $s = 2$ mass renormalization is required in the recoilless and relativistic recoil cases. For $s = 3$ mass and wavefunction renormalization appears in the recoilless and relativistic recoil cases. For $s = 3, 4$ the Galilean dressing operator is unitary, but weak convergence may be necessary to make sense of the dressed Hamiltonian even after mass renormalization. For $s = 5$, weak convergence and mass and wavefunction renormalization may suffice to make sense of the Galilean case.

V. CONCLUSION

In Papers I, II, and this paper we have shown that it is feasible to analyze models of quantum field theory without introducing operator-valued distributions. The methods developed provided enough simplification so that we could complicate a model by the inclusion of spin and charge, obtain self-adjointness, and discuss some of the physics in the model in a relatively few pages of analysis. At the same time, we have seen at what point we may as well turn to a distribution approach (as in the Galilean case for $s = 3$) and use weak convergence.

The asymptotic and interpolating fields for the model may be treated in this formalism by extending the results previously obtained in the spinless, chargeless case.[22] Since no further development of the formalism is required for such analysis, we will not discuss it here. The formalism is, therefore, sufficiently developed to be considered a viable alternative to the usual formalism of operator-valued distributions.

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Change of Petrov type under generation of solutions of Einstein's equations

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A method given by Geroch [J. Math. Phys. **12**, 918 (1971)] for generating new solutions of the vacuum gravitational field equations from known solutions is investigated in order to find out how the Petrov type of the new metric will be related to that of the old metric. Conditions are found under which algebraically special metrics will generate algebraically special metrics. It is shown how the Petrov type of these metrics will change under the generation method of Geroch.

1. INTRODUCTION

Various authors have discussed methods of generating new solutions of Einstein's equations from known solutions. In particular, Buchdahl,[1] Ehlers,[2] Harrison,[3] and Geroch[4] have shown how to obtain new stationary vacuum solutions from known stationary vacuum solutions. Their method has been extended to solutions of the Einstein–Maxwell equations.[5] Also ways of generating solutions of the vacuum Brans–Dicke equations have been found by Buchdahl,[6,7] McIntosh,[8] and Sneddon and McIntosh.[9]

It is known[3,4] that if the method of generation discussed by Geroch[4] is applied to the Schwarzschild solution, the result is the NUT metric.[10] This is an example where a metric whose Weyl tensor is of Petrov type D generates a family of type D metrics. In this note, this method is investigated more fully in order to discover in general how the Petrov type of the new metric will be related to the Petrov type of the old metric. In Sec. 2 some results due to Perjés[11] on a spinor treatment of stationary space–time metrics are summarised. In Sec. 3 Perjés' results are used to find conditions under which an algebraically special metric will generate algebraically special metrics. Section 4 describes in detail how the Petrov type of metrics may change under the generation of new solutions.

2. STATIONARY SPACE-TIME METRICS

Perjés[11] has given a spinor treatment of stationary space–time metrics. The necessary results may be summarised as follows. The line element of a stationary space–time can be written as

$$ds^2 = f(dt + \omega_i dx^i)^2 - f^{-1} g_{ij}\, dx^i dx^j \tag{1}$$

where i, j run from 1–3 and f, ω_i, and g_{ij} are time independent. Einstein's vacuum field equations imply that the rhs of

$$\phi_i = f^2 (g)^{1/2} \epsilon_{ijk}\, \omega^{j;k} \tag{2}$$

is curl-free and hence there exists, at least locally, a function ϕ such that $\phi_i = \phi_{,i}$. Following the notation of Ernst,[12] the "potential" $\mathcal{E}$ is defined as

$$\mathcal{E} = f + i\phi. \tag{3}$$

The metric g_{ij} of the 3-space can be described by a triad

$$z_m{}^i = (l^i, m^i, \bar{m}^i) \tag{4}$$

($m = 0, +, -$) where l^i is real, $\bar{m}^i$ is the complex conjugate of m^i, $l_i l^i = m_i \bar{m}^i = 1$ and $l_i m^i = m_i m^i = 0$. Then

$$g_{ij} = l_i l_j + m_i \bar{m}_j + \bar{m}_i m_j. \tag{5}$$

This triad can be used to define a null tetrad for the metric (1). One possibility is

$$\begin{aligned} \tilde{l}^\mu &= [f^{-1} - l_j \omega^j,\ l^i], \\ \tilde{m}^\mu &= f^{1/2}[-(m_j \omega^j),\ m^i], \\ \tilde{n}^\mu &= -\tfrac{1}{2} f \tilde{l}^\mu + a^\mu, \end{aligned} \tag{6}$$

where μ runs from 0–3, $t = x^0$, and $a^\mu = \delta^\mu_0$.

As in the null tetrad formalism of Newman and Penrose[13] Greek symbols are used to denote linear combinations of the Ricci notation coefficients

$$\gamma_{mnp} = z_{m\,i;j}\, z_n{}^i\, z_p{}^j. \tag{7}$$

In particular, if the congruence to which l^i is the tangent vector is geodesic, $\kappa = \gamma_{+00}$ is zero and $|\sigma| = |\gamma_{+0+}|$ is the shear of the congruence. The components of the conformal Weyl tensor for the tetrad (6) are

$$\begin{aligned} \Psi_0 &= 2[\delta G_+ - \sigma G_0 + \bar{\tau} G_+ + (2G_+ + G_+)\bar{G}_+], \\ \Psi_1 &= -(f)^{1/2}[DG_+ - \kappa G_0 - \epsilon G_+ + (2G_0 + \bar{G}_0)G_+], \\ \Psi_2 &= \tfrac{1}{2} f[DG_0 + \bar{\kappa} G_+ + \kappa G_- + (G_0 + \bar{G}_0)G_0 - 2G_+ G_-], \\ \Psi_3 &= \tfrac{1}{2} f^{3/2}[DG_- - \bar{\kappa} G_0 + \epsilon G_- + (2G_0 + \bar{G}_0)G_-], \\ \Psi_4 &= \tfrac{1}{2} f^2 [\bar{\delta} G_- - \bar{\sigma} G_0 + \tau G_- + (2G_- + \bar{G}_-)G_-], \end{aligned} \tag{8}$$

where $G_m = z_m{}^i \mathcal{E}_{,i}(2f)^{-1}$, $\partial_m = z_m{}^i \partial_i$, and $D = \partial_0$, $\delta = \partial_+$, $\delta = \partial_-$.

In this formalism the method referred to in Sec. 1 for generating new vacuum solutions from known vacuum solutions can be stated thus:

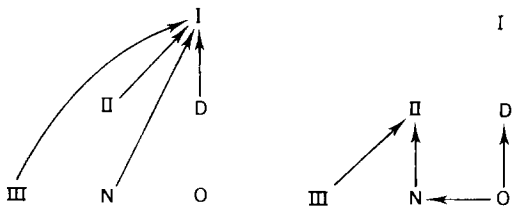
If $(\mathcal{E},\ z_m{}^i)$ is a solution of the vacuum field equations, then $(\mathcal{E}',\ z_m{}^i)$ is also a solution if

$$\mathcal{E}' = \{\mathcal{E}[\exp(2i\alpha) + 1] + [\exp(2i\alpha) - 1]\}/\{\mathcal{E}[\exp(2i\alpha) - 1] + [\exp(2i\alpha) + 1]\} \tag{9}$$

where α is a real constant.

3. GENERATION OF ALGEBRAICALLY SPECIAL METRICS

In order to investigate how the Petrov type of a metric will change under this generation it is convenient to consider how various quantities will change when the parameter α is small. Then conditions can be found under which a stationary metric will be algebraically special and any metric generated from it will also be



(a) (b)

FIG. 1(a) Metrics without a GSE will generate families of type I metrics under (9). (b) Metrics with a GSE may change Petrov type under (9) but will remain algebraically special.

algebraically special. For small α the new Weyl components are

$$\begin{aligned}
&\Psi_0' \simeq \Psi_0(1-2i\alpha f)+2i\alpha f(-6G_+^2),\\
&f^{-1/2}\Psi_1' \simeq f^{-1/2}\Psi_1(1-2i\alpha f)+2i\alpha f(3G_+G_0),\\
&f^{-1}\Psi_2' \simeq f^{-1}\Psi_2(1-2i\alpha f)+2i\alpha f(G_+G_- - G_0^2),\\
&f^{-3/2}\Psi_3' \simeq f^{-3/2}\Psi_3(1-2i\alpha f)+2i\alpha f(-\tfrac{3}{2}G_0G_-),\\
&f^{-2}\Psi_4' \simeq f^{-2}\Psi_4(1-2i\alpha f)+2i\alpha f(-\tfrac{3}{2}G_-^2).
\end{aligned} \tag{10}$$

The condition for the metric (1) to be algebraically special is that the polynomial

$$\Psi_0+4b\Psi_1+6b^2\Psi_2+4b^3\Psi_3+b^4\Psi_4 \tag{11}$$

has two coincident roots. This condition will be preserved (to order α) in the new metric if and only if the double root is also a root of

$$\begin{aligned}
&(f^{1/2}G_-b+G_0+(G_0^2+2G_+G_-)^{1/2})\\
&\times(f^{1/2}G_-b+G_0-(G_0^2+2G_+G_-)^{1/2}).
\end{aligned} \tag{12}$$

At this stage it is convenient to use some of the available triad freedom by choosing l^i to be an eigenray.[11] l^i then satisfies

$$fl_{i;j}l^j+f_{;i}-(f_{;j}l^j)l_i+\epsilon_{ijk}\phi^j l^k(g)^{1/2}=0 \tag{13}$$

(i.e., $G_+=0$). In this triad the roots of (12) are

$$b=0 \quad \text{and} \quad f^{1/2}b=2G_0/G_-. \tag{14}$$

In general there will be two solutions of (13). This freedom enables l^i to be chosen so that $G_+=0$ and the root of (12) corresponding to the double root of (11) is $b=0$.

These conditions imply that there exists a triad in which $G_+=0$ and $\Psi_1=\Psi_2=0$. Hence from (8) $\sigma G_0=\kappa G_0=0$. If either σ or κ is nonzero, then $G_+=G_0=0$ and the field equations imply that $G_-=0$ (i.e., $\mathcal{E}=$const), and the space–time is flat. Therefore, a necessary condition that the metric (1) and any metric generated from it by (9) be algebraically special is that (1) possess a geodesic, shear-free eigenray (GSE). The converse can easily be shown to be true, namely if the metric (1) has a GSE then it is algebraically special. Thus for stationary metrics it is only necessary to look at first order terms (in α) to decide if a metric will remain algebraically special under (9).

4. CHANGE OF PETROV TYPE

It is clear from the previous section that stationary metrics which do not possess a GSE will generate a family of algebraically general metrics under (9) [see Fig. 1(a)]. (Flat space–time metrics will always possess a GSE).

Suppose now that the metric (1) has a GSE and choose l^i to be this eigenray. The formulae (10) can now be used to show how the Petrov type will change under (9). Again it turns out that it is sufficient to consider terms of first order (in α). The results are displayed in Fig. 1(b) where the arrows indicate the possible changes of Petrov type.

It is important to realize that these changes depend not only on the metric itself, but also on the choice of Killing vector. As an example, a metric generated from flat space–time (which is type O) can be type O (if the Killing vector is chosen so that $\mathcal{E}=$const) type N (if $G_0=0$, $G_-\neq 0$) or type D (if $G_0\neq 0$). Thus metrics generated from

$$ds^2=dt^2-dx^2-dy^2-dz^2 \tag{15}$$

with Killing vector $\xi^\mu=\delta_0^\mu$ will be flat (type O), but if the Killing vector chosen is $\xi^\mu=(x,t,0,0)$ a family of type D metrics results. (These metrics are actually a family of metrics found in Ref. 10 with the parameter $\mu^\circ=0$).

Metrics generated from a metric of Petrov type N can be type II ($G_0\neq 0$) or type N ($G_0=0$). Also, for certain values of $\exp(2i\alpha)$ metrics in this latter class may be type O. (This is to be expected since some type N metrics can be generated from flat space). There can be at most a finite number of values of $\exp(2i\alpha)$ for which this will be true. Thus in general a type N metric will generate type N or type II metrics.

Type III metrics will generate type III metrics if $G_0=0$ or type II metrics otherwise.

In general type II metrics will generate type II metrics. However, in analogy with the type N metrics there may be certain type II metrics which [for specific values of $\exp(2i\alpha)$] will become type N, or type III.

The condition for a metric with a GSE to be type D is

$$\Psi_2\Psi_4=\tfrac{2}{3}\Psi_3^2. \tag{16}$$

An argument similar to that used in Sec. 3 can be used to show that this condition will be preserved if and only if

$$f^{-3/2}\Psi_3G_-=f^{-2}\Psi_4G_0 \tag{17}$$

or, equivalently,

$$3f^{-1}\Psi_2G_-=2f^{-3/2}\Psi_3G_0. \tag{18}$$

However, it can be shown[14] that Eqs. (17) and (18) will always be satisfied for type D metrics, and so all type D metrics with a GSE will generate a family of type D metrics under (9).

5. CONCLUSION

Metrics with a GSE will generate algebraically special metrics under the generation (9), and it has been shown how the Petrov type of these metrics will change

in general. All other stationary metrics will generate type I metrics.

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[14]To show this, the field equations for metrics with a GSE can be solved (cf. Ref. 11) to express the field variables in terms of two real functions of two variables (x^2 and x^3 say), each of which is the solution of a second order differential equation, and two arbitrary analytic functions of a complex variable ($z = x^2 + ix^3$). On substitution of these expressions into Eq. (16) it can be shown that the arbitrary analytic functions are constant and that Eq. (17) is automatically satisfied.

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