On trace-class operators of scattering theory and the asymptotic behavior of scattering cross section at high energy

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We investigate necessary and sufficient conditions under which the difference of the resolvents $R_z - R^0{}_z$ of two self-adjoint operators of the form $H_0{}^1 \equiv F(\mathbf{P})$ and $H \equiv F(\mathbf{P}) + V(\mathbf{Q})$ is nuclear. Here $F(\mathbf{P})$ denotes a positive and continuous function of the usual momentum observables P and $V(\mathbf{Q})$ a function of the conjugate coordinate observables. Roughly speaking, we prove that $R_z - R^0{}_z$ is nuclear if and only if $F(\mathbf{P})$ increases *faster* than $|\mathbf{P}|^{3/2}$ at large $|\mathbf{P}|$ and $V(\mathbf{Q})$ falls off to zero *faster* than $1/|\mathbf{Q}|^3$ at large $|\mathbf{Q}|$. (For a precise statement of this result Sec. 3.) In particular, it is noticed that if $H_0 = (|\mathbf{P}|^2 + m^2)^{1/2}$ the relativistic free Hamiltonian, then $R_z - R^0{}_z$ is *not* nuclear for any of the (suitably regular) potential $V(\mathbf{Q}_{N.W})$ where $\mathbf{Q}_{N.W}$ denotes the usual Newton-Wigner position operator of the relativistic particle. We also investigate in Sec. 3 the necessary and sufficient conditions for $R_z{}^\beta V R_z^{0\beta} (\beta > 0; \beta \neq 1)$ to be nuclear. The implications of these results for the asymptotic behavior of the total scattering cross sections at high energy is discussed in Sec. 4.

1. INTRODUCTION

In the mathematical theory of scattering processes the condition that certain pertinent operators are of trace class (nuclear) plays an important role. To cite some well-known instances one may only recall the results of Kato,[1] Birman and Krein,[2] etc. It is shown by these authors that the condition that the difference $R_z - R_z^0$ of the resolvents of the total and unperturbed Hamiltonian of the system belongs to the trace class (or somewhat more generally the condition that $R_z^n - R_z^{0n}$ is of trace-class for some integer n) is sufficient to ensure the existence and completeness of the Møller wave operators. It is also shown[2] that the above mentioned condition implies that the "energy shell" scattering operator $S(\lambda)$ differs from the identity operator by a trace-class operator which in turn implies that the total scattering cross sections at fixed energies are finite.

This latter result has been rederived recently by Jauch and Sinha,[3] who show also that if $R_z^n V R_z^{0m}$ is of trace class for some positive integers n and m then

$$\int \frac{\epsilon \sigma_{\text{tot}}(\epsilon)}{(\epsilon^2 + 1)^{n+m/2}} \, d\epsilon < \infty.$$

Here V denotes the interaction responsible for a single-channel nonrelativistic scattering process and $\sigma_{\text{tot}}(\epsilon)$ represents the total scattering cross section at energy ϵ.

It is clear that the finiteness of the above integral [together with certain additional regularity properties of $\sigma_{\text{tot}}(\epsilon)$] implies an upper bound on the high energy behavior of $\sigma_{\text{tot}}(\epsilon)$. For instance, as pointed out by Jauch and Sinha, if $R_z V R_z^0$ is itself of trace class, then $\sigma_{\text{tot}}(\epsilon)$ must decrease to zero as $\epsilon \to \infty$. As a last instance of the role of the trace-class condition on $R_z - R_z^0$ ($\equiv R_z V R_z^0$) in scattering theory we mention the recently developed theory of time delay of scattering processes[4] where this condition again plays an important part.

It is thus seen that a number of theoretically important results concerning elastic scattering processes can be derived from the abstract condition that $R_z V R_z^0$ or some related operator is nuclear.

In order to assess the range of application of these results, however, it is necessary to express this abstract condition in terms of explicit and easily verifiable properties of the interaction V and the unperturbed Hamiltonian H_0. Unfortunately, it seems that this latter problem has not received a systematic treatment in the literature. A systematic investigation of this problem is, therefore, one of the principal objects of the present paper.

In connection with the above mentioned question it seems that the only result that is readily available in the literature is the one which asserts that $R_z V R_z^0$ is nuclear if $H_0 = |\mathbf{p}|^2/2m$; the nonrelativistic free Hamiltonian and V is a suitably regular and sufficiently short ranged potential.[5] While this result insures that $R_z V R_z^0$ is nuclear in a number of physically interesting situations, it is also clear that it does not cover many other cases of physical interest. For instance, it is not known if a similar result holds when H_0 is the relativistic free Hamiltonian $(|\mathbf{p}|^2 + m^2)^{1/2}$ instead of being nonrelativistic Hamiltonian $|\mathbf{p}|^2/2m$.

With a view to answering such questions we have considered (elastic) potential scattering of a particle whose unperturbed Hamiltonian H_0 is a positive and continuous function $F(\mathbf{p})$ of the momentum observables. In this setting we investigate the necessary and sufficient conditions for $R_z V R_z^0$ to be nuclear. Our main result is the theorem 2 of Sec. 3 which formulates such a necessary and sufficient condition in terms of the asymptotic behavior of $H_0 \equiv F(\mathbf{p})$ and the potential $V(\mathbf{Q})$ (for large $|\mathbf{p}|$ and large $|\mathbf{Q}|$, respectively).

Two corollaries of Theorem 2 are of special interest in physical applications. They refer to the two special cases

$$H_0 = |\mathbf{p}|^2/2m \quad \text{(nonrelativistic)},$$

$$H_0 = (|\mathbf{p}|^2 + m^2)^{1/2} \quad \text{(relativistic)}.$$

For the nonrelativistic case Theorem 2 provides a complete characterization of the class of potentials for which $R_z V R_z^0$ is nuclear. This result, then, subsumes the result mentioned earlier.[5] For the relativistic Hamiltonian $H_0 = (|\mathbf{p}|^2 + m^2)^{1/2}$, on the other hand, our result reveals that $R_z V R_z^0$ is *not* nuclear for any of the interactions that are (suitably regular) functions of the Newton–Wigner position operator $\mathbf{Q}_{NW}$.[6]

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In Sec. 3 we also discuss the necessary and sufficient conditions for $R_z^\beta V R_z^{0\beta}$ ($\beta > 0$) to be nuclear. Our results (Proposition 5) (for $\beta \neq 1$) is not entirely satisfactory inasmuch as we have to make certain technical assumption which is not easily verifiable. But it is included in this paper on account of its application in the next section and with the hope that a similar result can be proven without the objectionable technical assumption in question.

Finally, in Sec. 4 we discuss the implications of these mathematical results for the asymptotic behaviour of scattering cross sections at high energy.

It may be observed, first, that since $R_z V R_z^0$ is not nuclear in "relativistic potential scattering"[7] there is no longer any compelling reason to conclude that the total cross section $\sigma_{tot}(\epsilon) \to 0$ as energy $\epsilon \to \infty$ in this case. In this connection it will be noted that according to the present experimental findings on the scattering of elementary particles the total elastic cross section does not tend to zero at high energy but tends, perhaps, to a nonzero constant.[8] It is thus interesting that although this observed behavior of the total elastic cross section is prohibited in nonrelativistic potential scattering (with short-ranged potential) it is no longer prohibited when the correct relativistic expression for the free Hamiltonian is used instead of the corresponding nonrelativistic expression.

Aside from the above general remark we prove specific upperbounds on the high energy behaviour of total scattering cross section of "relativistic" as well as nonrelativistic potential scattering. The relationship of our results to comparable results found in the literature will be discussed in Sec. 4. Here we mention only that our upperbound on the total scattering section of the "relativistic potential scattering" is very close to the well-known Froissart bound

$$\sigma_{tot}(\epsilon) < C(\log\epsilon)^2 \quad \text{as } \epsilon \to \infty,$$

which is derived from the axioms of quantum field theory.[9] It seems significant that the upperbound of the type in question results also from a potential model of scattering. It suggests that such upperbounds do not, perhaps, depend in any essential manner on the axioms of field theory.

Finally, we mention that although the analysis of the present paper is limited to elastic scattering processes it can be extended to scattering systems with *complex potentials* which takes into account the existence of elastic as well as nonelastic processes. This will be the subject of a forthcoming paper.

2. PROPERTIES OF A CLASS OF OPERATOR VALUED INTEGRALS

In this section we shall formulate and prove a mathematical result (Theorem 1, below) which will serve as the key lemma in our subsequent discussions. It should be noted here that the part (ai) of this theorem is only a slight generalization of a well-known lemma due to Kato,[10] whereas the parts (aii) and (b) generalize a result due to Jauch, Sinha and Misra.[4] Although the proof of Theorem 1 is identical with that found in the cited references except for some minor notational modifications necessary to take into account the generalization we are considering, we give an outline of this proof for the sake of ready reference.

Before formulating Theorem 1, we need to recall a few facts about the representations of locally compact Abelian groups G in order to establish our terminology and notations.

Let G be a locally compact Abelian group. Its character group will then be denoted by $\hat{G}$. If x is a character of G [i.e., if x is a continuous function on G which satisfies $|x(g)| = 1; x(g_1)\,x(g_2) = x(g_1 g_2)$ for all $g_1 g_2 \in G$], then we shall write $\langle x, g\rangle$ to denote the value of the function x at the point g of G. It is clear that if g is held fixed and x runs over $\hat{G}$, then $\langle x, g\rangle$ defines a character of the dual group $\hat{G}$.

Now let $g \to U_g$ be a strongly continuous unitary representation of G which acts on the Hilbert space H. We recall that with every such representation of G there is associated a unique projection-valued measure $E(\cdot)$, defined on the Borel sets of $\hat{G}$ such that

$$(\phi, U_g \psi) = \int_{\hat{G}} \langle x, g\rangle\, d(\phi, E(\cdot)\psi)$$

for every $g \in G$ and all ψ and ϕ in H (SNAG theorem).

If for every ψ in H the numerical valued measure $\|E(\cdot)\psi\|^2$ is absolutely continuous with respect to the Haar measure on $\hat{G}$, then we shall say that the representation $g \to U_g$ of G is *absolutely continuous*. In the following we shall consider such absolutely continuous representations only.

Let $g \to U_g$ be an absolutely continuous representation of G in H. Then it is well known[11] that there exists a direct-integral representation

$$H = \int_{\hat{G}}^{\oplus} H_x\, dx$$

of H over the measure space $(\hat{G}, dx)$(with dx denoting the Haar measure on $\hat{G}$), such that in this representation the operators U_g (with $g \in G$) are represented by the multiplication operators with the function $\langle x, g\rangle$. Somewhat more explicitly, there exists a family H_x of Hilbert spaces labelled by characters x of G and a correspondence $\psi \to \psi_x$ between vectors ψ in H and vector valued functions ψ_x (with $\psi_x \in H_x$) on $\hat{G}$ such that

$$(\psi, \phi) = \int_{\hat{G}} (\psi_x, \phi_x)_x\, dx$$

for all ψ, ϕ in H; and

$$U_g \psi \to \langle x, g\rangle \psi_x$$

for every $g \in G$ and all ψ in H. Here $(\psi_x, \phi_x)_x$ denotes the scalar product in the Hilbert space H_x. The direct integral representation of H just described is said to "diagonalize" the given representation $g \to U_g$ of the group G.

Finally, we need to recall a last result which is concerned with the theory of Fourier transform of functions on locally compact Abelian groups. Let $f(g)$ denote a function on G. Its Fourier transform $\hat{f}$ (when it exists) is a function on $\hat{G}$ which is defined by

$$\hat{f}(x) = \int_G \langle x, g\rangle f(g)\, dg.$$

Here dg denotes the Haar measure on G. It is known from Fourier–Plancherel theory (see Ref. 12) that if f_1 and f_2 are two square integrable functions on G with respect to its Haar measure, then their Fourier transforms $\hat{f}_1$ and $\hat{f}_2$ exist and are square integrable with respect to the Haar measure on $\hat{G}$. Moreover, if the Haar measures on G and $\hat{G}$ are suitably normalized relative to each other then the Parseval's *identity*

$\int \bar{f}_1(g) f_2(g)\, dg = \int_{\hat{G}} \bar{\hat{f}}_1(x) \hat{f}_2(x)\, dx$ holds.

By Haar measures on G and $\hat{G}$ we shall henceforward mean such normalized Haar measures.

With the above preliminary remarks out of the way we can now formulate

Theorem 1: Let $g \to U_g$ denote an absolutely continuous representation (in the Hilbert space H) of the locally compact Abelian group G and let the correspondence $\psi \to \psi_x$ yield the direct integral representation of H

$$H = \int_{\oplus \hat{G}} H_x\, dx$$

which diagonalizes the representation $g \to U_g$. Let D denote the set of all ψ in H for which

$$M_\psi = \operatorname*{ess.\,sup}_{x \in \hat{G}} \|\psi_x\|_x < \infty.$$

Then,

(a) For every nuclear operator T in H

(i) $B_T(\psi, \phi) = \int_G (\psi, U_g^* T U_g \phi)\, dg < \infty$ for all $\psi, \phi \in D$.

Moreover, for almost all $x \in \hat{G}$, there exists nuclear operators $Q_T(x)$ acting in H_x such that

(ii) $B_T(\psi, \phi) = \int_{\hat{G}} (\psi_x, Q_T(x)\phi_x)_x\, dx$ for all $\psi, \phi \in D$.

The family $Q_T(x)$ is essentially unique in the sense that if $Q_T'(x)$ is another family of nuclear operators satisfying (aii), then $Q_T(x) = Q_T'(x)$ for a.a. $x \in \hat{G}$.

(b) Furthermore, the following relations hold:

(i) $\mathrm{Tr}T = \int_{\hat{G}} \mathrm{Tr} Q_T(x)\, dx$,

(ii) $\int_{\hat{G}} \|Q_T(x)\|_1 dx \le \|T\|_1$.

Proof: The first step in the proof consists of a direct verification of the claims of the theorem for operators of rank one. Such an operator T is of the general form

$$Tf = \lambda(u, f)v, \quad f \in H, \tag{2.1}$$

where λ is a fixed positive number and u and v are two normalized vectors. We write symbolically

$$T = \lambda(u, \cdot)v.$$

For operators T of the form (2.1) we have

$$\int_G (\psi, U_g^* T U_g \phi)\, dg = \lambda \int_G (u, \phi_g)(\psi_g, v)\, dg, \tag{2.2}$$

where $\phi_g = U_g \phi$ and $\psi_g = U_g \psi$.

Since (u, ϕ_g) is the Fourier transform of $(u_x, \phi_x)_x$ which belongs to $L^2(\hat{G}, dx)$ whenever $\phi \in D$, (u, ϕ_g) is square integrable on G, and so is (v, ψ_g) for $\psi \in D$. It follows that the integral (2.2) is finite and an application of Parseval identity yields

$$\int_G (\psi, U_g^* T U_g \phi)\, dg = \lambda \int_{\hat{G}} (u_x, \phi_x)_x (\psi_x, v_x)_x\, dx = \int_{\hat{G}} (\psi_x, Q_T(x)\phi_x)_x\, dx,$$

where we have defined $Q_T(x) = \lambda(u_x, \cdot)_x v_x$ on H_x.

We verify now the properties (bi) and (bii):

From $\mathrm{Tr} Q_T(x) = \lambda(u_x, v_x)_x$ follows the relation

$$\int_{\hat{G}} \mathrm{Tr} Q_T(x)\, dx = \lambda(u, v) = \mathrm{Tr}T$$

and from $\|Q_T(x)\|_1 = \lambda \|u_x\|_x \|v_x\|_x$ the relation

$$\int_{\hat{G}} \|Q_T(x)\|_1\, dx = \lambda \int_{\hat{G}} \|u_x\|_x \|v_x\|_x\, dx \le \lambda \|u\| \|v\| = \|T\|_1.$$

We have thus verified all claims of Theorem 1 for operators of rank one [except the claim of essential uniqueness of the family $Q_T(x)$]. This result then immediately extends to all operators T of finite rank whose general form is

$$T = \sum_{i=1}^{n} \lambda_i (u^i, \ )v^i, \quad n < \infty, \tag{2.3}$$

where λ_i are fixed positive numbers and u^i and v^i are two finite systems of orthonormal vectors. The corresponding $Q_T(x)$ are given by

$$Q_T(x) = \sum_{i=1}^{n} \lambda_i (u_x^i, \cdot)_x v_x^i. \tag{2.4}$$

Finally, an arbitrary nuclear operator can be written in the canonical form

$$T = \lim_{n \to \infty} \sum_{i=1}^{n} \lambda_i (u^i, \cdot) v^i = \lim_{n \to \infty} T_n, \tag{2.5}$$

where λ_i is a sequence of positive numbers with $\sum_{i=1}^{\infty} \lambda_i < \infty$ and u^i and v^i are two orthonormal sets in H. The limit in (2.5) may be understood to be in either strong operator topology, operator-norm topology or trace-norm topology.

In order to verify part a(i) of the theorem for an arbitrary nuclear operator, we observe that

$$(\psi, U_g^* T U_g \phi) = \lim_{n \to \infty} (\psi, U_g^* T_n U_g \phi),$$

and the functions $(\psi, U_g^* T_n U_g \phi)$ are majorized by

$$|(\psi, U_g^* T_n U_g \phi)| \le \sum_{i=1}^{\infty} \lambda i\, |(u^i, \phi_g)| |(\psi_g, v^i)| \equiv F(g).$$

$F(g)$ is itself the limit of the monotone increasing sequence of positive functions

$$F_n(g) \equiv \sum_{i=1}^{n} \lambda^i |(u^i, g)|\, |(\psi_g, v^i)|.$$

Now, using again Schwartz inequality and Parseval identity, one establishes that

$$\int_G F_n(g) dg \le \left(\sum_{i=1}^{\infty} \lambda i \right) M_\phi M_\psi \quad \text{for } \phi, \psi \in D.$$

Thus, $F(g)$ is integrable according to the monotone convergence theorem, and we conclude from the dominated convergence theorem that

$$\int_G (\psi, U_g^* T U_g \phi)\, dg = \lim_{n \to \infty} \int_G (\psi, U_g^* T_n U_g)\, dg < \infty. \tag{2.6}$$

To verify part a(i) of the theorem for a general nuclear operator, we first show that in the trace-norm topology

$$\lim_{n \to \infty} Q_{T_n}(x) = Q_T(x) \quad \text{exists for a.a. } x \in \hat{G}.$$

To this end we consider the monotone increasing sequence of positive functions on $\hat{G}$,

$$K_n(x) = \sum_{i=1}^{n} \lambda_i \|u_x^i\|_x \|v_x^i\|_x.$$

Clearly the integrals $\int_{\hat{G}} K_n(x)dx$ are bounded by $\sum_{i=1}^{\infty} \lambda i$. Therefore, according to Beppo Levi's theorem, $K_n(x)$ converges a.e. in $\hat{G}$ to an integrable function, say, $K(x)$.

Now, for $n' > n$, one has

$$\|Q_{T_{n'}}(x) - Q_{T_n}(x)\|_1 \leq \sum_{i=n}^{n'} \lambda i \|u_x^i\|_x \|v_x^i\|_x = K_{n'}(x) - K_n(x)$$

which converges to zero as $n, n' \to \infty$ for a.e. x in $\hat{G}$.

This shows the existence of the trace-norm limit of $Q_{T_n}(x)$.

To conclude the proof of part (a) of the theorem, we have still to verify the equality (ii).

We notice that

$$|(\psi_x, Q_{T_n}(x)\phi_x)_x| \leq \sum_{i=1}^{n} \lambda i |(u_x^i, \phi_x)_x||(\psi_x, v_x^i)_x| \leq M_\phi M_\psi K(x).$$

Thus, the functions $(\psi_x, Q_{T_n}(x)\phi_x)_x$ are majorized by an integrable function, and consequently

$$\lim_{n\to\infty} \int_{\hat{G}} (\psi_x, Q_{T_n}(x)\phi_x)_x \, dx = \int_{\hat{G}} (\psi_x, Q_T(x)\phi_x) \, dx. \quad (2.7)$$

The desired equality follows from (2.6) and (2.7) and the fact that it holds for finite rank operators.

We now verify b(i) and b(ii) in the general case. We remark first that

$$\lim_{n\to\infty} \mathrm{Tr} T_n = \mathrm{Tr} T, \qquad \lim_{n\to\infty} \mathrm{Tr} Q_{T_n}(x) = \mathrm{Tr} Q_T(x),$$

$$\lim_{n\to\infty} \|Q_{T_n}(x)\|_1 = \|Q_T(x)\|_1$$

since all the involved operators converge in the respective trace-norm topologies.

We have b(i) since

$$\int \mathrm{Tr} Q_T(x) \, dx = \lim_{n\to\infty} \int \mathrm{Tr} Q_{T_n}(x) \, dx = \lim_{n\to\infty} \mathrm{Tr} T_n = \mathrm{Tr} T.$$

Here the first equality follows again from dominated convergence theorem since $|\mathrm{Tr} Q_{T_n}(x)| \leq \|Q_{T_n}(x)\|_1 \leq K(x)$ with $K(x)$ integrable.

We obtain b(ii) from the inequality

$$\int_{\hat{G}} \|Q_{T_n}(x)\|_1 dx \leq \|T_n\|_1 \leq \|T\|_1,$$

valid for all finite n and from an application of the Fatou lemma.

This completes the proof of all assertions of the theorem except the essential uniqueness of the family $Q_T(x)$.

If $Q_T'(x)$ is another family of nuclear operators such that

$$\int_{\hat{G}} (\psi_x, Q_T'(x)\phi_x)_x \, dx = \int_{\hat{G}} (\psi_x, Q_T(x)\phi_x)_x dx$$

for all ϕ and ψ in D,

then one has in particular,

$$\int_{\hat{G}} (\psi_x, Q_T'(x)\phi_x)_x \, b(x) \, dx = \int_{\hat{G}} (\psi_x, Q_T(x)\phi_x)_x b(x) \, dx$$

for all essentially bounded measurable functions $b(x)$ on $\hat{G}$, and for any $\phi, \psi \in D$. This implies

$$(\psi_x, Q_T'(x)\phi_x)_x = (\psi_x, Q_T(x)\phi_x)_x \quad \text{for a.a. } x \in \hat{G}$$

and all $\phi, \psi \in D$.

Thus,

$$Q_T'(x) = Q_T(x) \quad \text{for a.a. } x \in \hat{G},$$

since the vectors ψ_x and ϕ_x run over all the vectors in H_x as ψ and ϕ run over D.

3. NECESSARY AND SUFFICIENT CONDITIONS FOR THE DIFFERENCE OF THE RESOLVENTS OF TWO SELF-ADJOINT OPERATORS TO BE NUCLEAR

In this section we investigate the necessary and sufficient conditions for the difference of the resolvents of the total and the free Hamiltonian of a simple scattering system to be nuclear. Somewhat more specifically, we consider simple scattering systems that describe the scattering of spinless particles from local potentials. The Hilbert space of state vectors may thus be identified with the space $L^2(d^3\mathbf{p})$ of square integrable functions $\psi(\mathbf{p})$ of the three momentum variables $\mathbf{p}$ and the free Hamiltonian H_0 may be identified with the multiplication operator by a function $F(\mathbf{p})$

$$(H_0\psi)(\mathbf{p}) = F(\mathbf{p})\psi(\mathbf{p}) \quad \text{for all } \psi \in L^2(d^3\mathbf{p}), \qquad (3.1)$$

for which

$$\int_{R^3} |F(\mathbf{p})\psi(\mathbf{p})|^2 d^3\mathbf{p} < \infty.$$

The total Hamiltonian H will be of the form

$$H = H_0 + V(\mathbf{Q}), \qquad (3.2)$$

when $\mathbf{Q}$ denotes the usual position observables. They are the self-adjoint generators of the three-parameter unitary group U_λ,

$$(U_\lambda\psi)(\mathbf{p}) \equiv \psi(\mathbf{p} - \boldsymbol{\lambda}) \quad \text{for all } \psi \in L^2(d^3\mathbf{p}), \quad U_\lambda = e^{i\boldsymbol{\lambda}\cdot\mathbf{Q}}. \qquad (3.3)$$

It should be clear that the free and total Hamiltonians of both the "relativistic" as well as the nonrelativistic potential scattering are of the forms (3.1) and (3.2). The nonrelativistic case needs little comment. One has only to choose $F(\mathbf{p}) = |\mathbf{p}|^2/2m$.

For the "relativistic potential scattering", on the other hand, the free Hamiltonian H_R^0 is the multiplication operator [in $L^2(d^3\mathbf{p}/(|\mathbf{p}|^2 + m^2)^{1/2})$] by the function $(|\mathbf{p}|^2 + m^2)^{1/2}$ and the total Hamiltonian H_R is of the form $H_R = H_R^0 + V(\mathbf{Q}_{NW})$, where $\mathbf{Q}_{NW}$ is the well-known Newton–Wigner position operator [in $L^2(d^3\mathbf{p}/(|\mathbf{p}|^2 + m^2)^{1/2})$]. But it is evident that there exists a unitary mapping from $L^2(d^3\mathbf{p}/(|\mathbf{p}|^2 + m^2)^{1/2})$ on to $L^2(d^3\mathbf{p})$ which maps H_R^0 and H_R, respectively to the operators H_0 [with $F(\mathbf{p}) = (|\mathbf{p}|^2 + m^2)^{1/2}$] and H defined by (3.1) and (3.2). Thus, the free and total Hamiltonian of the "relativistic potential scattering" may also be taken to be of the form (3.1) and (3.2) with $F(\mathbf{p}) = (|\mathbf{p}|^2 + m^2)^{1/2}$ and all statements proved for H_0 [with $F(\mathbf{p}) = (|\mathbf{p}|^2 + m^2)^{1/2}$] and $H = H_0 + V(\mathbf{Q})$ will hold also for H_R^0 and $H_R \equiv H_R^0 + V(\mathbf{Q}_{NW})$.

With the preceding preliminary remarks out of the way, we now proceed to investigate the necessary and sufficient conditions for the difference of the resolvents of the self-adjoint operators of the forms (3.1) and (3.2) to be nuclear.

Our first proposition formulates such a *necessary* condition in terms of the asymptotic property of $F(\mathbf{p})$ at large $|\mathbf{p}|$.

Proposition 1: Let H_0 denote the (self-adjoint) operator of multiplication in $L^2(d^3\mathbf{p})$ by a continuous and positive function $F(\mathbf{p})$ for which there exist a constant $\alpha > 0$ such that[13] $\lim_{|\mathbf{p}|\to\infty}[F(\mathbf{p})/|\mathbf{p}|^\alpha] = 1$ and let H denote the self-adjoint operator $H_0 + V(\mathbf{Q})$, where $V(\mathbf{Q})(\neq 0)$ is assumed to be H_0-bounded with H_0-bound less than 1.[14] Then, for $R_z - R_z^0[z \in \rho(H) \Lambda \rho(H_0)]$ to be nuclear it is necessary that $\alpha > 3/2$.

Before proving Proposition 1, we remark that for the physically interesting case of potential scattering of a Klein–Gordon particle (i.e., a relativistic spinless particle) Proposition 1 yields immediately the

Corollary 1: For a Klein–Gordon particle in a local potential $V(\mathbf{Q}_{NW})$ the difference of the resolvents of the total and free Hamiltonian is *not nuclear* for any of the potentials $V(\mathbf{Q}_{NW})$ which is relatively bounded with respect to the free (relativistic) Hamiltonian H_R^0 with H_R^0-bound less than 1.

Now, a large class of physically interesting potentials, including the Yukawa potential

$$ge^{-\mu|\mathbf{Q}|}/|\mathbf{Q}| \quad \text{(for small } g\text{)},$$

can be shown to be H_R^0-bounded with H_R^0-bound less than 1. Thus, in relativistic potential scattering $R_z - R_z^0$ is precluded from being nuclear for a large class of physically interesting potentials. It is worth emphasizing that in this respect the potential scattering of a relativistic particle differs sharply from that of a nonrelativistic particle. In the latter case, it is known that $R_z - R_z^0$ is nuclear for a large class of potentials (cf. Ref. 5; see also Theorem 2 below).

We now turn to the *proof of Proposition 1.*

Since V is H_0-bounded with H_0-bound less than 1, it follows that $H = H_0 + V$ is self-adjoint on $D_{H_0}: D_H = D_{H_0}$ (cf. Ref. 1). This, in turn, implies that the operator $1 + VR_z^0$ is a bounded operator having a bounded inverse $(1 + VR_z^0)^{-1}$ and $R_z - R_z^0 = -R_z^0 V R_z^0 (1 + V R_z^0)^{-1}$. Hence $R_z - R_z^0$ is nuclear if and only if $R_z^0 V R_z^0$ is nuclear. It is, thus, sufficient to show that $R_z^0 V R_z^0$ is not nuclear unless $\alpha > 3/2$.

We shall now use part (a) of Theorem 1 to show that $R_z^0 V R_z^0$ is not nuclear unless $\alpha > 3/2$. Since the unitary operators U_λ defined by relation (3.3) provide an absolutely continuous representation of the additive group R^3, it follows that $R_z^0 V R_z^0$ is not nuclear unless

$$\int_{R^3} (\phi, U_\lambda R_z^0 V R_z^0 U_\lambda^* \phi)\, d^3\boldsymbol{\lambda} < \infty \tag{3.4}$$

for all $\phi \in L^2(d^3\mathbf{p})$ having essentially bounded Fourier transforms. In particular (3.4) must hold for all $\phi \in \mathcal{S}_\mathbf{p}$ for $R_z^0 V R_z^0$ to be nuclear. Here $\mathcal{S}_\mathbf{p}$ denotes the Schwartz space of infinitely differentiable and fast decreasing functions of $\mathbf{p}$. We now show that (3.4) holds for $\psi, \phi \in \mathcal{S}_\mathbf{p}$ only if $\alpha > 3/2$. To this end we need

Lemma 1: Let $z \in \rho(H_0)$ with $\mathrm{Re}\, z < 0$, and let R denote the set of all continuous functions $\phi(\mathbf{p})$ in $L^2(d^3\mathbf{p})$ for which

$$\lim_{|\mathbf{p}|\to\infty} |\mathbf{p}|^n \phi(\mathbf{p}) = 0 \quad \text{for all positive integers } n.$$

Then

$$\text{S-}\lim_{|\boldsymbol{\lambda}|\to\infty} |\boldsymbol{\lambda}|^\alpha U_\lambda R_z^0 U_\lambda^* \phi = \phi \quad \text{for all } \phi \in R.$$

A proof of Lemma 1 will be found in the Appendix. Now we assume its validity and use it to show that (3.4) holds [with z being a real point of $\rho(H_0)$ with $z < 0$] for all $\phi \in \mathcal{S}_\mathbf{p}$ only if $\alpha > 3/2$.

Since U_λ and V are both functions of $\mathbf{Q}$ and U_λ is unitary, it is clear that $U_\lambda V U_\lambda^* = V$.

By using this relation, the integrand of (3.4) can be rewritten in the form

$$(\phi, U_\lambda R_z^0 V R_z^0 U_\lambda^* \phi) = (1/|\boldsymbol{\lambda}|^{2\alpha})(\phi_\lambda, V\phi_\lambda), \tag{3.5}$$

where

$$\phi_\lambda = |\boldsymbol{\lambda}|^\alpha U_\lambda R_z^0 U_\lambda^* \phi.$$

Now according to Lemma 1

$$\text{S-}\lim_{|\boldsymbol{\lambda}|\to\infty} \phi_\lambda = \phi. \tag{3.6}$$

Moreover,

$$\begin{aligned}\|V(\phi_\lambda - \phi)\| &\le a\|H_0(\phi_\lambda - \phi)\| + b\|\phi_\lambda - \phi\| \\ &= a\|(|\boldsymbol{\lambda}|^\alpha U_\lambda R_z^0 U_\lambda^* - 1)H_0\phi\| + b\|\phi_\lambda - \phi\|. \end{aligned} \tag{3.7}$$

(The reader can easily verify that in the above all the involved vectors are in the domains of the relevant operators when $\phi \in \mathcal{S}_\mathbf{p}$.)

Here the first inequality merely expresses the assumption that V is the H_0-bounded, whereas the second equality follows owing to the fact that $H_0 \equiv F(\mathbf{p})$ and $U_\lambda R_z^0 U_\lambda^* = (F(\mathbf{p} - \boldsymbol{\lambda}) - z)^{-1}$ commute. Since $H_0\, \phi \in R$ when $\phi \in \mathcal{S}_\mathbf{p}$, the right-hand side of (3.7) tends to zero as $|\boldsymbol{\lambda}| \to \infty$ according to Lemma 1. Thus,

$$\text{s-}\lim_{|\boldsymbol{\lambda}|\to\infty} V\phi_\lambda = V\phi \quad \text{for } \phi \in \mathcal{S}_\mathbf{p}. \tag{3.8}$$

It thus follows from (3.5), (3.6) and (3.8) that for $z \in \rho(H_0)$ with z real and $z < 0$

$$(\phi, U_\lambda R_z^0 V R_z^0 U_\lambda^* \phi) \to (1/|\boldsymbol{\lambda}|^{2\alpha})(\phi, V\phi) \equiv C/|\boldsymbol{\lambda}|^{2\alpha}$$

as $|\boldsymbol{\lambda}| \to \infty$ for all $\phi \in \mathcal{S}_\mathbf{p}$, and this shows that if $C \equiv (\phi, V\phi) \neq 0$, then (3.4) can not hold unless $\alpha > 3/2$. Since there evidently exist $\phi \in \mathcal{S}_\mathbf{p}$ for which $(\phi, V\phi) \neq 0$ this establishes that $R_z - R_z^0$ [for real and negative z in $\rho(H) \Lambda \rho(H_0)$] is not of trace class unless $\alpha > 3/2$. But it is known that $R_z - R_z^0$ is of trace class for either all $z \in \rho(H)\Lambda\rho(H_0)$ or for none of these points. Hence, this completes the proof of Proposition 1.

In the next proposition we formulate another necessary condition for $R_z - R_z^0$ to be nuclear which is expressed in terms of the asymptotic behavior of the potential function $V(\mathbf{Q})$ at large $|\mathbf{Q}|$.

Proposition 2: Let the notations be the same as in Proposition 1. In addition to the assumptions of Proposition 1, assume further that:

(i) the function $F(\mathbf{p})$ is infinitely differentiable everywhere with the possible exception of isolated singularities;

(ii) the function $V(\mathbf{Q})$ is of the form

$$V = V_1 + V_2 \quad \text{with } V_1 \in L_2 \quad \text{and} \quad V_2 \in L^\infty;$$

(iii) there exists a constant $\gamma > 0$ such that $\lim_{|\mathbf{Q}|\to\infty} |\mathbf{Q}|^\gamma V(\mathbf{Q}) = C$, where C is any finite constant if $\gamma > 3$ and a *nonzero* constant if $\gamma \le 3$. Then, in order that $R_z - R_z^0(z \in \rho(H)\Lambda\rho(H_0)$ be nuclear, it is necessary that $\gamma > 3$.

Proof: Consider the unitary group $V_\lambda \equiv e^{i\boldsymbol{\lambda}\cdot\mathbf{p}}$ of space translation. As in the proof of Proposition 1 we

again conclude [from part (a) of Theorem 1] that $R_z - R_z^0$ is not nuclear unless

$$\int_{R^3}(\phi, V_\lambda R_z^0\, V R_z^0 V_\lambda^* \phi)\, d^3\lambda < \infty \tag{3.9}$$

for *all* $\phi \in \mathcal{S}_p$. Thus Proposition 2 will be established if we can exhibit a $\phi \in \mathcal{S}_p$ for which (3.9) does not hold unless $\gamma > 3$. Now choose a $\phi \in \mathcal{S}_p$ such that its support does not contain the points where $F(\mathbf{p})$ is not infinitely differentiable. We shall show that for such ϕ and a *real* $z \in \rho(H)\Lambda\rho(H_0)$

$$(\phi, V_\lambda R_z^0\, V R_z^0 V_\lambda^* \phi) \to \frac{C(\psi,\psi)}{|\lambda|^\gamma} \quad \text{as } |\lambda| \to \infty,$$

where $\psi \equiv R_z^0\phi$. (Since our assumptions imply that both H_0 and H are bounded from below, such real points exist.) This, then, leads to the desired conclusion.

Using the fact that V_λ commutes with R_z^0 and

$$V_\lambda V(\mathbf{Q}) V_\lambda^* = V(\mathbf{Q} + \lambda),$$

we obtain the equality

$$|\lambda|^\gamma (\phi, V_\lambda R_z^0\, V R_z^0 V_\lambda^* \phi) - C(\psi,\psi) = \int_{R^3}[\,|\lambda|^\gamma V(\mathbf{Q}+\lambda) - C]\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q} \tag{3.10}$$

where $\tilde\psi(\mathbf{Q})$ is the Fourier transform of $\psi(\mathbf{p}) \equiv (R_z^0\phi)(\mathbf{p}) = \phi(\mathbf{p})/F(\mathbf{p}) - z$.

To complete the proof, we have only to verify that the integral of (3.10) converges to zero as $|\lambda| \to \infty$. To this end we separate the integral (3.10) into the two integrals

$$\int_{R^3}[\,|\lambda|^\gamma V(\mathbf{Q}+\lambda) - C]\Theta_{|\lambda|/2}(\mathbf{Q})\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q} + \int_{|\mathbf{Q}|>|\lambda|/2}[\,|\lambda|^\gamma V(\mathbf{Q}+\lambda) - C]\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q}, \tag{3.11}$$

where $\Theta_{|\lambda|/2}(\mathbf{Q})$ is the characteristic function of the sphere

$$S_{|\lambda|/2} \equiv \{|\mathbf{Q}| < |\lambda|/2\}.$$

Now the first of these integrals converges to zero as $|\lambda| \to \infty$, since by our assumption the integrand tends to zero (pointwise) as $|\lambda| \to \infty$ and for a given $\epsilon > 0$ the absolute value of the integrand is bounded by the integrable function $(2^\gamma\epsilon + |C|(2^\gamma + 1))|\tilde\psi(\mathbf{Q})|^2$ for all $|\lambda|$ that are greater than a sufficiently large $\Lambda(\epsilon)$ independent of $\mathbf{Q}$.

As for the second integral of (3.11),

$$\int_{|\mathbf{Q}|>|\lambda|/2}[\,|\lambda|^\gamma V(\mathbf{Q}+\lambda) - C]\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q} \le \int_{|\mathbf{Q}|>|\lambda|/2}|\lambda|^\gamma |V(\mathbf{Q}+\lambda)|\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q} + \int_{|\mathbf{Q}|>|\lambda|/2}|C|\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q}.$$

The second integral of rhs evidently converges to zero as $|\lambda| \to \infty$. The first integral, on the other hand, satisfies the inequality

$$\int_{|\mathbf{Q}|>|\lambda|/2}|\lambda|^\gamma |V(\mathbf{Q}+\lambda)|\,|\tilde\psi(\mathbf{Q})|^2 d^3Q \le \int_{|\mathbf{Q}|>|\lambda|/2}|\lambda|^\gamma |V_1(\mathbf{Q}+\lambda)|\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q} + \int_{|\mathbf{Q}|>|\lambda|/2}|\lambda|^\gamma |V_2(\mathbf{Q}+\lambda)|\,|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q}.$$

But since $V_1 \in L_2$ and $V_2 \in L^\infty$, the first of the integral on the rhs of the above inequality is bounded by

$$|\lambda|^\gamma \|V_1\|_2 \Big(\int_{|\mathbf{Q}|>|\lambda|/2}|\tilde\psi(\mathbf{Q})|^4 d^3\mathbf{Q}\Big)^{1/2} \tag{3.12}$$

and the second integral is bounded by

$$|\lambda|^\gamma \|V_2\|_\infty \int_{|\mathbf{Q}|>|\lambda|/2}|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q}. \tag{3.13}$$

Since ϕ is assumed to have the property mentioned above, it follows that $\psi(\mathbf{p}) \equiv (R_z^0\phi)(\mathbf{p})$ and, hence also, $\tilde\psi(Q)$ are both in $\mathcal{S}$. Hence the integrals

$$\int_{|\mathbf{Q}|>|\lambda|/2}|\tilde\psi(\mathbf{Q})|^4 d^3\mathbf{Q} \quad \text{and} \quad \int_{|\mathbf{Q}|>|\lambda|/2}|\tilde\psi(\mathbf{Q})|^2 d^3\mathbf{Q}$$

both vanish, faster than any power of $|\lambda|$, as $|\lambda| \to \infty$. Thus (3.12) and (3.13) both tend to zero as $|\lambda| \to \infty$. And this completes the proof of Proposition 2.

Combining propositions (3.9) and (3.10), we find that for the difference of the resolvents of $H_0 = F(\mathbf{p})$ and $H = H_0 + V(\mathbf{Q})$ to be nuclear it is necessary that the kinematic energy H_0 increases, as a function of $\mathbf{p}$, faster than $|\mathbf{p}|^{3/2}$ at large $|\mathbf{p}|$ and the potential $V(\mathbf{Q})$ falls off to zero faster than $1/|\mathbf{Q}|^3$ for large $|\mathbf{Q}|$. The next proposition, which is a slight generalization of a known result,[5] shows that these conditions are also sufficient to insure the trace-class property of $R_z - R_z^0$.

Proposition 3: Let the assumptions and notations be the same as in Proposition 2. Assume further that $\alpha > 3/2$ and $\gamma > 3$. Then $R_z - R_z^0$ is nuclear for $z \in \rho(H)\Lambda(H_0)$.

Proof: In order to show that $R_z - R_z^0$ is nuclear if $\alpha > 3/2$ and $\gamma > 3$, it suffices (cf. Ref. 5) to prove that $V'R_z^0$ belongs to the Schmidt class, where V' is the multiplication operator by the function $V'(\mathbf{Q}) \equiv |V(\mathbf{Q})|^{1/2}$. According to our assumptions, $V(\mathbf{Q})$ belongs to $L^1(d^3Q)$ and, consequently, $V'(\mathbf{Q})$ belongs to $L^2(d^3Q)$.

In the Fourier transform representation V' acts as an integral operator with kernel $\tilde V'(\mathbf{p} - \mathbf{p}')$ where $\tilde V'(\mathbf{p})$ is the Fourier transformation of $V'(\mathbf{Q})$. It is a square integrable function since $V'(\mathbf{Q})$ is so. Now $V'R_z^0$ is an integral operator with kernel $\tilde V'(\mathbf{p} - \mathbf{p}')[1/F(\mathbf{p}') - z]$.

We notice that the function $[1/F(\mathbf{p}') - z]$ is also square integrable when $\alpha > 3/2$. If we consider $|\tilde V'(\mathbf{p})|^2$ and $|[1/F(\mathbf{p}') - z]|^2$ as two L^1 functions, the well-known inequality $\|f * g\|_1 \le \|f\|_1 \|g\|_1$ for the L^1 norm of the convolution of L^1 function yields, in our case,

$$\iint d^3p d^3p' \Big|\tilde V(\mathbf{p} - \mathbf{p}')\frac{1}{F(\mathbf{p}') - z}\Big|^2 \le \int d^3p \,\big|\tilde V'(\mathbf{p})\big|^2 \int d^3p' \Big|\frac{1}{F(\mathbf{p}') - z}\Big|^2 < \infty.$$

Therefore, the kernel representing the operator $V'R_z^0$ is square integrable and $V'R_z^0$ belongs to the Schmidt class. This concludes the proof of the Proposition 3.

If we combine propositions 1, 2 and 3 we find a complete characterization of the class of free Hamiltonians $H_0 = F(\mathbf{p})$ and the potentials $V(\mathbf{Q})$ for which $R_z - R_z^0$ is nuclear.

Theorem 2: Let the assumptions and notations be as in Proposition 2. Then $R_z - R_z^0$ is nuclear if and only if $\alpha > 3/2$ and $\gamma > 3$.

In the next section we shall see that the trace-class property of the operators $R_z^\beta\, V R_z^{0\beta}$ ($\beta > 0$) implies specific conclusions about the asymptotic behaviour of total scattering cross sections at high energy. We shall, therefore, conclude this section by mentioning certain conditions which ensure $R_z^\beta\, V R_z^{0\beta}$ to be nuclear.

It may be observed, first, that by a slight modification of the arguments employed in the proof of Propositions 1, 2 and 3, and that given in the Appendix, one can easily establish

Proposition 4: Let the notations and assumption be the same as in Propositions 1 and 2. Then $R_z^{0\beta} V R_z^{0\beta}$ (with $\beta > 0$) is nuclear if and only if $\alpha \cdot \beta > 3/2$ and $\gamma > 3$. (Since we are considering in general nonintegral powers of R_z^0, $R_z^{0\beta}$ should be suitably defined. Here and in the following we consider real and negative z so that R_z^0 is a positive self-adjoint operator. $R_z^{0\beta}$ may then be unambiguously defined by the functional calculus of R_z^0.)

Proposition 3 does not provide, however, any information about $R_z^\beta V R_z^{0\beta}$ when $\beta \neq 1$. For unlike the case with $\beta = 1$, the trace-class property of $R_z^\beta V R_z^{0\beta}$ does not in general follow from the corresponding property of $R_z^{0\beta} V R_z^{0\beta}$ when $\beta \neq 1$.

In order to conclude the trace-class property of $R_z^\beta V R_z^{0\beta}$ from that of $R_z^{0\beta} V R_z^{0\beta}$ it is, therefore, necessary to impose additional restrictions on H_0 and H. One such restriction is the requirement that, for a real and negative $c \in \rho(H) \Lambda \rho(H_0)$, $(H_0 - c)^\beta$ and $(H - c)^\beta$ have the same domain. It is easy to verify that under this condition the trace-class property of $R_c^\beta V R_c^{0\beta}$ follows from that of $R_c^{0\beta} V R_c^{0\beta}$. This result, together with the observation that if $R_c^\beta V R_c^{0\beta}$ is nuclear for some $\beta = \beta_0$ then it is so for all $\beta > \beta_0$, allows us to prove the following.

Proposition 5: Let the notations and assumptions be the same as in Proposition 2. Assume further that for a real and negative $c \in \rho(H) \Lambda \rho(H_0)$ $(H_0 - c)^\beta$ and $(H - c)^\beta$ have the same domain for $3/2\alpha \leq \beta < 3/2\alpha + \epsilon$, with ϵ being some positive number.

Then $R_z^\beta V R_z^{0\beta}$ is nuclear if and only if $\alpha\beta > 3/2$ and $\gamma > 3$. (Since the assumption concerning the domains of $(H_0 - c)^\beta$ and $(H - c)^\beta$ is not easily verifiable, it will be desirable to prove this result without such assumptions. Unfortunately, we are not able to do so at present.)

This proposition implies that in the relativistic case $[H_0 = (|\mathbf{p}|^2 + m^2)^{1/2}] R_c^\beta V R_c^{0\beta}$ is nuclear if $\beta > 3/2$ and $\gamma > 3$, whereas for the nonrelativistic situation $R_c^\beta V R_c^{0\beta}$ is nuclear if $\beta > 3/4$ and $\gamma > 3$. We shall see in the next section that this difference in the property of $R_z^\beta V R_z^{0\beta}$ in the relativistic and nonrelativistic case results in different asymptotic behavior of total cross sections in these two cases.

4. ASYMPTOTIC BEHAVIOR OF SCATTERING CROSS SECTION AT HIGH ENERGY

The mathematical results of the preceding sections will be used now to derive specific asymptotic behavior of the total scattering cross section of potential scattering.

For this we follow the analysis of Jauch and Sinha[3] and prove

Proposition 6: Let the self-adjoint operators H_0 and H represent (respectively) the free and the total Hamiltonian of a simple scattering system (i.e., let H_0 and H satisfy the usual asymptotic and completeness conditions of single-channel scattering theory[15]. Assume further that both H_0 and H are bounded from below; H_0 has absolutely continuous spectrum and $D_H = D_{H_0}$. If in addition $R_c^\beta(H - H_0)R_c^{0\beta}$ (with c a real and negative point of $\rho(H) \Lambda \rho(H_0)$] is nuclear for some given $\beta > 0$, then

$$\int_0^\infty \frac{\sigma_{\text{tot}}(\epsilon)\,|\mathbf{k}|^2}{(\epsilon - c)^{2\beta}} d\epsilon < \infty,$$

where $\sigma_{\text{tot}}(\epsilon)$ denotes the total scattering cross section at energy ϵ and $|\mathbf{k}|^2$ denotes the momentum square of the particle whose free (kinematic) energy is ϵ.

Proof: Under the stated assumption one proves that (cf. Ref. 16)

$$(\phi, T\psi) = -i \int_{-\infty}^{\infty} (\phi, e^{iH_0 t} \Omega_-^* V e^{iH_0 t} \psi) dt \tag{4.1}$$

for all $\phi \in H$ and all $\psi \in D_{H_0} = D_H$.

Here

$$\Omega_\mp \equiv \underset{t \to \pm\infty}{\text{s-lim}} e^{iHt} e^{-iH_0 t}; \quad V = H - H_0$$

and $T = S - I$ with S being the scattering operator $\Omega_-^* \Omega_+$. Relation (4.1) in conjunction with the intertwining property of Ω_-^* then yields

$$(\phi, R_c^{0\beta} T R_c^{0\beta} \psi) = -i \int_{-\infty}^{\infty} (\phi, e^{iH_0 t} \Omega_-^* R_c^\beta V R_c^{0\beta} e^{-iH_0 t} \psi), \tag{4.2}$$

which holds for all ϕ and ψ in some suitable dense manifold D. (D may be taken to be, for instance, the set of all ψ for which $\|\psi_\epsilon\|$ as functions of ϵ are continuous functions with compact support; here ψ_ϵ denotes, of course, the "components" of ψ in the Hilbert space H_ϵ appearing in the direct integral representation $H = \int_\oplus H_\epsilon d\epsilon$ which "diagonalizes" the operator H_0.) Since S and, therefore, T commutes with H_0, there exist the reduced "energy shell" operators S_ϵ and T_ϵ acting in the Hilbert spaces H_ϵ of the direct integral representation of H

$$H = \int_\oplus H_\epsilon d\epsilon$$

in which H_0 is "diagonalized". We have

$$T_\epsilon = S_\epsilon - I_\epsilon$$

and

$$(\phi, R_c^{0\beta} T R_c^{0\beta} \psi) = \int_0^\infty \frac{(\phi_\epsilon, T_\epsilon \psi_\epsilon)}{(\epsilon - c)^{2\beta}} d\epsilon.$$

On the other hand, since $R_c^\beta V R_c^{0\beta}$ is assumed to be nuclear and the operators $e^{iH_0 t}$ constitute an absolutely continuous representation of the additive group of real line, it follows from Theorem 1 that the right-hand side of (4.2) is of the form

$$\int_0^\infty (\phi_\epsilon, \tau_\epsilon \psi_\epsilon) d\epsilon$$

when τ_ϵ is a family of nuclear operators acting on H_ϵ. Relation (4.2) then implies (owing to the essential uniqueness of the family τ_ϵ) $\tau_\epsilon = T_\epsilon/(\epsilon - c)^{2\beta}$ for a.a. ϵ. Thus, from Theorem 1, we conclude

$$\int_0^\infty \frac{\text{Tr}_\epsilon T_\epsilon}{(\epsilon - c)^{2\beta}} d\epsilon = \text{Tr} \Omega_-^* R_c^\beta V R_c^{0\beta} < \infty.$$

In particular,

$$2\text{Re} \int \frac{\text{Tr}_\epsilon T_\epsilon}{(\epsilon - c)^{2\beta}} d\epsilon = \int \frac{\text{Tr}_\epsilon (T_\epsilon + T_\epsilon^*)}{(\epsilon - c)^{2\beta}} d\epsilon < \infty. \tag{4.3}$$

The desired relation then follows by relating $\text{Tr}_\epsilon(T_\epsilon + T_\epsilon^*)$ to $\sigma_{\text{tot}}(\epsilon)$ with the aid of the optical theorem. In fact the unitarity of S implies that

$$T_\epsilon + T_\epsilon^* = -T_\epsilon^* T_\epsilon \quad \text{for a.a. } \epsilon,$$

so that

$$\text{Tr}_\epsilon(T_\epsilon + T_\epsilon^*) = -\|T_\epsilon\|_{2\epsilon}^2$$

where $\| \ \|_2$ denotes the Hilbert–Schmidt norm of operators. But it is well known that $\|T_\epsilon\|_{2\epsilon}^2 = \sigma_{tot}(\epsilon)|\mathbf{k}|^2$ except for a constant factor. Relation (4.3) is thus equivalent to the desired relation

$$\int_0^\infty \frac{\sigma_{tot}(\epsilon)|\mathbf{k}|^2}{(\epsilon - c)^{2\beta}} d\epsilon < \infty. \tag{4.4}$$

It is clear that if $\sigma_{tot}(\epsilon)$ is continuous in ϵ and monotone for large ϵ, as is usually the case for scattering systems encountered in physics, then (4.4) implies specific asymptotic behavior for $\sigma_{tot}(\epsilon)$. In fact, for the nonrelativistic case where $\epsilon = |\mathbf{k}|^2/2m$ (4.4) implies

$$\frac{\sigma_{tot}(\epsilon)\epsilon}{(\epsilon - c)^{2\beta-1}} \simeq \frac{\sigma_{tot}(\epsilon)}{\epsilon^{2\beta-2}} \to 0 \quad \text{as } \epsilon \to \infty, \tag{4.5}$$

whereas in the relativistic case for which $\epsilon = (|\mathbf{k}|^2 + m^2)^{1/2}$ we find

$$\frac{\sigma_{tot}(\epsilon)\epsilon^2}{(\epsilon - c)^{2\beta-1}} \approx \frac{\sigma_{tot}(\epsilon)}{\epsilon^{2\beta-3}} \to 0 \quad \text{as } \epsilon \to \infty. \tag{4.6}$$

In order to find the best asymptotic estimate of $\sigma_{tot}(\epsilon)$ we have to substitute in (4.5) and (4.6) the minimum values of β for which $R_c^\beta V R_c^{0\beta}$ is nuclear. Now, according to Proposition 5 of Sec. 3 the permissible values of β are:

(i) $\frac{3}{4} < \beta$ for the nonrelativistic potential scattering;

(ii) $\frac{3}{2} < \beta$ for the relativistic case. Thus for the nonrelativistic potential scattering we find the asymptotic behavior

$$\lim_{\epsilon\to\infty} \epsilon^{1/2-\delta}\sigma_{tot}(\epsilon) = 0 \quad (\text{for any } \delta > 0) \tag{A_{NR}},$$

whereas in relativistic potential scattering we find only

$$\lim_{\epsilon\to\infty} \frac{\sigma_{tot}(\epsilon)}{\epsilon^\delta} = 0 \quad (\text{for any } \delta > 0) \tag{A_R}.$$

It should be emphasized that in our analysis the difference between the asymptotic behaviour A_{NR} and A_R is solely the result of the difference in the relativistic and nonrelativistic kinematics of free particles expressed by the differing functional dependence of the free Hamiltonian on momenta. And this difference of A_{NR} and A_R does not point to any essential difference of the interactions which produces the scattering in the two cases.

We conclude this section with a few remarks about the relation of the asymptotic properties A_{NR} and A_R to comparable results found in the literature.

For nonrelativistic potential scattering with spherically symmetric potential $V(r)$ satisfying

$$\int_0^\infty V(r) r^2 dr < \infty,$$

one concludes from a study of the dispersion relations that[17]

$$\epsilon^{1/2}\sigma_{tot}(\epsilon) \to 0 \text{ as } \epsilon \to \infty.$$

Thus, our result A_{NR} is a weaker version of this known result. Our method of proof, however, is independent of the known method. Although our method yields a weaker result for nonrelativistic potential scattering it has the advantage of being applicable to relativistic potential scattering as well.

As regards A_R, it seems that no such result has been rigorously established in the literature for relativistic potential scattering. It may be compared, however, with the well-known Froissart bound

$$\sigma_{tot}(\epsilon) < c(\log\epsilon)^2 \quad \text{as } \epsilon \to \infty \ (F),$$

which has been derived from the postulates of quantum field theory.[8]

The result A_R is, of course, weaker than (F) in two respects:

(1) Since our analysis in this paper is limited to simple scattering systems, the asymptotic property A_R refers to *elastic* cross section only, whereas the bound (F) applies to the total (i.e., elastic + nonelastic) cross section. As mentioned in the Introduction, we shall remedy this deficiency in a forthcoming publication where we extend the analysis of the present paper to scattering processes with *complex optical potentials*.

(2) Aside from the above, A_R is also a weaker result than (F) since an upper bound of the type

$$\sigma_{tot}(\epsilon) < c\,(\log\epsilon)^n \quad \text{as } \epsilon \to \infty$$

is consistent with A_R for any positive integer n, whereas Froissart bound specifies n to be 2.

APPENDIX

We demonstrate Lemma 1 stated at the beginning of the proof of the Proposition 1.

Proof of Lemma 1: Since $U_\lambda F(\mathbf{p})U_\lambda^* = F(\mathbf{p} - \boldsymbol{\lambda})$, one has

$$\| |\boldsymbol{\lambda}|^\alpha U_\lambda R_z^0 U_\lambda^* \phi - \phi \|^2 = \int \left| \frac{|\boldsymbol{\lambda}|^\alpha}{F(\mathbf{p} - \boldsymbol{\lambda}) - z} - 1 \right|^2 |\phi(\mathbf{p})|^2 d^3p. \tag{A1}$$

For fixed $\boldsymbol{\lambda}$, we integrate separately in (A1) over the sphere $S_{|\lambda|/2} = \{\mathbf{p} \mid |\mathbf{p}| \le |\boldsymbol{\lambda}|/2\}$ and over its exterior. Let $\Theta_{|\lambda|/2}(\mathbf{p})$ be the characteristic function of the sphere $S_{|\lambda|/2}$. We show that both parts converge to zero as $|\boldsymbol{\lambda}| \to \infty$.

(i) The integral over $S_{|\lambda|/2}$ reads

$$\int \left| \frac{|\boldsymbol{\lambda}|^\alpha}{F(\mathbf{p} - \boldsymbol{\lambda}) - z} - 1 \right|^2 \Theta_{|\lambda|/2}(\mathbf{p}) |\phi(\mathbf{p})|^2 d^3p. \tag{A2}$$

Its integrand converges pointwise to zero as $|\boldsymbol{\lambda}| \to \infty$ in view of the asymptotic behavior of $F(\mathbf{p})$. Moreover, for a given positive ϵ there exists a number Λ_ϵ such that

$$\left| \frac{|\boldsymbol{\lambda}|^\alpha}{F(\boldsymbol{\lambda})} \right| \le 1 + \epsilon \quad \text{for all } |\boldsymbol{\lambda}| \ge \Lambda_\epsilon.$$

We choose $|\boldsymbol{\lambda}| \ge 2\Lambda_\epsilon$ and obtain the following majorization (recall that $\mathrm{Re}z < 0$):

$$\begin{aligned}
\left| \frac{|\boldsymbol{\lambda}|^\alpha}{F(\mathbf{p} - \boldsymbol{\lambda}) - z} - 1 \right| \Theta_{|\lambda|/2}(\mathbf{p}) &\le \frac{|\boldsymbol{\lambda}|^\alpha}{|F(\mathbf{p} - \boldsymbol{\lambda}) - z|} \Theta_{|\lambda|/2}(\mathbf{p}) + 1 \\
&= \frac{|\boldsymbol{\lambda}|^\alpha}{\{[F(\mathbf{p} - \boldsymbol{\lambda}) - \mathrm{Re}z]^2 + (\mathrm{Im}z)^2\}^{1/2}} \Theta_{|\lambda|/2}(\mathbf{p}) + 1 \\
&\le \frac{|\boldsymbol{\lambda}|^\alpha}{F(\mathbf{p} - \boldsymbol{\lambda})} \Theta_{|\lambda|/2}(\mathbf{p}) + 1.
\end{aligned}$$

For $|\mathbf{p}| > |\boldsymbol{\lambda}|/2$ the first term of this last expression is zero, and for the $p \le |\boldsymbol{\lambda}|/2$, it is majorized by

$$\frac{|\lambda|^\alpha}{F(\mathbf{p}-\lambda)}\Theta_{|\lambda|/2}(\mathbf{p}) = \frac{|\mathbf{p}-\lambda|^\alpha}{F(\mathbf{p}-\lambda)}\frac{|\lambda|^\alpha}{|\mathbf{p}-\lambda|^\alpha} \leq (1+\epsilon)2^\alpha.$$

Since if $|\lambda| \geq 2\Lambda_\epsilon$ and $|\mathbf{p}| \leq |\lambda|/2$, one always has $|\mathbf{p}-\lambda| \geq |\lambda| - |\mathbf{p}| \geq |\lambda|/2 \geq \Lambda_\epsilon$. Therefore, for a given $\epsilon > 0$, the integrand in (A2) is bounded by the integrable function $(1 + (1+\epsilon)2^\alpha)|\phi(\mathbf{p})|^2$ for all $|\lambda|$ greater then the number $2\Lambda_\epsilon$ (which is independent of $\mathbf{p}$). The dominated convergence theorem implies that the part of the integral over $S_{|\lambda|/2}$ vanishes as $|\lambda| \to \infty$.

(ii) To evaluate the contribution of the exterior of $S_{|\lambda|/2}$, we consider the following inequality

$$\left|\frac{|\lambda|^\alpha}{F(\mathbf{p}-\lambda)-z} - 1\right| \leq \frac{|\lambda|^\alpha}{\{[F(\mathbf{p}-\lambda)-\mathrm{Re}z]^2 + (\mathrm{Im}z)^2\}^{1/2}} + 1 \leq \frac{|\lambda|^\alpha}{|\mathrm{Re}z|} + 1,$$

which is valid because $F(\mathbf{p})$ is positive and $\mathrm{Re}z < 0$.

We have now

$$\int_{|\mathbf{p}|>|\lambda|/2}\left|\frac{|\lambda|^\alpha}{F(\mathbf{p}-\lambda)-z} - 1\right|^2 |\phi(\mathbf{p})|^2 d^3\mathbf{p} \leq \left(\frac{\lambda^\alpha}{|\mathrm{Re}z|} + 1\right)^2 \int_{|\mathbf{p}|>|\lambda|/2} |\phi(\mathbf{p})|^2 d^3\mathbf{p}. \quad \text{(A3)}$$

If $\phi(\mathbf{p})$ belongs to R, the integral on rhs of (A3) vanishes faster than any power of $|\lambda|$ as $|\lambda| \to \infty$. And this concludes the proof of the lemma.

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Properties of matrix representations of $SU(3)$*

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Matrices representing the Lie algebra of $SU(3)$ can also serve as Clebsch–Gordan coefficients for the direct product of the basis states of the representation times their adjoints. This fact enables us to obtain a number of properties, both general and specific, of $SU(3)$ matrices. To carry out our program we develop a general formula for constructing a symmetric tensor of rank $(n+1)$ from the product of a tensor of rank n times an octet. We then deduce some general properties concerning the multiplicity of representations contained in the direct product of a representation and its adjoint. In the specific cases of the six- and ten-dimensional representations we obtain the characteristic equation for the $SU(3)$ matrices, and for the 27-dimensional representation we obtain other properties. We also compute the traces of products of two, three, and four matrices in any representation.

1. INTRODUCTION

There are two ways of looking at matrix representations of a Lie algebra: either as sets of matrices obeying the commutation rules of the algebra or as Clebsch–Gordan coefficients for the basis states of representations and their adjoints. The first viewpoint certainly gives us the tools with which to determine the properties of all representations of the algebra, but there are times when the second viewpoint is actually more convenient. This is particularly true of properties which are special to one representation and do not have simple counterparts in other representations, for example the anitcommutator of two matrices. Here we shall study this kind of property for the algebra of $SU(3)$.

The essential point we want to make is that the Clebsch–Gordan series for a representation times its adjoint can be used to deduce properties of the matrices that span the representation. If, for example, a certain representation does not appear in the Clebsch–Gordan series, then any combination of matrices corresponding to that representation must vanish. If a particular representation occurs only once in the series, then all combinations corresponding to it must be proportional to one another. Symmetry or antisymmetry under the exchange of the original representation and its adjoint also carry definite implications for the matrices.

To develop the point more precisely, we suppose that the $(n \times n)$ Hermitian matrices $B_\alpha (\alpha = 1, 2, \ldots, 8)$ obey the $SU(3)$ commutation rules[1]

$$[B_\alpha, B_\beta] = if_{\alpha\beta\gamma} B_\gamma \tag{1.1}$$

and that the state vectors $\psi_a (a = 1, \ldots, n)$ transform according to this representation under the action of abstract $SU(3)$ generators T_α:

$$\begin{aligned} [T_\alpha, T_\beta] &= if_{\alpha\beta\gamma} T_\gamma, \\ [T_\alpha, \psi_a] &= \psi_b (B_\alpha)_{ba}. \end{aligned} \tag{1.2}$$

The representation adjoint to B_α is given by the negative transpose of B_α,

$$\bar{B}_\alpha = -B_\alpha^T, \tag{1.3}$$

and the corresponding basis vectors $\bar{\psi}_a (a = 1, 2, \ldots, n)$ are such that

$$[T_\alpha, \bar{\psi}_a] = \bar{\psi}_b (\bar{B}_\alpha)_{ba} = -(B_\alpha)_{ab} \bar{\psi}_b. \tag{1.4}$$

Under the action of T_α, the product vector

$$\hat{R}_x = (R_x)_{ab} \psi_a \bar{\psi}_b, \tag{1.5}$$

where R_x is any $(n \times n)$ matrix, transforms according to the rule

$$\begin{aligned} [T_\alpha, \hat{R}_x] &= (R_x)_{ab} [\psi_c (B_\alpha)_{ca} \bar{\psi}_b + \psi_a \bar{\psi}_c (\bar{B}_\alpha)_{cb}] \\ &= [B_\alpha, R_x]_{ab} \psi_a \bar{\psi}_b. \end{aligned} \tag{1.6}$$

Thus the effect of the operator T_α upon the product vector $\hat{R}_x$ is governed by the commutator of the matrices B_α and R_x.

We can construct matrices R_x from the B_α themselves, from their dual matrices

$$\tilde{B}_\alpha = d_{\alpha\beta\gamma} B_\beta B_\gamma, \tag{1.7}$$

and from symmetrized products of two or more of these $SU(3)$ matrices. If R_x is one of the B_α, then, because of the commutation rules of Eqs. (1.1) and (1.7), the corresponding vector $\hat{R}_x$ behaves as a member of an octet. If R_x is a symmetric product of two B_α matrices, then $\hat{R}_x$ will be an admixture of (27)-plet, octet, and singlet; the last two components can be removed by adding suitable counter terms to R_x, and we are then left with a pure (27)-plet combination of ψ_a and $\bar{\psi}_b$. In a similar way, we can make (64)-plets, (125)-plets, and higher representations from $\psi_a \otimes \bar{\psi}_b$ by taking the R_x to be symmetrized products of three, four and more B_α and $\tilde{B}_\beta$ matrices.

This procedure for constructing R_x matrices of higher and higher rank can obviously go on *ad infinitum*, but at some point we reach the maximal representation contained in $\psi_a \otimes \bar{\psi}_b$. The next step in the procedure then takes us to a representation that does not exist for the particular vectors under consideration, and the only way to avoid a contradiction is for the corresponding R_x matrix to vanish. If, for example, the maximal representation is the $(k+1)^3$-fold one, the appropriate R_x is a symmetric product of k B_α matrices plus the counter terms necessary to remove lower representations; the R_x made from $(k+1)B_\alpha$ matrices plus counter terms corresponds to the $(k+2)^3$-fold representation, and so it must vanish in this case.

It is also possible to construct other R_x matrices for the $(k+1)^3$-fold representation by replacing one or more B_α by the dual $\tilde{B}_\alpha$. Now the maximal representation occurs once and only once in the Clebsch–Gordan series: consequently, these other ways of constructing it must all be equivalent to the first one, and the various R_x matrices must be proportional to one another. The same argument applies to any representation that occurs fewer times in the Clebsch–Gordan series than there are ways of making it from B_α and $\tilde{B}_\alpha$.

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The vanishing of R_x matrices which correspond to representations not contained in $\psi_a \otimes \bar{\psi}_b$, and the proportionality of others corresponding to representations that are unique both provide us with relations between products of B_α matrices. In the product $3 \otimes \bar{3}$, for example, the maximal representation is the octet, and so the combination of λ matrices corresponding to the (27)-plet must vanish:

$$\{\lambda_\alpha, \lambda_\beta\} - 2d_{\alpha\beta\gamma}\lambda_\gamma - \tfrac{4}{3}\delta_{\alpha\beta}I = 0. \tag{1.8}$$

In $8 \otimes 8$ the (27)-plet occurs only once, and so the appropriate combination of two F matrices must be proportional to the one obtained from two D matrices[2]; as a result we find that

$$\{F_\alpha, F_\beta\} + 3\{D_\alpha, D_\beta\} = 2\delta_{\alpha\beta}I. \tag{1.9}$$

Furthermore, this (27)-plet is symmetric under the exchange of the two octets, and so the (27)-plet formed from one F and one D matrix must vanish because it is antisymmetric:

$$\{F_\alpha, D_\beta\} + \{F_\beta, D_\alpha\} - 2d_{\alpha\beta\gamma}F_\gamma = 0. \tag{1.10}$$

These results for the 3- and 8-dimensional representations are of course well known,[1,3] and they have been derived in other ways. Nevertheless, they do illustrate the point that we can use the Clebsch–Gordan series for $\psi_a \otimes \bar{\psi}_b$ to obtain properties of the corresponding $SU(3)$ matrices. Here we shall use this observation to determine the characteristic equations for matrices in the 6- and 10-dimensional representations, to obtain a general property of (27)-plet matrices, and to compute the traces of products of B_α matrices.

In the next section of the paper we discuss some general properties of $SU(3)$ matrices that hold in all representations. We also consider two special classes of representation: the triangular class in which the dual matrix $\tilde{B}_\alpha$ is proportional[4] to B_α; and the self-adjoint class in which $\bar{B}_\alpha$ is unitarily equivalent to B_α. The third section deals with the basic technical problem of the paper, namely the construction of tensors belonging to the (k, k) representation of $SU(3)$ from symmetrized products of B_α and $\tilde{B}_\beta$ matrices. We solve it inductively: that is, given a tensor of rank $(k-1)$, we show how to combine it with one B_α or $\tilde{B}_\beta$ to form a tensor of rank k. Our formula enables us to build second-rank tensors from the B_α and $\tilde{B}_\beta$ matrices, and then to use them to construct third-rank ones; after that we use the third-rank tensors to construct fourth-rank ones and so on. We also prove a general result concerning the number of times the (k, k) representation occurs in the direct product of a representation times its adjoint.

In the fourth section we show that the third-rank tensor must vanish for 6-dimensional B_α matrices, and that the fourth-rank tensor must vanish for 10-dimensional ones. From these conditions we then deduce the characteristic equations for B_α matrices in the 6- and 10-dimensional representations, respectively. In the fifth section we observe that the direct product of two (27)-plet vectors contains one symmetric and one antisymmetric (64)-plet, and from this we obtain some general properties of B_α matrices in that representation. Lastly, we note that tensors we construct must have zero trace, and this enables us to compute the traces of products of B_α and $\tilde{B}_\beta$ for all representations.

2. GENERAL PROPERTIES

Our object in discussing the general properties of $SU(3)$ matrices is to demonstrate that, in any representation, B_α and $\tilde{B}_\alpha$ form a complete set with respect to octets; that is, any other octet matrix, for example $d_{\alpha\beta\gamma}B_\beta\tilde{B}_\gamma$, can be expressed as a linear combination of B_α and $\tilde{B}_\alpha$. This result is neither surprising nor new,[5] but the specific formulas to which it gives rise will be very useful in our subsequent analysis.

By definition, the matrices B_α satisfy the commutation rules of Eq. (1.1):

$$[B_\alpha, B_\beta] = if_{\alpha\beta\gamma}B_\gamma.$$

That the dual vectors $\tilde{B}_\beta$ satisfy a similar commutation rule, namely

$$[B_\alpha, \tilde{B}_\beta] = if_{\alpha\beta\gamma}\tilde{B}_\beta, \tag{2.1}$$

follows from the definition of $\tilde{B}_\beta$ in Eq. (1.7) and the Jacoby identity

$$if_{imk}d_{jlk} + if_{ilk}d_{mjk} + if_{ijk}d_{lmk} = 0. \tag{2.2}$$

Equations (1.1) and (2.1) mean that B_β and $\tilde{B}_\beta$ both transform as octets under the action of B_α.

Because the structure coefficients if_{ijk} are antisymmetric under the exchange of adjacent indices, the B_α matrices commute with the two Casimir operators[5,6]

$$M_2 \equiv 2B_\alpha B_\alpha = \mathfrak{M}_2(\mu_1, \mu_2)I$$
and
$$M_3 \equiv 2B_\alpha\tilde{B}_\alpha \equiv 2d_{\alpha\beta\gamma}B_\alpha B_\beta B_\gamma = -\mathfrak{M}_3(\mu_1, \mu_2)I, \tag{2.3}$$

where I is the unit matrix. The eigenvalues $\mathfrak{M}_2$ and $\mathfrak{M}_3$ are functions of the characteristic numbers[7] (μ_1, μ_2) of the representation,

$$\mathfrak{M}_2(\mu_1, \mu_2) = \tfrac{1}{3}[\mu_1^2 + \mu_2^2 + (\mu_1 + \mu_2)^2 + 6(\mu_1 + \mu_2)],$$

$$\mathfrak{M}_3(\mu_1, \mu_2) = \tfrac{1}{9}(\mu_2 - \mu_1)[(\mu_1 + 2\mu_2)(\mu_2 + 2\mu_1) + 9(\mu_1 + \mu_2 + 1)], \tag{2.4}$$

and the dimension of the representation is given by[7]

$$D(\mu_1, \mu_2) = \tfrac{1}{2}(\mu_1 + 1)(\mu_2 + 1)(\mu_1 + \mu_2 + 2). \tag{2.5}$$

As a special case we note that in the octet $(\mu_1 = \mu_2 = 1)$ the B_α can be represented by the structure constants

$$(B_\alpha)_{ab} = (F_\alpha)_{ab} = -if_{\alpha ab} \tag{2.6}$$

and the quadratic Casimir operator then becomes

$$F_\alpha F_\alpha = 3I. \tag{2.7}$$

From the antisymmetry of the structure constants, we find that for any representation

$$if_{\alpha\beta\gamma}B_\beta B_\gamma = \tfrac{1}{2}if_{\alpha\beta\gamma}[B_\beta, B_\gamma] = -\tfrac{1}{2}(F_\beta F_\beta)_{\alpha\tau}B_\tau.$$

Therefore, using Eq. (2.7) we obtain

$$if_{\alpha\beta\gamma}B_\beta B_\gamma = -\tfrac{3}{2}B_\alpha. \tag{2.8}$$

By the same argument we can show that

$$if_{\alpha\beta\gamma}(B_\beta\tilde{B}_\gamma + \tilde{B}_\beta B_\gamma) = -3\tilde{B}_\alpha. \tag{2.9}$$

In order to separate the two terms on the left-hand side of Eq. (2.9), we use the definition of $\tilde{B}_\alpha$ in Eq. (1.7), the identity of Eq. (2.2), and the trace condition[3]

$$\mathrm{Tr}(F_\alpha F_\beta D_\gamma) = \tfrac{3}{2} d_{\alpha\beta\gamma} \quad [(D_\gamma)_{ab} = d_{\gamma ab}] \tag{2.10}$$

to write

$$\begin{aligned} if_{\alpha\beta\gamma} B_\beta \tilde{B}_\gamma &= if_{\alpha\beta\gamma} d_{\gamma\rho\tau} B_\beta B_\rho B_\tau \\ &= if_{\alpha\beta\gamma} \tilde{B}_\beta B_\gamma - \tfrac{3}{2} \tilde{B}_\alpha - if_{\alpha\beta\gamma} B_\beta \tilde{B}_\gamma. \end{aligned} \tag{2.11}$$

Combining Eqs. (2.9) and (2.11), we have

$$if_{\alpha\beta\gamma} B_\beta \tilde{B}_\gamma = if_{\alpha\beta\gamma} \tilde{B}_\beta B_\gamma = -\tfrac{3}{2} \tilde{B}_\alpha. \tag{2.12}$$

Before we consider the effect of multiplying $\tilde{B}_\beta \tilde{B}_\gamma$ by $if_{\alpha\beta\gamma}$, we need a result involving the $d_{\alpha\beta\gamma}$ coefficients. If we multiply both sides of the identity[3]

$$\begin{aligned} d_{ij\alpha} d_{kl\alpha} + d_{ik\alpha} d_{lj\alpha} + d_{il\alpha} d_{jk\alpha} \\ = \tfrac{1}{3}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \end{aligned} \tag{2.13}$$

by $B_i B_j B_k$, we obtain

$$2d_{lk\alpha} \tilde{B}_\alpha B_k - \mathrm{Tr}(D_l F_\rho D_i) B_i B_\rho + d_{lk\alpha} B_k \tilde{B}_\alpha = \tfrac{1}{2}(M_2 - I) B_l. \tag{2.14}$$

Now because[3]

$$\begin{aligned} &\mathrm{Tr}(D_i D_l F_\rho) = \tfrac{5}{6} if_{il\rho}, \\ &\mathrm{Tr}(D_l F_m) = 0, \end{aligned} \tag{2.15}$$

we find from Eq. (2.14) that

$$d_{lk\alpha} \tilde{B}_\alpha B_k = d_{lk\alpha} B_k \tilde{B}_\alpha = (\tfrac{1}{6}\mathfrak{M}_2(\mu_1, \mu_2) + \tfrac{1}{4}) B_l. \tag{2.16}$$

With the aid of this result and the identity in Eq. (2.2), we can now show that

$$\begin{aligned} if_{\alpha\beta\gamma} \tilde{B}_\beta \tilde{B}_\gamma &= if_{\alpha\beta\gamma} d_{\gamma\rho\tau} \tilde{B}_\beta B_\rho B_\tau \\ &= -\tfrac{1}{4}(\mathfrak{M}_2(\mu_1, \mu_2) + \tfrac{3}{2}) B_\alpha. \end{aligned} \tag{2.17}$$

Lastly, by multiplying Eq. (2.13) first by $B_i B_j \tilde{B}_k$ and then by $B_i B_j B_k B_l$ we obtain the two results

$$d_{lk\alpha} \tilde{B}_k \tilde{B}_\alpha = -\tfrac{1}{3}\mathfrak{M}_3(\mu_1, \mu_2) B_l - (\tfrac{1}{6}\mathfrak{M}_2(\mu_1, \mu_2) - \tfrac{1}{4}) \tilde{B}_l \tag{2.18}$$

and

$$\tilde{B}_\alpha \tilde{B}_\alpha = \tfrac{1}{4}(\tfrac{1}{3}\mathfrak{M}_2(\mu_1, \mu_2) + \tfrac{1}{2})\mathfrak{M}_2(\mu_1, \mu_2) I. \tag{2.19}$$

This completes our demonstration that all octet matrices must be linear combinations of B_α and $\tilde{B}_\alpha$.

The results obtained above are valid for all representations of $SU(3)$, but their forms for two particular classes of representation, namely the triangular and the self-adjoint, are of particular interest to us. In triangular representations one of the two characteristic numbers is zero and the dual matrix $\tilde{B}_\alpha$ is proportional[8] to B_α

$$\tilde{B}_\alpha = \begin{cases} \dfrac{(2\mu_1 + 3)}{6} B_\alpha, & \mu_2 = 0, \\ -\dfrac{(2\mu_2 + 3)}{6} B_\alpha, & \mu_1 = 0. \end{cases} \tag{2.20}$$

It is not difficult to show that all the formulas in Eqs. (2.9)–(2.19) are consistent with Eq. (2.20) when either μ_1 or μ_2 vanishes; the dimensions and quadratic Casimir eigenvalues are given by

$$D = \tfrac{1}{2}(\mu + 1)(\mu + 2), \quad \mathfrak{M}_2 = \tfrac{2}{3}\mu(\mu + 3), \quad \mu = \mu_1 \text{ or } \mu_2. \tag{2.21}$$

In self-adjoint representations the matrix B_α is unitarily equivalent to its adjoint B_α (see Eq. 1.3),

$$UB_\alpha U^{-1} = \overline{B}_\alpha = -B_\alpha^T \tag{2.22}$$

and the characteristic numbers are equal to one another:

$$\mu_1 = \mu_2 = \hat{\mu}. \tag{2.23}$$

Hammermesh[9] has given general arguments to the effect that the transformation matrix U of Eq. (2.22) must either be symmetric or antisymmetric; and that when it is symmetric the matrix B_α can be chosen in such a way as to be equal to its adjoint. Biedenharn, Nyuts, and Ruegg[10] have shown that for self-adjoint representations of $SU(3)$, the matrix U is indeed symmetric: we shall therefore assume that for these cases

$$B_\alpha = -B_\alpha^T. \tag{2.24}$$

Being Hermitian, B_α must be antisymmetric and pure imaginary, while its dual $\tilde{B}_\alpha$ is symmetric and real:

$$\tilde{B}_\alpha = \tilde{B}_\alpha^T = (\tilde{B}_\alpha)^*. \tag{2.25}$$

The best known examples of this type are the F_α and D_α matrices of the octet (1, 1) representation. As in the triangular case, so here the results in Eqs. (2.9)–(2.19) are consistent with Eqs. (2.23)–(2.25); in particular, the dimension of these representations are perfect cubes, and the cubic Casimir eigenvalue is zero:

$$D(\hat{\mu}, \hat{\mu}) = (\hat{\mu} + 1)^3, \quad \mathfrak{M}_3(\hat{\mu}, \hat{\mu}) = 0, \quad \mathfrak{M}_2 = 2\mu(\mu + 2). \tag{2.26}$$

3. SYMMETRIC TENSORS

We turn now to the construction of symmetric tensors from products of $SU(3)$ matrices. Since our method is an inductive one, we begin by discussing the general properties of an nth-rank tensor. We then show how to combine it with B_α or with $\tilde{B}_\alpha$ to form a tensor of rank $(n + 1)$, and we give examples of tensors constructed from products of two, three, and four B_α and $\tilde{B}_\alpha$ matrices. Finally, we show that the representation (n, n) cannot occur more than $(n + 1)$ times in the direct product of a representation and its adjoint.

A. The general tensor of rank n

Let $T_{i_1 i_2 \cdots i_n}$ denote a tensor of rank n which is symmetric under the exchange of any two indices:

$$T_{i_1 \cdots i_r \cdots i_s \cdots i_n} = T_{i_1 \cdots i_s \cdots i_r \cdots i_n}. \tag{3.1}$$

Under commutation with B_α, each index of the tensor behaves as if it were an octet [see Eqs. (1.1) and (2.1)],

$$\begin{aligned} [B_\alpha, T_{i_1 i_2 \cdots i_n}] &= if_{\alpha i_1 \lambda} T_{\lambda i_2 \cdots i_n} \\ &+ if_{\alpha i_2 \lambda} T_{i_1 \lambda \cdots i_n} + \cdots + if_{\alpha i_n \lambda} T_{i_1 i_2 \cdots \lambda} \end{aligned} \tag{3.2}$$

and so the quadratic Casimir commutator is given by

$$\begin{aligned} &2[B_\alpha, [B_\alpha, T_{i_1 i_2 \cdots i_n}]] \\ &= 2 \sum_{r=1}^{n} (F_\alpha F_\alpha)_{i_r \mu} T_{i_1 \cdots i_{r-1} \mu i_{r+1} \cdots i_n} \\ &- 2 \sum_{r<s} \{F_{i_r}, F_{i_s}\}_{\lambda\mu} T_{i_1 \cdots i_{r-1} \lambda \cdots \mu i_{s+1} \cdots i_n}, \end{aligned} \tag{3.3}$$

where $\sum_{r<s}$ denotes the sum over all pairs of indices with $r < s$ and includes $\frac{1}{2}n(n-1)$ terms. Because of

the results in Eqs. (1.9), (2.7), and (2.13), the left-hand side of Eq. (3.3) can be rewritten as

$$2n(n+2)T_{i_1 i_2 \cdots i_n} - 2\sum_{r<s}\delta_{i_r i_s}T_{i_1\cdots i_{r-1}\lambda\cdots\lambda i_{s+1}\cdots i_n} - 6\sum_{r<s}d_{i_r i_s \rho}d_{\rho\lambda\mu}T_{i_1\cdots i_{r-1}\lambda\cdots\mu i_{s+1}\cdots i_n}. \quad (3.4)$$

One way of ensuring that $T_{i_1 i_2 \cdots i_n}$ be an eigentensor of the Casimir commutator is to require

$$T_{i'_1\cdots i'_{n-2}\lambda\lambda} = d_{\rho\lambda\mu}T_{i'_1\cdots i'_{n-2}\lambda\mu} = 0 \quad (3.5)$$

for any subset $(i'_1 \cdots i'_{n-2})$ of $(n-2)$ indices chosen from the original set $(i_1 \cdots i_n)$. Since these conditions also ensure that $T_{i_1 i_2 \cdots i_n}$ is an eigentensor of the cubic Casimir commutator with zero as its eigenvalue (see the Appendix for details), we shall henceforth assume that they are indeed satisfied. The eigenvalue equations

$$2[B_\alpha,[B_\alpha,T_{i_1 i_2\cdots i_n}]] = 2n(n+2)T_{i_1 i_2\cdots i_n},$$
$$2d_{\alpha\beta\gamma}[B_\alpha,[B_\beta,[B_\gamma,T_{i_1 i_2\cdots i_n}]]] = 0 \quad (3.6)$$

then imply that the nth rank tensor transforms according to the representation (n,n) of $SU(3)$ [see Eq. (2.26)].

The conditions of Eq. (3.5) can be understood by noting that the totally symmetric product of n octets contains (n,n) as the maximal, but not the only, irreducible representation in its Clebsch–Gordan series[11]; for example, in the case $n=2$, the series contains a singlet and an octet as well as the (27)-plet. Equations (3.5) serve to eliminate all representations other than (n,n) from the tensor $T_{i_1 i_2\cdots i_n}$. They also have the following very useful consequence.

Consider the quantity

$$Q \equiv d_{\lambda\alpha\rho}d_{\mu\beta\rho}T_{i_1\cdots i_{n-2}\lambda\mu}. \quad (3.7)$$

Because the tensor is symmetric in λ and μ we can rewrite Q as

$$Q = \tfrac{1}{2}(d_{\lambda\alpha\rho}d_{\mu\beta\rho} + d_{\mu\alpha\rho}d_{\lambda\beta\rho})T_{i_1\cdots i_{n-2}\lambda\mu}. \quad (3.8)$$

Then, using the identity of Eq. (2.13) and the conditions of Eq. (3.5) we obtain

$$Q = \tfrac{1}{3}T_{i_1\cdots i_{n-2}\alpha\beta}. \quad (3.9)$$

There will be many opportunities to use this result in the calculations of the next subsection.

B. Constructing the tensor of rank $(n+1)$

To construct a tensor of rank $(n+1)$ which satisfies Casimir conditions equivalent to Eq. (3.6) with n replaced by $(n+1)$, we consider the product

$$\hat{T} = \sum_{c\cdot p(i_1\cdots i_{n+1})}T_{i_1\cdots i_n}C_{i_{n+1}}, \quad (3.10)$$

where the summation runs over all cyclic permutations of the indices $(i_1,\ldots,i_{n+1})$, and $C_{i_{n+1}}$ can be either $B_{i_{n+1}}$, or $\tilde{B}_{i_{n+1}}$, or any other octet matrix. After some manipulation like that used in Eqs. (3.3) and (3.4), we obtain the basic result

$$2[B_\alpha,[B_\alpha,\hat{T}]] = 2(n+1)(n+3)\hat{T} - 12\hat{L} - 4\hat{N}, \quad (3.11)$$

where

$$\hat{L} = \sum_{r<s}d_{i_r i_s \rho}d_{\rho\lambda\mu}T_{i'_1\cdots i'_{n-1}\lambda}C_\mu,$$
$$\hat{N} = \sum_{r<s}\delta_{i_r i_s}T_{i'_1\cdots i'_{n-1}\lambda}C_\lambda. \quad (3.12)$$

The sum $\sum_{r<s}$ runs over all pairs $(i_r i_s)$ with $r<s$ and it contains $\frac{1}{2}n(n+1)$ terms; the indices $(i'_1\ldots i'_{n-1})$ are those remaining when i_r and i_s have been removed from the original set.

If we multiply Eq. (3.11) by $\delta_{i_n,i_{n+1}}$, sum over all values of these indices, and make use of Eqs. (3.5) and (3.9) we find that

$$2[B_\alpha,[B_\alpha,T_{i_1\cdots i_{n-1}\lambda}C_\lambda]] = 2(n-1)(n+1)T_{i_1\cdots i_{n-1}\lambda}C_\lambda. \quad (3.13)$$

Consequently the quantity $\hat{N}$ of Eq. (3.12) is also an eigentensor of the Casimir operator:

$$2[B_\alpha,[B_\alpha,\hat{N}]] = 2(n^2-1)\hat{N}. \quad (3.14)$$

We now multiply Eq. (3.11) by $d_{i'_n i_n i_{n+1}}$, sum over all values of the indices (i_n, i_{n+1}), and then sum over all permutations of $(i_1,\ldots,i_{n-1},i'_n)$. With the aid of Eqs. (3.5) and (3.9), and of the identity (2.13) written in the form

$$\{D_i,D_j\}_{\alpha\beta} = -d_{ijk}(D_k)_{\alpha\beta} + \tfrac{1}{3}(\delta_{ij}\delta_{\alpha\beta} + \delta_{i\alpha}\delta_{j\beta} + \delta_{i\beta}\delta_{j\alpha}), \quad (3.15)$$

we obtain the result

$$2[B_\alpha,[B_\alpha,\sum_{c\cdot p(i_1\cdots i_n)}d_{i_n\lambda\mu}T_{i_1\cdots i_{n-1}\lambda}C_\mu]] = 2n(n+2)\sum_{c\cdot p(i_1\cdots i_n)}d_{i_n\lambda\mu}T_{i_1\cdots i_{n-1}\lambda}C_\mu - 4\sum_{r<s}d_{i_r i_s \tau}T_{i'_1\cdots i'_{n-2}\tau\lambda}C_\lambda, \quad (3.16)$$

where $(i'_1\cdots i'_{n-2})$ represents the indices remaining when i_r and i_s are removed from $(i_1\cdots i_n)$. Equations (3.16) and (3.13) imply that the tensor

$$\tilde{T}_{i_1\cdots i_n} = \sum_{c\cdot p(i_1\cdots i_n)}d_{i_n\lambda\mu}T_{i_1\cdots i_{n-1}\lambda}C_\mu - \frac{2}{(2n+1)}\sum_{r<s}d_{i_r i_s \tau}T_{i'_1\cdots i'_{n-2}\tau\lambda}C_\lambda \quad (3.17)$$

transforms according to the (n,n) representation of $SU(3)$:

$$2[B_\alpha,[B_\alpha,\tilde{T}_{i_1\cdots i_n}]] = 2n(n+2)\tilde{T}_{i_1\cdots i_n}. \quad (3.18)$$

To determine the effect of the Casimir commutator upon $\hat{L}$ we must multiply Eq. (3.11) by $d_{i'_n i'_{n+1}\rho}d_{\rho i_n i_{n+1}}$, sum over all values of i_n and i_{n+1}, and then sum over all permutations of $(i_1\cdots i_{n-1}i'_n i'_{n+1})$. In addition to Eqs. (3.5) and (3.9) we need an identity, namely

$$2\sum_{\substack{\text{all perms}\\(a\,b\,c)}}(D_aD_bD_c)_{\alpha\beta} = \sum_{c\cdot p(a\,b\,c)}[\delta_{ab}(D_c)_{\alpha\beta} + \tfrac{1}{3}\delta_{a\alpha}d_{bc\beta} + \tfrac{1}{3}\delta_{a\beta}d_{bc\alpha}] - d_{abc}\delta_{\alpha\beta}, \quad (3.19)$$

which can be proved by applying Eq. (3.15) to the double anticommutator $\sum_{c\cdot p(a\,b\,c)}\{D_a,\{D_b,D_c\}\}$. We then find that

$$2[B_\alpha,[B_\alpha,\hat{L}]] = 2(n^2+n+1)\hat{L} + 2\hat{M} - \tfrac{2}{3}(n-1)\hat{N}, \quad (3.20)$$

where

$$\hat{M} = \sum_{r<s<t} \sum_{c\cdot p(rst)} d_{i_r i_s \nu} d_{i_t \lambda \mu} T_{i'_1 \cdots i'_{n-2} \nu \lambda} C_\mu \quad (3.21)$$

and the summations in $\hat{M}$ involve $\frac{1}{2}(n+1)n(n-1)$ terms corresponding to the permutations $(i_r i_s i_t i'_1 \cdots i'_{n-2})$ of the original indices $(i_1 \cdots i_{n+1})$.

Multiplying Eq. (3.16) by $d_{i'_n i'_{n+1} i_n}$ and using the same techniques as in the case of $\hat{L}$, we have that

$$2[B_\alpha, [B_\alpha, \hat{M}]] = 2(n^2+2n-1)\hat{M} + 2(n-1)\hat{L} - \tfrac{2}{3}(n-1)\hat{N} - 8\hat{P}, \quad (3.22)$$

where

$$\hat{P} = \sum_{r<s<t<p} \sum_{c\cdot p(rst)} d_{i_r i_s \lambda} d_{i_t i_p \mu} T_{i_1 \cdots i'_{n-3} \lambda \mu \nu} C_\nu. \quad (3.23)$$

It follows from Eq. (3.13) that

$$2[B_\alpha, [B_\alpha, \hat{P}]] = 2(n^2-1)\hat{P}. \quad (3.24)$$

Putting all of these results together we can show that the $(n+1)$th-rank tensor defined by

$$T_{i_1 \cdots i_{n+1}} = \hat{T} - \frac{4(n+2)}{(n+1)(2n+3)}\hat{L} - \frac{2}{(n+1)(2n+3)}\hat{M} - \frac{(2n^2+6n+7)}{3(n+1)^2(2n+3)}\hat{N} + \frac{2}{(n+1)^2(2n+3)}\hat{P} \quad (3.25)$$

[where T, L, M, N, P are as in Eqs. (3.10), (3.12), (3.21), and (3.23)] is the desired eigentensor:

$$2[B_\alpha, [B_\alpha, T_{i_1 \cdots i_{n+1}}]] = 2(n+1)(n+3)T_{i_1 \cdots i_{n+1}}. \quad (3.26)$$

It is straightforward to demonstrate that

$$T_{i_1 \cdots i_{n-1} \lambda\lambda} = d_{\rho\lambda\mu} T_{i_1 \cdots i_{n-1}\lambda\mu} = 0 \quad (3.27)$$

and so, as shown in the Appendix, the cubic Casimir operator has zero as its eigenvalue:

$$d_{\alpha\beta\gamma}[B_\alpha, [B_\beta, [B_\gamma, T_{i_1 \cdots i_{n+1}}]]] = 0. \quad (3.28)$$

Thus $T_{i_1 \cdots i_{n+1}}$ transforms according to the $(n+1, n+1)$ representation of $SU(3)$.

C. Some second- and third-rank tensors

The simplest application of the formula for $T_{i_1 \cdots i_{n+1}}$ in Eq. (3.25) is to the case $n=1$, with the first-rank tensor T_{i_1} being either B_{i_1} or $\tilde{B}_{i_1}$. Since there are only two indices available and the quantities $\hat{M}$ and $\hat{P}$ require at least three and four, respectively [see Eqs. (3.21) and (3.23)], they do not come into play. The general formula then becomes

$$T_{i_1 i_2} = \hat{T} - \tfrac{6}{5}\hat{L} - \tfrac{1}{4}\hat{N}. \quad (3.29)$$

There are three basic choices for the pair of first-rank tensors (T_{i_1}, C_{i_2}):

$(T_{i_1}, C_{i_2}) = (B_{i_1}, B_{i_2})$:

$$T_{i_1 i_2} = \{B_{i_1}, B_{i_2}\} - \tfrac{6}{5} d_{i_1 i_2 \rho}\tilde{B}_\rho - \tfrac{1}{8}\mathfrak{M}_2 \delta_{i_1 i_2} I; \quad (3.30a)$$

$(T_{i_1}, C_{i_2}) = (\tilde{B}_{i_1}, B_{i_2})$:

$$T_{i_1 i_2} = \tilde{B}_{i_1} B_{i_2} + \tilde{B}_{i_2} B_{i_1} - \tfrac{1}{10}(2\mathfrak{M}_2 + 3) d_{i_1 i_2 \rho} B_\rho + \tfrac{1}{8}\mathfrak{M}_3 \delta_{i_1 i_2} I; \quad (3.30b)$$

$(T_{i_1}, C_{i_2}) = (\tilde{B}_{i_1}, \tilde{B}_{i_2})$:

$$T_{i_1 i_2} = \{\tilde{B}_{i_1}, \tilde{B}_{i_2}\} + \tfrac{1}{10}(2\mathfrak{M}_2 - 3) d_{i_1 i_2 \rho}\tilde{B}_\rho + \tfrac{2}{5}\mathfrak{M}_3 d_{i_1 i_2 \rho} B_\rho - \tfrac{1}{96}\mathfrak{M}_2(2\mathfrak{M}_2 + 3)\delta_{i_1 i_2} I, \quad (3.30c)$$

where I is a unit matrix of appropriate dimensions, $\mathfrak{M}_2$ and $\mathfrak{M}_3$ are the eigenvalues of Eq. (2.4), and use has been made of the identities of Eq. (2.16) and (2.18).

When $n=2$, the quantity $\hat{M}$ [see Eq. (3.21)] does contribute to the third-rank tensor $T_{i_1 i_2 i_3}$ of Eq. (3.25), but $\hat{P}$ [see Eq. (3.23)] still does not. The general formula for the tensor is given by

$$T_{i_1 i_2 i_3} = \hat{T} - \tfrac{16}{21}\hat{L} - \tfrac{2}{21}\hat{M} - \tfrac{1}{7}\hat{N} \quad (3.31)$$

and there are four basic choices for the components from which $T_{i_1 i_2 i_3}$ is constructed. They are

(a) *three B_i matrices:*

$$T^{(a)}_{i_1 i_2 i_3} = \sum_{\substack{\text{allperms} \\ i_1 i_2 i_3}} B_{i_1} B_{i_2} B_{i_3} - \tfrac{16}{7} \sum_{c\cdot p(i_1 i_2 i_3)} d_{i_1 i_2 \rho}\tilde{B}_\rho B_{i_3} - \tfrac{2}{7} \sum_{c\cdot p(i_1 i_2 i_3)} d_{i_1 i_2 \rho}\tilde{B}_{i_3} B_\rho - \tfrac{3}{14}(\mathfrak{M}_2 - 2) \times \sum_{c\cdot p} \delta_{i_1 i_2} B_{i_3} - \tfrac{9}{35}\mathfrak{M}_3 d_{i_1 i_2 i_3} I; \quad (3.32a)$$

(b) *two B_i and one $\tilde{B}_i$:*

$$T^{(b)}_{i_1 i_2 i_3} = \sum_{\text{allperms}\,(i_1 i_2 i_3)} B_{i_1}\tilde{B}_{i_2} B_{i_3} - \tfrac{1}{7}(2\mathfrak{M}_2 + 3) \sum_{c\cdot p(i_1 i_2 i_3)} d_{i_1 i_2 \rho} B_\rho B_{i_3} - \tfrac{2}{21} \sum_{c\cdot p(i_1 i_2 i_3)} d_{i_1 i_2 \rho}(8\tilde{B}_{i_3}\tilde{B}_\rho + \tilde{B}_\rho \tilde{B}_{i_3}) - \tfrac{1}{3} \sum_{c\cdot p(i_1 i_2 i_3)} d_{i_1 i_2 \rho}(D_\rho F_{i_3})_{\mu\tau}[\tilde{B}_\tau B_\mu - \tilde{B}_\mu B_\tau] - \tfrac{1}{42}(3\mathfrak{M}_2 - 11) \sum_{c\cdot p} \delta_{i_1 i_2}\tilde{B}_{i_3} + \tfrac{1}{7}\mathfrak{M}_3 \sum_{c\cdot p} \delta_{i_1 i_2} B_{i_3} + \tfrac{3}{140}\mathfrak{M}_2(2\mathfrak{M}_2 + 3) d_{i_1 i_2 i_3} I; \quad (3.32b)$$

(c) *two $\tilde{B}_i$ and one B_i:*

$$T^{(c)}_{i_1 i_2 i_3} = \sum_{\substack{\text{allperms} \\ (i_1 i_2 i_3)}} \tilde{B}_{i_1} B_{i_2}\tilde{B}_{i_3} - \tfrac{1}{42} \sum_{c\cdot p(i_1 i_2 i_3)} d_{i_1 i_2 \rho}[(10\mathfrak{M}_2 + 17) B_\rho \tilde{B}_{i_3} - (4\mathfrak{M}_2 - 10)\tilde{B}_\rho B_{i_3} - 12\mathfrak{M}_3 B_\rho B_{i_3}] - \tfrac{1}{3} \sum_{c\cdot p(i_1 i_2 i_3)} d_{i_1 i_2 \rho}(D_\rho F_{i_3})_{\mu\tau}[\tilde{B}_\tau, \tilde{B}_\mu] - \tfrac{1}{504}(2\mathfrak{M}_2 + 3)(3\mathfrak{M}_2 - 11) \sum_{c\cdot p} \delta_{i_1 i_2} B_{i_3} + \frac{\mathfrak{M}_3}{7} \sum_{c\cdot p} \delta_{i_1 i_2}\tilde{B}_{i_3} - \tfrac{3}{140}\mathfrak{M}_3(2\mathfrak{M}_2 + 3) d_{i_1 i_2 i_3} I; \quad (3.32c)$$

(d) *three $\tilde{B}_i$:*

$$T^{(d)}_{i_1 i_2 i_3} = \sum_{\substack{\text{allperms} \\ (i_1 i_2 i_3)}} \tilde{B}_{i_1}\tilde{B}_{i_2}\tilde{B}_{i_3} - \tfrac{16}{21} \sum_{\substack{c\cdot p \\ (i_1 i_2 i_3)}} d_{i_1 i_2 \rho} d_{\rho\lambda\mu}\tilde{B}_\lambda \tilde{B}_{i_3}\tilde{B}_\mu$$

$$
\begin{aligned}
&- \tfrac{2}{21} \sum_{c\cdot p\,(i_1 i_2 i_3)} d_{i_1 i_2 \alpha} d_{i_3 \lambda \mu} \tilde{B}_\lambda \tilde{B}_\alpha \tilde{B}_\mu \\
&+ \tfrac{1}{14}(2\mathfrak{M}_2 + 3) \sum_{c\cdot p\,(i_1 i_2 i_3)} d_{i_1 i_2 \rho} \{\tilde{B}_\rho, \tilde{B}_{i_3}\} \\
&+ \frac{4\mathfrak{M}_3}{63} \sum_{c\cdot p\,(i_1 i_2 i_3)} d_{i_1 i_2 \rho} (8 B_\rho \tilde{B}_{i_3} + \tilde{B}_\rho B_{i_3}) \\
&- \tfrac{1}{56}(2\mathfrak{M}_2^2 - 3\mathfrak{M}_2 - 3) \sum_{c\cdot p} \delta_{i_1 i_2} \tilde{B}_{i_3} \\
&+ \tfrac{1}{14}\mathfrak{M}_3 \sum_{c\cdot p} \delta_{i_1 i_2} B_{i_3} \\
&+ \tfrac{1}{560}[48\mathfrak{M}_3^2 - \mathfrak{M}_2(4\mathfrak{M}_2^2 - 9)] d_{i_1 i_2 i_3} I. \qquad (3.32d)
\end{aligned}
$$

As a check on these formulas, we note that in the triangular representation $(\mu, 0)$ they are all proportional to

$$
\begin{aligned}
T^{(R)}_{i_1 i_2 i_3} = &\sum_{\substack{\text{allperms} \\ (i_1 i_2 i_3)}} B_{i_1} B_{i_2} B_{i_3} - \tfrac{3}{7}(2\mu + 3) \sum_{c\cdot p} d_{i_1 i_2 \rho} B_\rho B_{i_3} \\
&+ \tfrac{1}{7}(3 - \mu(\mu + 3)) \sum_{c\cdot p} \delta_{i_1 i_2} B_{i_3} \\
&+ \tfrac{1}{35}\mu(\mu + 3)(2\mu + 3) d_{i_1 i_2 i_3} I. \qquad (3.33)
\end{aligned}
$$

The first occasion on which the term $\hat{P}$ of Eq. (3.23) contributes to the symmetric tensor of Eq. (3.25) occurs when $n = 3$. In general there are five basic choices of tensor corresponding to the different numbers of B_i and $\tilde{B}_i$ matrices from which it may be constructed. For the triangular representation $(\mu, 0)$ they all reduce to

$$
\begin{aligned}
T^{(R)}_{i_1 i_2 i_3 i_4} = &\sum_{\substack{\text{allperms} \\ (i_1 i_2 i_3 i_4)}} B_{i_1} B_{i_2} B_{i_3} B_{i_4} \\
&- \tfrac{2}{3}(2\mu + 3) \sum_{r<s} d_{i_r i_s \rho} B_\rho \{B_{i_3'}, B_{i_4'}\} \\
&+ \tfrac{1}{12}\mu(\mu + 3) \sum_{r<s} d_{i_r i_s \alpha} d_{i_3' i_4' \tau} \{B_\alpha, B_\tau\} \\
&- \tfrac{1}{36}(7\mu^2 + 21\mu - 54) \sum_{r<s} \delta_{i_r i_s} \{B_{i_3'}, B_{i_4'}\} \\
&+ \tfrac{1}{630}(2\mu + 3)(48\mu^2 + 144\mu - 25) \sum_{c\cdot p} d_{i_1 i_2 i_3} B_{i_4} \\
&+ \frac{1}{6 \times 630}(2\mu + 3)(99\mu^2 + 297\mu - 940) \\
&\times \sum_{r<s} d_{i_r i_s \rho} \delta_{i_3' i_4'} B_\rho - \tfrac{1}{1260}(2\mu + 3)(21\mu^2 + 63\mu + 40) \\
&\times \sum_{r<s} d_{i_1 i_2 \rho} d_{i_3' i_4' \tau} d_{\rho\tau\beta} B_\beta \\
&+ \tfrac{1}{216}\mu(\mu + 3)(\mu^2 + 3\mu - 18) \sum_{r<s} \delta_{i_r i_s} \delta_{i_3' i_4'} I, \qquad (3.34)
\end{aligned}
$$

where (i_3', i_4') denote the pair of indices remaining when (i_r, i_s) is removed from $(i_1 i_2 i_3 i_4)$. For other representations the fourth-rank tensors are much more complicated, and we have not worked them out.

D. Multiplicity of representations

Since the symmetric tensors of rank n are constructed from some number, say r, of B_α matrices and a complementary number $(n - r)$ of $\tilde{B}_\alpha$ matrices, the largest number of independent tensors is $(n + 1)$ corresponding to the number of ways of choosing r. In the case of the third-rank tensors, for example, there are four different forms [see Eq. (3.32)]; for some representations all four will be independent of one another, and for others, such as the triangular ones, they will not [see Eq. (3.33)]. Now each tensor can be used to pick out an $SU(3)$ representation (n, n) in the direct product of a basis vector ψ_a and its adjoint $\bar{\psi}_b$ [see Eq. (1.6)]. Consequently the maximum number of times that (n, n) occurs in $\psi_a \otimes \bar{\psi}_b$ is $(n + 1)$.

The best known example of this result is the octet (1, 1) which never occurs more than twice in $\psi_a \otimes \bar{\psi}_b$, and sometimes only once. The same is true for the general case: sometimes the maximum number is realized, and at other times it is not. Generally speaking, the representation (n, n) occurs a maximum number of times when ψ_a belongs to the $SU(3)$ representation (p, q) with both p and q greater than or equal to n.

4. CHARACTERISTIC EQUATIONS FOR TRIANGULAR REPRESENTATIONS

If the basis vector ψ_a transforms according to the triangular representation $(\mu, 0)$ of $SU(3)$ and its adjoint $\bar{\psi}_b$ according to $(0, \mu)$, then the maximal representation contained in the direct product $\psi_a \otimes \bar{\psi}_b$ is (μ, μ). Consequently, the tensor $T_{i_1 \cdots i_n}$ of rank $n = \mu + 1$ corresponding to the $\psi_a \otimes \bar{\psi}_b$ state $(\mu + 1, \mu + 1)$ must vanish when the B_i matrices from which it is constructed belong to the representation $(\mu, 0)$. For the six-dimensional representation $\mu = 2$ and so the third-rank tensor vanishes; for the ten-dimensional representation $\mu = 3$ and the fourth-rank tensor is zero. We now use these results to obtain the characteristic equations for B_i belonging to these representations.[12]

A. The six dimensional representation

The third-rank tensor that must vanish is the one in Eq. (3.33) with $\mu = 2$:

$$
\begin{aligned}
T^{(R)}_{i_1 i_2 i_3} = &\sum_{\text{allperms}} B_{i_1} B_{i_2} B_{i_3} - 3 \sum_{c\cdot p} d_{i_1 i_2 \rho} B_\rho B_{i_3} \\
&- \sum_{c\cdot p} \delta_{i_1 i_2} B_{i_3} + 2 d_{i_1 i_2 i_3} I = 0. \qquad (4.1)
\end{aligned}
$$

We introduce the octet vector $\pi_i (i = 1, 2, \ldots, 8)$, define the quantities[12]

$$
\Pi_i = d_{ijk} \pi_j \pi_k, \quad X = \pi_i \pi_i, \quad Y = d_{ijk} \pi_i \pi_j \pi_k, \quad (B\pi) \equiv (B_i \pi_i), \quad (B\Pi) \equiv (B_i \Pi_i) \qquad (4.2)
$$

and then multiply Eq. (4.1) by $\pi_{i_1} \pi_{i_2} \pi_{i_3}$ to obtain

$$
6(B\pi)^3 - 9(B\Pi)(B\pi) - 3X(B\pi) + 2YI = 0 \qquad (4.3a)
$$

or, equivalently,

$$
9(B\Pi)(B\pi) = 6(B\pi)^3 - 3X(B\pi) + 2YI. \qquad (4.3b)
$$

Next we multiply Eq. (4.1) by $\Pi_{i_1} \pi_{i_2} \pi_{i_3}$ and make use of the results

$$
d_{ijk} \pi_j \Pi_k = \tfrac{1}{3} X \pi_k \qquad (4.4)
$$

to obtain

$$
\begin{aligned}
&6(B\pi)^2(B\Pi) - 2X(B\pi)^2 - 3(B\Pi)^2 \\
&\qquad - 2Y(B\pi) - X(B\Pi) + \tfrac{2}{3} X^2 I = 0. \qquad (4.5)
\end{aligned}
$$

Finally, we multiply Eq. (4.5) by $(B\pi)^2$ and eliminate $(B\Pi)$ with the aid of Eq. (4.3b); we find that the matrix $(B\pi)$ satisfies the equation

$$
\begin{aligned}
&36(B\pi)^6 - 45X(B\pi)^4 - 21Y(B\pi)^3 + 9X^2(B\pi)^2 \\
&\qquad + 3XY(B\pi) - 2Y^2 I = 0. \qquad (4.6)
\end{aligned}
$$

To check that this is the correct eigenvalue equation for $(B\pi)$ we consider two special cases. When π_i is a so-

called s vector[13] ($X = 1$, $Y = 0$), $(B\pi)$ behaves like the z component of isospin and it should have an eigenvalue spectrum corresponding to the isospin content $T = 0, \frac{1}{2}, 1$ of the six-dimensional representation. Setting $X = 1$, $Y = 0$ in Eq. (4.6), we can rewrite it in a form

$$9(B\pi)^2(4(B\pi)^2 - 1)[(B\pi)^2 - 1] = 0, \tag{4.7}$$

which indicates that its roots are 0 (twice), $\pm\frac{1}{2}$, ± 1, and so it does indeed have the correct spectrum for the s vector case.

When π_i is a q vector[13] ($X = 1$, $Y = -1/\sqrt{3}$) the matrix $Q \equiv (2/\sqrt{3})(B\pi)$ behaves like a hypercharge operator and in the six-dimensional representation it must have a spectrum corresponding to the relation $T = \frac{2}{3} + \frac{1}{2}Q$. Setting $X = 1$, $Y = -1/\sqrt{3}$ in Eq. (4.6) we obtain an equation, namely

$$(3Q)^6 - 15(3Q)^4 + 14(3Q)^3 + 36(3Q)^2 - 24(3Q) - 32 = 0, \tag{4.8}$$

which after some manipulation reduces to one with the desired eigenvalue spectrum:

$$(3Q - 2)^3(3Q + 1)^2(3Q + 4) = 0. \tag{4.9}$$

Thus Eq. (4.6) behaves like the characteristic equation for six-dimensional B_i matrices in the special cases of s and q vectors, and so we can be confident that it is indeed the characteristic equation for the general case.

B. The decuplet

For the decuplet the vanishing fourth-rank tensor is a special case of Eq. (3.34) with $\mu = 3$. We follow the same procedure as above and multiply the tensor first by $\pi_{i_1}\pi_{i_2}\pi_{i_3}\pi_{i_4}$ and then by $\pi_{i_1}\pi_{i_2}\pi_{i_3}\pi_{i_4}$. This gives us two equations, namely

$$4(B\pi)^4 + 3(B\Pi)^2 - 12(B\pi)^2(B\Pi) - 4X(B\pi)^2 + 6Y(B\pi) + 3X(B\Pi) = 0, \tag{4.10}$$

$$4(B\pi)^3(B\Pi) - 2X(B\pi)^3 - 6(B\Pi)^2(B\pi) - 2Y(B\pi)^2 - X(B\pi)(B\Pi) + 3Y(B\Pi) + 2X^2(B\pi) = 0, \tag{4.11}$$

which, as we have shown elsewhere,[12] yield an equation of tenth degree for $(B\pi)$ when $(B\Pi)$ is eliminated from them. With $X = 1$, $\sqrt{3}\,Y = \sin\psi$, this equation is

$$(B\pi)[(4(B\pi)^3 - 3(B\pi))^2 - 1 + 3Y^2] \times [4(B\pi)^3 - 9(B\pi) - 9Y] = 0 \tag{4.12}$$

and it has the correct spectrum of eigenvalues for the s and q vector cases. Thus Eq. (4.12) is the characteristic equation for matrices belonging to the triangular representation (3, 0) of $SU(3)$.

It is evident from the examples of the 6- and 10-dimensional representations that we can obtain the characteristic equation for any triangular representation $(\mu, 0)$ by setting the symmetric tensor of rank $(\mu + 1)$ equal to zero, and then multiplying it by products of the octet vector π_i. Products involving the dual vector, for example $B\cdot\Pi$, can be eliminated with the aid of identities like Eq. (4.4) and other techniques used above. The resulting equation for $(B\cdot\pi)$ will be valid in the special cases in which π_i is either an s or a q vector, as well as in the general case when it is neither one nor the other.

5. SELF-ADJOINT REPRESENTATIONS

At the end of Sec. 2 we pointed out that in self-adjoint representations ($\mu_1 = \mu_2 = \mu$) the matrices B_α can always be chosen to be antisymmetric, and their duals $\tilde{B}_\alpha$ to be symmetric. We shall now illustrate how this fact can be used to deduce other properties of the matrices by considering the special case of the (27)-dimensional representation.

In general we can represent the basis vectors of self-adjoint representations by symmetric tensors with exactly the same properties as the tensor operators constructed from $SU(3)$ matrices[7] [see Eqs. (3.1) and (3.5)]:

$$\psi_A \equiv \psi_{j_1 j_2 \cdots j_\mu} = \psi_{j_2 j_1 \cdots j_\mu}, \tag{5.1}$$

where

$$\psi_{j_1 j_2 \cdots j_{\mu-2}\gamma\gamma} = d_{\alpha\beta\gamma}\psi_{j_1 \cdots j_{\mu-2}\beta\gamma} = 0. \tag{5.2}$$

For the (27)-plet there are two such indices ($\mu = 2$), and for the (64)-plet there are three ($\mu = 3$).

Let us form the direct product $\bar{\psi}_B \otimes \psi_A$ in which both basis vectors transform according to the (27)-dimensional representation, and let us pick out the (64)-plets contained in it. Since we require tensors with three indices, we can construct them from two basic elements, namely

$$(\bar{\psi}_B \otimes \psi_A)^{(D)} = \sum d_{k i_1 j_1}\bar{\psi}_{i_1 i_2}\psi_{j_1 j_2}, \qquad (\bar{\psi}_B \otimes \psi_A)^{(F)} = \sum i f_{k i_1 j_1}\bar{\psi}_{i_1 i_2}\psi_{j_1 j_2}, \tag{5.3}$$

where the sum is carried out to symmetrize the products with respect to the indices (k, i_2, j_2). Because the f and d coefficients are respectively antisymmetric and symmetric under the permutation of their indices, the (64)-plet $(\bar{\psi}_B \otimes \psi_A)^{(F)}$ is antisymmetric under the interchange of $\bar{\psi}_B$ and ψ_A, and $(\bar{\psi}_B \otimes \psi_A)^{(D)}$ is symmetric.

An alternative way of constructing these (64)-plets is to form the third-rank tensors $T_{i_1 i_2 i_3}$ from the $SU(3)$ matrices and then sandwich them between the states of the (27)-plets $\bar{\psi}_B$ and ψ_A. Now as shown in Eq. (3.32), there are four such tensors; in the self-adjoint case, two of them, (3.22a) and (3.32c), are antisymmetric, and the other two (3.32b) and (3.32d) are symmetric. But we have just shown that in the product of two (27)-plets there are only two (64)-plets, one symmetric and the other antisymmetric. Therefore, the two antisymmetric tensors from Eq. (3.32) must be proportional to one another, and likewise for the two symmetric ones. To compute the coefficients of proportionality we multiply the antisymmetric tensors by $B_{i_1}B_{i_2}B_{i_3}$, and the symmetric ones by $\tilde{B}_{i_1}B_{i_2}B_{i_3}$. After much manipulation we find that

$$T^{(c)}_{i_1 i_2 i_3} = -\frac{383}{768}T^{(a)}_{i_1 i_2 i_3}, \qquad T^{(d)}_{i_1 i_2 i_3} = \frac{31838}{3^7}T^{(b)}_{i_1 i_2 i_3} \tag{5.4}$$

when the B_i and $\tilde{B}_i$ matrices belong to the (27)-dimensional representation.

To generalize this result, we note that when ψ_A belongs to the (μ, μ) representation its direct product with its adjoint $\bar{\psi}_B$ contains the representation $(2\mu - 1, 2\mu - 1)$ only twice, once in symmetric form and once in antisymmetric form. However, there are 2μ distinct tensors $T_{i_1 \cdots i_{2\mu-1}}$ of rank $(2\mu - 1)$, and in the self-adjoint case half of them are symmetric and the other half antisymmetric. Obviously then, the symmetric ones must be proportional to one another when the B_i are in the (μ, μ)

representation and so must the antisymmetric ones. The computation of the coefficients of proportionality is, however, an extremely tedious affair.

In conclusion, we note that similar arguments can also be applied to lower rank tensors contained in $\bar{\psi}_B \otimes \psi_A$. In the particular case of the (27)-plet, we learn nothing new from this, but for other representations we do.

6. CALCULATION OF TRACES

As a final application of our results we use them to compute the traces of products of $SU(3)$ matrices belonging to an arbitrary representation. We show that the traces of both the symmetric tensors of Sec. 3, and of certain other tensors must vanish; then by working our way through the second- and third-rank tensors, we are able to compute the traces of products of two, three, and four matrices. We can handle larger products in a similar way, but we shall not do so here.

A. General

Because the trace of the product of any two matrices is independent of their order, the trace of their commutator must vanish:

$$\mathrm{Tr}([G,H]) = 0. \tag{6.1}$$

Therefore, it follows from the commutation rule for two B matrices [see Eq. (1.1)] that

$$\mathrm{Tr}(if_{\alpha\beta\gamma}B_\gamma) = 0. \tag{6.2}$$

Multiplying by $if_{k\beta\alpha}$ and using the property [see Eq. (2.7)]

$$if_{k\alpha\beta}if_{\alpha\beta\gamma} = 3\delta_{k\gamma}, \tag{6.3}$$

we find that the B matrices themselves must be traceless. Similarly, the trace of $\tilde{B}_k$ must also be zero. Thus,

$$\mathrm{Tr}(B_k) = \mathrm{Tr}(\tilde{B}_k) = 0. \tag{6.4}$$

Now consider a symmetric second-rank tensor T_{ij} which satisfies the commutation rule

$$[B_\alpha, T_{ij}] = if_{\alpha i\beta}T_{\beta j} + if_{\alpha j\beta}T_{i\beta}. \tag{6.5}$$

If we multiply both sides by $if_{ki\alpha}$, and make use of the symmetry of T_{ij} as well as Eq. (6.3), we obtain

$$if_{ki\alpha}[B_\alpha, T_{ij}] = 3T_{kj} - \tfrac{1}{2}\{F_i, F_\beta\}_{kj}T_{i\beta}. \tag{6.6}$$

With the aid of Eqs. (1.9) and (3.15) for $\{F_i, F_\beta\}$ and the general properties [see Eq. (3.5)]

$$T_{\beta\beta} = d_{k\alpha\beta}T_{\alpha\beta} = 0, \tag{6.7}$$

we can reduce Eq. (6.6) to

$$if_{ki\alpha}[B_\alpha, T_{ij}] = 4T_{kj}. \tag{6.8}$$

Consequently, the trace of T_{kj} vanishes:

$$\mathrm{Tr}(T_{kj}) = 0. \tag{6.9}$$

It is not difficult to see that this argument applies to a symmetric tensor of any rank, and so we have

$$\mathrm{Tr}(T_{i_1 i_2 \cdots i_n}) = 0 \tag{6.10}$$

as long as $T_{i_1 i_2 \cdots i_n}$ satisfies Eq. (3.5).

Suppose next that S_{ij} is an antisymmetric tensor which obeys the commutation rules

$$[B_\alpha, S_{ij}] = if_{\alpha i\beta}S_{\beta j} + if_{\alpha j\beta}S_{i\beta} \tag{6.11}$$

and the subsidiary conditions

$$S_{ij} = -S_{ji}, \quad if_{k\alpha\beta}S_{\alpha\beta} = 0. \tag{6.12}$$

The second condition ensures that S_{ij} contains no octet component, and so it is some combination of the (10) and (10*) representations. If we multiply both sides of Eq. (6.11) by $if_{ki\alpha}$ and make use of the antisymmetry of S_{ij}, we find that

$$if_{ki\alpha}[B_\alpha, S_{ij}] = 3S_{kj} - \tfrac{1}{2}[F_i, F_\beta]_{kj}S_{i\beta}. \tag{6.13}$$

From the commutation rule for F-matrices and the subsidiary condition of Eq. (6.12), we obtain

$$if_{ki\alpha}[B_\alpha, S_{ij}] = 3S_{kj} \tag{6.14}$$

and hence

$$\mathrm{Tr}(S_{ij}) = 0. \tag{6.15}$$

This argument can be combined with the previous one for symmetric tensors to show that the trace of a tensor of rank m and with mixed symmetry will vanish as long as it obeys all subsidiary conditions like those in Eqs. (3.5) and (6.12). These subsidiary conditions serve to limit the irreducible representations occurring in the tensor, but from our point of view their important effect is to ensure that the tensor contains no $SU(3)$ singlet. Since the singlet always commutes with the B_i matrices, its trace need not vanish, and in fact it does not. All $SU(3)$ singlets are proportional to the unit matrix and their traces are proportional to the dimensions of the representation being studied. Thus any tensor containing a singlet will have nonzero trace, while the trace of any tensor not containing a singlet will always be zero.

We emphasize this point because we find it useful to apply it to products of symmetric tensors $T_{i_1 \cdots i_n}$ with matrices B_j and $\tilde{B}_j$. For n greater than or equal to two the product $T_{i_1 \cdots i_n}B_j$ (or $\tilde{B}_j$) does not contain an $SU(3)$ singlet and so its trace must vanish; the same is true of the product $T_{i_1 \cdots i_n}B_jB_{j'}$ as long as $n \geq 3$, and so on. This provides us with a useful labor-saving device in practical calculations.

B. Products of two matrices

The three basic second-rank tensors are given in Sec. 3C. Setting the trace of the tensor in Eq. (3.30a) equal to zero, we obtain

$$\mathrm{Tr}(B_iB_j) = \tfrac{1}{16}\mathfrak{M}_2 D\delta_{ij}, \tag{6.16}$$

where D is the dimension of the representation (μ_1, μ_2) given in Eq. (2.5), and $\mathfrak{M}_2$ is the Casimir eigenvalue of Eq. (2.4). Similarly, from Eq. (3.30c) we obtain

$$\mathrm{Tr}(\tilde{B}_i\tilde{B}_j) = \tfrac{1}{192}\mathfrak{M}_2(2\mathfrak{M}_2 + 3)D\delta_{ij}. \tag{6.17}$$

Setting the trace of Eq. (3.30b) equal to zero, we find that

$$\mathrm{Tr}(\tilde{B}_iB_j + \tilde{B}_jB_i) = -\tfrac{1}{8}\mathfrak{M}_3 D\delta_{ij}. \tag{6.17'}$$

Now $(\tilde{B}_iB_j - \tilde{B}_jB_i)$ is an antisymmetric tensor which contains octet, (10), and (10*) components but no singlet;

consequently its trace vanishes. We therefore conclude from Eq. (6.17) that

$$\mathrm{Tr}(\tilde{B}_i B_j) = -\tfrac{1}{16}\mathfrak{M}_3 D\delta_{ij}. \tag{6.18}$$

C. Products of three matrices

The simplest way of computing the traces of three matrices is to observe that, since the direct products $T_{ij}B_k$ and $T_{ij}\tilde{B}_k$ contain no $SU(3)$ singlets, their traces are zero. Taking the second-rank tensor of Eq. (3.30a) times B_k and using Eq. (6.18), we find in this way that

$$\mathrm{Tr}[\{B_i, B_j\}B_k] = -\tfrac{3}{40}\mathfrak{M}_3 D d_{ijk}. \tag{6.19}$$

But

$$\mathrm{Tr}[[B_i, B_j]B_k] = if_{ijl}\,\mathrm{Tr}[B_l B_k] = \tfrac{1}{16}\mathfrak{M}_2 D i f_{ijk} \tag{6.20}$$

and so

$$\mathrm{Tr}(B_i B_j B_k) = \frac{D}{16}\left(-\tfrac{3}{5}\mathfrak{M}_3 d_{ijk} + \tfrac{1}{2}\mathfrak{M}_2 i f_{ijk}\right). \tag{6.21}$$

In a similar way we obtain

$$\mathrm{Tr}(B_i B_j \tilde{B}_k) = \frac{D}{32}\left(\tfrac{1}{10}\mathfrak{M}_2(2\mathfrak{M}_2 + 3)d_{ijk} - \mathfrak{M}_3 i f_{ijk}\right) \tag{6.22}$$

from the product of Eq. (3.30a) with $\tilde{B}_k$.

If we take T_{ij} to be the tensor of Eq. (3.30b) and multiply it by $\tilde{B}_k$, we have

$$\mathrm{Tr}(B_j \tilde{B}_k \tilde{B}_i + B_i \tilde{B}_k \tilde{B}_j) = -\frac{D}{160}\mathfrak{M}_3(2\mathfrak{M}_2 + 3)d_{ijk}. \tag{6.23}$$

If we take T_{jk} to be the tensor of Eq. (3.30c) and multiply by B_i, we find that

$$\mathrm{Tr}(B_i \tilde{B}_j \tilde{B}_k + B_i \tilde{B}_k \tilde{B}_j) = -\frac{D}{160}\mathfrak{M}_3(2\mathfrak{M}_2 + 3)d_{ijk}. \tag{6.24}$$

Subtracting Eq. (6.23) from (6.24), we have

$$\mathrm{Tr}(B_j \tilde{B}_k \tilde{B}_i) = \mathrm{Tr}(B_i \tilde{B}_j \tilde{B}_k) \tag{6.25}$$

and so we can rewrite Eq. (6.23) as

$$\mathrm{Tr}[\{B_i, \tilde{B}_j\}\tilde{B}_k] = -\frac{D}{160}\mathfrak{M}_3(2\mathfrak{M}_2 + 3)d_{ijk}. \tag{6.26}$$

Because

$$\mathrm{Tr}[[B_i, \tilde{B}_j]\tilde{B}_k] = if_{ijl}\,\mathrm{Tr}[\tilde{B}_l \tilde{B}_k] = \frac{D}{192}\mathfrak{M}_2(2\mathfrak{M}_2 + 3)if_{ijk}, \tag{6.27}$$

we conclude that

$$\mathrm{Tr}(B_i \tilde{B}_j \tilde{B}_k) = \frac{D}{1920}(2\mathfrak{M}_2 + 3)(-6\mathfrak{M}_3 d_{ijk} + 5\mathfrak{M}_2 i f_{ijk}). \tag{6.28}$$

To determine the trace of three $\tilde{B}$-matrices, we multiply the tensor of Eq. (3.30c) by $\tilde{B}_k$; thus

$$\mathrm{Tr}[\{\tilde{B}_i, \tilde{B}_j\}\tilde{B}_k] = \frac{D}{1920}(48\mathfrak{M}_3^2 - \mathfrak{M}_2(4\mathfrak{M}_2^2 - 9))d_{ijk}. \tag{6.29}$$

Now

$$\mathrm{Tr}[[\tilde{B}_i, \tilde{B}_j]\tilde{B}_k] = d_{i\alpha\beta} i f_{\beta j\rho}\,\mathrm{Tr}[(B_\alpha \tilde{B}_\rho + \tilde{B}_\rho B_\alpha)\tilde{B}_k]$$

and from Eqs. (6.24) and (2.15), this becomes

$$\mathrm{Tr}[[\tilde{B}_i, \tilde{B}_j]\tilde{B}_k] = -\frac{D}{192}\mathfrak{M}_3(2\mathfrak{M}_2 + 3)if_{ijk}. \tag{6.30}$$

Therefore, we have

$$\mathrm{Tr}(\tilde{B}_i \tilde{B}_j \tilde{B}_k) = \frac{D}{3840}\{(48\mathfrak{M}_3^2 + 9\mathfrak{M}_2 - 4\mathfrak{M}_2^3)d_{ijk} - 10\mathfrak{M}_3(2\mathfrak{M}_2 + 3)if_{ijk}\}. \tag{6.31}$$

This completes the calculation of traces of products of three $SU(3)$ matrices and we turn to products of four matrices.

D. Products of four matrices

We can calculate the traces of products of four $SU(3)$ matrices either by noting that the traces of T_{ijk} times either B_l or $\tilde{B}_l$ vanish when T_{ijk} is any one of the symmetric tensors in Eq. (3.32), or by using the following result due to Dittner.

Dittner[14] has shown that the most general fourth-rank tensor of $SU(3)$ is a linear combination of eight terms, namely

$$R_{ijkl} = a\delta_{ij}\delta_{kl} + b\delta_{ik}\delta_{jl} + c\delta_{il}\delta_{jk} + \alpha d_{ij\rho}d_{kl\rho} + \beta d_{ik\rho}d_{jl\rho} + \lambda d_{ij\rho}if_{jk\rho} + \mu d_{ik\rho}d_{jl\rho} + \nu d_{il\rho}if_{jk\rho}. \tag{6.32}$$

Therefore, the trace of the product of any four matrices, $B_i B_j B_k B_l$, for example, must be of the general form given in Eq. (6.32). To compute the coefficients $a, b, \ldots, \nu$ we contract both sides with $SU(3)$ coefficients like δ_{ij}, $d_{jk\sigma}$, $if_{kl\sigma}$ and then use the results of the previous sections for the products of two and three matrices. This method is somewhat more straightforward than the other one, but it involves just as much tedious algebra.

We shall not give the details of computation, but instead we quote the results for the coefficients of the right-hand side of Eq. (6.32).

They are:

$\mathrm{Tr}(B_i B_j B_k B_l)$:

$$a = c = \frac{\mathfrak{M}_2}{960}(3\mathfrak{M}_2 + 7)D, \quad b = \frac{\mathfrak{M}_2}{960}(3\mathfrak{M}_2 - 13)D,$$
$$\alpha = 0, \quad \beta = -\frac{\mathfrak{M}_2}{32}D, \quad \lambda = \mu = \nu = -\frac{3}{160}\mathfrak{M}_3 D; \tag{6.33a}$$

$\mathrm{Tr}(B_i B_j B_k \tilde{B}_l)$:

$$a = c = -\frac{\mathfrak{M}_3}{960}(3\mathfrak{M}_2 + 7)D, \quad b = -\frac{\mathfrak{M}_3}{960}(3\mathfrak{M}_2 - 13)D$$
$$\alpha = 0, \quad \beta = \frac{\mathfrak{M}_3}{32}D, \quad \lambda = \mu = \nu = \frac{D}{640}\mathfrak{M}_2(2\mathfrak{M}_2 + 3); \tag{6.33b}$$

$\mathrm{Tr}(B_i B_j \tilde{B}_k \tilde{B}_l)$:

$$a = \frac{D}{1440}\left(-\mathfrak{M}_3^2 + \frac{1}{24}\mathfrak{M}_2(2\mathfrak{M}_2 + 3)(11\mathfrak{M}_2 + 21)\right),$$
$$b = \frac{D}{360}\left(\mathfrak{M}_3^2 + \frac{1}{96}\mathfrak{M}_2(2\mathfrak{M}_2 + 3)(\mathfrak{M}_2 - 39)\right),$$
$$c = \frac{D}{360}\left(\mathfrak{M}_3^2 + \frac{1}{96}\mathfrak{M}_2(2\mathfrak{M}_2 + 3)(\mathfrak{M}_2 + 21)\right),$$
$$\alpha = \frac{D}{240}\left(\mathfrak{M}_3^2 - \frac{1}{12}\mathfrak{M}_2^2(2\mathfrak{M}_2 + 3)\right),$$
$$\beta = -\frac{1}{384}\mathfrak{M}_2(2\mathfrak{M}_2 + 3),$$
$$\lambda = \mu = \nu = -\frac{D}{640}\mathfrak{M}_3(2\mathfrak{M}_2 + 3); \tag{6.33c}$$

$\mathrm{Tr}(B_i\tilde{B}_j\tilde{B}_k\tilde{B}_l)$:

$$a = c = -\frac{D}{12\times 960}\,\mathfrak{M}_3(2\mathfrak{M}_2+3)(3\mathfrak{M}_2+7),$$

$$b = -\frac{D}{12\times 960}\,\mathfrak{M}_3(2\mathfrak{M}_2+3)(3\mathfrak{M}_2-13),$$

$$\alpha = 0, \quad \beta = \frac{D}{384}\,\mathfrak{M}_3(2\mathfrak{M}_2+3),$$

$$\lambda = \nu = \frac{D}{320}\left(\mathfrak{M}_3^2 + \tfrac{1}{8}\mathfrak{M}_2(2\mathfrak{M}_2+3)\right),$$

$$\mu = \frac{D}{320}\left(3\mathfrak{M}_3^2 - \frac{1}{24}\,\mathfrak{M}_2(2\mathfrak{M}_2+3)(4\mathfrak{M}_2-3)\right); \tag{6.33d}$$

$\mathrm{Tr}(\tilde{B}_i\tilde{B}_j\tilde{B}_k\tilde{B}_l)$:

$$a = c = \frac{D}{2880}\times\left(\mathfrak{M}_3^2 + \frac{1}{48}\,\mathfrak{M}_2(2\mathfrak{M}_2+3)(6\mathfrak{M}_2^2+19\mathfrak{M}_2+21)\right),$$

$$b = \frac{D}{2880}\times\left(11\mathfrak{M}_3^2 + \frac{1}{48}\,\mathfrak{M}_2(2\mathfrak{M}_2+3)(6\mathfrak{M}_2^2-61\mathfrak{M}_2-39)\right),$$

$$\alpha = 0, \quad \beta = -\frac{D}{240}\times\left(\mathfrak{M}_3^2 + \frac{1}{96}\,\mathfrak{M}_2(2\mathfrak{M}_2+3)(2\mathfrak{M}_2+15)\right),$$

$$\lambda = \mu = \nu = -\frac{D}{8\times 960}\,\mathfrak{M}_3(2\mathfrak{M}_2+3)^2. \tag{6.33e}$$

These results are valid for any representation (μ_1, μ_2) and as far as we know at this point, they are new ones.

7. SUMMARY AND CONCLUSIONS

We have completed the program set forth in the introduction and we hope that by now the reader is convinced that a knowledge of the Clebsch–Gordan series for the basis vectors $\psi_a \otimes \bar{\psi}_b$ enables us to determine many properties of the matrices B_i belonging to the appropriate representation of $SU(3)$. The particular examples we have used are by no means exhaustive, but they do illustrate the power of our method and the ways in which it may be applied. Other examples may, of course, require some variation in the approach.[15]

Besides specific results such as the characteristic equations for the six- and ten-dimensional representations [see Eqs. (4.6) and (4.12)] and the relationships among matrices of the (27)-dimensional representation [see Eq. (5.4)], there are several results of a general nature. The first is the formula for the $(n+1)$-rank symmetric tensor $T_{i_1 i_2 \cdots i_{n+1}}$ constructed from the n-rank tensor $T_{i_1 i_2 \cdots i_n}$ and an octet C_j [see Eq. (3.5)]. Another is the fact that the representation (n, n) occurs at most $(n+1)$ times in the direct product of ψ_a and its adjoint $\bar{\psi}_b$ (see Sec. 3D). When B_i belongs to the triangular representation $(\mu, 0)$ the symmetric tensor of rank $(\mu+1)$ constructed from products of B matrices must vanish identically (Sec. 4B); and when B_i belongs to the self-adjoint representation (μ, μ), only two of the 2μ tensors of rank $(2\mu-1)$ constructed from B_i and B_j are independent [see Sec. 5 below Eq. (5.4)]. The formula for $T_{i_1 i_2 \cdots i_{n+1}}$ does not depend on our remark about the Clebsch–Gordan series for $\psi_a \otimes \bar{\psi}_b$, but it does provide the basic tool for applications; this is also true of our trace calculations in Sec. 6.

In conclusion, we note that the general observation upon which our work is based, namely that matrices representing the algebra of $SU(3)$ also serve as Clebsch–Gordan coefficients for the group, is valid not only for $SU(3)$, but for all other Lie algebras. Consequently, we can apply the approach to many other groups.

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APPENDIX: THE CUBIC CASIMIR OPERATOR

We wish to show that the conditions of Eq. (3.5) ensure that the symmetric tensor $T_{i_1 \cdots i_n}$ has zero for its eigenvalue of the cubic Casimir operator. We begin by considering a tensor of rank one, namely an octet:

$$\begin{aligned} d_{abc}[B_a,[B_b,[B_c,C_i]]] &= d_{abc} f_{ci\lambda} f_{b\lambda\mu} f_{a\mu\nu} C_\nu \\ &= \mathrm{Tr}(F_i F_\mu D_a) f_{a\mu\nu} C_\nu \\ &= \tfrac{3}{2} d_{i\mu a} f_{a\mu\nu} C_\nu \\ &= 0. \end{aligned} \tag{A1}$$

The last two lines are consequences of Eqs. (2.10) and (2.15), respectively.

When we apply the Casimir operator to a second-rank tensor T_{ij} we encounter two types of terms. In one type, all three B matrices act upon the index in one fixed position; and in the other, two of the B matrices act upon the index in one position, and the third matrix acts upon the index in the other position. The first type vanishes by virtue of the argument in Eq. (A1), and the typical term of the second type is

$$\begin{aligned} & d_{abc} f_{ci\lambda} f_{b\lambda\mu} f_{aj\nu} T_{\mu\nu} \\ &\quad = \mathrm{Tr}(F_i F_\mu D_a) f_{aj\nu} T_{\mu\nu} = \tfrac{3}{2} d_{i\mu a} f_{aj\nu} T_{\mu\nu}. \end{aligned} \tag{A2}$$

Because $T_{\mu\nu}$ is symmetric under $\mu \leftrightarrow \nu$, and because the f and d coefficients satisfy the Jacobi identity of Eq. (2.2), we can write the right-hand side of Eq. (A2) as

$$\tfrac{3}{4}(d_{i\mu a} f_{aj\nu} + d_{i\nu a} f_{aj\mu}) T_{\mu\nu} = f_{ija} d_{a\mu\nu} T_{\mu\nu} = 0, \tag{A3}$$

where the second step is an immediate consequence of Eq. (3.5). Thus the second type of term also vanishes and so we have the general result

$$d_{abc}[B_a,[B_b,[B_c,T_{ij}]]] = 0. \tag{A4}$$

In the case of a third-rank tensor T_{ijk}, the Casimir operator gives rise to three types of term: the two types already encountered in the second-rank case, and a third in which each B-matrix acts on an index in a different position. Since the first two have already been shown to be zero, we need only consider the third type, a typical term being:

$$\begin{aligned} & d_{abc} f_{ci\lambda} f_{bj\mu} f_{ak\nu} T_{\lambda\mu\nu} \\ &\quad = -(F_\lambda D_a F_\mu)_{ij} f_{ak\nu} T_{\lambda\mu\nu} \\ &\quad = -(F_\lambda [D_k, F_\nu] F_\mu)_{ij} T_{\lambda\mu\nu} \\ &\quad = \tfrac{1}{2}[(\{F_\lambda, F_\nu\} D_k F_\mu)_{ij} - (F_\lambda D_k \{F_\nu, F_\mu\})_{ij}] T_{\lambda\mu\nu}, \end{aligned} \tag{A5}$$

where we have used the symmetry of $T_{\lambda\mu\nu}$ under permutations of its indices to obtain the last line of Eq. (A5). From the identity [see Eqs. (1.9) and (3.15)]

$$\{F_\lambda, F_\mu\} = \delta_{\lambda\mu} I + 3d_{\lambda\nu\tau} D_\tau - R_{\lambda\mu},$$
$$(R_{\lambda\mu})_{ab} = \delta_{\lambda a}\delta_{\mu b} + \delta_{\lambda b}\delta_{\mu a} \tag{A6}$$

and the conditions of Eq. (3.5), the Eq. (A5) becomes

$$-\tfrac{1}{2}[\delta_{\lambda i}(D_\nu F_\mu)_{kj} + \delta_{\nu i}(D_\lambda F_\mu)_{kj} - \delta_{\mu j}(F_\lambda D_\nu)_{ik} - \delta_{\nu j}(F_\lambda D_\mu)_{ik}]T_{\lambda\mu\nu}. \tag{A7}$$

Because $T_{\lambda\mu\nu}$ is symmetric under the exchange of μ and ν, we can rewrite the first term in the square bracket as

$$-\tfrac{1}{2}\delta_{\lambda i}[\tfrac{1}{2}(D_\nu F_\mu)_{kj} + \tfrac{1}{2}(D_\mu F_\nu)_{kj}]T_{\lambda\mu\nu}$$

and then use the Jacobi identity of Eq. (2.2) to rewrite it as

$$\tfrac{1}{2}\delta_{\lambda i} i f_{\rho kj} d_{\rho\mu\nu} T_{\lambda\mu\nu} = 0. \tag{A8}$$

Similarly, the other three terms in Eq. (A7) are all zero, and so we conclude that all terms of the third type are also zero. Therefore, we have

$$d_{abc}[B_a, [B_b, [B_c, T_{ijk}]]] = 0. \tag{A9}$$

When we apply the Casimir operator to tensors of rank greater than three we do not encounter any new types of term, and so the arguments given above can be used to show that

$$d_{abc}[B_a, [B_b, [B_c, T_{i_1 i_2 \cdots i_n}]]] = 0 \tag{A10}$$

for any symmetric tensor obeying the conditions of Eq. (3.5).

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On the radial wave equation in Schwarzschild's space-time

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The radial factor of a separable solution of the wave equation in Schwarzschild's space-time satisfies a second-order linear differential equation. This equation is studied in detail. The behavior of the solutions near the singular points (the origin, the horizon, and infinity) of the equation is analyzed. By an appropriate transformation two simpler differential equations are obtained corresponding to retarded and advanced solutions with characteristic asymptotic expansions. Their properties permit the expression of the general solution of the radial equation in terms of a single contour integral. Finally, through a "matching" technique, the behavior of a solution at the singular points is determined from its behavior at a single singular point.

1. INTRODUCTION

In curved space-times the detailed mathematical study of the wave equation must precede any systematic investigation of wave phenomena, exactly as in flat space-time. However, even in the simple space-time of Schwarzschild, separation of variables in the wave equation leads to a second order linear differential equation, *the radial wave equation*, which is not related to any known differential equation of mathematical physics. Expression of the solution in closed form is not possible. Even methods containing infinite steps[1,2] have not given satisfactory expressions and have raised unanswered questions of convergence. In fact, the solution of the radial wave equation has not gone essentially beyond the stage of writing down the differential equation.[1,3] In all physical problems, which lead to the radial wave equation[3,4,5] (or similar second order differential equations[6,7]), techniques of "effective potential" tailored to the specific requirements of the problem have been used.

In this paper we set and reach a limited objective, that is, the investigation of those properties of the solutions which are essential for the study of time-dependent wave phenomena around a Schwarzschild black hole. These essential properties of the solutions can be considered in two groups. The first group concerns the behavior of the solutions at the origin of the coordinate system and the horizon of the black hole. It is intimately related with the radiation of multipole moments[4,8] and the possibility of destruction of the black hole. The second group concerns the behavior of the solution at infinity, the retarded and advanced contributions to the wave solution, and is related to the observations of a distant observer.

In Sec. 2 we review briefly the radial wave equation in flat space-time. In Secs. 3 and 4 we consider the radial wave equation in Schwarzschild's space-time, and we study the behavior of the solution at the origin and the horizon (Sec. 3) and at infinity in terms of retarded and advanced solutions (Sec. 4). In Sec. 5 we derive certain linear relationships among the characteristic solutions of the differential equation. These relations enable us to find the behavior of a solution near a singular point from its behavior near another singular point.

2. THE RADIAL WAVE EQUATION IN FLAT SPACE-TIME

We present briefly the solution of the radial wave equation in flat space-time in a way which avoids the use of Bessel functions. The method of solution will indicate the generalization needed to derive the retarded and advanced solutions in Schwarzschild's space-time (see Sec. 4). Moreover, the formulas presented in this section will help in demonstrating the correspondence between the flat-space and the Schwarzschild-space solutions.

In flat space-time the metric tensor in spherical coordinates is

$$g_{\mu\nu} = \mathrm{diag}[c^2, -1, -r^2, -r^2 \sin^2\theta], \tag{1}$$

and the scalar wave equation[9]

$$\Box\Psi \equiv g^{\mu\nu}\Psi_{;\mu\nu} = 0 \tag{2}$$

is separable[10] (the semicolon denotes covariant differentiation).

If

$$\Psi = R(r)Y(\theta,\varphi)e^{-i\omega t}, \tag{3}$$

then $Y(\theta,\varphi)$ is a spherical harmonic and $R(r)$ satisfies the equation

$$r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + [k^2r^2 - l(l+1)]R = 0, \tag{4}$$

where $k = \omega/c$.

A change of the dependent variable to $r^{1/2}R$ will give a Bessel equation[10] of fractional order. However, we can avoid the Bessel functions. If we set

$$R(r) = e^{\mp ix}F_{\pm}(x), \tag{5}$$

where $x = kr$, Eq. (4) reduces to

$$x^2\frac{d^2F_{\pm}}{dx^2} + 2(x \mp ix^2)\frac{dF_{\pm}}{dx} + [\mp 2ix - l(l+1)]F_{\pm} = 0. \tag{6}$$

This equation has an irregular singular point at $x = +\infty$, but we can obtain closed-form solutions (one F_+ and one F_-), which are polynomials of x^{-1} of degree $l+1$. In fact, we have[11]

$$F_{l\pm} = (\pm i)^{l+1}x^{-1}\sum_{n=0}^{l}\frac{(l+n)!}{(l-n)!n!}(\pm 2ix)^{-n}, \tag{7}$$

with F_{l-} corresponding to retarded waves and F_{l+} to advanced waves. Usually we consider the two linearly independent combinations[12]

$$j_l = \tfrac{1}{2}(e^{ix}F_{l-} + e^{-ix}F_{l+}) \tag{8}$$

and

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$$h_l = e^{ix} F_{l-}, \tag{9}$$

which are finite at $r = 0$ and $r = +\infty$ respectively.

In Sec. 4 a generalization of transformation (5) will result in equations similar to Eq. (6).

3. THE RADIAL WAVE EQUATION IN SCHWARZSCHILD'S SPACE-TIME

We consider now the wave equation (2) in Schwarzschild's space–time with metric tensor

$$g_{\mu\nu} = \mathrm{diag}\left[\left(1 - \frac{r_s}{r}\right)c^2, -\left(1 - \frac{r_s}{r}\right)^{-1}, -r^2, -r^2 \sin^2\theta\right], \tag{10}$$

where r_s is the *Schwarzschild radius* (a constant related to the mass M by the relation $r_s = 2GMc^{-2}$).

Assuming a solution[13] of Eq. (2) of the form (3), we have for $R(r)$ the *radial wave equation*[14]

$$x(x - x_s)^2 \frac{d^2R}{dx^2} + (x - x_s)(2x - x_s)\frac{dR}{dx} + [x^3 - l(l+1)(x - x_s)]R = 0, \tag{11}$$

where

$$x = kr, \quad x_s = kr_s. \tag{12}$$

Eq. (11) has two regular singular points[15,16] at $x = 0$ and $x = x_s$ and an irregular singular[17] point at $x = +\infty$.

A. Behavior near the origin

In the neighborhood of $x = 0$ we try a power series of x as a solution of Eq. (11). The indicial equation has a double root equal to zero and, consequently, two linearly independent solutions are[17]

$$\mathcal{R}_1(x) = \sum_{n=0}^{\infty} a_n x^n \tag{13}$$

and

$$\mathcal{R}_2(x) = \left(\sum_{n=0}^{\infty} a_n x^n\right)\ln x + \sum_{n=0}^{\infty} b_n x^n. \tag{14}$$

Substituting these expressions into Eq. (11), we find that a_n and b_n satisfy the recurrence relations

$$n^2 x_s^2 a_n + [l(l+1) - (n-1)(2n-1)]x_s a_{n-1} + [(n-1)(n-2) - l(l+1)]a_{n-2} + a_{n-4} = 0 \tag{15}$$

and

$$n^2 x_s^2 b_n + [l(l+1) - (n-1)(2n-1)]x_s b_{n-1} + [(n-1)(n-2) - l(l+1)]b_{n-2} + b_{n-4} + 2nx_s^2 a_n - (4n-3)x_s a_{n-1} + (2n-3)a_{n-2} = 0. \tag{16}$$

The coefficients a_0 and b_0 are not specified by Eqs. (15) and (16) and have to be chosen arbitrarily. We must choose $a_0 \neq 0$; otherwise $\mathcal{R}_1(x) \equiv 0$ (trivial solution.[18] Any arbitrary pair (a_0, b_0) with $a_0 \neq 0$ will give two linearly independent solutions. We choose $a_0 = b_0 = 1$, thus making $\mathcal{R}_1(x)$ and $\mathcal{R}_2(x)$ particular solutions of Eq. (11). The general solution of Eq. (11) is an arbitrary linear combination of $\mathcal{R}_1(x)$ and $\mathcal{R}_2(x)$.

The series in Eqs. (13) and (14) converge for $x < x_s$ $(x = kr > 0)$. Hence, *there is one solution finite at the origin* [expression (13)], which can be regarded as "physically preferable."[19]

B. Behavior near the horizon

We consider the solutions of Eq. (11) in the neighborhood of the other regular singular point $x = x_s$. Expanding in powers of $x - x_s$, we obtain an indicial equation with roots $\pm ix_s$. Consequently, two linearly independent solutions are

$$\mathcal{R}_3(x) = e^{ix_s \ln|x - x_s|} \sum_{n=0}^{\infty} c_n (x - x_s)^n \tag{17}$$

and

$$\mathcal{R}_4(x) = e^{-ix_s \ln|x - x_s|} \sum_{n=0}^{\infty} d_n (x - x_s)^n, \tag{18}$$

where

$$(n + 2ix_s)nx_s c_n + [(n+l)(n-l-1) + 2x_s^2 + (2n-1)ix_s]c_{n-1} + 3x_s c_{n-2} + c_{n-3} = 0 \tag{19}$$

and

$$(n - 2ix_s)nx_s d_n + [(n+l)(n-l-1) + 2x_s^2 - (2n-1)ix_s]d_{n-1} + 3x_s d_{n-2} + d_{n-3} = 0. \tag{20}$$

The coefficients c_0 and d_0 must be different than zero,[18] but are otherwise arbitrary. We choose $c_0 = d_0 = 1$. Thus, $\mathcal{R}_3(x)$ and $\mathcal{R}_4(x)$ are particular solutions of Eq. (11) and the general solution is an arbitrary linear combination of them.

From expressions (17) and (18) we derive two important properties of the solutions of Eq. (11). First, *every solution remains bounded on the horizon* $r = r_s$ (and, consequently, every solution is "physically acceptable"[19]). Second, *no solution goes to zero as* $r \to r_s$. The proof of these properties is simple, since near $x = x_s$ any solution behaves as $A(x - x_s)^{ix_s} + B(x - x_s)^{-ix_s}$, which remains absolutely smaller than $|A| + |B|$ and does not have a limit as $x \to x_s$.

The importance of these two properties is due to the fact[8] that they are intimately connected with the possibility of destruction of the black hole and the radiation of higher multipole moments during the fall of a small scalar particle into the black hole.

4. RETARDED AND ADVANCED SOLUTIONS AT INFINITY

We ask now for a generalization[20] of transformation (5), which will "separate" the retarded and advanced solutions of Eq. (11). Two remarks indicate the generalization. First expressions (17) and (18) indicate that a factor $e^{\pm ix_s \ln|x - x_s|}$ should be removed from R. Second, the retarded (advanced) solution would have been reached, if we had worked from the beginning in a retarded[21] (advanced) coordinate system. This means that a factor $e^{-i\omega u}$ would have been removed from Ψ instead of $e^{-i\omega t}$. Hence the new transformation is

$$R_{l\pm}(x, x_s) = e^{\mp i(x + x_s \ln|x - x_s|)} F_{l\pm}(x, x_s). \tag{21}$$

Obviously, for $x_s = 0$ we have again Eq. (5).

Replacing $R_{l\pm}$ in Eq. (11) we find two equations satisfied by F_{l+} and F_{l-}, respectively. At this point the consideration of complex values for the independent variable appears to be useful. If $F_l(z, x_s; \epsilon)$ is a solution of

$$z(z - x_s)\frac{d^2F_l}{dz^2} + (-\epsilon z^2 + 2z - x_s)\frac{dF_l}{dz} - [\epsilon z + l(l+1)]F_l = 0, \tag{22}$$

then

$$F_{l\pm}(x, x_s) = F_l(x, x_s; \pm 2i), \tag{23}$$

namely, Eq. (19) for $z = x$ gives the differential equations for F_{l+} ($\epsilon = 2i$) and F_{l-} ($\epsilon = -2i$). Note also that for $x_s = 0$ we rediscover Eq. (6).

The solutions of Eq. (22) present the following important property. *If $F_l(z, x_s; \epsilon)$ is a solution of Eq. (22), then*

$$e^{\epsilon[z+x_s \ln(z-x_s)]} F_l(z, x_s; -\epsilon) \tag{24}$$

is also a solution. This property can be proved easily by substituting expression (24) into Eq. (22).

We will express now the retarded and advanced solutions as contour integrals. According to the theory of contour integration[15,16] of ordinary linear differential equations, the integral

$$\int_C G_l(w) e^{zw} dw \tag{25}$$

will be a solution of Eq. (22), if $G_l(w)$ satisfies the equation[22]

$$w(w-\epsilon)\frac{d^2G}{dw^2} + (x_s w^2 + 2w - \epsilon)\frac{dG}{dw} + [x_s w - l(l+1)]G = 0. \tag{26}$$

The contour C consists of a straight line parallel to the real axis from $\mathrm{Re}\, w = -\infty$ to $w = 0$ (or $w = \epsilon$), a circle around $w = 0$ (or $w = \epsilon$) described positively, and a straight line also parallel to the real axis from $w = 0$ (or $w = \epsilon$) to $\mathrm{Re}\, w = -\infty$. At $w = 0$ the indicial equation of Eq. (26) has a double root equal to zero; hence of the two solutions only the one containing $\ln w$ (the nonanalytic at $w = 0$) will contribute to the integral. Specifically, let $G_l(w, x_s; \epsilon)$ be the solution of Eq. (26), which near $w = 0$ is given by

$$G_l(w, x_s; \epsilon) = \sum_{n=0}^{\infty} g_n w^n, \tag{27}$$

with $g_0 = 1$ and

$$n^2 \epsilon g_n + (l+n)(l-n+1)g_{n-1} - (n-1)x_s g_{n-2} = 0. \tag{28}$$

Then a solution of Eq. (22) is

$$F_l(z, x_s; \epsilon) = \frac{i}{2\pi}\left(\frac{\epsilon}{2}\right)^{l+1} \int_C G_l(w, x_s; \epsilon) \ln w e^{zw} dw, \tag{29}$$

with C surrounding the negative real axis $\mathrm{Re}\, w < 0$. Its asymptotic expansion[23] for $\mathrm{Re}\, z > 0$ is

$$F_l(z, x_s; \epsilon) \sim \left(\frac{\epsilon}{2}\right)^{l+1} \sum_{n=0}^{\infty} \tau_n z^{-(n+1)}, \tag{30}$$

with $\tau_0 = 1$ and[18]

$$n\epsilon\tau_n - (l+n)(l-n+1)\tau_{n-1} - (n-1)^2 x_s \tau_{n-2} = 0. \tag{31}$$

Equations (27) and (28) have been normalized so that when $x_s = 0$, G_l becomes equal[24] to $P_l(1 - 2w/\epsilon)$ and F_l equal to F_{l+} and F_{l-} of Eq. (7) for $\epsilon = 2i$ and $\epsilon = -2i$, respectively.

From F_l we determine a second solution F_l' of Eq. (22) using expression (24). *F_l and F_l' are linearly independent* (for $\epsilon \neq 0$), since they are independent in the special case $x_s = 0$.

The solution F_l' is related to the second contour-integral solution given by the integral (25), say F_l'', when C starts and ends at $\mathrm{Re}\, w = -\infty$ surrounding the point $w = \epsilon$. In fact, *F_l' gives that integral* (up to a constant factor). The proof of this statement consists of two steps. First, we show that F_l' and F_l'' have the same asymptotic expansion (up to a factor). Secondly, we argue that F_l' and F_l'' cannot be linearly independent because in that case every solution would have the same asymptotic expansion, which is not correct for F_l. Consequently, F_l' and F_l'' are proportional to each other.

Reviewing the results of the present section, we see that two linearly independent solutions of Eq. (11) have been determined in terms of the contour integral (29). These solutions are

$$\mathcal{R}_5 = R_{l-} \quad \text{and} \quad \mathcal{R}_6 = R_{l+}. \tag{32}$$

They are defined by Eqs. (21), (23), and (29), and have asymptotic expansions given by Eqs. (30) and (31). The notation R_{l-} and R_{l+} has been adopted to indicate the retarded and advanced character of the solutions, while the notation $\mathcal{R}_5$ and $\mathcal{R}_6$ has been adopted to show the association of the asymptotic expansions with the third singular point at $x = +\infty$.

5. GLOBAL PROPERTIES OF THE SOLUTIONS

In the mathematical formulation of a physical problem the differential equations obeyed by the field are supplemented by a set of boundary conditions. In our case, in addition to Eq. (2), Ψ will have to satisfy some conditions containing Ψ and/or its derivatives evaluated on some surfaces, most probably[19] $r = 0$, $r = r_s$, and $r = +\infty$. Consequently, we must know how a particular solution of Eq. (11) behaves over all space-time. In fact, it will suffice to know the behavior of a particular solution at the singular points of Eq. (11), since every solution is analytic at the regular points. To put it differently, we have to know to what linear combination of $\mathcal{R}_3$ and $\mathcal{R}_4$ (or $\mathcal{R}_5$ and $\mathcal{R}_6$) a given linear combination of $\mathcal{R}_1$ and $\mathcal{R}_2$ corresponds.

In principle, we face the general problem of finding the analytic continuation of a given solution of a differential equation.[25] However, here we are interested in practical answers, which can be used in numerical computations. In what follows we will limit ourselves to the real axis $z = \mathrm{Re}\, z = x$.

The matching of the solutions can be attained through the use of some linear relationships among $\mathcal{R}_i$ ($i = 1, 2, 3, 4, 5, 6$). If

$$W[\mathcal{R}_i, \mathcal{R}_j] = \mathcal{R}_i \frac{d\mathcal{R}_j}{dx} - \mathcal{R}_j \frac{d\mathcal{R}_i}{dx} \tag{33}$$

is the *Wronskian* of any two of the six solutions given by Eqs. (13), (14), (17), (18), and (32), then a constant K_{ij} exists such that

$$W[\mathcal{R}_i, \mathcal{R}_j] = K_{ij}/x(x - x_s), \tag{34}$$

as it can be proved easily from Eq. (11). Moreover, the identities

$$K_{ij}\mathcal{R}_k + K_{jk}\mathcal{R}_i + K_{ki}\mathcal{R}_j = 0 \tag{35}$$

and

$$K_{ij}K_{kl} + K_{ik}K_{lj} + K_{il}K_{jk} = 0 \tag{36}$$

are direct consequencies of Eq. (34). Equation (35) is obviously the key in relating the solutions among them-

selves. It is enough to find the fifteen K_{ij} ($K_{ij} = -K_{ji}$), although they are not all independent.

We start by evaluating the simplest of them, namely K_{12}, K_{34}, K_{56}, using the definition (34) and the series expansions for $\mathcal{R}_i$. Since K_{ij} is a constant, it can be evaluated at any point, where the respective series converge. However, the expressions become simpler when we consider the limit of K_{ij} as x goes to one of the singular points $0, x_s, +\infty$. We find

$$K_{12} = -x_s, \quad K_{34} = -2ix_s^2, \quad K_{56} = -2i. \tag{37}$$

Note that K_{56} can be evaluated only by taking the limit as $x \to +\infty$ because $\mathcal{R}_5$ and $\mathcal{R}_6$ have asymptotic expansions only.

We come now to the evaluation of $K_{13}, K_{14}, K_{23}, K_{24}$. The expansions of the needed $\mathcal{R}_i$ converge for $0 < x < x_s$ and, consequently, we can take the limits as x goes to x_s from below. We find

$$K_{A3} = ix_s^2 \lim_{x \to x_s -} \left[e^{ix_s \ln|x - x_s|} \left(\mathcal{R}_A + i \frac{x - x_s}{x_s} \frac{d\mathcal{R}_A}{dx} \right) \right], \tag{38}$$

where $A = 1, 2$. K_{14} and K_{24} are found to be the complex conjugates of K_{13} and K_{23}, respectively. Note that the coefficients c_n and d_n of the expansions for $\mathcal{R}_3$ and $\mathcal{R}_4$ do not appear in expression (38).

The evaluation of $K_{35}, K_{36}, K_{45}, K_{46}$ requires a more elaborate scheme of matching. The series in Eqs. (17) and (18) converge for $0 < x < 2x_s$ only, and the point $x = +\infty$ lies far from the circle of convergence. Hence, we have to reexpress $\mathcal{R}_3$ and $\mathcal{R}_4$ so that the expansion of the solution around $x = x_s$ will converge up to $x = +\infty$. Using the transformation $y = x^{-1}$, we rewrite Eq. (11) as

$$y^4(y - y_s)^2 \frac{d^2R}{dy^2} + y^4(y - y_s) \frac{dR}{dy} + [y_s^2 + y_s l(l+1)(y - y_s)y^2]R = 0. \tag{39}$$

Its solutions $\mathcal{R}'_3$ and $\mathcal{R}'_4$ in the neighborhood of the regular singular point $y = y_s = x_s^{-1}$ are (after resubstitution of y and y_s with x^{-1} and x_s^{-1})

$$\mathcal{R}'_3(x) = \exp[ix_s \ln|(x_s^2/x) - x_s|] \cdot \mathcal{R}''_3(x), \tag{40}$$

$$\mathcal{R}''_3(x) = \sum_{n=0}^{\infty} c'_n \left(\frac{1}{x} - \frac{1}{x_s} \right)^n, \tag{41}$$

with $\mathcal{R}'_4(x)$ and $\mathcal{R}''_4(x)$ given by the complex conjugates of expressions (40) and (41), respectively. The coefficients c'_n are related by the recurrence relation ($c'_0 = 1$)

$$\begin{aligned} &y_s^4(n + 2ix_s)nc'_n + [4(n - 1 + ix_s)^2 + l(l+1)]y_s^3 c'_{n-1} \\ &+ [3(n - 2 + ix_s)^2 + l(l+1)]2y_s^2 c'_{n-2} \\ &+ [4(n - 3 + ix_s)^2 + l(l+1)]y_s c'_{n-3} \\ &+ (n - 4 + ix_s)^2 c'_{n-4} = 0. \end{aligned} \tag{42}$$

An easy calculation shows that the Wronskians of $\mathcal{R}_3, \mathcal{R}'_3$ and of $\mathcal{R}_4, \mathcal{R}'_4$ are zero and, consequently, $\mathcal{R}'_3$ and $\mathcal{R}'_4$ are proportional to $\mathcal{R}_3$ and $\mathcal{R}_4$, respectively. In fact, in Eqs. (40) and (41) we have normalized $\mathcal{R}'_3$ and $\mathcal{R}'_4$ so that (when $c_0 = c'_0 = 1$)

$$\mathcal{R}_3 = \mathcal{R}'_3, \quad \mathcal{R}_4 = \mathcal{R}'_4. \tag{43}$$

However, the expressions for $\mathcal{R}''_3$ and $\mathcal{R}''_4$ [Eq. (41) and its complex conjugate] converge for $0 < y < 2y_s$ or $x > x_s/2$, namely for x up to $+\infty$. Hence, we can take the limits of $K_{35}, K_{45}, K_{36}, K_{46}$ as $x \to +\infty$ and use the asymptotic expansions for $\mathcal{R}_5$ and $\mathcal{R}_6$. The result is

$$K_{3B} = (\mp i)^l e^{ix_s \ln x_s} \lim_{x \to \infty} \left[x e^{\pm i(x + x_s \ln|x - x_s|)} \left(\mathcal{R}''_3 \pm i \frac{d\mathcal{R}''_3}{dx} \right) \right], \tag{44}$$

where the upper sign is to be taken when $B = 5$ and the lower sign when $B = 6$. K_{45} and K_{46} are the complex conjugates of K_{36} and K_{35}, respectively.

An attempt to calculate $K_{15}, K_{25}, K_{16}, K_{26}$ along the same lines as above results in highly complicated formulas, because no simple transformation[26] exists, which will bring $x = +\infty$ on the circumference of the circle of convergence of the solution around $x = 0$. However, $K_{15}, K_{16}, K_{25}, K_{26}$ can be calculated indirectly from the relation (36) in terms of the remaining eleven K_{ij}, for which formulas have already been given.

In the numerical evaluation of K_{ij}, the formulas (38) and (44) can be simplified by choosing appropriately the values through which x goes to the limit. If, for example, we set

$$x_\nu = x_s - \exp(-2\pi\nu/x_s), \quad x'_\nu = x_s + \exp(2\pi\nu/x_s), \tag{45}$$

where ν is a positive integer, then

$$K_{A3} = ix_s^2 \lim_{\nu \to +\infty} \left[\mathcal{R}_A + i \frac{x - x_s}{x_s} \frac{d\mathcal{R}_A}{dx} \right]_{x = x_\nu} \quad (A = 1, 2) \tag{46}$$

and

$$K_{3B} = (\mp i)^l e^{ix_s \ln x_s} \lim_{\nu \to +\infty} \left[x e^{\pm ix} \left(\mathcal{R}''_3 \pm i \frac{d\mathcal{R}''_3}{dx} \right) \right]_{x = x'_\nu} \tag{47}$$

(the upper sign if $B = 5$, the lower if $B = 6$). A different choice of x'_ν can eliminate completely the factor $e^{\pm ix}$ in Eq. (47).

The next step in solving the complete boundary value problem will be the selection of two solutions $R_l^{(i)}$ and $R_l^{(e)}$ to represent the field in the "near zone" and the "far zone", respectively. $R_l^{(i)}$ and $R_l^{(e)}$ will be called "interior" and "exterior" and will play the roles of j_l and h_l of Eqs. (8) and (9). The interior and exterior solutions will be linear combinations of R_{l+} and R_{l-} and in view of the results of the present section can be expressed as linear combinations of $\mathcal{R}_1$ and $\mathcal{R}_2$ or $\mathcal{R}_3$ and $\mathcal{R}_4$. However, their selection has to be done after the exact formulation of the physical problem we wish to solve, since the boundary conditions will determine the appropriate $R_l^{(i)}$ and $R_l^{(e)}$.

Some final remarks should be added here. Contrary to the flat-space case, in a curved space the electromagnetic 4-potential does not satisfy the same wave equation [Eq. (2)] as the scalar field Ψ. Consequently, the radial factor of the electromagnetic potential will satisfy a radial wave equation[19] different from Eq. (11).

The study of the solutions of this new radial equation can be accomplished[27] along the lines of this paper. Beyond that, the methods of this paper can be used in studying radial equations which are derived from equations similar to Eq. (2) (as the Klein–Gordon equation) in spherically symmetric spaces. These spaces can satisfy the Einstein or similar equations, e.g., in the Brans–Dicke and Weyl theories.[28] However, in these

more general cases the study of the static field[28] should be completed before going to time-dependent situations.

ACKNOWLEDGMENTS

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[21]In a retarded coordinate system, u, r, θ, φ, the only nonzero components of the metric tensor are $g_{00} = (1 - r_s/r)c^2$, $g_{01} = g_{10} = c$, $g_{22} = -r^2$, $g_{33} = -r^2 \sin^2\theta$. The transformation is $u = t - rc^{-1} - r_s c^{-1} \ln(r/r_s - 1)$ with r, θ, φ unchanged.
[22]If $F_l(z, x_s, \epsilon)$ is a solution of Eq. (22), then $F_l(w, \epsilon; -x_s)$ is a solution of Eq. (26). From this property an integral equation can be obtained for F or G.
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[24]P_l is the Legendre polynomial normalized so that $P_l(1) = 1$.
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[26]In fact we must find a transformation $y = f(x)$ which will map $x = x_s$ to $y = y_s$ and $x = +\infty$ to $y = y_\infty$ so that (a) *no* other singular point lies *inside* the circle $(y_s, |y_s - y_\infty|)$ and (b) there is a large positive number x_0 such that all finite $x > x_0$ are mapped *inside* the circle $(y_s, |y_s - y_\infty|)$. It can be proved that a (complex) bilinear transformation cannot satisfy these conditions. A more involved transformation, such as a complex Schwarz–Christoffel transformation or a highly nonlinear transformation, can be found to satisfy the above conditions.
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Note on Green's functions for open lattices*

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The method of Horiguchi is modified to discuss the case in which functions become infinite. The modified method is then used to derive Green's functions for the diamond lattice from those for the face-centered-cubic lattice.

In a recent publication[1] Horiguchi has shown how to derive the Green's functions for the honeycomb net from those for the triangular net. His method is essentially as follows: The difference equation for an unbiased random walk on a triangular net with probability of motion ν along each of the six possible directions,

$$F(x,y) = \delta_{x0}\delta_{y0} + \nu\,[\,F(x+2,y) + F(x-2,y) + (F(x+1,y+3) + F(x+1,y-3) + F(x-1,y+3) + F(x-1,y-3)], \quad (1)$$

is satisfied by a certain complicated integral. Horiguchi showed that, for the source and the two nearest neighbors, the integral may be evaluated in terms of complete elliptic integrals whose arguments are complicated algebraic functions of ν. Then, using the fact that the honeycomb net is composed of two interpenetrating triangular nets (see Fig. 1), he demonstrated that for those positions of the honeycomb net which coincide with those of the triangular net containing the source,

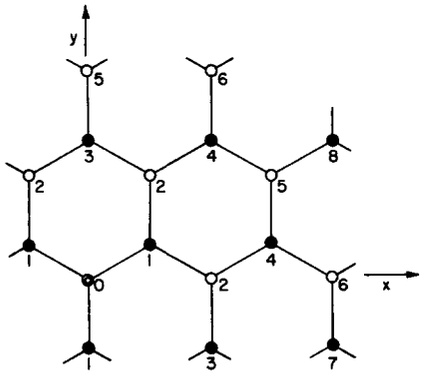

FIG. 1. The honeycomb net.

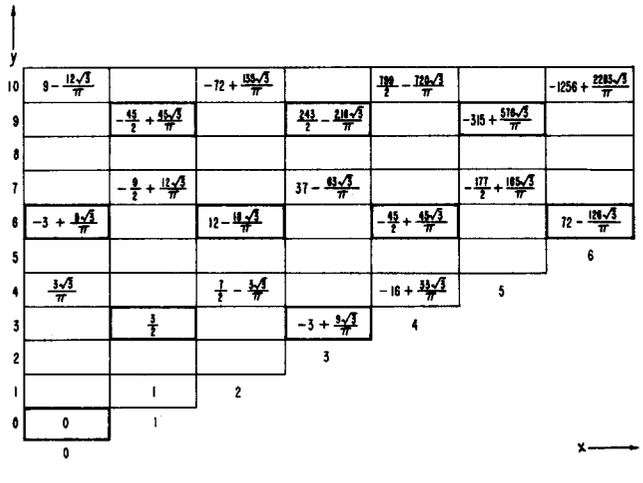

FIG. 2. Difference Green's functions for the honeycomb net.

the Green's functions for the honeycomb net are proportional to those for the triangular net; furthermore, the Green's functions for the other positions may be found from the difference equations for the honeycomb net. It follows from this that the Green's functions for the triangular and honeycomb nets may be expressed in terms of complete elliptic integrals.

It is unfortunate, in a sense, that the solutions are all infinite for the physically important case, $\nu = 1/6$; in that case the arguments of the elliptic integrals are unity and the integrals diverge. It is the purpose of this note to propose an alternate treatment of this case, and to show how this treatment may be used to express the Green's functions of the diamond lattice in terms of those for the face-centered-cubic lattice.

It is known[2,3] that the difficulties with divergence may be overcome by defining a difference Green's function,

$$G(x,y) \equiv F(0,0) - F(x,y), \quad (2)$$

where, in the case of the triangular lattice, $F(x,y)$ is a solution of Eq. (1). The functions $G(x,y)$ have been evaluated for the square[2] and the triangular[3] nets. As is obvious from the definition,

$$G(0,0) \equiv 0; \quad (3)$$

furthermore, for unbiased random walks in which the probability of motion is the inverse of the number of nearest neighbors (i.e., $\nu = 1/3$ for the honeycomb net; $\nu = 1/4$ for the square net and the diamond lattice; $\nu = 1/6$ for the triangular net and simple-cubic lattice), the difference equations insure that

$$G(1) = 1, \quad (4)$$

where $G(1)$ is the difference Green's function for the nearest neighbors of the source. It is easy to show that, for the open honeycomb net, the difference equations require

$$G_h(2) = \tfrac{3}{2}, \quad (5)$$

where the subscript h is to remind that this result is valid only for the honeycomb net. The result[1] of Horiguchi is equivalent to the statement that, for those sites of the honeycomb net which coincide with those of the triangular net containing the source,

$$G_h(x,y) = \tfrac{3}{2}\,G_t(x,y), \quad (6)$$

where the $G_t(x,y)$ are given in Ref. 3. This follows from the fact that if the G's for the two nets are proportional where the sites coincide, the proportionality factor must be given by the ratio $G_h(2)/G_t(1) = 3/2$. Again, the $G_h(x,y)$ for the other sites are found from the appropriate difference equation. The results of this procedure are given in Fig. 2, which shows the difference Green's functions for the positions near the origin. The

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table could be extended with little effort but numerical values are most easily found by using the accurate asymptotic formula for $G_t(x,y)$ given in Ref. 3.

In extending the method to the diamond lattice, we remark first that Eqs. (3) and (4) still apply whereas Eq. (5) is replaced by

$$G_d(2) = \tfrac{4}{3}. \tag{7}$$

The diamond lattice is composed of two interpenetrating face-centred-cubic lattices, one centered at (0, 0, 0), the source, the other centered at (1, 1, 1), one of the four first neighbours; the odd neighbors of the diamond lattice are located on the fcc lattice centered at (1, 1, 1) and the even neighbors of the diamond lattice are located on the fcc lattice centered at (0, 0, 0). In accord with the prescription above, the Green's function for one half of the diamond sites are given by

$$F_d(2k, 2l, 2m) = \tfrac{4}{3} F_f(2k, 2l, 2m), \tag{8}$$

where F_d is the Green's function for the diamond lattice and F_f is the Green's function for the face-centered-cubic lattice. The Green's function for the odd-neighbor sites are found from the appropriate difference equation. The calculations are sketched below:

$$F_d(0) \equiv F_d(0,0,0) = \tfrac{4}{3}\ F_f(0,0,0) = \tfrac{4}{3} \times 1.344\ 661\ 183 = 1.792\ 881\ 58,$$

$$F_d(2) \sim F_d(2,2,0) = \tfrac{4}{3} \times 0.344\ 661\ 183 = 0.459\ 548\ 24,$$

$$F_d(4) \sim F_d(4,0,0) = \tfrac{4}{3} \times 0.229\ 936\ 054 = 0.306\ 581\ 41,$$

$$F_d(6) \sim F_d(4,2,2) = \tfrac{4}{3} \times 0.195\ 466\ 708 = 0.260\ 622\ 28,$$

$$F_d(8) \sim F_d(4,4,0) = \tfrac{4}{3} \times 0.170\ 889\ 341 = 0.227\ 852\ 45.$$

The values of $F_f(2k, 2l, 2m)$ are taken from Ref. 4, wherein they are designated $F(k, l, m)$.

The difference equation

$$F(0) = 1 + F(1)$$

yields

$$F_d(1) \sim F_d(1,1,1) = 0.792\ 881\ 58.$$

The difference equation

$$F(3) = \tfrac{1}{2}F(2) + \tfrac{1}{4}F(4) + \tfrac{1}{4}F(6)$$

yields

$$F_d(3) \sim F_d(3,1,-1) = 0.371\ 575\ 04.$$

The difference equation

$$F(2) = \tfrac{1}{4}F(1) + \tfrac{1}{2}F(3) + \tfrac{1}{4}F(5)$$

yields

$$F_d(5) \sim F(3,3,1) = 0.302\ 161\ 31.$$

The difference equation

$$F(4) = \tfrac{1}{2}F(3) + \tfrac{1}{2}F(7)$$

yields

$$F_d(7) \sim F(5,1,1) = 0.241\ 587\ 78.$$

These values are complete through the first eight neighbor shells except for a seventh neighbor of the second kind, $F_d(7') \sim F_d(-3,-3,-3)$, which requires a knowledge of $F_f(4,4,4)$, or $F(2,2,2)$, not tabulated in Ref. 4. $F(2,2,2)$ is, however, known in integral form and the integral may be evaluated by the methods discussed in Ref. 4; thus, the tabulation may be extended in an obvious manner. The values obtained may be checked by various relations derived from the difference equations. The most interesting of these is

$$G_d(4) + 2G_d(5) + G_d(6) = 6,$$

which is satisfied identically.

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Electromagnetic wave propagation in inhomogeneous multilayered structures of arbitrarily varying thickness—Generalized field transforms*

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To provide a suitable basis for the expansion of electromagnetic fields in multilayered structures of arbitrarily varying thickness we derive, in this paper, the appropriate transform pairs for the transverse electric and magnetic field components. Applying the technique utilized earlier for two semi-infinite media, we first derive the transform pairs for the three-medium problem. Building on these expressions for the transform pairs, we systematically extend our results for structures with an arbitrary number of layers. The generalized transforms derived consist of two infinite integrals (continuous spectrum) which correspond to the radiation and the lateral wave terms as well as a finite number of terms (discrete spectrum) which correspond to the surface waves. Exact boundary conditions are employed rather than surface impedance boundary conditions. In the analysis, the sources and the observation point may be located in any of the structure's layers. Thus for instance, the derived field expressions are suitable for the study of antennas embedded in the earth's crust or submerged underwater.

1. INTRODUCTION

A full wave solution to the problem of electromagnetic wave propagation over nonuniform boundaries was derived recently using a Fourier-type transform pair that provides a suitable basis for the expansion of the electromagnetic fields above and below the nonuniform interface.[1,2] In order to solve the problem of propagation in inhomogeneous multilayered structures of arbitrarily varying thickness (see Fig. 1), we derive, in this paper, the appropriate transform pairs for the transverse components of the electromagnetic fields. To this end, we first apply the familiar Fourier transform method to derive the fields for a three-medium problem, with source and observer in any of the three layers. Using the techniques employed earlier, we deform the path of integration in the complex plane to obtain the desired transforms which consist of two branch-cut integrals and a finite number of contributions due to the poles of the integrand. Building on these expressions for the three-medium transform pair, we systematically construct the generalized transform pairs for structures with an arbitrary number of layers, without any recourse to the familiar Fourier transforms.

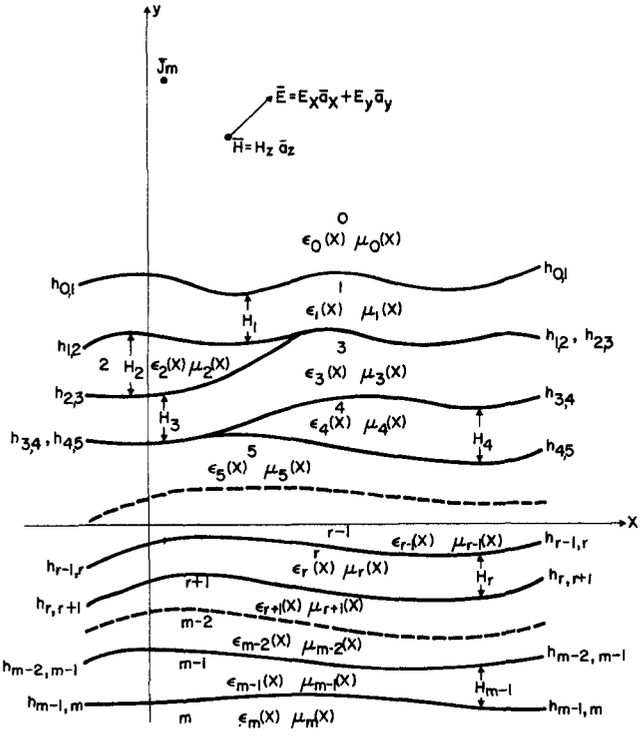

FIG. 1. Inhomogeneous multilayered structure of variable thickness.

If the electromagnetic parameters of the uppermost or lowermost layers are such that $(\mu/\epsilon)^{1/2} \to 0$ or $(\epsilon/\mu)^{1/2} \to 0$ (perfect electric or magnetic walls respectively) or if one of the boundaries of the multilayered structure is characterized by a (approximate) surface impedance, the electromagnetic fields are expressed in terms of a finite number of surface wave modes and only one branch-cut integral. However, if both boundary media are characterized by electromagnetic parameters $(\mu/\epsilon)^{1/2} \to 0$ or $(\epsilon/\mu)^{1/2} \to 0$, or both boundaries of the multilayered structure are characterized by surface impedances, the electromagnetic fields are expressed in terms of an infinite set of waveguide modes. There are no contributions from branch-cut integrals in this case.

These solutions are not restricted by approximate surface impedance boundary conditions and, since in this analysis the source and the observer may be located in any of the structure's layers, the transforms may be used to study the performance of antennas embedded in a nonuniform environment such as the earth's crust or the ionosphere.

2. TRANSFORM PAIR FOR A THREE-MEDIUM UNIFORM STRUCTURE

In this paper we consider in detail the case of vertically polarized waves and assume that there are no field variations in the z direction (see Fig. 2). Using duality considerations for electromagnetic fields, these solutions can be applied directly to the case of horizontally polarized waves.

For an $\exp(i\omega t)$ time dependence, the horizontal magnetic field $H_z\,\bar{a}_z$ generated by a z directed magnetic line source $J_m\,\bar{a}_z$ (analogous to the electric line current) satisfies the wave equation

$$\frac{\partial^2 H_z}{\partial x^2} + \frac{\partial^2 H_z}{\partial y^2} + k^2 H_z = i\omega\epsilon J_m = i\omega\epsilon K\delta(x-x_0)\delta(y-y_0), \tag{2.1a}$$

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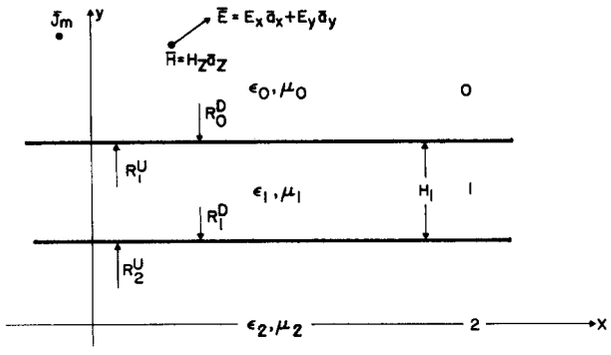

FIG. 2 Three-medium uniform structure.

where the magnetic line source, of intensity K volts, is located anywhere in medium $0(\mu_0, \epsilon_0), 1(\mu_1, \epsilon_1)$, or $2(\mu_2, \epsilon_2)$ and $\delta(x - x_0)$ and $\delta(y - y_0)$ are Dirac delta functions. The wavenumber is

$$k = \omega(\mu\epsilon)^{1/2}, \quad \mathrm{Im}(k) \leq 0, \tag{2.1b}$$

$$\epsilon(y) = \begin{cases} \epsilon_0 \\ \epsilon_1, \\ \epsilon_2 \end{cases} \quad \mu(y) = \begin{cases} \mu_0 \\ \mu_1, \\ \mu_2 \end{cases} \quad \text{for} \begin{cases} y > h_{01} \\ h_{01} > y > h_{12}. \\ h_{12} > y \end{cases} \tag{2.1c}$$

For $\rho = (x^2 + y^2)^{1/2} \to \infty$, H_z satisfies the radiation condition and at the surfaces $y = h_{01}$ and $y = h_{12}$ the boundary conditions are

$$H_z(x, h^+_{i,i+1}) = H_z(x, h^-_{i,i+1}) \tag{2.2a}$$

and

$$\frac{1}{\epsilon_i}\frac{\partial}{\partial y} H_z(x, h^+_{i,i+1}) = \frac{1}{\epsilon_{i+1}}\frac{\partial}{\partial y} H_z(x, h^-_{i,i+1}), \quad i = 0 \text{ and } 1. \tag{2.2b}$$

Using the familiar Fourier transforms with respect to the unbounded variable x, we seek a solution of the form

$$H_z(x, y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(\beta, y)\, \exp[-i\beta(x - x_0)]d\beta, \tag{2.3a}$$

where $H(\beta, y)$ satisfies

$$\frac{\partial^2 H(\beta, y)}{\partial y^2} + u^2 H(\beta, y) = i\omega\epsilon K\delta(y - y_0) \tag{2.3b}$$

and

$$u = (k^2 - \beta^2)^{1/2}, \quad \mathrm{Im}(u) \leq 0. \tag{2.3c}$$

On applying the boundary conditions (2.2), the solution for $H(\beta, y)$ in the three layers 0, 1, and 2, respectively, are, for $y_0 > h_{0,1}$,

$$H(\beta, y) = \frac{-K\omega\epsilon_0}{2u_0} \times \begin{cases} \exp[-iu_0|y - y_0|] + R_0^{Dh}\exp[-iu_0(y + y_0)], \\ (T_0^D/T_1^{DH})\exp[-iu_0(y_0 - h_{01})] \\ \times \{\exp[iu_1(y - h_{01})] + R_1^{Dh}\exp[-iu_1(y - h_{01})]\}, \\ (T_0^D T_1^D/T_1^{DH})\exp[-iu_0(y_0 - h_{01}) - iu_1H_1] \\ \times \exp[iu_2(y - h_{12})], \end{cases} \quad \text{for } h_{01} > y_0 > h_{12}, \tag{2.4a}$$

$$H(\beta, y) = \frac{-K\omega\epsilon_1}{2u_1} \times \begin{cases} (1 + A)T_1^u[\exp - iu_1(h_{01} - y_0)]\exp[-iu_0(y - h_{01})], \\ \exp[-iu_1|y - y_0|] + A\exp[-iu_1(y - y_0)] \\ + B\exp[iu_1(y - y_0)], \\ (1 + B)T_2^D\exp[iu_1(h_{12} - y_0)] \\ \times \exp[iu_2(y - h_{12})], \end{cases} \tag{2.4b}$$

and, for $h_{12} > y_0$,

$$H(\beta, y) = \frac{-K\omega\epsilon_2}{2u_2} \times \begin{cases} (T_2^U T_1^U/T_1^{UH})\exp[iu_2(y_0 - h_{12}) - iu_1H_1] \\ \times \exp[-iu_0(y - h_{01})], \\ (T_2^U/T_1^{UH})\exp[iu_2(y_0 - h_{12})]\{\exp[-iu_1(y - h_{12})] \\ + R_1^{Uh}\exp[iu_1(y - h_{12})]\}, \\ \exp[-iu_2|y - y_0|] + R_2^{Uh} \\ \times \exp[iu_2(y + y_0)], \end{cases} \tag{2.4c}$$

where R_i^U and R_i^D, the reflection coefficients in the ith layer looking in the positive and negative y directions, respectively, are given by

$$R_0^D = (R_{1,0} + R_1^{DH})/(1 + R_{1,0}R_1^{DH}), \quad R_1^D = R_{2,1},$$
$$R_i^{DH} = R_i^D\exp(-i2u_iH_i), \quad R_i^{Dh} = R_i^D\exp(i2u_ih_{i,i+1}),$$
$$R_2^U = (R_{1,2} + R_1^{UH})/(1 + R_{1,2}R_1^{UH}), \quad R_1^U = R_{0,1},$$
$$R_i^{UH} = R_i^U\exp(-i2u_iH_i), \quad R_i^{Uh} = R_i^U\exp(-i2u_ih_{i-1,i}). \tag{2.5a}$$

The coefficients A and B are

$$A = [R_1^{Dh}\exp(-i2u_1y_0) - R_{1,0}R_1^{DH}]/(1 + R_{1,0}R_1^{DH}),$$
$$B = [R_1^{Uh}\exp(i2u_1y_0) - R_{1,2}R_1^{UH}]/(1 + R_{1,2}R_1^{UH}),$$

and $R_{i,i+1}$, the two-medium Fresnel reflection coefficients, are

$$R_{i+1,i} = -R_{i,i+1} = (u_i\epsilon_{i+1} - u_{i+1}\epsilon_i)/(u_i\epsilon_{i+1} + u_{i+1}\epsilon_i). \tag{2.5b}$$

The transmission coefficients are

$$T_i^U = 1 + R_i^U, \quad T_i^D = 1 + R_i^D, \quad T_i^{UH} = 1 + R_i^{UH}, \quad T_i^{DH} = 1 + R_i^{DH} \tag{2.5c}$$

and the thickness of the ith layer is (see Fig. 2)

$$H_i = h_{i-1,i} - h_{i,i+1}, \tag{2.5d}$$

where $i = 1$ and 2.

The above Fourier expansion of $H_z(x, y)$ [(2.3a)] is not suitable for the full wave analysis of problems in which the layers are inhomogeneous ($\epsilon_i(x)$, $\mu_i(x)$) or when all the surfaces $y = h_{i,i+1}$ are not planes parallel to the (x, z) plane. To obtain a suitable expansion, we deform the path of integration ($-\infty < \beta < \infty$) in the lower and

upper half β plane for $x \geq x_0$ and $x \leq x_0$, respectively, as indicated in Fig. 3.[3,4] We note that, in all the expressions (2.4), $u_0 = 0$ and $u_2 = 0$ are branch points; however, $u_1 = 0$ is not a branch point since $H(\beta, y)$ in (2.4) is the same for the values of u_1 on both Rieman sheets. The poles of the integrand are at $1/R_0^D = 0$ (or $1/R_2^U = 0$). Thus the modal equation for the surface waves is

$$R_1^U R_1^{DH} = R_{0,1} R_{2,1} \exp(-iu_1 H_1) = \exp(-i2n\pi) \tag{2.6}$$

subject to the condition (2.3c), $\mathrm{Im}(u) \leq 0$.

Accounting for the residues at the N poles $\beta = \beta_n$ ($\mathrm{Im}\,\beta_n \leq 0$) and the contributions along the branch cuts $\mathrm{Im}(u_0) = 0$ and $\mathrm{Im}(u_2) = 0$, we get, after some tedious algebraic manipulations,

$$\begin{aligned} H_z(x,y) &= H_0(x,y) + H_2(x,y) + \sum_{n=1}^{N} H_s^n(x,y) \\ &= -\frac{K}{2}\left(\int_0^\infty \exp(-i\beta|x-x_0|)\Psi_0(u,y_0)\psi_0(u,y)du_0 \right. \\ &\quad + \int_0^\infty \exp(-i\beta|x-x_0|)\Psi_2(u,y_0)\psi_2(u,y)du_2 \\ &\quad \left. + \sum_{n=1}^{N} \exp(-i\beta_n|x-x_0|)\Psi_s(u,y_0)\psi_s(u,y)\right) \\ &\equiv -\frac{K}{2}\sum_m \exp(-i\beta|x-x_0|)\Psi_m(u,y_0)\psi_m(u,y), \\ &\qquad m = 0, 2, \text{or } s, \end{aligned} \tag{2.7a}$$

where

$$\begin{aligned} 2\pi Z_0 \Psi_0(u,y) &= R_0^{Dh}\psi_0(u,y) \\ &= \begin{cases} \exp(iu_0 y) + R_0^{Dh}\exp(-iu_0 y), \\ (T_0^D/T_1^{DH})\exp[i(u_0-u_1)h_{01}][\exp(iu_1 y) \\ \quad + R_1^{Dh}\exp(-iu_1 y)], \\ (T_0^D T_1^D/T_1^{DH})\exp[i(u_0-u_1)h_{01} \\ \quad + i(u_1-u_2)h_{12}]\exp(iu_2 y), \end{cases} \end{aligned} \tag{2.7b}$$

$$\begin{aligned} 2\pi Z_2 \Psi_2(u,y) &= R_2^{Uh}\psi_2(u,y) \\ &= \begin{cases} (T_2^U T_1^U/T_1^{UH})\exp[i(u_1-u_2)h_{12} + i(u_0-u_1)h_{01}] \\ \quad \times \exp(-iu_0 y), \\ (T_2^U/T_1^{UH})\exp[i(u_1-u_2)h_{12}][\exp(-iu_1 y) + R_1^{Uh} \\ \quad \times \exp(iu_1 y)], \\ \exp(-iu_2 y) + R_2^{UH}\exp(iu_2 y), \end{cases} \end{aligned} \tag{2.7c}$$

and for the nth surface wave mode

$$\begin{aligned} \Psi_s^n(u,y) &= \psi_s^n(u,y) = \Psi_s^n(u,h_{01}) \\ &\times \begin{cases} \exp[-iu_0^n(y-h_{01})], \\ (1/T_1^{DH})\exp(-iu_1^n h_{01})[\exp(iu_1^n y) + R_1^{Dh}\exp(-iu_1^n y)], \\ (T_1^D/T_1^{DH})\exp(-iu_1^n H_1)\exp[iu_2^n(y-h_{12})]. \end{cases} \end{aligned} \tag{2.7d}$$

The transverse wave impedance is

$$Z(u,y) = \beta/\omega\epsilon(y) = \begin{cases} Z_0, & y > h_{01} \\ Z_1, & h_{01} > y > h_{12} \\ Z_2, & h_{12} > y \end{cases} \tag{2.8a}$$

and

$$[\Psi_s^n(u,h_{01})]^2 = \left[\beta\left(iu_0 Z_0 \frac{d}{d\beta}\frac{1}{R_0^D}\right)^{-1}\right]_{\beta=\beta_n} \tag{2.8b}$$

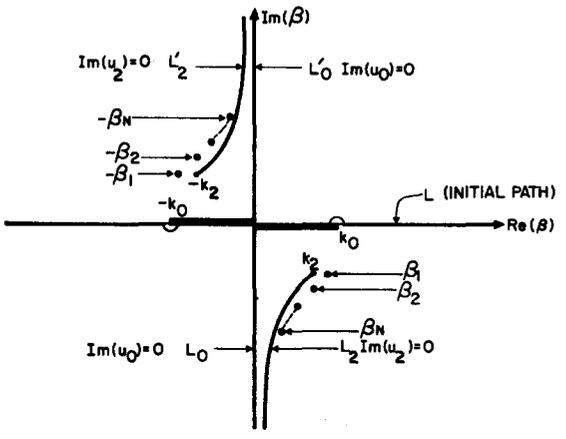

FIG. 3. Paths of integration in the complex β plane.

It can be shown that

$$\begin{aligned} [\Psi_s^n(u,h_{12})]^2 &= \left[\Psi_s^n(u,h_{01})\frac{T_1^D}{T_1^{DH}}\exp(-iu_1^n H_1)\right]^2 \\ &= \left[\beta\left(iu_2 Z_2 \frac{d}{d\beta}\frac{1}{R_2^U}\right)^{-1}\right]_{\beta=\beta_n} \end{aligned} \tag{2.8c}$$

Substituting the expression (2.7a) for $H_z(x,y)$ into the wave equation (2.1a) and noting that the one-dimensional Green's function $\exp[-i\beta|x-x_0|]$ satisfies the differential equation

$$\left(\frac{\partial^2}{\partial x^2} + \beta^2\right)\exp[-i\beta|x-x_0|] = -i2\beta\delta(x-x_0), \tag{2.9a}$$

we get the following complete expansion for $\delta(y-y_0)$:

$$\sum_m Z(y_0)\Psi_m(u,y_0)\psi_m(u,y) = \delta(y-y_0) \tag{2.9b}$$

where the summation symbol $\sum$ is interpreted as in (2.7a). To derive the desired transform pair for the three-medium problem, we multiply (2.9b) by $H_z(x,y_0)$ and integrate with respect to y_0 over the interval $(-\infty, \infty)$. Thus

$$\begin{aligned} H_z(x,y) &= H_0(x,y) + H_2(x,y) + \sum H_s^n(x,y) \\ &\equiv \sum H_p(x,u)\psi_p(u,y), \quad p = 0, 2, \text{or } s \end{aligned} \tag{2.10a}$$

and the transform functions $H_p(x,u)$ are

$$H_p(x,u) = \int_{-\infty}^{\infty} H_z(x,y)Z(u,y)\Psi_p(u,y)dy, \qquad p = 0, 2, \text{or } s. \tag{2.10b}$$

Using the transform pair (2.10), we derive the important orthogonal relationship

$$\begin{aligned} &\int_{-\infty}^{\infty} Z(u,y)\Psi_p(u,y)\psi_q(u^*,y)dy \\ &= \delta_{p,q}\Delta(u-u^*) = \delta_{p,q}\begin{cases} \delta(u-u^*), & \beta \neq \beta_s, \\ \delta_{u,u_s}, & \beta^* = \beta_s, \end{cases} \end{aligned} \tag{2.11}$$

where p and q are equal to 0, 2, or s and $\delta_{a,b}$ is the Kronecker delta. The expressions for the functions $H_{0,2}(x,y)$ in (2.10a) can be written in forms that are more convenient for integration by the method of steepest descent.

Noting that

$$H_0(x,u_0) = R_0^{Dh} H_0(x,-u_0) \tag{2.12a}$$

and

$$H_2(x,u_2) = R_2^{Uh} H_2(x,-u_0), \tag{2.12b}$$

we get

$$H_0(x,y) = \int_{-\infty}^{\infty} H_0(x,u)\exp(-iy,u_0)du_0, \quad y > h_{01}, \tag{2.12c}$$

and

$$H_2(x,y) = \int_{-\infty}^{\infty} H_2(x,y)\exp(iy,u_2)du_2, \quad y < h_{12}. \tag{2.12d}$$

In the analysis of the two-medium problem,[1,2] it has been shown that the above expressions (2.11) correspond to the radiation and the lateral wave terms. We now derive the corresponding transform pair for the transverse component of the electric field E_y. Noting that

$$E_y(x,y) = \frac{i}{\omega\epsilon}\frac{\partial H_z}{\partial x} \tag{2.13}$$

the appropriate basis function for $E_y(x,y)$ is $Z(u,y)\psi(u,y)$; thus

$$E_y(x,y) = \sum_p E_p(x,u)\,Z(u,y)\psi_p(u,y), \tag{2.14a}$$

where

$$E_p(x,u) = \int_{-\infty}^{\infty} E_y(x,y)\Psi_p(u,y)dy, \quad p = 0, 2, \text{and } s, \tag{2.14b}$$

and $\sum$ is interpreted as in (2.7a).

To obtain the corresponding transform pairs for the dual problem (electric line current excitation I) in which the waves are horizontally polarized, we make the following substitutions in the above-derived transform pairs:

$$H_z \to E_z, \quad E_y \to -H_y, \quad \mu \to \epsilon,$$
$$\epsilon \to \mu, \quad K \to I.$$

As a result, the reflection coefficients for vertical polarization R_v are replaced by the reflection coefficient for horizontally polarized waves R_h, and $Z(u,y)$ is replaced by $Y(u,y) = \beta/\omega\mu$.

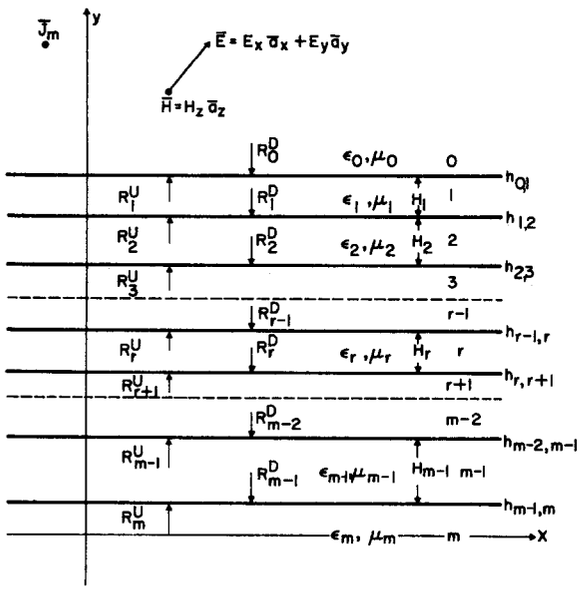

FIG. 4. Multilayered uniform structure.

3. GENERALIZED TRANSFORMS FOR MULTILAYERED MEDIA

On the basis of the derivations in the preceding section, we systematically construct the expressions for the generalized transforms for stratified media with an arbitrary number of layers (see Fig. 4). We shall do this directly, without recourse to the familiar Fourier transforms (with respect to the x variable).

The $m+1$ layers are characterized by the electromagnetic parameters ϵ_i and μ_i with $i = 0,1,\ldots,m$. The wave parameters k_i and u_i are defined as in Sec. 2, Eqs. (2.1b) and (2.3c). Likewise, all the reflection and transmission coefficients in the ith layer are denoted by the subscript i (see Fig. 4).

As in the case of the three-medium problem, the expressions for the transforms for the multilayered case consist of two infinite branch cut integrals [$\mathrm{Im}(u_0) = 0$ and $\mathrm{Im}(u_m) = 0$] corresponding to the branch points $u_0 = 0$ and $u_m = 0$. In addition the transforms consist of a finite number of surface-wave (or trapped) waveguide modes, characterized by the modal equation

$$1/R_0^D = 0 \quad \text{or} \quad 1/R_m^U = 0. \tag{3.1a}$$

The reflection coefficient R_i^D is the reflection coefficient at the $i, i+1$ interface for waves incident from above and R_i^U is the reflection coefficient at the $i, i-1$ interface for waves incident from below. Thus

$$R_0^U = 0, \quad R_i^U = (R_{i-1,i} + R_{i-1}^{UH})/(1 + R_{i-1,i}R_{i-1}^{UH}), \quad i = 1,2,\ldots,m, \tag{3.1b}$$

and

$$R_m^D = 0, \quad R_i^D = (R_{i+1,i} + R_{i+1}^{DH})/(1 + R_{i+1,i}R_{i+1}^{DH}), \quad i = 0,1,\ldots,m-1, \tag{3.1c}$$

where $R_{i+1,i}$ and $R_{i-1,i}$ are the Fresnel reflection coefficients (2.5b) and $R_i^{Uh}, R_i^{UH}, R_i^{Dh}$ and R_i^{DH} are defined as in Sec. 2, Eq. (2.5a). The transmission coefficients T_i^U, T_i^{UH}, T_i^D and T_i^{DH} are given by (2.5c).

To obtain the expression for the basis function $\psi_0(u,y)$ [corresponding to the branch cut integral $Im(u_0) = 0$], we begin with the expressions for the fields for $y > h_{01}$ and $y_0 > h_{01}$ and work downward (in the negative y direction), satisfying at each interface the boundary conditions

$$\psi(u,h_{i,i+1}^+) = \psi(u,h_{i,i+1}^-) \tag{3.2a}$$

and

$$\frac{1}{\epsilon_i}\frac{\partial}{\partial y}\psi(u,h_{i,i+1}^+) = \frac{1}{\epsilon_{i+1}}\frac{\partial}{\partial y}\psi(u,h_{i,i+1}^-). \tag{3.2b}$$

Thus we obtain directly

$$2\pi Z_0\Psi_0(u,y) = R_0^{Dh}\psi_0(u,y)$$

$$= \begin{cases} \exp(iu_0y) + R_0^{Dh}\exp(-iu_0y), & \text{for medium 0,} \\ \prod_{p=1}^{r}\left(T_{p-1}^D/T_p^{DH}\right)\exp\left\{i\sum_{n=1}^{r}u_{p-1,p}h_{p-1,p}\right\} \\ \times[\exp(iu_ry) + R_r^{Dh}\exp(-iu_ry)], \\ \qquad \text{for medium } r = 1,2,3,\ldots,m, \end{cases} \tag{3.3a}$$

where

$$u_{n-1,n} = u_{n-1} - u_n. \tag{3.3b}$$

Similarly, to derive the basis functions $\psi_m(u,y)$ [corresponding to the branch cut integral $\mathrm{Im}(u_m) = 0$], we begin with the fields for $y < h_{m-1,m}$ and $y_0 < h_{m-1,m}$ and work upward (in the positive y direction), satisfying at each interface the boundary conditions (3.2). Thus we obtain directly

$$2\pi Z_m \Psi_m(u,z) = R_m^{Uh}\psi_m(u,y)$$

$$= \begin{cases} \prod_{p=1}^{m-r} \dfrac{T_{m+1-p}^{U}}{T_{m-p}^{UH}} \exp\{i\textstyle\sum u_{m-p,m+1-p} h_{m-p,m+1-p}\} \\ \times [\exp(-iu_r y) + R_r^{Uh} \exp(iu_r y)], \\ \qquad\qquad \text{for medium } r = 0,1,2,\ldots,m-1, \\ \exp(-iu_m y) + R_m^{Uh} \exp(iu_m y), \quad \text{for medium } m. \end{cases} \tag{3.3c}$$

To derive the basis functions $\psi_s(u,y)$ for the (trapped) waveguide modes, we can begin with the field expression in either the uppermost or lowermost medium (0 or m) and work downward or upward respectively, satisfying the boundary conditions (3.2) at each interface. Thus for the nth waveguide mode, working downward from medium 0, we get

$$\Psi_s^n(u,y) = \psi_s^n(u,y) = \Psi_s^n(u,h_{01})$$

$$\times \begin{cases} \exp[-iu_0^n (y - h_{01})], \quad \text{for medium 0} \\ \dfrac{1}{T_1^{DH}} \exp(-iu_1^n h_{01})[\exp(iu_1^n y) + R_1^{Dh} \exp(-iu_1^n y)], \\ \qquad\qquad \text{for medium 1} \\ \dfrac{1}{T_1^{DH}} \exp(-iu_1^n h_{01}) \prod_{p=2}^{r} \dfrac{T_{n-1}^{D}}{T_n^{DH}} \exp\left(i \sum_{p=2}^{r} u_{p-1,p}^n h_{p-1,p}\right) \\ \times [\exp(iu_r^n y) + R_r^{Dh} \exp(-iu_r^n y)], \\ \qquad\qquad \text{for medium } r = 2,3,\ldots,m, \end{cases} \tag{3.4a}$$

where

$$[\Psi_s^n(u,h_{01})]^2 = \left[\beta\left(iZ_0 u_0 \frac{d}{d\beta}\frac{1}{R_0^D}\right)^{-1}\right]_{\beta=\beta_n} \tag{3.4b}$$

Alternatively, working upward starting with medium m, we get an equivalent expression for $\Psi_s^n(u,y)$,

$$\Psi_s^n(u,y) = \psi_s^n(u,y) = \Psi_s^n(u,h_{m-1,m})$$

$$\times \begin{cases} \dfrac{1}{T_{m-1}^{UH}} \exp(iu_{m-1,m}^n) \prod_{p=2}^{m-r} \dfrac{T_{m+1-p}^{U}}{T_{m-p}^{UH}} \\ \times \exp(iu_{m-p,m+1-p}^n h_{m-p,m+1-p}). \\ \times [\exp(-iu_r^n y) + R_r^{Uh} \exp(iu_r^n y)] \\ \text{for medium } r, \text{ where } r = 0,1,2,\ldots,m-2, \\ \dfrac{1}{T_{m-1}^{UH}} \exp(iu_{m-1}^h h_{m-1,m})[\exp(-iu_{m-1}^n y) \\ + R_{m-1}^{Uh} \exp(iu_{m-1}^n y)], \quad \text{for medium } m-1, \\ \exp[iu_m^n (y - h_{m-1,m})], \quad \text{for medium } m, \end{cases} \tag{3.4c}$$

where

$$[\Psi_s^n(u,h_{m-1,m})]^2 = \left[\beta\left(iZ_m u_m \frac{d}{d\beta}\frac{1}{R_m^U}\right)^{-1}\right]_{\beta=\beta_n}. \tag{3.4d}$$

Using the expression (3.3a), (3.3c), and (3.4a) (or 3.4c) for the basis functions, we can now write complete expansions for $H_z(x,y)$ and $E_y(x,y)$ in terms of their transforms $H(u,y)$ and $E(u,y)$ as in (2.10) and (2.14), respectively. Thus noting that here the subscript 2 (for medium 2) must be replaced by m, we get

$$H_z(x,y) = H_0(x,y) + H_m(x,y) + \sum_{n=1}^{N} H_s^n(x,y)$$

$$= \textstyle\sum H_p(x,u)\psi_p(x,u), \quad p = 0,m, \text{ or } s, \tag{3.5a}$$

where

$$H_p(x,u) = \int_{-\infty}^{\infty} H_z(x,y)\, Z(u,y)\Psi_p(u,y)dy, \quad p = 0,m, \text{ or } s, \tag{3.5b}$$

and

$$E_y(x,y) = \textstyle\sum E_p(x,u)\, Z(u,y)\psi_p(u,y), \tag{3.6a}$$

where

$$E_p(x,u) = \int_{-\infty}^{\infty} E_y(x,y)\Psi_p(u,y)dy. \tag{3.6b}$$

Similarly the orthogonal relationship (2.11) is satisfied for the $(m+1)$-layer medium. In this case we let p and q equal $0, m$, or s in (2.11). Note that all the normalization coefficients are obtained automatically without actual integration with respect to y over the interval $(-\infty, \infty)$.

4. THE MODAL EQUATION

It was intuitively assumed in Sec. 3 that, for the waveguide modes, $1/R_0^D = 0$ or $1/R_m^U = 0$ [(3.1a)]. In Sec. 2, this was explicitly shown to be the case for the three-medium problem. We demonstrate in this section that the same holds when the structure has an arbitrary number of layers $(m+1)$. Beginning with the condition

$$1/R_0^D = 0, \tag{4.1a}$$

it follows directly from (3.1c) that, for the waveguide modes,

$$1 + R_{10}R_1^{DH} = 1 - R_1^U R_1^{DH} = 0. \tag{4.1b}$$

By substituting for R_1^{DH}, using the recurrence formula (3.1c), the above equation (4.1b) can also be written as

$$[(1 - R_1^{UH}R_{21}) + (R_{21} - R_1^{UH})R_1^{DH}]/(1 + R_{21}R_2^{DH}) = 0. \tag{4.1c}$$

To satisfy (4.1c), the necessary and sufficient condition is

$$1 - R_2^U R_2^{DH} = 0, \tag{4.2}$$

where we have used the definition of R_2^U given in (3.1b). In a straightforward manner it can be shown that, in general, the necessary and sufficient condition can be expressed as

$$1 - R_p^U R_p^D \exp(-i2u_p H_p) = 0, \quad p = 1,2,3,\ldots,m-1. \tag{4.3}$$

Thus for $p = m-1$ we get from (4.3)

$$1 - R_{m-1}^U R_{m-1}^D \exp(-i2u_{m-1}H_{m-1}) = 1 + R_{m-1}^{UH}R_{m,m-1} = 0. \tag{4.4a}$$

The above modal equation corresponds precisely to the condition

$$1/R_m^U = 0. \tag{4.4b}$$

Thus, the roots of Eqs. (4.1a), (4.3), and (4.1b) are identical. Equation (4.3), which is satisfied in each of the layers of finite thickness, is equivalent to the statement that the waves associated with the trapped waveguide modes undergo constructive interference in each layer of the structure.

5. CONCLUDING REMARKS

In this paper, we have derived a systematic method for constructing the transform pairs for the transverse components of the electromagnetic fields in a multilayered structure. The complete expansion consists of two infinite (branch cut) integrals—the continuous part of the wavenumber spectrum, as well as a finite number of trapped waveguide modes—the discrete part of the wavenumber spectrum.

The method also provides all the important orthogonality relationships (2.11) that are satisfied by the basis functions and determines all the normalization coefficients without performing any integrations.

In an earlier analysis of the two-medium problem,[1,2] the infinite integrals are identified as the radiation and the lateral wave terms.

The transforms derived in this paper for uniform multilayered media provide a suitable basis for the expansion of electromagnetic fields in an inhomogeneous multilayered structure of arbitrarily varying thickness.[5]

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Electromagnetic wave propagation in inhomogeneous multilayered structures of arbitrary thickness—Full wave solutions*

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In this paper, we derive full wave solutions to the problem of electromagnetic wave propagation in inhomogeneous multilayered structures of arbitrarily varying thickness. To this end, we employ generalized transforms that provide an appropriate basis for the complete expansion of the transverse components of the electromagnetic fields. The continuous parts of the wavenumber spectrum are the radiation and the lateral wave terms while the discrete part is identified as the finite set of trapped waveguide modes (surface waves). When the bounding media are characterized by perfect electric or magnetic walls ($\mu/\epsilon \to 0$ or $\epsilon/\mu \to 0$, respectively) or surface impedances, the fields are expressed exclusively in terms of an infinite set of waveguide modes. These solutions are not restricted by the approximate surface impedance concept and the sources and observation point may be located in any of the nonuniform layers of the structure. Exact boundary conditions are imposed and the solutions satisfy the reciprocity relationships. Thus, the solutions are applicable to artificial layered structures as well as natural structures such as the inhomogeneous ionosphere and the earth's crust. These solutions can also be used to determine the scattering from objects of finite cross section in free space or embedded in the earth's crust.

1. INTRODUCTION

Full wave solutions are derived to the problem of propagation of electromagnetic waves in multilayered structures of arbitrarily varying thickness (see Fig. 1). The electromagnetic parameters ϵ and μ, characterizing the medium of propagation in each layer, are also assumed to vary along the propagation path (the x axis). The sources and observation point may be located in any of the $(m + 1)$ media of the structure.

Exact boundary conditions are imposed and the solutions are not restricted by the approximate surface impedance concept.

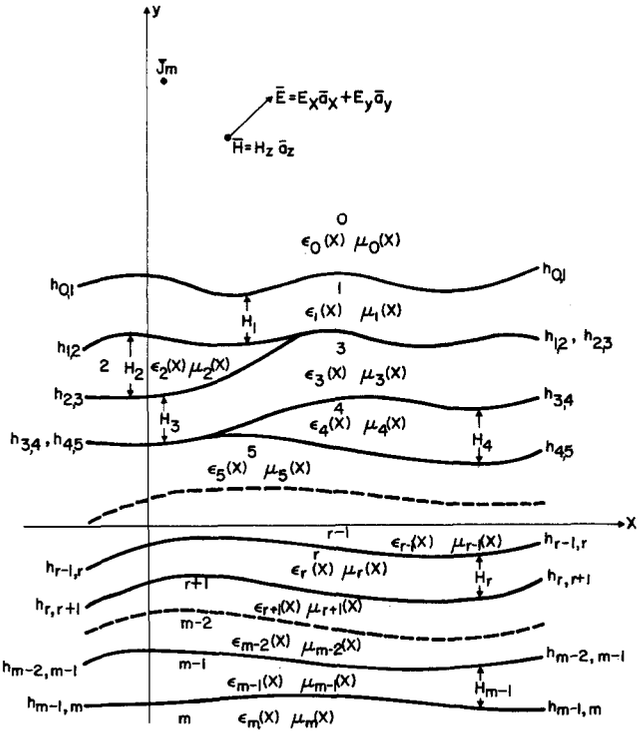

FIG. 1. Line source over a nonuniform multilayered structure.

For the purpose of the full wave analysis, generalized transforms[1] are used to provide a suitable complete expansion for the transverse components of the electromagnetic fields. The continuous parts of the wavenumber spectrum (two infinite integrals) correspond to the radiation and the lateral wave terms, while the discrete part is identified as the finite set of trapped waveguide modes or surface waves. These solutions satisfy the reciprocity relationships in electromagnetic theory.

A wide class of problems such as propagation in the nonuniform and inhomogeneous ionosphere layers or the earth's crust as well as artificial layered structures may be solved using the analysis derived in this paper. In the special case when the bounding media of the structure are regarded as perfect electric or magnetic walls ($\mu/\epsilon \to 0$ or $\epsilon/\mu \to 0$, respectively) or when they are characterized by surface impedances, the electromagnetic fields are expressed exclusively in terms of an infinite set of waveguide modes and the radiation and lateral wave terms vanish. Thus, in these cases, when $m = 2$ and the electromagnetic parameters ϵ, μ are constant, our problem reduces to the problem of propagation in a waveguide of variable height which has been treated extensively in the technical literature. On the other hand, when only one of the bounding media is regarded as an electric or magnetic wall or if it is characterised by a surface impedance, only one of the infinite integrals in the field expansions vanishes.

In the special case when $m = 1$, our solutions reduce to those derived recently[2] for the two-medium problems. The solutions can also be used to determine the scattering of electromagnetic waves from objects of finite cross-section embedded in the earth's crust or in free space (see Fig. 2).

2. FORMULATION OF THE PROBLEM

Propagation of vertically polarized waves in the nonuniform multilayered structure shown in Fig. 1 is considered in detail in this paper. The solutions for horizontally polarized waves may be derived in a similar manner or obtained directly from our present analysis, through duality considerations in electromagnetic theory ($\epsilon \to \mu$, $\mu \to \epsilon$, $\bar{H} \to \bar{E}$, and $\bar{E} \to -\bar{H}$). The height of the

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interface between medium r and medium $r+1$ from a reference plane $y=0$ is $h_{r,r+1}(x)$ and the thickness of the rth layer is

$$H_r(x) = h_{r-1,r}(x) - h_{r,r+1}(x). \tag{2.1}$$

Furthermore, the electromagnetic parameters for the rth layer (ϵ_r, μ_r) are also assumed to vary arbitrarily along the propagation path (the x axis). It is assumed here that the excitation is independent of the z axis; thus, the problem is two-dimensional and the scattered fields are also vertically polarized. We assume, without loss of generality, that the vertically polarized waves are generated by a z-directed line source $\bar{J}_m$ (dual to the electric line current $\bar{J}$) located at $x = x_0$ and $y = y_0$ (see Fig. 1):

$$J_m(x,y) = K\delta(x-x_0)\delta(y-y_0), \tag{2.2}$$

where $\delta(x-x_0)$ and $\delta(y-y_0)$ are Dirac delta functions and the intensity of the line source K is measured in volts. For an assumed $\exp(i\omega t)$ time dependence, the nonvanishing components of the electric and magnetic fields $\bar{E}$ and $\bar{H}$, respectively, are

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -i\omega\mu H_z - J_m, \tag{2.3a}$$

$$\frac{\partial H_z}{\partial y} = i\omega\epsilon E_x, \tag{2.3b}$$

and

$$-\frac{\partial H_z}{\partial x} = i\omega\epsilon E_y, \tag{2.3c}$$

where the electromagnetic coefficients are

$$\left.\begin{aligned}\epsilon(x,y) &= \epsilon_r(x)\\ \mu(x,y) &= \mu_r(x)\end{aligned}\right\}, \quad h_{r,r+1} < y < h_{r-1,r}, \quad r = 1,\ldots,m-1,$$

and

$$\begin{aligned}&\epsilon(x,y) = \epsilon_0(x), \quad \mu(x,y) = \mu_0(x), && y > h_{01},\\ &\epsilon(x,y) = \epsilon_m(x), \quad \mu(x,y) = \mu_m(x), && h_{m-1,m} < y.\end{aligned} \tag{2.4}$$

For $\rho = (x^2+y^2)^{1/2} \to \infty$, the electromagnetic fields satisfy the radiation condition and at each varying interface $y = h_{r,r+1}(x)$, the boundary conditions are

$$H_z(x, h^+_{r,r+1}) = H_z(x, h^-_{r,r+1}) \tag{2.5a}$$

and

$$\begin{aligned}&E_y(x, h^+_{r,r+1})\sin\theta_{r,r+1} + E_x(x, h^+_{r,r+1})\cos\theta_{r,r+1}\\ &\quad = E_y(x, h^-_{r,r+1})\sin\theta_{r,r+1} + E_x(x, h^-_{r,r+1})\cos\theta_{r,r+1},\end{aligned} \tag{2.5b}$$

where

$$\tan\theta_{r,r+1} = h'_{r,r+1} = \frac{dh_{r,r+1}(x)}{dx}. \tag{2.5c}$$

Using (2.3b) to eliminate E_x from (2.5b) and (2.3a), we get

$$[E_y^+ - E_y^-]h'_{r,r+1} = \frac{i}{\omega}\frac{\partial}{\partial y}\left(\frac{1}{\epsilon_r}H_z^+ - \frac{1}{\epsilon_{r+1}}H_z^-\right) \tag{2.5d}$$

and

$$-\frac{\partial E_y}{\partial x} = \frac{i}{\omega\epsilon}\left[k^2 H_z + \frac{\partial^2 H_y}{\partial y^2}\right] + J_m, \tag{2.5e}$$

where the wavenumber is

$$k(x,y) = \omega(\mu\epsilon)^{1/2}, \quad \mathrm{Im}(k) \le 0. \tag{2.5f}$$

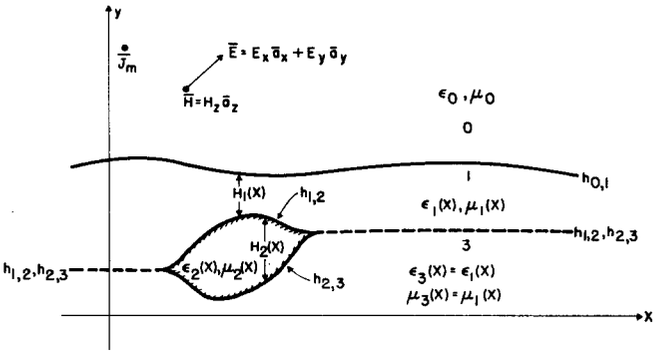

FIG. 2. Line source over a nonuniform structure with a layer of finite cross section

In our analysis, we employ the following generalized transform pair to obtain a complete expansion for the magnetic field component[1] H_z:

$$\begin{aligned}H_z(x,y) &= H_0(x,y) + H_m(x,y) + H_s(x,y)\\ &\equiv \sum H_p(x,u)\psi_p(u,y)\\ &= \int_0^\infty H_0(x,u)\psi_0(u,y)du_0 + \int_0^\infty H_m(x,u)\psi_m(x,u)du_m\\ &\quad + \sum_{n=1}^{N} H_s^n(x,u)\psi_s^n(x,u)\end{aligned} \tag{2.6a}$$

and

$$H_p(x,u) = \int_{-\infty}^{\infty} H_z(x,y)Z(u,y)\psi_p(u,y)dy, \qquad p = 0, m, \text{or } s. \tag{2.6b}$$

The basis functions satisfy the differential equation

$$\left(\frac{\partial^2}{\partial y^2} + u^2\right)\psi(u,y) = 0 \tag{2.7a}$$

and the boundary conditions at each interface, $y = h_{r,r+1}$,

$$\psi(u,h^+) = \psi(u,h^-)$$

and

$$\frac{\partial}{\partial y}\left(\frac{1}{\epsilon_r}\psi(u,h^+) - \frac{1}{\epsilon_{r+1}}\psi(u,h^-)\right) = 0. \tag{2.7b}$$

The boundary condition (2.7b) corresponds to (2.5d) only for the special case $h_{r,r+1} = \text{const}$. Thus, in general the expansion (2.6) for $H_z(x,y)$ does not uniformly converge at the interfaces $y = h_{r,r+1}$. In general, the basis functions are explicitly functions of x (through the height functions $h_{r,r+1}$ and the electromagnetic parameters ϵ and μ).

The expressions for the basis functions $\psi_q(u,y)$ are, for $q = 0$, given by

$$2\pi Z_0\Psi_0(u,y) = R_0^{Dh}\psi_0(u,y)$$

$$= \begin{cases}\exp(iu_0y) + R_0^{Dh}\exp(-iu_0y), & \text{for medium 0}\\ \prod_{p=1}^{r}\dfrac{T_{p-1}^{D}}{T_p^{DH}}\exp\left(i\sum_{p=1}^{r}u_{p-1,p}h_{p-1,p}\right)\\ \times[\exp(iu_ry) + R_r^{Dh}\exp(-iu_ry)],\\ \text{for medium } r = 1,2,\ldots,m,\end{cases} \tag{2.8a}$$

for $q = m$,

$$2\pi Z_m\Psi_m(u,y) = R_m^{Uh}\psi_m(u,y)$$

$$= \begin{cases} \prod_{p=1}^{m-r} \frac{T^U_{m+1-p}}{T^{UH}_{m-p}} \exp\left(i \sum_{p=1}^{m-r} u_{m-p,\,m+1-p} h_{m-p,\,m+1-p}\right) \\ \times [\exp(-iu_r y) + R^{Uh}_r \exp(iu_r y)], \\ \text{for medium } r = 0, 1, 2, \ldots, m-1, \\ \exp(-iu_m y) + R^{Uh}_m \exp(iu_m y), \\ \text{for medium } m, \end{cases} \tag{2.8b}$$

and for the nth surface-wave mode ($q = s$),

$$\Psi^n_s(u, y) = \psi^n_s(u, y) = \Psi^n_s(u, h_{01})$$

$$\times \begin{cases} \exp[-iu^n_0(y - h_{01})], \quad \text{for medium 0,} \\ \frac{1}{T^{DH}_1} \exp(-iu^n_1 h_{01})[\exp(iu^n_1 y) + R^{Dh}_1 \\ \times \exp(-iu^n_1 y)], \quad \text{for medium 1,} \\ \frac{1}{T^{DH}_1} \exp(-iu^n_1 h_{01}) \prod_{p=2}^{r} \frac{T^D_{n-1}}{T^{DH}_n} \\ \times \exp\left(i \sum_{p=2}^{r} u^n_{p-1,p} h_{p-1,p}\right) \\ \times [\exp(iu^n_r y) + R^{Dh}_r \exp(-iu^n_r y)], \\ \text{for medium } m = 2, 3, \ldots, m, \end{cases} \tag{2.8c}$$

where

$$[\Psi^n_s(u, h_{01})]^2 = \left[\beta\left(iZ_0 u_0 \frac{d}{d\beta} \frac{1}{R^D_0}\right)^{-1}\right]_{\beta=\beta_n} \tag{2.8d}$$

and β_n [$\mathrm{Im}(\beta_n) \leq 0$] is one of the finite set of surface wave modes that satisfies the modal equation

$$1/R^D_0 = 0. \tag{2.8e}$$

In the above expressions, the reflection coefficients at the $i, i+1$ interface, for waves incident from above and below, are respectively (see Fig. 1),

$$R^D_m = 0, R^D_i = (R_{i+1,i} + R^{DH}_{i+1})/(1 + R_{i+1,i} R^{DH}_{i+1}), \quad i = 1, 2, \ldots, m, \tag{2.9a}$$

$$R^U_0 = 0, R^U_i = (R_{i-1,i} + R^{UH}_{i-1})/(1 + R_{i-1,i} R^{UH}_{i-1}), \quad i = 0, 1, \ldots, m-1, \tag{2.9b}$$

where $R_{i+1,i}$ and $R_{i-1,i}$ are the Fresnel reflection coefficients

$$R_{i+1,i} = -R_{i,i+1} = (u_i \epsilon_{i+1} - u_{i+1} \epsilon_i)/(u_i \epsilon_{i+1} + u_{i+1} \epsilon_i) \tag{2.9c}$$

and

$$R^{DH}_i = R^D_i \exp(-i2u_i H_i), \quad R^{Dh}_i = R^D_i \exp(i2u_i h_{i,i+1}), \tag{2.9d}$$

$$R^{UH}_i = R^U_i \exp(-i2u_i H_i), \quad R^{Uh}_i = R^U_i \exp(-i2u_i h_{i-1,i}). \tag{2.9e}$$

The transmission coefficients are

$$T^D_i = 1 + R^D_i, \quad T^U_i = 1 + R^U_i, \quad T^{DH}_i = 1 + R^{DH}_i, \quad \text{and} \quad T^{UH}_i = 1 + R^{UH}_i. \tag{2.9f}$$

The wave parameter for medium r is

$$u_r(x) = [k^2_r - \beta^2]^{1/2}, \quad \mathrm{Im}(u_r) \leq 0, \tag{2.10a}$$

and

$$u_{p,p+1} = u_p - u_{p+1}. \tag{2.10b}$$

The transverse wave impedance is, for all y,

$$Z(u, y) = \beta/\omega\epsilon(x, y) \tag{2.10c}$$

and for medium r

$$Z(u, y) = \beta/\omega\epsilon_r(x) = Z_r(u). \tag{2.10d}$$

In a similar manner, the transverse component of the electric field E_y can be expressed in terms of its transform $E(x, u)$. In this case, the appropriate basis function is $Z(x, y)\psi(u, y)$; thus,

$$E_y(x, y) = \sum E_p(x, u) Z(u, y) \psi_p(u, y) \tag{2.11a}$$

and

$$E_p(x, u) = \int_{-\infty}^{\infty} E_y(x, y) \Psi(u, y) dy, \tag{2.11b}$$

where $\sum$ is to be interpreted as in (2.6).

The transform functions $H(u, y)$ and $E(u, y)$ can be expressed in terms of the forward and backward wave amplitudes $a(x, u)$ and $b(x, u)$, respectively.

Thus we define

$$H(x, u) = a(x, u) + b(x, u), E(x, u) = a(x, u) - b(x, u). \tag{2.12}$$

3. THE FORWARD AND BACKWARD WAVE AMPLITUDES

The transform pairs (2.6) and (2.11) provide a convenient basis for converting the partial differential equations (2.3c) and (2.5e) for $E_y(x, y)$ and $H_z(x, y)$ [in conjunction with the exact boundary conditions (2.5a) and (2.5d)] into a coupled set of ordinary differential equations for the wave amplitudes (2.12). To this end, we derive (directly from the transform pairs) the following completeness and orthogonal relationships. Thus the Dirac delta function $\delta(y - y_0)$ can be expressed in terms of the transforms (2.6) as

$$\delta(y - y_0) = \sum Z(u, y) \Psi_p(u, y_0) \psi_p(u, y), \tag{3.1a}$$

where $\sum$ is interpreted as in (2.6). Using (2.7a), the orthogonal relationship between the basis functions can be shown to be

$$\int_{-\infty}^{\infty} Z(u, y) \Psi_p(u^*, y) \psi_q(u, y) dy = \frac{1}{\beta^{*2} - \beta^2} \left[\psi_q(u, y) Z(u, y) \frac{\partial}{\partial y} \Psi_p(u^*, y) - \Psi_p(u^*, y) Z(u, y) \frac{\partial}{\partial y} \Psi_q(u, y)\right]_{-\infty}^{\infty}$$

$$= \delta_{p,q} \Delta(u, u^*) = \delta_{p,q} \begin{cases} \delta(u, u^*), & \beta^* \neq \beta_n, \\ \delta_{u,u^*}, & \beta^* = \beta_n, \end{cases} \tag{3.1b}$$

where β_n is a solution for the modal equation (2.8e), p and q are equal to 0, m, or s and $\delta_{p,q}$ is the Kronecker delta.

To obtain the desired ordinary differential equations for the wave amplitudes $a(x, u)$ and $b(x, u)$, multiply

(2.5e) by $\Psi_p(u^*, y)$ and (2.1c) by $Z(u^*, y)\Psi_p(u^*, y)$ and integrate with respect to y over the interval $(-\infty, \infty)$. Thus, for $p = 0, m$, or s we get

$$-\int_{-\infty}^{\infty} \frac{\partial E_y}{\partial x}\,\Psi_p dy = i\int_{-\infty}^{\infty} \frac{1}{\omega\epsilon}\left(\frac{\partial^2 H_z}{\partial y^2} + k^2 H_z\right) \times \Psi_p dy + \int_{-\infty}^{\infty} J_m \Psi_p dy \qquad (3.2a)$$

and

$$-\int_{-\infty}^{\infty} \frac{\partial H_z}{\partial x}\, Z\Psi_p dy = i\int_{-\infty}^{\infty} \omega\epsilon E_y Z\Psi_p dy. \qquad (3.2b)$$

In (3.2) we express $E_y(x, y)$ and $H_z(x, y)$ in terms of their respective transforms (2.6) and (2.11). However, since the basis functions $\psi(u, y)$ and $Z(u, y)\psi(u, y)$ do not in general satisfy the boundary conditions for the field components $H_z(x, y)$ and $E_y(x, y)$, respectively, the expansions (2.6a) and (2.11a) do not converge uniformally at the interfaces $h_{r-1,r}$ $(r = 1, \ldots, m)$. Hence, since it is not permissible in general to interchange orders of integration and differentiation, we apply Green's theorem in one dimension (or integration by parts) to the terms in (3.2) that involve differentiation. Thus, for instance, the first term in (3.2a) is given by

$$-\int_{-\infty}^{\infty} \frac{\partial E_y}{\partial x}\,\Psi_p dy = -\frac{d}{dx}\int_{-\infty}^{\infty} E_y\Psi_p dy + \int_{-\infty}^{\infty} E_y \frac{\partial \Psi_p}{\partial x}\, dy - \sum_{r=1}^{m}\{[E_y\Psi_p]_{h^+_{r-1,r}} - [E_y\Psi_p]_{h^-_{r-1,r}}\}h'_{r-1,r} \qquad (3.3a)$$

and for the second term in (3.2a) we can use the identity

$$\int_{-\infty}^{\infty} \frac{1}{\epsilon}\,\frac{\partial^2 H_z}{\partial y^2}\,\Psi_p dy = \int_{-\infty}^{\infty} \frac{1}{\epsilon}\, H_z \frac{\partial^2 \Psi_p}{\partial y^2}\, dy - \sum_{r=1}^{m}\left\{\left[\frac{1}{\epsilon}\,\frac{\partial H_z}{\partial y}\,\Psi_p\right]_{h^+_{r-1,r}} - \left[\frac{1}{\epsilon}\, H_z \frac{\partial \Psi_p}{\partial y}\right]_{h^-_{r-1,r}}\right\}h'_{r-1,r}. \qquad (3.3b)$$

On applying the boundary conditions (2.5d) for $H_z(x, y)$ and $E_y(x, y)$ as well as (2.7) for $\psi(u, y)$ and using the orthogonal relationship (3.1b), (3.2a) reduces to

$$-\frac{dE_p(x, u^*)}{dx} = i\beta^* H_p(x, u^*) - \sum G_{pq}(u^*, u)E_q(x, u) + J_p(x, u^*), \qquad (3.4a)$$

where the summation is interpreted as in (2.6). We have

$$G_{pq}(u^*, u) = \int_{-\infty}^{\infty} \frac{\partial \Psi_p(u^*, y)}{\partial x}\, Z(u, y)\psi_q(u, y)dy \qquad (3.4b)$$

and

$$J_p(x, u^*) = \int_{-\infty}^{\infty} J_m(x, y)\Psi_p(u^*, y)dy = K\Psi_p(u^*, y)\delta(x - x_0). \qquad (3.4c)$$

A similar treatment of (3.2b) yields the equation

$$\frac{-dH_p(x, u^*)}{dx} = i\beta^* E_p(x, u^*) + \sum \frac{N_p(u^*)}{N_q(u)}\, G_{pq}(u, u^*)H_q(x, u), \qquad (3.5a)$$

where

$$N_p(u) = \Psi_p(u, y)/\psi_p(u, y) = \begin{cases} R_0^{Dh}/2\pi Z_0, & p = 0, \\ R_m^{Uh}/2\pi Z_m, & p = m, \\ 1, & p = s, \end{cases} \qquad (3.5b)$$

and the following relationship derived from (3.1b) has been used for $u^* \neq u$:

$$\frac{d}{dx}\int_{-\infty}^{\infty} Z(u^*, y)\Psi_p(u^*, y)\psi_q(u, y)dy = 0 = \frac{\beta^*}{\beta}\, G_{pq}(u^*, u) + \frac{N_p(u^*)}{N_q(u)}\, G_{qp}(u, u^*) + \int_{-\infty}^{\infty} \frac{\partial Z(u^*, y)}{\partial x}\,\Psi_p(u^*, y)\psi_q(u, y)dy - \sum_{r=1}^{m} h'_{r-1,r}\Psi_p(u^*, h_{r-1,r})\psi_q(u, h_{r-1,r}) \times [Z_{r-1}(u^*) - Z_r(u^*)]. \qquad (3.6a)$$

Similarly, for $u^* = u = \mu_s^n$ it can be shown that

$$\frac{d}{dx}\int_{-\infty}^{\infty} Z(u, y)\Psi_s^n(u, y)\psi_s^n(u, y)dy = 0 = 2G_{ss}^{nn} + \int_{-\infty}^{\infty} \frac{\partial Z(u, y)}{\partial x}\,[\Psi_s^n(u, y)]^2 dy - \sum_{r=1}^{m} h'_{r-1,r}[\Psi_s^n]^2_{h_{r-1,r}}[Z_{r-1}(u) - Z_r(u)], \qquad (3.6b)$$

where

$$\int_{-\infty}^{\infty} \frac{\partial Z(u, y)}{\partial x}\,[\Psi_s^n(u, y)]^2 dy = \frac{\beta_n'}{\beta_n} - \frac{Z_0\epsilon_0'}{2iu_0\epsilon_0}\,[\Psi_s^n]^2_{h_{01}} + \frac{Z_m\epsilon_m'}{2iu_m\epsilon_m}\,[\Psi_s^n]^2_{h_{m-1,m}} - \sum_{r=1}^{m-1} \frac{Z_r\epsilon_r'}{2u_r^2\epsilon_r}\,[y(\Psi_s^{n\prime})^2 + yu_r^2(\Psi_s^n)^2 - \Psi_s^n\Psi_s^{n\prime}]^{h_{r-1,r}}_{h_{r,r+1}}. \qquad (3.6c)$$

Thus (3.6b) can be used to determine $G_{ss}^{nn}(u_s^n, u_s^n)$.

We utilize the relationship between (3.1b) and (3.4b) to determine the general expression for $G_{pq}(u^*, u)$. Thus, for $u \neq u^*$,

$$G_{pq}(u^*, u) = \left[\frac{Z(u, y)}{\beta^{*2} - \beta^2}\left(\psi_q(u, y)\,\frac{\partial^2}{\partial x\partial y}\,\Psi_p(u^*, y) - \frac{\partial}{\partial y}\,\psi_q(u, y)\,\frac{\partial}{\partial x}\,\Psi_p(u^*, y)\right)\right]^{h^-_{m-1,m}}_{h^+_{01}} + \sum_{r=1}^{m-1}\left[\frac{Z(u, y)}{\beta^{*2} - \beta^2}\left(\psi_q(u, y)\,\frac{\partial^2}{\partial x\partial y}\,\Psi_p(u, y) \times \frac{\partial}{\partial y}\,\psi_q(u, y)\,\frac{\partial}{\partial x}\,\Psi_p(u^*, y)\right)\right]^{h^-_{r-1,r}}_{h^+_{r,r+1}}. \qquad (3.7)$$

Expressing the transforms $H(x, u)$ and $E(x, u)$ in terms of the wave amplitudes $a(x, u)$ and $b(x, u)$ [(2.12)], we obtain from (3.4a) and (3.5a) a set of coupled ordinary differential equations. Thus, for $p, q = 0, m$, or s,

$$-\frac{d}{dx}\,a_p(x, u^*) - i\beta^* a_p(x, u^*) = \sum S_{pq}^{BA}(u^*, u)a_q(x, u) + \sum S_{pq}^{BB}(u^*, u)b_q(x, u) + J_p(x, u^*)/2 \qquad (3.8a)$$

and

$$-\frac{d}{dx}\,b_p(x, u^*) + i\beta^* b_p(x, u^*) = \sum S_{pq}^{AB}(u^*, u)b_q(x, u) + \sum S_{pq}^{AA}(u^*, u)a_q(x, u) - J_p(x, u^*)/2, \qquad (3.8b)$$

where $\sum$ is interpreted as in (2.6a) and the transmission and reflection scattering coefficients are defined respectively as

$$S^{BA}_{pq}(u^*, u) = S^{AB}_{pq}(u^*, u) = \frac{1}{2}\left(\frac{N_p(u^*)}{N_q(u)}\, G_{qp}(u, u^*) - G_{pq}(u^*, u)\right) \tag{3.9a}$$

and

$$S^{BB}_{pq}(u^*, u) = S^{AA}_{pq}(u^*, u) = \frac{1}{2}\left(\frac{N_p(u^*)}{N_q(u)}\, G_{qp}(u, u^*) + G_{pq}(u^*, u)\right)_{p,q=0,m,\text{or } s.} \tag{3.9b}$$

In view of the normalization used in this paper, it can be shown that

$$S^{BA}_{pq}(u^*, u) = -\, S^{AB}_{qp}(u, u^*) N_p(u^*)/N_q(u) \tag{3.9c}$$

and

$$S^{CC}_{pq}(u^*, u) = S^{CC}_{qp}(u, u^*) N_p(u^*)/N_q(u) \tag{3.9d}$$

for $p, q = 1, m$, or s and $C = A$ or B. Thus, (2.8) satisfies the reciprocity relationships in electromagnetic theory. The scattering coefficients (2.9) may also be derived by imposing the continuity of $H_z(x, y)$ and $E_y(x,y)$ for any plane $x =$ const. separating two multilayered structures whose electromagnetic parameters are $\epsilon(x)$, $\mu(x)$ and $\epsilon(x) + \epsilon'(x)dx$, $\mu(x) + \mu'(x)dx$, respectively, and with layer boundaries at $h_{r,r+1}(x)$ and $h_{r,r+1}(x) + h'_{r,r+1}(x)dx$, respectively. This procedure has been show to be rigorous.[3]

For any specific problem, $G_{pq}(u^*, u)$ depends upon variations of the parameters ϵ_r, μ_r, and $h_{r,r+1}$. Thus, for example we can express $\partial\Psi_p/\partial x$ in (3.4b) as follows:

$$\frac{\partial}{\partial x}\Psi_p(u, y) = \left[\sum_{r=0}^{m}\left(\epsilon'_r \frac{\partial}{\partial \epsilon_r} + \mu'_r \frac{\partial}{\partial \mu_r}\right) + \sum_{r=1}^{m} h'_{r-1,r} \frac{d}{dh_{r-1,r}}\right]\Psi_p(u, y) \tag{3.10}$$

and a similar expression can be written for $\partial^2\Psi_p(u, y)/\partial x \partial y$.

4. THE SURFACE IMPEDANCE AND THE RELATED WAVEGUIDE PROBLEM

In electromagnetic wave propagation problems, one often encounters layered structures in which one or both the bounding layers are regarded as perfect electric or magnetic walls, $\mu/\epsilon \to 0$ or $\epsilon/\mu \to 0$, respectively. Thus, from (2.9) we get

$$R^U_1 = R_{0,1} = \begin{cases} 1, & y = h_{0,1}, \quad \text{perfect electric wall,} \\ -1, & y = h_{0,1}, \quad \text{perfect magnetic wall.} \end{cases} \tag{4.1a}$$

In this case, $u_0 = 0$ is not a branch point and the contribution from the branch cut integral $\mathrm{Im}(u_0) = 0$ vanishes.[1]

Similarly for

$$R^D_{m-1} = R_{m,m-1} = \begin{cases} 1, & y = h_{m-1,m}, \quad \text{perfect electric wall,} \\ -1, & y = h_{m-1,m}, \quad \text{perfect magnetic wall,} \end{cases} \tag{4.1b}$$

the contribution from the branch cut integral $\mathrm{Im}(u_m) = 0$ vanishes since $u_m = 0$ is not a branch point.

Furthermore, in problems of propagation over good conducting earth (or sea water) for instance, it is convenient to characterize the interface $h_{0,1}$ (or $h_{m-1,m}$) by an approximate surface impedance (tangential electric to magnetic field ratio) which is assumed to be independent of the particular excitation. Thus, if Z_{s0} is the surface impedance looking upward into the boundary $y = h_{0,1}$,

$$R^U_1 = (u_1/\omega\epsilon_1 - Z_{s0})/(u_1/\omega\epsilon_1 + Z_{s0}), \tag{4.2a}$$

and the contribution from the branch cut $\mathrm{Im}(u_0) = 0$ vanishes. Similarly, when Z_{sm} is the surface impedance looking downward into the boundary $y = h_{m-1,m}$,

$$R^D_{m-1} = (u_{m-1}/\omega\epsilon_{m-1} - Z_{sm})/(u_{m-1}/\omega\epsilon_{m-1} + Z_{sm}), \tag{4.2b}$$

and the contribution from the branch cut $\mathrm{Im}(u_m) = 0$ vanishes. Thus, when the bounding media are characterized by surface impedances (including perfect electric or magnetic walls for which $Z_s = 0$ or $Y_s = 1/Z_s = 0$, respectively), the fields are expressed exclusively in terms of an infinite set of waveguide modes that satisfy the modal equation[1]

$$R^U_i R^{DH}_i = 1, \quad i = 1, \ldots, m = 1. \tag{4.3}$$

For the special case when ϵ and μ are independent of x and y and in addition $Z_s = 0$, the structure is a waveguide of varying height (a structure that is treated extensively in the literature). It is interesting to note that the present analysis also provides a full wave solution to the problem of scattering by objects of finite cross section embedded in the earth's crust ($\epsilon_1 \neq \epsilon_0$, $\mu_1 \neq \mu_0$) or in free space ($\epsilon_1 = \epsilon_0$, $\mu_1 = \mu_0$) (See Fig. 2).

5. FAR FIELD SOLUTIONS

To obtain the expressions for the magnetic field in a multilayered medium, it is necessary to solve the coupled ordinary differential equations for the wave amplitudes $a_p(x, u)$ and $b_p(x, u)$ [(3.8)] and substitute these results into the complete expansion for $H_z(x, y)$ given by (2.6a). This procedure simplifies considerably if the sources and observation point are at large distances from the principal regions of wave scattering. Noting that

$$H_0(x, -u) = H_0(x, u)/R^{Dh}_0 \tag{5.1a}$$

and

$$H_m(x, -u) = H_m(x, u)/R^{Dh}_m, \tag{5.1b}$$

we can write the fields radiated into the semi-infinite media 0 and m as

$$H_0(x, y) = \int_{-\infty}^{\infty} H_0(x, u) \exp(-iyu_0)du_0, \quad y > h_{0,1}, \tag{5.2a}$$

and

$$H_m(x, y) = \int_{-\infty}^{\infty} H_m(x, u) \exp(iyu_m)du_m, \quad y < h_{m-1,m}. \tag{5.2b}$$

The above exact expressions for the radiated fields are particularly conducive to integration by the method of steepest descent. In this section, we shall consider only far field solutions that are derived through an iterative method.[2] The line source is assumed to be in free space (medium 0) at a large distance $\rho_0 = (x_0^2 + y_0^2)^{1/2} \gg 1/k_0$ from the nonuniform region $-L < x < L$, where $x_0 < -L$.

The boundary conditions for the wave amplitudes are

$$a_p(-\infty, u) = 0, \quad b_p(\infty, u) = 0, \quad p = 0, m, \text{ or } s, \tag{5.3a}$$

and in view of the line source excitation, the wave amplitudes are discontinuous at $x = x_0$. Thus, we have

$$a_p(x,u)\,|_{x_0^-}^{x_0^+} = -\,b_p(x,u)\,|_{x_0^-}^{x_0^+} = -\tfrac{1}{2}K\Psi_p(u,y), \quad p = 0, m, \text{ and } s. \tag{5.3b}$$

Thus, neglecting wave scattering due to the nonuniformities of the structure, we solve (3.8a) for $a_p(x,u)$ and substitute into (5.2a). Integration of (5.2a), using the steepest descent method yields the following expression for the primary fields in the nonuniform region[2] $(-L < x < L)$:

$$H_z^P(x,y) = H_0^i \exp(-i\beta^i x) R_0^{Dh}\Psi_0(u,y). \tag{5.4a}$$

In (5.4a) $R_0^{Dh}\psi_0(u,y)$ is given by (2.8a). The amplitude of the primary wave is

$$H_0^i = -\frac{K\omega\epsilon_0}{2(2\pi k_0\rho_0)^{1/2}} \exp[-i(k_0\rho_0 - \tfrac{1}{4}\pi], \tag{5.4b}$$

$$x_0 = \rho_0 \sin\theta_0^i, \quad y_0 = \rho_0 \cos\theta_0^i, \tag{5.4c}$$

and as a result of Snell's law

$$\beta^i = k_r \sin\theta_r^i \quad \text{and} \quad u_r^i = k_r \cos\theta_r^i, \quad r = 0, 1, \ldots, m. \tag{5.4d}$$

In the expression (5.4a), $R_0^{Dh}\Psi_0(u,y)$ is implicitly a function of x since ϵ, μ and $h_{r,r+1}$ are functions of x in the nonuniform region. Using (2.6b), we determine the wave amplitude $a_p(x,u)$ corresponding to the primary field (5.4a). Thus,

$$a_p^P(x,u) = H_0^i R_0^{Dh} \exp(-i\beta^i x)\delta(u-u')\delta_{p,0} \equiv a_0^i(x,u)\delta(u-u')\delta_{p,0}. \tag{5.5}$$

Substituting the above expression for a_p on the right-hand side of (3.8), we obtain the following solutions for the scattered wave amplitudes:

$$a_p(x,u) = -\exp[-i\beta(x-L)] \int_{-L}^{L} S_{p0}^{B}(u,u^i)a_0^i(x',u) \times \exp\left(i\int_L^{x'}\beta dx''\right)dx' \equiv \exp[-i\beta(x-L)]\,A_{p0}(u,u^i) \tag{5.6a}$$

for $x > L$, and

$$b_p(x,u) = \exp[+i\beta(x+L)] \int_{-L}^{L} S_{p0}^{AA}(u,u^i)a_0^i(x,u) \times \exp(-i\int_{-L}^{x'}\beta dx'')dx' \equiv \exp[i\beta(x+L)][i\beta(x+L)] \times B_{p0}(u,u^i). \tag{5.6b}$$

for $x < -L$.

To obtain the expression for the forward scattered radiation field $H_0^f(x,y)$, we substitute the expression $a_0(x,u)$ from (5.6a) into (5.2a) and integrate using the method of steepest descent.[2] Thus, provided that $A_{00}(u, u^i)$ can be regarded as a slowly varying function of u, it can be shown that

$$H_0^f(x,y) = A_{00}(u^f,u^i)\beta^f(2\pi/k_0\rho)^{1/2} \times \exp(i\pi/4)\exp(-ik_0\rho), \tag{5.7a}$$

where

$$(x-L) = \rho\sin\theta_0^f, \quad y = \rho\cos\theta_0^f \tag{5.7b}$$

and

$$\beta^f = k_r \sin\theta_r^f, \quad u_r^f = k_r\cos\theta_r^f. \tag{5.7c}$$

Hence, $A_{00}(u^f, u^i)\beta^f$ is the radiation pattern for the forward scattered waves. Similarly, the backward scattered radiation field is

$$H_0^b(x,y) = B_{00}(u^b,u^i)\beta^b(2\pi/k_0\rho)^{1/2}\exp(i\pi/4)\exp(-ik_0\rho), \tag{5.8a}$$

where

$$-(x+L) = \rho\sin\theta_0^b, \quad y = \rho\cos\theta_0^f \tag{5.8b}$$

and

$$\beta^b = k_r\sin\theta_r^b, \quad u_r^b = k_r\cos\theta_r^b. \tag{5.8c}$$

In general the terms $A_{00}(u,u^i)$ and $B_{00}(u,u^i)$ [(5.6)] may be expressed in terms of infinite series.[4] The expression for $H_m(x,y)$ [(5.2b)] is identified as the lateral wave term.[2] For nondissipative media, for instance, this term corresponds to waves that emerge in medium m, traveling parallel to the interface $h_{m-1,m}(\beta = k_m, u_m = 0)$. This contribution to the total magnetic field is associated with the phenomenon of total internal reflection.

The expression for the nth surface wave excited by the nonuniform structure is

$$H_s^n(x,y) = A_{s0}^n(u_s^n,u^i)\exp[-i\beta_s(x-L)\psi_s^n(u,y), \quad x > L, \tag{5.9}$$

where $\psi_s^n(u,y)$ is given by (2.8c), and similar expressions may be written for the backward scattered surface waves.

By placing the line source far from the nonuniform region, it was only necessary to consider the scattering of uniform plane waves into the radiation, the lateral wave and the surface wave terms. In general, however, when the source is located near the nonuniform region, it is necessary to consider the entire spectrum of primary waves excited by the source. These are obtained from (3.8b) on neglecting the coupling terms and noting that the basis functions are also implicitly functions of x. Thus,

$$a_p^P(x,u) = -\frac{K}{2}\exp\left(-i\int_{x_0}^{x}\beta dx\right)\Psi_p(u,y_0)U(x-x_0) \tag{5.10a}$$

and

$$b_p^P(x,u) = -\frac{K}{2}\exp\left(i\int_{x_0}^{x}\beta dx\right)\Psi_p(u,y)U(x_0-x), \quad p = 0, m, \text{ and } s, \tag{5.10b}$$

where $U(x-x_0)$ is the unit step function. The above expressions (5.10) determine the primary fields $H^P(x,y)$ in this case.

6. CONCLUDING REMARKS

Full wave expressions for the electromagnetic fields in nonuniform multilayered structures are derived. The electromagnetic parameters ϵ and μ as well as the boundaries between the layers of the structure are assumed to vary along the path of propagation. The analysis employs generalized transforms[1] that provide a suitable basis for a complete expansion of the transverse components of the electromagnetic fields. In general, the

field expansion consists of two infinite integrals (the continuous part of the wavenumber spectrum) which are identified as the radiation and the lateral wave terms as well as a finite set of surface wave modes (the discrete part of the wavenumber spectrum). In certain special cases, the contributions from one or both the infinite integrals vanish. When both the radiation and lateral wave terms vanish, the fields are expressed completely in terms of an infinite set of trapped waveguide modes. In some special cases (two-medium problems or propagation over a nonuniform impedance boundary), no surface wave may exist and the fields can be expressed in terms of the one or two infinite integrals.

By using the analysis derived in this paper a vast variety of propagation problems such as propagation through the nonuniform layers of the ionosphere and the earth's crust may be solved. Coupling into and out of artificial surface structures as well as mode coupling in nonuniform waveguides can also be determined by using the full wave solutions. The analysis also provides full wave solutions to the problems of scattering by objects of finite cross section embedded in the earth's crust or in free space (see Fig. 2).

No restrictive impedance boundary conditions are used, and the sources and observation point may be located anywhere in the structure; thus, the analysis is particularly suited to the investigation of hardened communication systems. It can readily be shown that the solutions are consistent with the reciprocity relationships in electromagnetic theory.

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On the necessity of nearly-best-possible methods for analytic continuation of scattering data

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In the present paper we discuss some mathematical methods which are nearly-best-possible in order to extract as much as possible information from the numerical analytic continuation of the scattering data. All the questions related to the stability are analyzed; in this sense we explicitly show some cases where the continuity of the solutions on the data is very poor. Finally the error-bounds are extensively explored.

1. INTRODUCTION

The purpose of this article is to explore in a quantitative manner the rather precarious stability of analytic continuation problems for scattering data (including some in attempted use, which probably should not be); to expose in the specific case of scattering problems some nearly best possible methods of the first author and others which are in use in the general mathematical field of ill-posed problems, and to give a critical analysis of some of the expansion methods found in the physical literature.

Chew[1] and Chew-Low[2] were the first to emphasize the role of analytic continuation of scattering data in determination of the pion-nucleon coupling constant[1] and of cross sections with unstable particles as targets.[2] Following these two initial papers Frazer[3] and Ciulli-Fisher[4] pointed out the advantages of using conformal mapping techniques; more precisely, they mapped the cosine complex cut-plane into the unit circle. Thereafter, many authors applied the methods of analytic continuation to various phenomenological problems; among these we recall Lovelace,[5] Ashmore *et al.*,[6] the Hamilton group,[7,8] Atkinson,[9] and Levinger, Peierls, and Wong.[10,11] Of course in these works the authors went far beyond the original proposals of Chew and Chew-Low. In fact, some phenomenological problems were attempted which would have required analytic continuation of the data up to the cuts, i.e., up to the boundary of the analyticity domain.

Bertero and Viano[12] (in a short note which appeared in 1965) recalled that analytic continuation of complex-valued functions is one of the classical improperly-posed problems in the sense of Hadamard;[13] i.e., it is completely unstable. However, this is one of the large class of improperly-posed problems which can be stabilized by restricting attention to those solutions satisfying a certain prescribed global bound (see Ref. 14 for references to the mathematical literature).

In Ref. 12 the Hadamard three-circle theorem and its extension (the Carlemann inequality) were used to give stability estimates for extrapolation of experimental data for nucleon form factors. Thereafter, Ciulli,[15,16] Cutkosky and Deo,[17,18] and Cutkosky[19] returned to these questions and proposed improved methods. Of course this list of references does not pretend to be exhaustive and we apologize to the authors who are not mentioned here. In these papers the authors, after mapping the analyticity domain into an annulus (Ciulli) or an ellipse (Cutkosky-Deo), devise methods with much greater care regarding analysis of the stability.

We feel, however, that several relevant points need a deeper analysis. In Sec. 2 we give a general mathematical formulation (which includes most of the continuation problems occurring in the physical literature) and introduce the concept of "best-possible stability estimate". In Sec. 3 we analyze this best possible stability estimate for many of our examples of physical interest.

In certain cases stability can be shown to be so extremely poor that we feel that such continuations from physical data should never be attempted. For example, the best possible stability estimate for continuation up to the boundary, with a prescribed global bound on the derivative of the boundary functions, is at best only logarithmic, i.e., proportional to $|\log\epsilon|^{-1}$, where ϵ is the data accuracy. On the other hand, continuation to points well within the domain of analyticity usually has a fairly satisfactory ϵ^{λ} Hölder type stability ($0 < \lambda < 1$). In all cases it becomes evident, however, that even the best possible stability is sufficiently precarious that one should proceed with great caution and use only numerical continuation methods which are in a certain sense "nearly-best-possible."

In Secs. 4-6 we discuss two general classes of numerical methods of the first author, least-squares methods,[20] and method of partial eigenfunction expansions,[14,21] which turn out to be "nearly-best-possible." Various portions of these methods were also introduced by Backus[22-25] and by Cutkosky.[19] One fortunate property of these methods is that only one of the two numbers ϵ (the data accuracy) and E (the global bound) is required for the computation. We should emphasize, however, that it is necessary to have knowledge of E in order to have error bounds on the accuracy of our approximation; moreover, this knowledge must come from information completely outside anything which can be discerned from the data itself. In Sec. 6 we point out the inflexibility of polynomial expansion methods, and in Sec. 7 we will try some conclusions.

2. MATHEMATICAL FORMULATION AND EXAMPLES

The usual problem is to approximately determine by analytic continuation certain values of a function $f^0(x)$ which is holomorphic in the domain Ω shown in Fig. 1a, a cut x plane, but where measurements for f^0 are possible only at data points in the segment $\Gamma = [-1, 1]$ (or $[-a, b]$ in general) of the real axis, which segment is called the physical region. We let $\tilde{\Gamma}$, the data set, de-

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note the set of data points actually available and used in any particular instance. $\dot{\Gamma}$ may be all of $[-1, 1]$ but in physically realistic situations it is quite often a finite subset of $[-1, 1]$. The boundary $\partial\Omega$ should be thought of as consisting of both sides of both cuts, plus $x_{\infty+}$ and $x_{\infty-}$ (the points at ∞ for the upper and lower half-planes).

Physically $f^0(x)$ may correspond to the differential cross section for a certain scattering process $d\sigma/d\Lambda$, where Λ denotes the solid angle. One also encounters references in the literature to analytic continuation of the scattering amplitude $A(s, x)$ itself, where s in the barycentric energy squared and x is the cosine of the center of mass scattering angle. In actual practice the $f^0(x)$ which we consider, however, will usually not be exactly either of the above. One usually first adjusts the considered function and data quite a bit; one first subtracts off poles with known locations, or divides by nonzero analytic functions of the proper form to reduce certain unbounded behavior of our function at $x \to \infty$ to more nearly bounded behavior, etc. (see Cutkosky-Deo[17]). In this way one hopes to apply analytic continuation only to an unknown "background" function f^0 which is as small and as decently behaved as possible.

Of course, other physically interesting analytic continuation problems, with different domains Ω and physical regions Γ, also occur in scattering theory. Henceforth, for the next several sections, we will attempt to refrain as much as possible from physical interpretations and terminology and to limit ourselves to purely mathematical considerations.

Merely as a notational and mathematical convenience, we choose to work in certain bounded geometries obtained from the unbounded x-plane geometry by conformal mapping. In Fig. 1b we show the unit disc z-plane geometry, which seems most notationally convenient in many instances. In Fig. 1c we show the elliptical y-plane geometry employed by Cutkosky and Deo.[17,18] In Fig. 1d we show the annular ζ-plane geometry employed by Ciulli.[15] The specific details and formulas for these three mappings are available in the literature.[26] A function $f(x)$ holomorphic in the x-geometry transforms into functions $f(x(z))$, $f(x(y))$, and $f(x(\zeta))$ holomorphic in the z, y, and ζ geometries. However, to avoid notational proliferation we adopt the rather loose convention of using the same symbol f for all three functions, and speak of the functions $f(z)$, $f(y)$, and $f(\zeta)$. Likewise, we employ the same symbols for

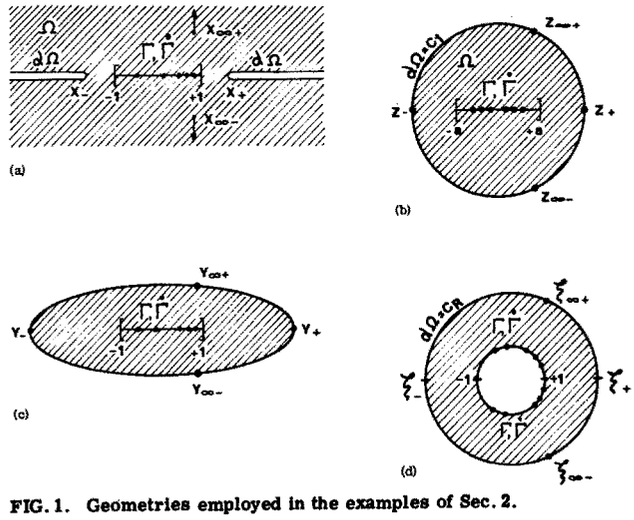

FIG. 1. Geometries employed in the examples of Sec. 2.

the sets Ω, $\partial\Omega$, Γ, and $\dot{\Gamma}$ in the x plane and for their images under the z, y, and ζ mappings.

The general mathematical formulation may be stated as follows: we desire to approximately determine an unknown element f^0 of a certain space X of functions f holomorphic on the given complex domain Ω; we call X the solution space. For each f in X, Af denotes a certain function on the data set $\dot{\Gamma}$ which can be approximately measured physically. Let h denote the data function actually measured on $\dot{\Gamma}$ as an approximation to Af^0. The possible Af and h lie in a certain space Y of functions on $\dot{\Gamma}$; we call A the data operator and Y the data space. Of course Af and h are "vectors" or "discrete functions" when the data set $\dot{\Gamma}$ has finitely many points. In order to stabilize the problem one usually requires some sort of global bound on f^0; in most cases this can be interpreted as a bound on the boundary values of f^0. For each f in X, let Bf denote certain "boundary values" of f on $\partial\Omega$ (this sometimes has to be interpreted in a rather generalized sense, and it is sometimes worthwhile to consider other B, such as the tangential derivative of the boundary values for example). The possible Bf lie in a certain space Z of functions (or generalized functions) on $\partial\Omega$; we call B the constraint operator and Z the constraint space.

We limit ourselves to a completely linear formulation; this includes most of the methods found in the literature. That is, we assume that X, Y, and Z are normed linear spaces, with norms $\| \ \|_X$, $\| \ \|_Y$, and $\| \ \|_Z$, that A is a continuous linear operator mapping X into Y, and that B is a continuous linear operator mapping X into Z.

We let $\langle \ \rangle$ denote a norm or seminorm on X (or sometimes a family of seminorms) which will be employed to measure the solution accuracy. For example, $\langle f \rangle$ might denote the magnitude $|f(z_0)|$, where z_0 is a fixed point of interest in Ω.

Problem: Suppose that f^0 satisfies

$$\|Af^0 - h\|_Y \leq \epsilon, \tag{2.1}$$

$$\|Bf^0\|_Z \leq E, \tag{2.2}$$

where E is a "fixed" number and ϵ is a "small" number. We assume, but only for the moment, that both ϵ and E are known. We want to find an element f^1 in X which "approximates" f^0, in the sense that $\langle f^1 - f^0 \rangle$ is small when ϵ is small (and when the number of data points in $\dot{\Gamma}$ is sufficiently high, although we choose not to explicitly indicate in our notation the possible variability of $\dot{\Gamma}$).

Suppose f^1 is any other element of X satisfying the constraints (2.1) and (2.2). The error function $f^1 - f^0$ then satisfies $\langle f^1 - f^0 \rangle \leq 2M(\epsilon, E)$, where

$$M(\epsilon, E) \equiv \sup\{\langle f \rangle : f \in X \text{ and } \|Af\|_Y \leq \epsilon, \ \|Bf\|_Z \leq E\}, \tag{2.3}$$

and there is essentially nothing further that can be said about the size of $\langle f^1 - f^0 \rangle$. We call any decent upper bound for $M(\epsilon, E)$ a stability estimate for problem (2.1), (2.2), and $M(\epsilon, E)$ itself we call the best possible stability estimate.

Before proceeding to the specific examples, it is worthwhile to mention several common features of them all. The holomorphic functions $f(x)$ [or $f(z), f(y), f(\zeta)$] are all real on the intersection of Ω with the real x axis (or z axis, y axis, ζ axis) in the physical problems we are considering. In the z-geometry such functions have the Taylor series representation.

$$f(z) = \sum_{j=0}^{\infty} x_j z^j, \tag{2.4}$$

convergent for $z \in \Omega$ with real coefficients x_j. In the y-geometry they have the representation

$$f(y) = \sum_{j=0}^{\infty} x_j \mathcal{P}_j(y), \tag{2.5}$$

convergent for $y \in \Omega$ with real coefficients x_j and where the $\mathcal{P}_j(y)$ are the normalized Legendre polynomials P_j {orthonormal with respect to the weight $\beta(y) = 1$ on $[-1, 1]$}, or the normalized Chebyshef polynomials T_j {orthonormal with respect to the weight $\beta(y) = (1-y^2)^{-1/4}$ on $[-1, 1]$}, or some other system of orthogonal polynomials. In the ζ-geometry the image $\Gamma = \{\zeta : |\zeta| = 1\}$ is a symmetric 2-1 image of the original segment $[-1, 1]$ in the x-plane. The functions $f(\zeta)$ of interest must therefore be holomorphic on $\Omega = \{\zeta : 1 \leq \zeta < R\}$, real on Γ, symmetric on Γ about the real axis, and (as stated previously) real on the intersection of Ω with the real ζ axis. Such functions have the representation

$$f(\zeta) = \sum_{j=0}^{\infty} x_j(\zeta^j + \zeta^{-j}), \tag{2.6}$$

convergent for $\zeta \in \Omega$, with real coefficients x_j.

In all the following examples Af and Bf will denote the restriction of the function f to its values on $\dot{\Gamma}$ and $\partial\Omega$, respectively. Many other choices are, of course, possible; Af could denote, for example, the derivative f' restricted to $\dot{\Gamma}$.

Our solution space X will always then be the space of all functions $f(z)$ [or $f(y)$, $f(\zeta)$] of the form (2.4) [or (2.5), (2.6)] and for which also a certain "boundary value norm" $\|Bf\|_Z$ is finite. Notice that X will then be a real linear space, that is, a linear space over the real scalar field. Also Y and Z must be considered as real linear spaces, even though we are often dealing with complex valued functions. This sometimes leads to slightly more complicated notation than would be required if complex coefficients were allowed in (2.4)-(2.6).

Possible norms or seminorms $\langle f \rangle$ in all the following specific examples are the magnitude $|f(z_0)|$ of f at a given point z_0 in Ω, or the magnitude $|f'(z_0)|$ of the derivative at z_0, or the magnitude $|l(f)|$ of any continuous linear functional l on X, or the uniform norm $\|f\|_K$ of f on a given closed bounded subset K in Ω, etc. Also, the particular norm used on X is not of great importance, since it enters into the problem only qualitatively; we may, therefore, always choose

$$\|f\|_X = \|Bf\|_Z. \tag{2.7}$$

We begin with examples using the supremum norms on $\dot{\Gamma}$ and $\partial\Omega$.

Example 1a: Let Ω and Γ be the unit disc and the real segment $[-a, +a]$ in the z plane as shown in Fig. 1b. Let $\dot{\Gamma} = \Gamma$ and let X be the space of all functions $f(z)$ holomorphic in Ω, real on the real z axis, and continuous on $\overline{\Omega}$. Let Y be the space of all continuous real-valued functions on $\dot{\Gamma}$, and Z the space of all continuous complex-valued functions on $\partial\Omega$. Let the norms for Y and Z by the supremum norms on $\dot{\Gamma}$ and $\partial\Omega$, respectively.

That is,

$$\|Af\|_Y = \sup_{z\in\Gamma} |f(z)|, \qquad \|f\|_X = \|Bf\|_Z = \sup_{z\in\partial\Omega} |f(z)|. \tag{2.8}$$

Example 1b: As in (1a), except let the data set $\dot{\Gamma}$ be only a finite subset $\{d_1, \ldots, d_k\}$ of k evenly spaced points on the segment Γ. In this case, Af and h are real-valued discrete functions on $\dot{\Gamma}$.

Example 1c: As in (1a) and (1b) above except replace the supremum norms by weighted supremum norms, with certain continuous positive weight functions β and γ defined on Γ and on $\partial\Omega$, respectively. That is

$$\|Af\|_Y = \sup_{z\in\dot{\Gamma}} \beta(z)|f(z)| \quad \text{and} \qquad \|f\|_X = \|Bf\|_Z = \sup_{z\in\partial\Omega} \gamma(z)|f(z)|. \tag{2.9}$$

We next consider examples using inner product norms on $\dot{\Gamma}$ and $\partial\Omega$.

Example 2a: Let Ω and Γ once again be the unit disc and segment $[-a, a]$, as shown in Fig. 1b, and let $\dot{\Gamma} = \Gamma$. Let X be the Hilbert space of all functions $f(z)$ holomorphic in Ω, real on the real z axis, and having L_2 boundary values on $\partial\Omega$ (in the sense of radial limits). Let Y be the Hilbert space of all real-valued L_2 functions on Γ, equipped with the usual L_2 norm and inner product. Let Z be the Hilbert space of all complex-valued L_2 functions on $\partial\Omega$, but considered as a real linear space, with an inner product equal the real part of the usual complex inner product.

Let X borrow its inner product from Z; i.e., $(f, g)_X = (Bf, Bg)_Z$. It is convenient to normalize so that the constant function $f(z) \equiv 1$ has norm 1 in all three spaces. Notice that X consists of all Taylor series of the form (2.4) with real coefficients x_j such that $\sum_{j=0}^{\infty} |x_j|^2 < \infty$.

Example 2b: As in (2a), except let $\dot{\Gamma}$ be the discrete data set $\{d_1, \ldots, d_k\}$ and replace on $\dot{\Gamma}$ the L_2 integral norm of (2a) by the l_2 sum norm here.

Example 2c: As in (2a) or (2b), except replace the norms there by weighted norms. That is,

$$(Af, Ag)_Y = \int_{z\in\dot{\Gamma}} f(z)g(z)\beta^2(z)\,|dz| \tag{2.10}$$

or

$$(Af, Ag)_Y = \sum_{j=1}^{k} f(d_j)g(d_j)\beta^2(d_j) \tag{2.11}$$

when $\dot{\Gamma}$ is discrete, and

$$(f, g)_X = (Bf, Bg)_Z = \mathrm{Re}\left\{\int_{z\in\partial\Omega} f(z)\overline{g(z)}\gamma^2(z)\,|dz|\right\}, \tag{2.12}$$

where $\beta^2(z)$ and $\gamma^2(z)$ are normalized to have total integral (or sum) equal 1 on $\dot{\Gamma}$ and $\partial\Omega$. Usually $\beta(z)$ and $\gamma(z)$ are assumed to be continuous and positive on all $\dot{\Gamma}$ and $\partial\Omega$. It is sometimes convenient, however, to let $\beta(z)$ and $\gamma(z)$ tend to ∞ or 0 at a few special points such as $-a$ and $+a$; z_-, z_+; $z_{\infty+}, z_{\infty-}$. In this case, the detailed specification of what the space Z of boundary functions is, or in what sense f assumes its boundary value Bf, becomes somewhat obscure. It suffices for our purposes to define the Hilbert space X to be the completion, with respect to the norm (2.12) of the space of "polynomials" $\sum_{j=1}^{n} x_j z^j$ with real coefficients.

Example 2d: Under conformal mapping of Examples (2a)-(2c) back into the x-geometry, one introduces an additional factor of $|dz/dx|$ into the integral inner pro-

duct involved in (2.10) and (2.12). For example, $f(x)$ and $g(x)$ have the inner product

$$(f,g)_X = (Bf, Bg)_Z = \mathrm{Re} \int_{x\in\partial\Omega} f(x)\overline{g(x)}\,\gamma^2(z(x)) \left|\frac{dz}{dx}\right| |dx|. \tag{2.13}$$

Notice that the required behavior of $f(z)$ as z tends to $\partial\Omega$ in the z-geometry imposes a restriction on the type of singularities which $f(x)$ may have as $x \to \infty$ in the lower or upper half-planes. Thus, for example, the function $f(x) = \sin x$, will not be in X, even though its boundary integral (2.13) in the x-geometry may happen to be finite. Once again, it is best to keep in mind that X is the completion, with respect to the norm (2.13), of the space of "polynomials" $\sum_{j=1}^{n} x_j(z(x))^j$ with real coefficients.

Example 3a: In the annular ζ-plane geometry of Fig. 1d, let $\Omega = \{\zeta : 1 \leq |\zeta| < R\}$, $\Gamma = \{\zeta : |\zeta| = 1\}$, and $\partial\Omega = \{\zeta : |\zeta| = R\}$. Let $\dot{\Gamma} = \Gamma$ and let X be the space of analytic functions $f(\zeta)$ of form (2.6), with real coefficients x_j and with finite L_2-norm on $\partial\Omega$. Let $\|Af\|_Y$ and $\|f\|_X = \|Bf\|_Z$ be the L_2 norms of f on $\dot{\Gamma}$ and $\partial\Omega$ respectively, and let Y be the space of real L_2 functions on $\dot{\Gamma}$ which are symmetric about the real axis.

This example, is, of course, a special case of Example (2c) after conformal mapping, but it is particularly simple and well suited to expansion methods since the basis functions $(\zeta^j + \zeta^{-j})$ are orthogonal with respect to both the Y and the Z inner products. The norms involved can thus be written as simple quadratic sums of the Fourier coefficients x_j. That is,

$$f(\zeta) = \sum_{j=0}^{\infty} x_j(\zeta^j + \zeta^{-j}), \tag{2.14}$$

$$\|Af\|_Y = \left(\sum_{j=0}^{\infty} 2|x_j|^2\right)^{1/2} \tag{2.15}$$

$$\|f\|_X = \|Bf\|_Z = \left(\sum_{j=0}^{\infty} (R^{2j} + R^{-2j})|x_j|^2\right)^{1/2}. \tag{2.16}$$

Example 3b: Under conformal mapping into the y-geometry of Fig. 1c, the basis functions $\zeta^j + \zeta^{-j}$ transform into the Chebyshef polynomials $T_j(y)$ and the unweighted L_2 inner product integrals on Γ and $\partial\Omega$ transform into inner product integrals in the y-geometry with the weight functions $\beta^2(y) = |d\zeta/dy|$ and $\gamma^2(y) = |d\zeta/dy|$. Now $\beta(y)$ is bounded, positive and smooth on $\partial\Omega$, but $\gamma(y)$ on Γ equals a constant times $(1-y^2)^{-1/4}$.

Next we consider examples introduced by Ciulli and by Cutkosky-Deo, which use integral inner product norms on $\dot{\Gamma}$ and which (at least implicitly) employ various other norms on $\partial\Omega$.

Example 4a: In the y-geometry Cutkosky and Deo[17] consider a weighted L_2 inner product on $\dot{\Gamma} = \Gamma$ with weight function $\beta(y)$. Functions $f(y)$ holomorphic on the ellipse Ω can then be expanded as $f(y) = \sum_{j=0}^{\infty} x_j\mathcal{P}_j(y)$, where the $\mathcal{P}_j(y)$ are the polynomials orthonormal for this inner product. The classical theory of polynomial expansions, as described by Walsh,[27] then establishes convergence properties for such expansions which are closely analogous to the well-known convergence properties of the Taylor series expansions. The regions of convergence, now, instead of being circles of radius ρ, are the ellipses E_ρ with foci ± 1 and "radius" ρ = semimajor + semiminor axis. The moduli $|\mathcal{P}_j(y)|$ are essentially proportional to ρ^j on E_ρ. The expansion converges inside the largest ellipse within which f is holomorphic. Let us say this ellipse is $E_R = \partial\Omega$ for our f of interest. For each $\delta > 0$ and each $1 \leq \rho < R - \delta$ there exists a constant $M = M_{\delta,\rho,f}$ such that the truncation error after n terms is bounded on E_ρ by $M[\rho/(R-\delta)]^n$. Moreover, the jth coefficient then satisfies $\lim \sup(x_j)^{1/j} = 1/R$.

Cutkosky and Deo assume that the x_j are Gaussian random variables with mean zero and variance v_0R^{-2j} (See Ref. 17). They also assume that the coefficients h_j of the data function $h(y)$ on $\dot{\Gamma}$ are Gaussian random variables. Moreover one is implicitly dealing here with the conditions.

$$\|Af^0 - h\|_Y = \left(\int_{\dot{\Gamma}} \beta^2(y)\,|f^0(y) - h(y)|^2|dy|\right)^{1/2} = \left(\sum_{j=0}^{\infty} |x_j^0 - h_j|^2\right)^{1/2} \leq \epsilon, \tag{2.17}$$

$$\|f^0\|_X = \|Bf^0\|_Z = \left(\sum_{j=0}^{\infty} |x_j^0|^2R^{2j}\right)^{1/2} \leq E. \tag{2.18}$$

Example 4b: Ciulli[15,16] considers the conformally equivalent problem in the ζ geometry. In Ref. 15 his norm on $\dot{\Gamma}$ is the supremum norm; in Ref. 16 the norm on $\dot{\Gamma}$ is the L_2-norm. He works with linear combinations of the basis functions $(\zeta^j + \zeta^{-j})$; these transform, under mapping into the y plane, into the Chebyshef polynomials. Moreover, the basis functions $(\zeta^j + \zeta^{-j})$ behave asymptotically like ζ^j as $\zeta \to \infty$, or $j \to \infty$ for $|\zeta| > 1$, and this suffices in the proofs for much of Walsh's theory.

Ciulli[16] assumes that the pth derivative of the boundary function $Bf^0(\zeta)$ is a Hölder continuous function on $\partial\Omega$ with exponent $0 < \alpha < 1$. In other words, he is dealing with the Hölder norm

$$\|Bf\|_Z = \sup_{\zeta_1,\zeta_2\in\partial\Omega} \frac{|f^{(p)}(\zeta_1) - f^{(p)}(\zeta_2)|}{|\zeta_1 - \zeta_2|^\alpha}. \tag{2.19}$$

In this case, Ciulli is interested in analytic continuation with uniform accuracy all the way to the boundary; in other words, he is using the supremum norm on Ω, as the norm to measure solution accuracy.

In example (4a) it is quite possible that the boundary function $Bf(y) = \sum_{j=0}^{\infty} x_j\mathcal{P}_j(y)$, where the coefficients satisfy (2.18), does not converge anywhere on $\partial\Omega$. Mathematically speaking, this should not bother us at all, Bf is then merely some sort of "generalized function" on $\partial\Omega$. It is a well-known mathematical device to define generalized functions on $\partial\Omega$ in terms of formal series which converge in Ω, but perhaps not on $\partial\Omega$. Identical considerations hold for Example (4b).

3. QUANTITATIVE ANALYSIS OF THE THEORETICALLY BEST POSSIBLE STABILITY

At the outset, we point out that stability can be proved for the above example, in every single instance, by employing the following elementary theorem on compactness (Kelley[28]): Let σ be a continuous map on a compact topological space into a Hausdorff topological space. If σ is one-to-one, then its inverse map σ^{-1} is continuous. That is, we may prove that $M(\epsilon, E)$ tends to zero as $\epsilon \to 0$ (and as the number of data points tends to ∞ when $\dot{\Gamma}$ is discrete), with E being fixed. See Miller[20] and Miller-Viano[29] for two worked out examples. Such results are essentially useless, however, for they are completely qualitative and can give no estimate at all on the smallness or largeness of $M(\epsilon, E)$. In fact,

such results may often give the wrong impression indicating stability in situations where the stability is so poor as to be almost nonexistent. The purpose of this section is to quantitatively examine the stability of the analytic continuation examples mentioned above and to draw certain conclusions from that examination. We assume now that the solution error seminorm of interest is the pointwise error $\langle f \rangle = |f(z)|$ at various points z in Ω. We begin with problems of analytic continuation to points well inside Ω.

Consider first the example (1a) using the unweighted supremum norms and with $\dot{\Gamma}$ being the whole arc Γ, rather than a finite subset. Here we may apply the Carlemann inequality[12]: if $f(z)$ is analytic on Ω-Γ, continuous on $\overline{\Omega}$, and $|f(z)| \leq \epsilon$ on Γ, $|f(z)| \leq E$ on $\partial\Omega$, then

$$|f(z)| \leq \epsilon^{\omega(z)} E^{(1-\omega(z))}; \quad z \in \Omega, \tag{3.1}$$

where $\omega(z)$ is the harmonic function on Ω-Γ which is continuous on $\overline{\Omega}$ and equals 1 and 0 on Γ and $\partial\Omega$, respectively. This inequality gives the best-possible stability estimate for Example (1a) (or any conformally equivalent example) except for a factor of at most 2 (at least at points z on the real axis and for a whole sequence of values ϵ/E tending to zero). To see this it suffices to consider the functions $f(\zeta) = (1/2R^j)(\zeta^j + \zeta^{-j})$ in the conformally equivalent ζ-plane geometry of Fig. 1d. These satisfy $|f(\zeta)| \leq \epsilon \equiv R^{-j}$ on Γ, $|f(\zeta)| \leq E \equiv 1$ on $\partial\Omega$, and yet for $1 \leq \zeta \leq R$ on the real axis we have $|f(\zeta)| \geq \frac{1}{2}(|\zeta|/R)^j = \frac{1}{2}\epsilon^{\omega(\zeta)}$, since $\omega(\zeta) = \log(R/|\zeta|)/\log R$ in this geometry. For ζ off the real axis with $1 < |\zeta| \leq R$, we have $|f(\zeta)| \geq \frac{1}{2}(1 - |\zeta|^{2j})\epsilon^{\omega(\zeta)}$ which is nearly the same.

With unweighted L_2-norms on $\partial\Omega$ and on $\dot{\Gamma} = \Gamma = [-a, a]$ in the z-plane geometry [i.e., with conditions of Example (2a)], Miller[20] obtains the stability estimate

$$|f(z)| \leq [c \log(E/\epsilon) + (1 - |z|^2)^{-1/2}]\epsilon^{\omega(z)} E^{[1-\omega(z)]}, \tag{3.2}$$

where c is a computable constant depending only on a.

The method of partial eigenfunction expansions allows one to evaluate the best possible stability estimate exactly (except for a factor of at most 2) in certain cases with particularly simple orthogonal expansions. In Sec. 6 we apply this technique to Example (3a) and obtain a bound [see (6.28)], which after simplification looks much like (3.2). Prescribed L_2 bounds on derivatives of f on $\partial\Omega$, it can also be seen, do not improve the stability estimate greatly.

Notice that the error-bounds obtained by Ciulli[15] and by Cutkosky and Deo,[17] in all their work using the Walsh theory of optimal polynomial convergence, contain a dominant term of $\approx E(|\zeta|/R)^{\alpha}$ [consider the geometry of Example (3a)], where the truncation order α is usually chosen such that $(1/R)^{\alpha} \approx \epsilon/E$; thus the dominant term is once again $\approx \epsilon^{\omega(\zeta)} E^{[1-\omega(\zeta)]}$.

We continue next to problems involving analytic continuation all the way to the boundary. Ciulli[15] obtains stability estimates for $f(\zeta)$ on $\partial\Omega$ [Example (4b)]; the complicated derivation somewhat obscures the fact that the stability obtained is extremely poor. The results of Miller[14] yield stability estimates to the boundary in the geometry of Example (3a), but with the L_2 bound $\|D^k f\| \leq E \equiv 1$ for the kth derivative with respect to $\vartheta = \arg\zeta$ on $\partial\Omega$ (the estimates there were actually for harmonic continuation on the unit disc, but the changes needed are minor). The bound obtained for $|f(\zeta)|$ on $\partial\Omega$ is essentially proportional to $[|\log\epsilon|/\log R]^{1/2-k}$.

To prove that the best possible stability is truly as poor as our bounds seem to indicate, we switch to a simple pathological example. In the ζ plane geometry the function $f(\zeta) = (E/2j^k R^j)(\zeta^j + \zeta^{-j})$ satisfies $|D^k f| \leq E$ on $\partial\Omega$, and $|f| \leq \epsilon \equiv ER^{-j}$ on Γ. Nevertheless,

$$|f(\zeta)| \simeq E/2j^{-k} = \frac{E}{2}\left(\frac{|\log(\epsilon/E)|}{\log R}\right)^{-k}$$

on $\partial\Omega$. Such logarithmic continuity is so poor as to be intolerable in any physical problem. For example, with $k = 1, E$ fixed, and ϵ/E initially equal 10^{-1}, an increase in solution accuracy by factor of $2, 3, 4, \cdots$ would require increase in the data accuracy to $\epsilon/E = 10^{-2}, 10^{-3}, 10^{-4}, \cdots$, etc.

Let us obtain an estimate of R for the specific case of the nucleon-nucleon scattering. In this case the thresholds of the branch-cuts are located at $x_{\pm} = \pm[1 + (2\mu^2/k^2)]$ (see Ref. 1), where μ is the pion rest-mass and k is the barycentric momentum. For geometries with the thresholds $x_{\pm}$ of the cuts quite close to ± 1 (i.e., for high energies) we may use the approximate formulas (10) and (24) of Cutkosky-Deo[18], to approximate the parameter R of our conformal mapping. In this way, we get for the parameter R the value $R \simeq 1.77$ for an energy of 300 Mev in the Lab. system, the value $R \simeq 1.4$ for an energy of 10^3 Mev and the value $R \simeq 1.14$ at an energy of 10^4 Mev.

Now we can try some conclusions.

(A) Analytic continuation all the way to the boundary has such poor stability that it should not be attempted in a physical situation. The authors can think of no reasonable conditions for f^0 on $\partial\Omega$, other than assumptions (which are not considered in the present discussion) that f^0 be bounded and holomorphic on a much larger domain, which would raise this stability to a tolerable level.

(B) The best possible stability estimate in all our examples can never be much better than $\epsilon^{\omega(z)} E^{[1-\omega(z)]}$ (which is nearly the best possible estimate in case of supremum norms on $\dot{\Gamma} = \Gamma$ and $\partial\Omega$). This stability is also very poor at points near the boundary (i.e., at z where $\omega(z)$ is fairly small). Therefore, one should not attempt analytic continuation to points near the boundary.

(C) At points well interior to Ω, it is sufficient in all the above examples to assume that the best possible stability estimate is essentially of the form $C\epsilon^{\omega(z)} \times E^{[1-\omega(z)]}$ (provided enough data points are used).

Let us return to the nucleon-nucleon scattering considered above and obtain an estimate for $\omega(x)$ in this case. Here the position of the poles in the $\cos\vartheta$ plane is given by $x_{\pm}^{p} = \pm(1 + \mu^2/2k^2)$ (see Ref. 1). The exact $\omega(x)$ is the harmonic function which takes the value 1 on the physical region (i.e., on the interval $[-1, +1]$) and the value zero on the left and right cuts [recall that the position of the cut thresholds is given by $x_{\pm} = \pm(1 + 2\mu^2/k^2)$]. Let us estimate the value $\omega(x_{+}^{p})$ at high energies where the thresholds of the cuts become nearer to the physical region. In this case we may approximate $\omega(x)$ (in the gap between $+1$ and x_{+}) by the harmonic function $\omega^*(x)$ which takes boundary value $\omega^*(x) \equiv 1$ on $(-\infty, +1]$ and boundary value $\omega^*(x) \equiv 0$ on the right-hand cut. Since the boundary values of ω^* differ from those of ω only at boundary points on $(-\infty, -1]$, which are relatively speaking quite distant from this gap, simple estimates reveal that the error $\omega^* - \omega$ is small in the gap.

Now we can say by symmetry that the value $\omega^*(x)$ on the vertical line at the middle of the gap is $\omega(x) = \frac{1}{2}$. A simple use of the maximum principle on the vertical strip $1 \leq \mathrm{Re}x \leq \frac{1}{2}(1 + x_+)$ then establishes that $\frac{1}{2} < \omega^*(x_+^p) < 1$. Thus at high energies the Hölder coefficient ω at the point of interest x_+^p is nearly equal the value $\omega^*(x_+^p)$ which can be reasonable estimated $\simeq \frac{3}{4}$.

(D) The stability of all analytic continuation problems of scattering data is sufficiently precarious that it is necessary to use "nearly-best-possible" methods, both for generating the approximation f^1 and for generating bounds on the error $\langle f^1 - f^0 \rangle$.

A method is "nearly-best-possible" if it always gives us a f^1 for which the error $\langle f^1 - f^0 \rangle$ is nearly bounded by the best possible stability estimate [i.e., it is $\leq CM(\epsilon, E)$ where C is a constant not too much greater than unity]. Since the stability derives exclusively from the constraints (2.1) and (2.2), one way to insure this is to design methods which always give us a solution satisfying nearly the same constraints ϵ, E as the unknown f^0. Such methods will then be completely independent of the particular seminorm $\langle\ \rangle$ used to measure the solution error. In the next sections we consider two such methods which are computationally efficient.

4. LEAST-SQUARES METHODS

The proofs of the following results may be found in Ref. 20. Consider the general problem (2.1), (2.2) when X, Y, Z are real Hilbert spaces, with (2.7) also holding for the moment. We will keep Example (2c) in the back of our mind as the typical example. We begin first with the methods in an infinite dimensional setting because the exposition is clearest in that setting, later we discretize to a finite dimensional problem and all computations reduce to simple matrix calculations.

A. The method in general Hilbert space

If f^0 satisfies (2.1) and (2.2), then it also satisfies

$$\|Af^0 - h\|_Y^2 + (\epsilon/E)^2 \|Bf^0\|_Z^2 \leq 2\epsilon^2. \tag{4.1}$$

Conversely, any f satisfying (4.1) satisfies (2.1) and (2.2) except for factors of at most $\sqrt{2}$. If we let $M_1(\epsilon, E)$ denote the supremum of $\langle f \rangle$ with respect to (4.1) with $h = 0$, then

$$M(\epsilon, E) \leq M_1(\epsilon, E) \leq \sqrt{2}\, M(\epsilon, E). \tag{4.2}$$

Method 1: Let our approximation f^1 be that element of X which minimizes

$$\|Af - h\|_Y^2 + \lambda^2 \|Bf\|_Z^2 \tag{4.3}$$

with $\lambda = \epsilon/E$. It is the solution of the normal equation

$$Cf \equiv (A^*A + \lambda^2 B^*B)f = A^*h. \tag{4.4}$$

In the present case, (2.7) implies $B^*B = I$; this is not at all necessary in general, it merely insures that C is invertible.

If there does exist an f^0 satisfying (2.1), (2.2) as claimed, then f^1 must satisfy the *a posteriori* compatibility check.

$$\|Af^1 - h\|_Y^2 + (\epsilon/E)^2 \|Bf^1\|_Z^2 \leq 2\epsilon^2. \tag{4.5}$$

Moreover, $(f^1 - f^0)$ satisfies (4.1) with $h = 0$, so

$$\langle f^1 - f^0 \rangle \leq M_1(\epsilon, E) \leq \sqrt{2}\, M(\epsilon, E). \tag{4.6}$$

Hence this is a "nearly-best-possible" method.

Suppose $\langle f \rangle$ is of the form $|l(f)|$, where l is a real continuous linear functional on X. The Riesz representation theorem says that every continuous linear functional on a Hilbert space has a unique representation as an inner product, i.e., there exists a unique v in X such that

$$l(f) = (f, v)_X. \tag{4.7}$$

Moreover, $M_1(\epsilon, E)$ is exactly computable in terms of v and C^{-1}. We have

$$M_1(\epsilon, E) = \sqrt{2}\, \epsilon (C^{-1}v, v)_X^{1/2}. \tag{4.8}$$

The preceding formulation has the disadvantage that the error bound ϵ and the constraint E must both be known. We show now that a satisfactory approximation policy requires a knowledge of only one of these numbers. Let us call a pair of numbers (ϵ, E) permissible if there exists a f in X satisfying (2.1) and (2.2), and let $\mathcal{E}$ denote the set of permissible pairs in the plane. It turns out now that the solutions f_λ of the normal equation, as λ increases from 0 to ∞, give complete information concerning which pairs are permissible. Let

$$\epsilon_\lambda \equiv \|Af_\lambda - h\|_Y, \tag{4.9}$$

$$E_\lambda \equiv \|Bf_\lambda\|_Z, \tag{4.10}$$

where f_λ is the solution of (4.4). Clearly f_λ minimizes $\|Af - h\|_Y$ with respect to the constraint $\|Bf\|_Z \leq E_\lambda$ and likewise minimizes $\|Bf\|_Z$ with respect to the constraint $\|Af - h\|_Y \leq \epsilon_\lambda$. Also, ϵ_λ and E_λ are continuously increasing and decreasing functions of λ. Thus, $\mathcal{E}$ is exactly the set of points which are above and to the right of the curve $(\epsilon_\lambda, E_\lambda)$, $0 \leq \lambda \leq \infty$, as shown in Fig. 2. Moreover, $\mathcal{E}$ is a convex set, hence computation of only a few points $(\epsilon_\lambda, E_\lambda)$ on its boundary curve should give a good idea of its shape.

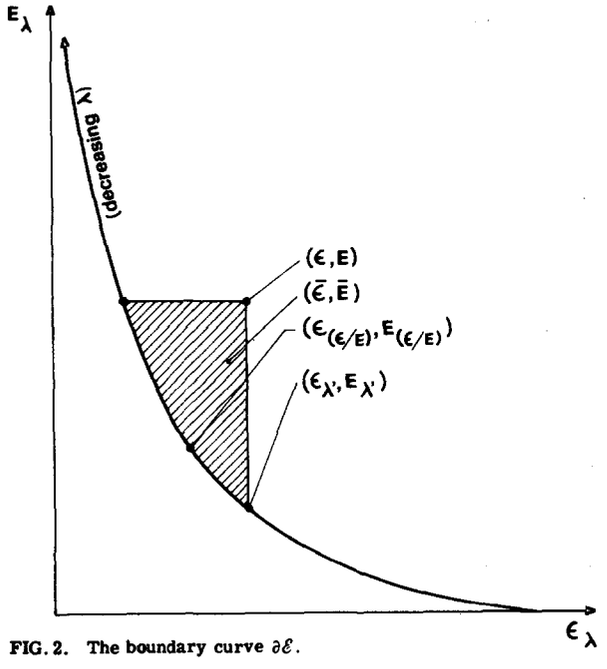

FIG. 2. The boundary curve $\partial\mathcal{E}$.

Recall that we are considering a particular element

f^0. Let $\bar{\epsilon}$ and $\bar{E}$ denote the exact values $\|Af^0 - h\|_Y$ and $\|Bf^0\|_Z$, respectively.

If good upper bounds ϵ and E are known for both $\bar{\epsilon}$ and $\bar{E}$, then we may either let our approximation be $f_{(\epsilon/E)}$ as in Method 1, or

Method 2: Let our approximation f^1 be any f_λ whose corresponding $(\epsilon_{\lambda'}, E_{\lambda'})$ touches the shaded area in Fig. 2. The error is then bounded by $\langle f^1 - f^0\rangle \leq M \times (\epsilon + \bar{\epsilon}, E + \bar{E}) \leq 2M(\epsilon, E)$.

Method 3: Suppose a good upper bound ϵ for $\bar{\epsilon}$ is known, but none for $\bar{E}$. Let our approximation f^1 be that element in X which minimizes $\|Bf\|_Z$ with respect to $\|Af - h\|_Y \leq \epsilon$. That is, let $f^1 = f_{\lambda'}$, where λ' is the value such that $\epsilon_{\lambda'} = \epsilon$ as shown in Fig. 2. Since ϵ_λ is monotone and continuous we can solve for the desired Lagrangian multiplier λ' by a variety of iterative root solving methods, interval halving for example. Now $\bar{E} \geq E_{\lambda'}$, thus the error is bounded by $\langle f^1 - f^0\rangle \leq M(\epsilon + \bar{\epsilon}, E_{\lambda'} + \bar{E}) \leq 2M(\epsilon, \bar{E})$, which is essentially optimal with respect to the given information, even though $\bar{E}$ is unknown.

B. The discretized problem and methods in general

We replace the infinite dimensional X by an $(n+1)$-dimensional "approximating subspace" $X_{n+1} \subset X$, with basis elements $\varphi^0, \varphi^1, \varphi^2, \ldots, \varphi^n$. By "approximating subspace" we mean that every f of interest has an approximation $\underline{f}$ in X_{n+1} such that $A\underline{f} \approx Af$ and $\langle \underline{f} - f\rangle \approx 0$ (for all $\langle\ \rangle$ of interest) to within desired accuracy, and such that $\|B\underline{f}\|_Z$ is either $\leq$ or $\approx \|Bf\|_Z$. Thus $\underline{f}^0$, for example, might satisfy

$$\|A\underline{f}^0 - h\|_Y \leq 1.1\epsilon, \qquad \|B\underline{f}^0\|_Z \leq 1.1E, \tag{4.11}$$

and the best-possible stability estimate on X_{n+1} will be approximately that on X.

We are going to neglect all these discretization errors since they can be made negligibly small by making n sufficiently large. That is, we assume that f^0 and all f of interest actually lie in X_{n+1}, and that f^0 still satisfies (2.1), (2.2). One then merely proceeds with the above least squares method but with X replaced by X_{n+1}; this is the general discretized method.

All computations reduce to linear calculations involving the basis coefficients. The general f has the form

$$f = x_0\varphi^0 + x_1\varphi^1 + \cdots + x_n\varphi^n, \tag{4.12}$$

where the coefficient vectors x vary over the parameter space R^{n+1} of all $(n+1)$-dimensional column vectors with real components x_j. We equip R^{n+1} with its usual Euclidean inner product and norm. We define maps $\mathfrak{A}$ from R^{n+1} into Y, and $\mathfrak{B}$ from R^{n+1} into Z, in the natural way

$$\mathfrak{A}x = A(x_0\varphi^0 + x_1\varphi^1 + \cdots + x_n\varphi^n),$$
$$\mathfrak{B}x = B(x_0\varphi^0 + x_1\varphi^1 + \cdots + x_n\varphi^n), \tag{4.13}$$
$$\langle x\rangle = \langle x_0\varphi^0 + x_1\varphi^1 + \cdots + x_n\varphi^n\rangle.$$

Conditions (2.1) and (2.2) now become

$$\|\mathfrak{A}x^0 - h\|_Y \leq \epsilon, \qquad \|\mathfrak{B}x^0\|_Z \leq E, \tag{4.14}$$

where x^0 is the coefficient vector of f^0. The $(n+1) \times (n+1)$ real matrix $\mathfrak{A}^*\mathfrak{A}$ is defined by

$$(\mathfrak{A}^*\mathfrak{A}x, y)_{R^{n+1}} = (A(x_0\varphi^0 + \cdots + x_n\varphi^n), A(y_0\varphi^0 + y_1\varphi^1 + \cdots + y_n\varphi^n))_Y \tag{4.15}$$

for all x, y in R^{n+1}. Letting x and y be all zero except for values 1 in their ith and jth component, respectively, we have

$$(\mathfrak{A}^*\mathfrak{A})_{ij} = (A\varphi^j, A\varphi^i)_Y. \tag{4.16}$$

Likewise $\mathfrak{B}^*\mathfrak{B}$ is the $(n+1) \times (n+1)$ real matrix such that

$$(\mathfrak{B}^*\mathfrak{B})_{ij} = (B\varphi^j, B\varphi^i)_Z. \tag{4.17}$$

$\mathfrak{A}^*h$ is the vector in R^{n+1} defined by

$$(\mathfrak{A}^*h, y)_{R^{n+1}} = (h, \mathfrak{A}y)_Y \quad \text{for all } y \text{ in } R^{n+1}, \qquad (\mathfrak{A}^*h)_i = (h, A\varphi^i)_Y. \tag{4.18}$$

Any linear functional on X_{n+1} has an immediate representation as an inner product on R^{n+1}

$$l(f) = x_0 l(\varphi^0) + \cdots + x_n l(\varphi^n) = (x, y)_{R^{n+1}}, \tag{4.19}$$

where y is the vector in R^{n+1} with components

$$y_0 = l(\varphi^0), \cdots, y_n = l(\varphi^n). \tag{4.20}$$

We assume that one can somehow evaluate the above terms by numerical means, and also $\|h\|_Y^2$. All else is merely matrix computation on R^{n+1}, replacing the $X, f, f^0, A^*A, B^*B, A^*h, f$, and v of (4.1)-(4.10) by R^{n+1}, $x, x^0, \mathfrak{A}^*\mathfrak{A}, \mathfrak{B}^*\mathfrak{B}, \mathfrak{A}^*h, x_\lambda$, and y here.

Notice that evaluation of the $(\epsilon_\lambda, E_\lambda)$ is also just a calculation in R^{n+1}:

$$\epsilon_\lambda^2 = \|\mathfrak{A}x_\lambda - h\|_Y^2 = (\mathfrak{A}^*\mathfrak{A}x_\lambda, x_\lambda)_{R^{n+1}} - 2(x_\lambda, \mathfrak{A}^*h)_{R^{n+1}} + \|h\|_Y^2, \tag{4.21}$$
$$E_\lambda^2 = \|\mathfrak{B}x_\lambda\|_Z^2 = (\mathfrak{B}^*\mathfrak{B}x_\lambda, x_\lambda)_{R^{n+1}}.$$

Example: We work out Example (2c) in detail, with the discrete data set $\Gamma = \{d_1, \ldots, d_k\}$ and with $\langle f\rangle = |\mathrm{Re} f(z_0)|$ at some fixed z_0 of interest. We introduce the functions $\varphi^0(z) = 1, \varphi^1(z) = z, \ldots, \varphi^n(z) = z^n$ as our approximate basis. If $\beta(z)$ is nonzero and very smooth, then n usually does not have to be very large at all to make the discretization errors completely negligible, for example see Ref. 20, p. 65. We can also allow singularities like $(z - z_+)^{-1/2}$ in $\beta(z)$, but this tends to make n quite a bit larger; we therefore feel it would be best to take care of these singularities in the original formulation of the problem, by adjusting appropriately the function $f(z)$ originally.

One initially computes

$$(\mathfrak{A}^*\mathfrak{A})_{ij} = \sum_{\nu=1}^{k} (d_\nu)^{i+j}\beta^2(d_\nu), \qquad i, j = 0, 1, \ldots, n, \tag{4.22}$$

$$(\beta^*\beta)_{ij} = \mathrm{Re}\int_{z\in\partial\Omega} z^j\bar{z}^i\gamma^2(z)\,|\,dz\,|, \qquad i, j = 0, 1, \ldots, n, \tag{4.23}$$

$$\|h\|_Y^2 = \sum_{\nu=1}^{k} |h(d_\nu)|^2\beta^2(d_\nu), \tag{4.24}$$

$$(\mathfrak{A}^*h)_i = \sum_{\nu=1}^{k} h(d_\nu)(d_\nu)^i\beta^2(d_\nu), \qquad i = 0, 1, \ldots, n, \tag{4.25}$$

$$(y)_i = \mathrm{Re}((z_0)^i), \qquad i = 0, 1, \ldots, n \tag{4.26}$$

using numerical integration on (4.23). All else is matrix calculations; one proceeds to solve the canonical equations

$$C_\lambda x_\lambda \equiv (\mathfrak{A}^*\mathfrak{A} + \lambda^2\mathfrak{B}^*\mathfrak{B})x_\lambda = \mathfrak{A}^*h \tag{4.27}$$

by a Gaussian elimination computer program (Cholesky elimination would be better here).

Since a decent upper bound E for the true $\overline{E}$ will usually not be known, we adopt the strategy of Method 3. We solve (4.27) for a variety of λ and plot the $(\epsilon_\lambda, E_\lambda)$ obtained on a diagram like Fig. 2 with linear interpolation in between, to get a precise idea of the shape of the boundary curve of $\mathcal{E}$. Since the matrix C_λ^{-1} will be readily available from the direct elimination solution of (4.27), we can also compute the best-possible (but for a factor of $\sqrt{2}$) stability estimate $M_1(\epsilon, (\epsilon/\lambda)) = \sqrt{2}\,\epsilon(C_\lambda^{-1}y, y)^{1/2}_{R^{n+1}}$ perhaps at many points z_0. Interval on λ, then gives us a good approximate value of λ', and we take $x_{\lambda'}$ as our approximation.

Notice that we cannot discover an upper bound for $\overline{E}$ from the data, but only the exact lower bound $E_{\lambda'}$.

5. EXACT DISCRETIZATION USING REPRODUCING KERNEL[30]

There is one discretization which is exact for our least-square methods when Y has finite dimension k. It is imperative in this section that the two norms $\|f\|_X$ and $\|Bf\|_Z$ be equal. Let $(Af)_j$ denote the jth component of the k-dimensional vector Af; since it is a real continuous linear function of f, there must exist a unique element u^j in X such that

$$(Af)_j = (f, u^j)_X \qquad \text{for all } f \text{ in } X. \tag{5.1}$$

Let $\mathcal{L}$ be the subspace of all linear combination of these $u^1, \ldots, u^k$. Now for each f in X, let $\underline{f}$ denote its orthogonal projection onto $\mathcal{L}$. Since $\underline{f} - f$ is orthogonal to $\mathcal{L}$, we have

$$(A\underline{f})_j = (Af)_j + (A(\underline{f} - f))_j = (Af)_j + (\underline{f} - f, u^j)_X = (Af)_j, \quad \forall j. \tag{5.2}$$

In other words, for every f not in $\mathcal{L}$, its projection $\underline{f}$ onto $\mathcal{L}$ has the same value $A\underline{f} = Af$ and, moreover, has smaller norm.

It is thus immediately obvious that the solutions f_λ of the least squares problem (4.3) all lie in the finite dimensional subspace $\mathcal{L}$. Thus, if one discretizes by using $u^1, \ldots, u^k$ as our approximate basis, and solves the canonical equations for the discretized problem, then the solution f_λ obtained is the exact least-squares solution not only for $\mathcal{L}$ but also for X.

For the sake of error analysis we may want also to include in our approximate basis the element v associated with our linear functional l and corresponding seminorm $\langle f \rangle = |l(f)| = (f, v)_X$. More generally, we may have several linear functionals of interest, say $l_1, \ldots, l_p$. These then also have representations as inner product

$$l_j(f) = (f, v^j)_X \qquad \text{for all } f \text{ in } X,\ j = 1, \ldots, p. \tag{5.3}$$

Let $\mathcal{L}_1$ be the subspace of all linear combinations of $u^1, \ldots, u^k, v^1, \ldots, v^p$; one sees immediately that for every f not in $\mathcal{L}_1$, its projection $\underline{f}$ onto $\mathcal{L}_1$ has the same values $A\underline{f} = Af, l_1(\underline{f}) = l_1(f), \ldots, l_p(\underline{f}) = l_p(f)$ and, moreover has smaller norm. Thus, if one discretizes by using $u^1, \ldots, u^k, v^1, \ldots, v^p$ as our approximate basis, and solves the canonical equations and computes the stability estimates $M_1(\epsilon, E) = \sqrt{2}\,\epsilon(C_\lambda^{-1}v^jv^j)^{1/2}, j = 1, \ldots, p$ for this discretized problem, then the f_λ and $M_1(\epsilon, E)$ obtained are the exact least squares solution and the best-possible stability estimates not only for $\mathcal{L}_1$, but also for X.

A. Numerical computation of $u^1, \cdots, u^k \quad v^1, \cdots, v^p$

Consider any linear functional l which we wish to represent as an inner product $l(f) = (f, v)_X$. If an orthonormal basis $\psi_0, \psi_1, \ldots$ for X is available, the computation of the coefficients $y_0, y_1 \ldots$ of v with respect to this basis is automatic; as in (4.19)-(4.20), we have

$$l(f) = l\left(\sum_{\nu=0}^{\infty} x_\nu\psi^\nu\right) = \sum_{\nu=0}^{\infty} x_\nu l\psi^\nu) = \sum_{\nu=0}^{\infty} x_\nu y_\nu = (f, v)_X. \tag{5.4}$$

Thus the coefficients y_ν must be given by

$$y_0 = l(\psi^0), \qquad y_1 = l(\psi^1), \cdots. \tag{5.5}$$

If an exact orthonormal basis is not available then we can proceed to construct an approximate one by numerical orthogonalization. That is, we begin with an "approximate basis" $\varphi^0, \varphi^1, \ldots, \varphi^n$ as before. Using Gram-Schmidt orthogonalization, one then construct on orthonormal bases $\psi^0, \psi^1, \ldots, \psi^n$ for X_{n+1}. Therefore, the element

$$\underline{v} = l(\psi^0)\psi^0 + l(\psi^1)\psi^1 + \cdots + l(\psi^n)\psi^n \tag{5.6}$$

is the projection onto X_{n+1} of the desired v, and $l(\underline{f}) = (\underline{f}, \underline{v})_X$ for all $\underline{f}$ in X_{n+1}.

In this way we can construct $\underline{u}^1, \ldots, \underline{u}^k, \underline{v}^1, \ldots, \underline{v}^p$ which are the projections onto X_{n+1} of the desired $u^1, \ldots, v^p$. If $(k + p) < (n + 1)$, then we can use $\underline{u}^1, \ldots, \underline{v}^p$ as our approximate basis and work the discretized problem. Clearly, the results f_λ and $M_1(\epsilon, E)$ obtained will be exactly those which would have been obtained if one had instead worked the discretized problem using $\varphi^0, \ldots, \varphi^n$ as our approximate basis; the advantage is that the dimensionality of the canonical equations has been reduced with little effort from $(n + 1)$ to $(k + p)$.

Example: Consider Example 2b. The ith component of Af is $(Af)_i = f(d_i), i = 1, \ldots, k$, where d_i is the ith data point in Γ. Now $\psi^0 = 1$, $\psi^1 = z$, $\psi^2 = z^2, \cdots$ is an orthonormal basis, thus

$$f(d_i) = \sum_{\nu=0}^{\infty} x_\nu(d_i)^\nu = \left(\sum_{\nu=0}^{\infty} x_\nu z^\nu, \sum_{\nu=0}^{\infty} (\bar{d}_i)^\nu z^\nu\right) = (f, u^i)_X. \tag{5.7}$$

The function u^i

$$u^i(z) = u(d_i, z) = \sum_{\nu=0}^{\infty} (\bar{d}_i)^\nu z^\nu = \frac{1}{1 - \bar{d}_i z}, \tag{5.8}$$

is called the reproducing kernel[31] for the point d_i, because of the property that integration with respect to it on $\partial\Omega$ reproduces the value of f at d_i, i.e.,

$$f(d_i) = \int_{\partial\Omega} f(z)\,\overline{u(d_i, z)}\,dz. \tag{5.9}$$

Despite the fact that use of the reproducing kernels $u^1, \ldots, u^k$, $v^1, \ldots, v^k$ as basis yields an exact discretization of the least squares methods, it is often much more convenient (at least in the case of Example 2b to use the approximate basis $\varphi^0 = 1$, $\varphi^1 = z$, $\varphi^2 = z^2, \ldots$, $\varphi^n = z^n$ instead). We need only take n proportional to $\log(E/\epsilon)$ to make the truncation error essentially negligible. On the other hand it seems that we should take k proportional to $[\log(E/\epsilon)]^2$ in order to make negligible the effect of using a finite data set $\dot{\Gamma} \neq \Gamma$ (see Ref. 20 for details).

6. METHODS OF PARTIAL EIGENFUNCTIONS EXPANSIONS

Suppose that we have available for X a basis $\psi^0, \psi^1, \cdots$ which is simultaneously orthogonal with respect to both the Y and the Z norms, i.e.,

$$(A\psi^i, A\psi^j)_Y \equiv (A^*A\psi^i, \psi^j)_X = a_j^2\delta_{ij}, \tag{6.1}$$

$$(B\psi^i, B\psi^j)_Z \equiv (B^*B\psi^i, \psi^j)_X = b_j^2\delta_{ij}. \tag{6.2}$$

In that case, f^0, the general f, and also h can be expanded in terms of this basis, with Fourier coefficients $\{x_j^0\}$, $\{x_j\}$, and $\{h_j\}$:

$$\begin{aligned} &f^0 = \sum_{j=0}^{\infty} x_j^0\psi^j \qquad f = \sum_{j=0}^{\infty} x_j\psi^j, \\ &h = \underline{h} + \underline{\underline{h}} = \sum_{a_j\neq 0} h_j(A\psi^j) + \underline{\underline{h}}, \end{aligned} \tag{6.3}$$

where $\underline{h}$ is in the range of A and $\underline{\underline{h}}$ is in its orthogonal complement.

Thus (2.1) and (2.2) become

$$\begin{aligned} \|Af^0 - h\|_Y^2 &= \|Af^0 - \underline{h}\|_Y^2 + \|\underline{\underline{h}}\|_Y^2 \\ &= \Big\|\sum_{a_j\neq 0} (x_j^0 - h_j)A\psi^j\Big\|_Y^2 + \|\underline{\underline{h}}\|_Y^2 \leq \epsilon^2, \end{aligned} \tag{6.4}$$

$$\|Bf^0\|_Z^2 = \Big\|\sum_{j=0}^{\infty} x_j^0 B\psi^j\Big\|_Z^2 \leq E^2. \tag{6.5}$$

Thus the analysis reduces completely to a consideration of Fourier coefficients. We have the weighted quadratic sums

$$\left(\sum_{j=0}^{\infty} (a_j/\epsilon)^2(x_j^0 - h_j)^2\right)^{1/2} \leq 1, \tag{6.6}$$

$$\left(\sum_{j=0}^{\infty} (b_j/E)^2(x_j^0 - 0)^2\right)^{1/2} \leq 1, \tag{6.7}$$

and we assume that the basis has been prearranged such that the ratios a_j/b_j are decreasing and also $\downarrow 0$ as $j \to \infty$.

We now decompose each f in X precisely into a low order part f_L and a high order part f_H,

$$f = f_L + f_H = \sum_{j=0}^{\alpha} x_j\psi^j + \sum_{j=\alpha+1}^{\infty} x_j\psi^j, \tag{6.8}$$

where α is the largest integer such that $(a_\alpha/\epsilon) \geq (b_\alpha/E)$. With this decomposition we notice, using (6.6) and (6.7), that

$$\|Af_L\|_Y \leq \epsilon \quad \text{implies} \quad \|Bf_L\|_Z \leq E \tag{6.9}$$

for every low order part f_L and

$$\|Bf_H\|_Z \leq E \quad \text{implies} \quad \|Af_H\|_Y \leq \epsilon \tag{6.10}$$

for every high order part f_H.

Method 1': We let our approximation f^1 be the low order part h_α of the Fourier expansion of the data

$$f^1 \equiv h_\alpha = \sum_{j=0}^{\alpha} h_j\psi^j. \tag{6.11}$$

In other words, we have used the Fourier coefficients h_j from (6.6) for the components where the weight (a_j/ϵ) is the larger, and we have used the Fourier coefficients 0 from (6.7) for the components where the weight (b_j/E) is the larger.

From (6.9) and (6.10) one obtains the following results:

$$\max\{L(\epsilon, E), H(\epsilon, E)\} \leq M(\epsilon, E) \leq L(\epsilon, E) + H(\epsilon, E), \tag{6.12}$$

where

$$L(\epsilon, E) = \sup\{\langle f_L\rangle : \|Af_L\|_Y \leq \epsilon\}, \tag{6.13}$$

$$H(\epsilon, E) = \sup\{\langle f_H\rangle : \|Bf_H\|_Z \leq E\}. \tag{6.14}$$

Moreover, if $\langle f\rangle$ is a linear functional $|l(f)|$, then $L(\epsilon, E)$ and $H(\epsilon, E)$ can be exactly evaluated. We have, using the Schwartz inequality

$$\langle f_L\rangle = \left|\sum_{j=0}^{\alpha} x_j l(\psi^j)\right| \leq \epsilon\left(\sum_{j=0}^{\alpha}\left[\frac{l(\psi^j)}{a_j}\right]^2\right)^{1/2} \equiv L(\epsilon, E), \tag{6.15}$$

$$\langle f_H\rangle = \left|\sum_{j=\alpha+1}^{\infty} x_j l(\psi^j)\right| \leq E\left(\sum_{j=\alpha+1}^{\infty}\left[\frac{l(\psi^j)}{b_j}\right]^2\right)^{1/2} \equiv H(\epsilon, E). \tag{6.16}$$

Moreover, our approximation satisfies

$$\|A(h_\alpha - f^0)_L\|_Y \leq \epsilon, \qquad \|B(h_\alpha - f^0)_H\|_Z \leq E, \tag{6.17}$$

and hence

$$\langle h_\alpha - f^0\rangle \leq L(\epsilon, E) + H(\epsilon, E) \leq 2M(\epsilon, E), \tag{6.18}$$

which is the best possible error bound, but for a factor of 2.

In general, let h_N denote the $N$the order truncated expansion (6.11) of the data function h, and let ϵ_N and E_N denote the fit to data, and the global bound of h_N

$$\epsilon_N \equiv \|Ah_N - h\|_Y = \left(\|h\|_Y^2 - \sum_{j=0}^{N} (a_jh_j)^2\right)^{1/2}, \tag{6.19}$$

$$E_N = \|Bh_N\|_Z = \left(\sum_{j=0}^{N} (b_jh_j)^2\right)^{1/2}. \tag{6.20}$$

From (6.9) and (6.10) one can obtain

$$\epsilon_\alpha \leq 2\epsilon, \qquad E_\alpha \leq 2E. \tag{6.21}$$

Hence, our method is the best possible but for a factor of 2 in this sense also.

A plot of the (ϵ_N, E_N), $N = 0, 1, 2, \cdots$ as the truncation order is increased now yields nearly complete information as to which constraints (ϵ, E) are in the set $\mathcal{E}$ of permissible pairs. Instead of Fig. 2, we now have Fig. 3; as this diagram illustrates, each point in the set $2\mathcal{E}$ is above and to the right of at least one point (ϵ_N, E_N).

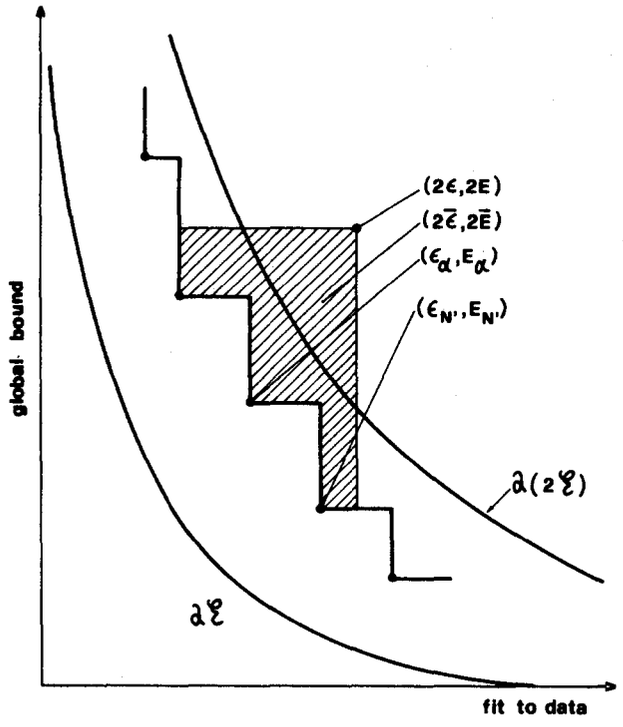

FIG. 3. A plot of the (ϵ_N, E_N), $N = 0, 1, 2, \cdots$.

Method 2': Take h_N as our approximation, where N is any integer such that the point (ϵ_N, E_N) touches the shaded area in Fig. 3. The error is then limited by $\langle h_N - f^0 \rangle \leq M(\epsilon_N + \bar{\epsilon}, E_N + \bar{E}) \leq 3M(\epsilon, E)$.

Method 3': If a good upper bound ϵ for $\bar{\epsilon}$ is known, but no good upper bound E for $\bar{E}$, then take $h_{N'}$ as our approximation, where N' is the first integer such that $\epsilon_{N'} \leq 2\epsilon$. Then $E_{N'} \leq 2\bar{E}$. Thus this approximation has the error bound

$$\langle h_{N'} - f^0 \rangle \leq M(\epsilon_{N'} + \epsilon, E_{N'} + \bar{E}) \leq 3M(\epsilon, \bar{E}) \qquad (6.22)$$

which is essentially best-possible but for a factor of three, even though $\bar{E}$ is unknown.

Example: Consider Example 3a. The basis $\psi^0 = 2$, $\psi^1 = \zeta + \zeta^1, \psi^2 = \zeta^2 + \zeta^{-2}, \cdots$ is orthogonal with respect to both the Y and Z inner products. Expanding both the unknown $f^0(\zeta)$ and the data function $h(\zeta)$ on $\Gamma = \dot{\Gamma}$ in terms of this basis, we have

$$f^0(\zeta) = \sum_{j=0}^{\infty} x_j^0(\zeta^j + \zeta^{-j}), \quad 1 \leq |\zeta| \leq R, \qquad (6.23)$$

$$h(\zeta) = \sum_{j=0}^{\infty} h_j(\zeta^j + \zeta^{-j}) \quad \text{on } |\zeta| = 1, \qquad (6.24)$$

and the conditions (2.1), (2.2) can be written in terms of the coefficients

$$\|Af^0 - h\|_Y = \left(\sum_{j=0}^{\infty} 2(x_j^0 - h_j)^2 \right)^{1/2} \leq \epsilon, \qquad (6.25)$$

$$\|Bf^0 - 0\|_Z = \left(\sum_{j=0}^{\infty} (R^{2j} + R^{-2j})(x_j - 0)^2 \right)^{1/2} \leq E. \qquad (6.26)$$

Our approximation by Method 1' is the αth partial expansion

$$h_\alpha(\zeta) = \sum_{j=0}^{\alpha} h_j(\zeta^j + \zeta^{-j}), \quad 1 \leq |\zeta| \leq R, \qquad (6.27)$$

where α is the largest integer such that $2/\epsilon^2 \geq (R^{2\alpha} + R^{-2\alpha})/E^2$, i.e., $R^\alpha \simeq E/\epsilon$. If f in X satisfies $\|Af\|_Y \leq \epsilon$ and $\|Bf\|_Z \leq E$, then we have

$$\langle f \rangle \equiv |f(\zeta)| \leq \left| \sum_{j=0}^{\alpha} x_j(\zeta^j + \zeta^{-j}) \right| + \left| \sum_{j=\alpha+1}^{\infty} x_j(\zeta^j + \zeta^{-j}) \right|$$

$$\leq \epsilon \left(\frac{1}{2} \sum_{j=0}^{\alpha} (|\zeta|^j + |\zeta|^{-j})^2 \right)^{1/2}$$

$$+ E \left(\sum_{j=\alpha+1}^{\infty} \frac{(|\zeta|^j + |\zeta|^{-j})^2}{(R^{2j} + R^{-2j})} \right)^{1/2} \qquad (6.28)$$

This equals $L(\epsilon, E) + H(\epsilon, E)$ when ζ is real, and hence is the best-possible stability estimate but for a factor of two.

A. The simultaneous diagonalization (6.1) and (6.2) in general

The simultaneous diagonalization (6.1) and (6.2) is theoretically always possible in general. To begin with, we may always assume that X borrows its inner product from Z by (2.7), thus making B^*B the identity. Then A^*A is self-adjoint and so has a spectral representation; in Ref. 20 the general case using the spectral integral representation is treated. However, in every case of interest A^*A is also compact; its spectrum is discrete and X has an orthonormal basis of eigenfunctions $\psi^0, \psi^1, \cdots$ for A^*A with corresponding eigenvalues $a_0^2 \geq a_1^2 \geq a_2^2 \geq \cdots \geq 0$ tending to zero, as desired.

B. Discretization in general of these expansion methods

We discretize these methods just as in Sec. 6. That is, we introduce an "approximate basis" $\varphi^0, \varphi^1, \ldots, \varphi^n$ spanning the "approximating subspace" X_{n+1}; we assume that f^0 and all f of interest actually lie in X_{n+1}, and we then merely proceed with our previous expansion methods, but with X replaced by X_{n+1}.

The advantage is that calculation of the basis $\psi^0, \psi^1, \ldots, \psi^n$ for X_{n+1} which simultaneously diagonalizes the quadratic forms A^*A and B^*B in (6.1) and (6.2) now becomes merely a matrix eigenvalue problem. Let the $(n+1) \times (n+1)$ matrices $\mathfrak{A}^*\mathfrak{A}$ and $\mathfrak{B}^*\mathfrak{B}$ be defined and numerically computed just as in Sec. 6. It suffices then to find vectors $y^0, y^1, \ldots, y^n$ in R^{n+1} such that

$$(\mathfrak{A}^*\mathfrak{A}y^i, y^j)_{R^{n+1}} = a_j^2 \delta_{ij},$$

$$(\mathfrak{B}^*\mathfrak{B}y^i, y^j)_{R^{n+1}} = b_j^2 \delta_{ij} = \delta_{ij} \qquad (6.29)$$

(with $b_j \equiv 1$ for the sake of normalization); for these are then the coefficient vectors of a basis $\psi^0 = y_0^0\varphi^0 + y_1^0\varphi^1 + \cdots + y_n^0\varphi^n, \psi^1 = y_0^1\varphi^0 + y_1^1\varphi^1 + \cdots + y_n^1\varphi^n$ satisfying (6.1) and (6.2) as desired. This simultaneous diagonalization of two quadratic forms, with the second

positive definite, is a well-known matrix computation. In this first place, one may use the Gram-Schmidt orthogonalization to exchange the original basis for one which is orthonormal with respect to the Z inner product. To avoid a bit of notational complexity, let us assume that this has been done in advance and that $\varphi^0, \varphi^1, \ldots, \varphi^n$ is already orthonormal; $\mathfrak{B}^*\mathfrak{B}$ is thus the identity matrix. Secondly, one must then compute the eigenvalues $a_0^2 \geq a_1^2 \geq \cdots \geq a_n^2 \geq 0$ and corresponding orthonormal eigenvectors $y^0, y^1, \ldots, y^n$ of $\mathfrak{A}^*\mathfrak{A}$, (6.29) will then be satisfied as desired.

C. Exact discretization using reproducing kernels

When Y has finite dimension k and $\|f\|_X = \|Bf\|_Z$, as in Sec. 5, recall that X decomposes into the two subspaces $\mathcal{L}^\perp = \{f \in X : Af = 0\}$ and its orthogonal complement $\mathcal{L}$. Notice, however, that this is exactly the orthogonal decomposition of X which occurs when one divides the orthonormal basis of eigenvectors $\psi^0, \psi^1, \cdots$ into those $\psi^0, \psi^1, \ldots, \psi^{r-1} (r = \text{dim range } (A) \leq k)$ for which $a_0^2 \geq \cdots \geq a_{r-1}^2 \geq 0$ and those $\psi^r, \psi^{r+1}, \cdots$ for which $a_r^2 = a_{r+1}^2 = \cdots = 0$. That is span $\{\psi^r, \psi^{r+1}, \psi^{r+2}, \cdots\}$ is clearly equal $\mathcal{L}^\perp$ and hence its orthogonal complement span $\{\psi^0, \psi^1, \ldots, \psi^{r-1}\}$ must equal $(\mathcal{L}^\perp)^\perp = \mathcal{L}$, which then equals span $(u^1, \ldots, u^k)$.

It is then easy to see that if we perform the discretized version 6B of our expansion methods using $u^1, \ldots u^k$ as our "approximate basis," then the eigenfunctions $\psi^0, \ldots, \psi^{r-1}$, the eigenvalues $a_0^2 \geq \cdots \geq a_{r-1}^2 \geq 0$, the partial expansions $h_N, N = 0, 1, \ldots$, the fits to data, and the global bounds (ϵ_N, E_N) obtained are exactly what would have been obtained with no discretization at all. Similarly, if we perform the discretized version of our expansion methods using $u^1, \ldots, u^k$ and $v^1, \ldots, v^p$, as our "approximate basis," then the stability estimates $M(\epsilon, E)$, $L(\epsilon, E)$, and $H(\epsilon, E)$ for the discretized problem are also exactly what would have occurred with no discretization at all.

D. Inflexibility of polynomial expansions

The classical theory (Walsh[27]) of orthogonal polynomial expansions, with data given on a fairly arbitrary data set Γ and with respect to a fairly arbitrary positive weight function β on Γ, establishes convergence properties for such expansions which are closely analogous to the well-known convergence properties (on circles) of the Taylor series expansion. According to this theory, the shape of the regions of convergence is completely and rigidly determined by the shape of Γ. We mentioned a special case in Example 4a, where $\Gamma = [-1, +1]$ and the regions of convergence are confocal ellipses. This difficulty can be circumvented by conformal mapping of the original region of holomorphy of the physical problem into one of these regions of convergence, as pointed out by Cutkosky-Deo[17] and Ciulli.[15]

However, there is then the further difficulty that, given the weight function β on Γ, the orthogonal polynomials are then uniquely determined and, in general, these will not be orthogonal with respect to any natural norm on $\partial\Omega$.

The method of partial eigenfunction expansions is instead much more flexible. One is free to choose natural inner product norms independently on both Γ and $\partial\Omega$. Then, instead of expanding the data in polynomials, we expand them in eigenfunctions of the operator A^*A (see also Cutkosky[19] at this point).

7. CONCLUSIONS

Various portions of the least-squares, partial expansions, reproducing kernel techniques of the preceding sections have been discovered independently by several different authors. The methods of Backus[22-25] are essentially equivalent to the least-squares Method 1, combined always with the reproducing kernel discretization. He gives a probabilistic interpretation to the data accuracy (2.1), the prescribed bound (2.2), and the error bound (4.8).

The partial eigenfunction expansion Method 1′ (with exactly the same choice of truncation order) occurs in Cutkosky.[19] Cutkosky[19] also uses the reproducing kernel technique. This corresponds to a "minimal decomposition" of the operator A in his terminology. However, much of the complication of his paper can probably be attributed to the fact that he seeks explicit integral formulas for the kernel functions, rather than the more simple device of Sec. 5A.

The approach of Cutkosky[19] as to choice of truncation point when the "scale factor" E is unknown seems to differ from that of Method 3′. Cutkosky assumes that the coefficients of $(Af - h)$ are independent Gaussian random variables. He also assumes that f is a Gaussian random variable in the Hilbert space X. From these assumptions he derives a series truncation order N (and also error estimates for $\langle f - h_N \rangle$) using a statistical test involving ratios of the computed Fourier coefficients.

This Gaussian hypothesis may be too restrictive for some of the problems mentioned in Sec. 2. There is some reason to believe that the ratio test of Cutkosky would lead to a choice of truncation point similar to that of Method 3′ if the coefficients of f truly have a Gaussian type distribution. However, it is unclear to us what effect departures from Gaussian behavior will have in this ratio test. Can this ratio test lead to truncation point N with E_N much larger than $E_{N'}$? If so, we fear for the stability of the process.

The authors prefer to take a much more conservative and pessimistic point of view. Ultimately, it seems to us, that any knowledge of the value E of the global bound (in order to have error bounds) must come from *a priori* sources, that is, sources completely outside anything which can be discerned from the data itself. The data h can only disclose that E below a certain value $E_{\lambda'} = E(\epsilon)$ (given by Method 3) is impossible. For the purpose of computing error estimates one may then wish to make the assumption that $E \approx E(\epsilon)$; however, there is no reliable basis for this assumption. On the other hand, there always remains the possibility that fits to data of greater accuracy would reveal greater oscillation and pathology in f.

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Perturbation solution of the Kirkwood–Salsburg equation*

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A formal series solution to the Kirkwood–Salsburg equation and its radius of convergence are derived. This solution leads naturally to the establishment of an approximate hierarchy of equations for the distribution functions which needs no closure. The asymptotic behavior of the solutions to this approximate hierarchy is studied as well as the behavior of the derivatives of the pair function with respect to the interparticle distance.

I. INTRODUCTION

In order to facilitate the study of the N particle distribution functions, many hierarchies of equations have been developed which admit the set of distribution functions as a solution. These equations have been studied from various points of view. For pairwise additive potentials the Kirkwood–Salsburg[1] equations have yielded both approximate numerical information[2] and rigorous results.

Ruelle[3a,b] has made progress by formulating the Kirkwood–Salsburg as an operator equation in a Banach space. Iterating the equation generates a power series in the activity z, which Ruelle proved converged in a region of the complex z plane centered about $z = 0$.

The purpose of this paper is to present an alternate solution to the Kirkwood–Salsburg (K–S) equation which shows some promise of having a larger radius of convergence and of yielding some information about properties of the distribution functions such as their asymptotic behavior.

We also consider the K–S equation as an operator equation in a Banach space. By making some modifications to the equation and separating the operator into an unperturbed part and a perturbation, we obtain a series solution to the equation. This method of solution, which for positive potentials generates a resummation of the activity series of Ruelle, leads naturally to the establishment of an approximate hierarchy which is identical to the first covering sphere approximation of Sabry[2]. The solution for $\rho_{NA}(\{\mathbf{x}_N\})$ of the approximate hierarchy is shown to be the first nonzero contribution to $\rho_N(\{\mathbf{x}_N\})$, the solution to the exact hierarchy, generated by the perturbation expansion.

Various properties of the approximate hierarchy are studied. We also argue that certain of these properties studied are identical in the solution of both approximate and exact hierarchies.

II. INTRODUCTION OF THE BANACH SPACE APPROACH

The N particle distribution functions are defined in the grand canonical ensemble as

$$\rho_N(\{\mathbf{x}_N\}) = \sum_{m=N+1}^{n} \frac{z^m}{m!} \int_{\Lambda m} d\mathbf{x}_{N+1} \cdots d\mathbf{x}_m \exp[-\beta U(\{\mathbf{x}_{m+n}\})]/\Xi,$$

$$\Xi = \sum_{m=0}^{n} \int_{\Lambda m} d\mathbf{x}_1 \cdots d\mathbf{x}_m \exp[-\beta U(\{\mathbf{x}_m\})],$$

$$z = e^{\beta\mu}/\lambda^3, \qquad \beta = 1/KT, \qquad \lambda = h/(2\pi mKT)^{1/2}.$$

Λ^m is the m particle configuration space. $\rho_N(\{\mathbf{x}_N\})$ can be shown, for pairwise additive potentials, to be a solution of the K–S equation

$$\rho_1(\mathbf{x}_1) = z\left(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int \rho_n(\mathbf{x}_2 \cdots \mathbf{x}_{n+1}) \prod_{j=2}^{n+1} f_{1j} d\mathbf{x}_j\right),$$

$$\rho_N(\{\mathbf{x}_N\}) = z \prod_{j=2}^{N} (1 + f_{1j})\left(\rho_{N-1}(\mathbf{x}_2 \cdots \mathbf{x}_N) + \sum_{n=1}^{\infty} \frac{1}{n!} \int \rho_{N+n-1}(\mathbf{x}_2 \cdots \mathbf{x}_{N+n}) \prod_{j=N+1}^{N+n} f_{1j} d\mathbf{x}_j\right),$$

$$f_{ij} = \exp[-\beta\phi(\mathbf{x}_i - \mathbf{x}_j)] - 1, \qquad \text{(II. 1)}$$

$$\phi(\mathbf{x}_i - \mathbf{x}_j) = \text{two particle potential.}$$

We require, with Ruelle,[3b] three properties of the interaction potential.

(1) The N particle potential

$$U_N(\mathbf{x}_1 \cdots \mathbf{x}_N) = \sum_{i \neq j} \phi(|\mathbf{x}_i - \mathbf{x}_j|) \geq -NB,$$

where B is a positive constant.

(2)

$$\int |f_{ij}|\, d\mathbf{x}_{ij} = C(\beta) < \infty.$$

(3)

$$\phi(\mathbf{x}_i - \mathbf{x}_j) = \phi(|\mathbf{x}_i - \mathbf{x}_j|) > -A,$$

where A is a positive constant.

The K–S equation can be considered as an operator equation in a Banach space[4] composed of the vectors

$$f = \begin{pmatrix} f_1(\mathbf{x}_1) \\ \cdot \\ \cdot \\ \cdot \\ f_N(\{\mathbf{x}_N\}) \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

with the norm

$$\|f\| = \sup_{\substack{\forall i \\ \forall\{x_i\}}} \frac{|f_i(\{\mathbf{x}_i\})|}{S^i}.$$

The $f_i(\{\mathbf{x}_i\})$ are bounded measurable functions and S is an arbitrary positive constant. The K–S operator is defined by its effect on an arbitrary vector in the Banach space

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$$zKf = \begin{pmatrix} f_1'(\mathbf{x}_1) \\ \cdot \\ \cdot \\ \cdot \\ f_N'(\{\mathbf{x}_N\}) \end{pmatrix},$$

$$f_1'(\mathbf{x}_1) = z\left(\sum_{n=1}^{\infty} \frac{1}{n!} \int fn(\mathbf{x}_2 \cdots \mathbf{x}_{n+1}) \prod_{j=2}^{n+1} f_{1j} d\mathbf{x}_j\right),$$

$$f_N'(\mathbf{x}_1 \cdots \mathbf{x}_N) = z \prod_{j=2}^{N} (1 + f_{1j}) \left(f_{N-1}(\mathbf{x}_2 \cdots \mathbf{x}_N) + \sum_{n=1}^{\infty} \frac{1}{n!} \int f_{n+N-1}(\mathbf{x}_2 \cdots \mathbf{x}_{n+N}) \prod_{j=N+1}^{N+n} f_{1j} d\mathbf{x}_j\right). \quad \text{(II. 2)}$$

Employing definition (II. 2), we can write (II. 1) as

$$\rho = z + zK\rho, \quad \text{(II. 3)}$$

where

$$\rho = \begin{pmatrix} \rho_1(\mathbf{x}_1) \\ \cdot \\ \cdot \\ \cdot \\ \rho_N(\{\mathbf{x}_N\}) \end{pmatrix}$$

is the vector of N particle distribution functions.

From their definition we usually understand that the N particle distribution functions are invariant under the interchange of particles. Arbitrary vectors in the Banach space, however, need not have this property. Consequently, the Kirkwood–Salsburg operator must be specified with more care. The first term in each of the sums of the right-hand side of Eq. (II. 2) is of the form

$$\int f_N(\mathbf{x}_2 \cdots \mathbf{x}_{N+1}) f_{1,N+1} d\mathbf{x}_{N+1}.$$

These terms can be considered as operators which, in addition to the integration with a kernel $f_{1,N+1}$, replace particle 1 by particle $N + 1$. They will be written as

$$\int f_N(\mathbf{x}_{N+1}, \mathbf{x}_2 \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}.$$

Terms with kernels which are constructed from products of two or more f_{ij} will be considered as operators which replace particle i with $i + 1$:

$$\theta f_N(\mathbf{x}_1 \cdots \mathbf{x}_N) = \int f_{1,N} f_{1,N+1} f_N(\mathbf{x}_2 \cdots \mathbf{x}_N, \mathbf{x}_{N+1}) d\mathbf{x}_N d\mathbf{x}_{N+1}.$$

Due to the symmetry of the distribution functions under particle interchange they will be a solution of Eq. (II. 3) with the above modifications.

K is clearly a linear operator. By generally following Ruelle, a bound for the norm of zK can be obtained as follows

$$\sup_{\forall\{x_N\}} |f_N'(\mathbf{x}_1 \cdots \mathbf{x}_N)| \leq |z| e^{2\beta BN} \left[\sup_{\forall\{x_{N-1}\}} |f_{N-1}(\mathbf{x}_2 \cdots \mathbf{x}_N)| \frac{S^{N-1}}{S^{N-1}} + \sum_{n=1}^{\infty} \frac{1}{n!} \sup_{\forall\{x_{N+n-1}\}} |f_{N+n-1}(\mathbf{x}_2 \cdots \mathbf{x}_{N+n})| C(\beta)|^n \frac{S^{N+n-1}}{S^{N+n-1}}\right],$$

$$\sup_{\forall\{x_N\}} \frac{|f_N'(\mathbf{x}_1 \cdots \mathbf{x}_N)|}{S^N} \leq |z| e^{2\beta BN} \|f\| \exp\frac{[C(\beta)S]}{S}.$$

The term $e^{2\beta BN}$ is obtained by bounding:

$$\prod_{j=2}^{N} (1 + f_{1j}) = \exp\left(-\beta \sum_{j=2}^{N} \phi(\mathbf{x}_i - \mathbf{x}_j)\right) \leq \exp\left(-\beta \inf_{\substack{\forall\{x_i\} \\ \forall\{x_j\}}} \sum_{j=1}^{N} \sum_{i=1}^{N} \phi(\mathbf{x}_i - \mathbf{x}_j)\right) \leq \exp[-2\beta U_N(\mathbf{x}_1 \cdots \mathbf{x}_N)] \leq \exp(2\beta BN). \quad \text{(II. 4)}$$

For positive potentials $B = 0$ and zK is bounded. If the potential has an attractive part, Eq. (II. 4) becomes infinite as $N \to \infty$.

For $B \neq 0$ the operator cannot be bounded in this manner. Ruelle[5] avoided this difficulty by defining a permutation operator π which permutes particle 1 with that particle which makes

$$\prod_{j \neq i}^{N} (1 + f_{ij}) < e^{2\beta B}.$$

By virtue of their symmetry under particle interchange the distribution functions will also satisfy.

$$\rho = z + z\pi K\rho.$$

In addition to the disadvantages of the series expansion mentioned in Sec. I, the permutation operator employed by Ruelle complicates the equation in such a way that its utility for numerical computation is greatly reduced.

We avoid the divergence of Eq. (II. 4) by limiting the class of potentials considered to those which satisfy

$$\phi(|\mathbf{x}|) = \infty, \quad |\mathbf{x}| < \sigma,$$

$$\phi(|\mathbf{x}|) = 0, \quad |\mathbf{x}| < a, \; a > \sigma.$$

This class, of course, includes repulsive potentials.

We take advantage of this restriction by multiplying the Kirkwood–Salsburg operator by a projection operator

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & P_2(\mathbf{x}_2, \mathbf{x}_3) & 0 & \cdots \\ 0 & 0 & 0 & P_3(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) & \cdots \end{pmatrix},$$

where

$$P_N = 1 \quad \text{for } |\mathbf{x}_i - \mathbf{x}_j| > \sigma,$$

$$\forall i_j j \in \{\mathbf{x}_N\}, \; i \neq j,$$

$$P_N = 0 \quad \text{if } |\mathbf{x}_i - \mathbf{x}_j| < \sigma$$

for some i and $j \in \{\mathbf{x}_N\}$, $i \neq j$.

Since the distribution functions are symmetric under particle interchange, they will also be solutions of

$$\rho = z + zPK\rho$$

with these modifications

$$P_N \prod_{j=2}^{N} (1 + f_{1j}) = P_N \exp\left(-\beta \sum_{j=2}^{N} \phi(\mathbf{x}_1 - \mathbf{x}_j)\right) \leq e^{2\beta B'}. \quad \text{(II. 5)}$$

The role of P_N is to insure that in a finite region of space there can be only a finite number of particles. The finite range of the potentials considered limits the volume within which a particle can have a nonzero interaction with particle 1. Therefore the sum

$$\sum_{j=2}^{N} \phi(\mathbf{x}_1 - \mathbf{x}_j)$$

in the exponential of (II. 5) will truncate at a finite $N = N_0$ and will be finite.

The modified K–S operator has a norm bounded by

$$\| zPK \| \leq e 2\beta B'/\exp[C(\beta)S]/S.$$

The value of B' depends on the details of the potential. The relationship between B' and the B of Ruelle is also potential dependent. It is clear, however, that

$$B' \geq B$$

and that, for potentials for which the lower bound for the energy per particle is achieved in the close packed configuration,

$$B' = B.$$

III. PERTURBATION SERIES SOLUTION

The K–S operator (II. 2) can be written as the sum of two operators. Including the projection operator P, we define

$$zPK' \begin{pmatrix} f_1(\mathbf{x}_1) \\ \cdot \\ \cdot \\ \cdot \\ f_N(\{\mathbf{x}_N\}) \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = zP \begin{pmatrix} 0 \\ (1 + f_{12}) f_1(\mathbf{x}_2) \\ \cdot \\ \cdot \\ \prod_{j=2}^{N} (1 + f_{1j}) f_{N-1}(\mathbf{x}_2 \ldots \mathbf{x}_N) \end{pmatrix}, \tag{III. 1}$$

$$zPK_0 \begin{pmatrix} f_1(\mathbf{x}_1) \\ \cdot \\ \cdot \\ \cdot \\ f_N(\{\mathbf{x}_N\}) \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} = zP \begin{pmatrix} f'_1(\mathbf{x}_1) \\ \cdot \\ \cdot \\ \cdot \\ f'_N(\{\mathbf{x}_N\}) \\ \cdot \\ \cdot \\ \cdot \end{pmatrix},$$

$$f'_1(\mathbf{x}_1) = \sum_{n=1}^{\infty} \frac{1}{n!} \int fn(\mathbf{x}_2 \ldots \mathbf{x}_{n+1}) \prod_{j=2}^{n} f_{1j} d\mathbf{x}_j,$$

$$f'_N(\mathbf{x}_1 \ldots \mathbf{x}_N) = \prod_{j=2}^{N} (1 + f_{1j}) \left(\sum_{n=1}^{\infty} \frac{1}{n!} \int f_{N+n-1}(\mathbf{x}_2 \ldots \mathbf{x}_{N+n}) \prod_{j=N+1}^{N+n} f_{1j} d\mathbf{x}_j \right),$$

$$f'' = zPKf = zPK_0 f + zPK' f.$$

The contribution to $f''_N(\mathbf{x}_N)$ from $zPK'f$ is

$$ZP_N \prod_{j=1}^{N} (1 + f_{1j}) f_{N-1}(\mathbf{x}_2 \ldots \mathbf{x}_N). \tag{III. 2}$$

Outside of a finite range, small in comparison to the remainder of configuration space,

$$\prod_{j=2}^{N} (1 + f_{1j}) = 1.$$

In addition $f_{N-1}(\mathbf{x}_2 \ldots \mathbf{x}_N)$ is only defined over a subspace of the N particle configuration space. These considerations suggest that the contribution of (III. 2) to $f_N''(\mathbf{x}_N)$ is small compared to the contribution of $zPK_0 f$ and that zPK' might be treated as a perturbation.

Multiplying zPK' by an arbitrary perturbation parameter ϵ gives

$$\rho = z + zPK_0 f + \epsilon zPK' f. \tag{III. 3}$$

We assume that ρ can be expanded in a power series in ϵ,

$$\rho = \sum_{n=0}^{\infty} \epsilon^n \phi_n. \tag{III. 4}$$

Inserting (III. 4) in (III. 3) and equating powers of ϵ gives the recursion relation

$$\begin{aligned} \phi_0 &= z + zPK_0 \phi_0, \\ \phi_N &= zPK' \phi_{N-1} + zPK_0 \phi_N. \end{aligned} \tag{III. 5}$$

Equation (III. 4) will be a solution of the K–S equation if each of the equations of (III. 5) has a solution and the expansion (III. 4) is uniformly convergent for $\epsilon \leq 1$.

Satisfaction of the first condition can be guaranteed[6] if

$$\| zPK_0 \| < 1.$$

Since

$$\begin{aligned} \| zPK_0 \| &\leq |z| \| P \| \| K_0 \| \\ &\leq |z| \| K_0 \| \end{aligned}$$

and $\| K_0 \|$ can be bound by the same procedure outlined in Sect. II to bound the entire Kirkwood–Salsburg operator,

$$\| zPK_0 \| \leq |z| e^{\beta B^1} \{\exp[C(\beta)S] - 1\}/S. \tag{III. 6}$$

Choosing

$$S = C(\beta)^{-1},$$

$$\| zPK_0 \| \leq |z| e^{\beta B^1} (e - 1) C(\beta).$$

Restricting z so that

$$|z| < [e^{\beta B^1} (e - 1) C(\beta)]^{-1}, \tag{III. 7}$$

we find that each of the equations of (III. 5) has a unique solution. From (III. 5)

$$\phi_0 = (1 - zPK_0)^{-1} z,$$

$$\phi_N = [(1 - zPK_0)^{-1} zPK']^N \phi_0.$$

The second condition will be satisfied[6] if

$$\| (1 - zPK_0)^{-1} zPK' \| < 1.$$

We assume z satisfies (III. 7). Expanding and taking the norm of both sides, we have

$$\begin{aligned} \| (1 - zPK_0)^{-1} \| &= \| \sum_{n=0}^{\infty} (zPK_0)^n \| \\ &\leq \sum_{n=0}^{\infty} \| zPK_0 \|^n \\ &\leq 1/(1 - \| zPK_0 \|). \end{aligned}$$

Therefore,

$$\|(1 - zPK_0)^{-1}\| \leq 1/[1 - |z| e^{\beta B^1}(e-1)C(\beta)].$$

$\|zPK'\|$ can be bounded by noting that if for an arbitrary vector ϕ

$$\sup_{\substack{\forall i \\ \forall\{x_i\}}} \frac{|\phi_i(\mathbf{x}_1 \ldots \mathbf{x}_i)|}{S_i} = \sup_{\forall\{x_i\}} \frac{|\phi_{i0}(\mathbf{x}_1 \ldots \mathbf{x}_{i0})|}{S^{i0}},$$

then

$$\sup_{\substack{\forall i \\ \forall\{x_i\}}} \frac{|P_i \prod_{j=2}^{i} (1 + f_{1j})\, \phi_{i-1}(\mathbf{x}_2 \ldots \mathbf{x}_i)|}{S^i} < \sup_{\forall\{x_i\}} e^{\beta B'} \frac{|\phi_{i0}(\mathbf{x}_2 \ldots \mathbf{x}_{i0+1})|}{S^{i0+1}}.$$

Therefore,

$$\|zPK'\| \leq |z| e^{\beta B'}/S = |z| e^{\beta B'} C(\beta).$$

Since

$$\|AB\| \leq \|A\|\, \|B\|,$$

for the second condition to be satisfied,

$$\frac{|z| e^{\beta B'} C(\beta)}{1 - |z| e^{\beta B^1}(e-1)C(\beta)} < 1$$

or

$$|z| < (e^{\beta B'} e C(\beta))^{-1},$$

which is consistent with (III. 7).

Therefore the only solution to the K–S equation for

$$|z| < (e^{(\beta B'+1)} C(\beta))^{-1}$$

can be written as

$$\rho = \sum_{N=0}^{\infty} \left[(1 - zPK_0)^{-1} zPK'\right]^N (1 - zPK_0)^{-1} z.$$

IV. THE STRIP OPERATOR APPROXIMATION

The perturbation series solution defined in the previous section leads very naturally to the definition of an approximate hierarchy. The components of the solution vector of this hierarchy are the first nonzero perturbation corrections to the corresponding distribution functions.

To derive this approximate hierarchy, one must note that for the range of z we are considering

$$|z| < [\exp(\beta B' + 1) C(\beta)]^{-1}$$

operators of the form

$$zP_N \prod_{j=2}^{N} (1 + f_{1j}) \int \rho_N(\mathbf{x}_{N+1}, \mathbf{x}_2 \ldots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}$$

have a norm less than 1.

This coupled with Eq. (III. 6) allows us to construct the solution to

$$\phi_0 = z + zPK_0\phi_0$$

by requiring that all components of ϕ_0 except the first are 0; and the first component satisfies

$$\rho_{1s} = z + z \int \rho_{1s}(\mathbf{x}_2) f_{12} d\mathbf{x}_2. \tag{IV. 1}$$

The same procedure can be used to solve

$$\phi_1 = zPK'\phi_0 + zPK_0\phi_1.$$

We demand that all components of the solution vector except the first two be zero and that they satisfy

$$\rho_{1s1}(\mathbf{x}_1) = z \int \rho_{1s1}(\mathbf{x}_2) f_{12} d\mathbf{x}_2 + z \int \rho_{2s}(\mathbf{x}_2, \mathbf{x}_3) f_{i2} f_{13} d\mathbf{x}_2 d\mathbf{x}_3,$$

$$\rho_{2s}(\mathbf{x}_1, \mathbf{x}_2) = z(1 + f_{12})\left(\rho_{1s}(\mathbf{x}_2) + \int \rho_{2s}(\mathbf{x}_3, \mathbf{x}_2) f_{13} d\mathbf{x}_3\right). \tag{IV. 2}$$

This procedure can be continued to all orders of the perturbation expansion.

Two points can be made about the above 'solution' to the K–S hierarchy. First: ρ_{1s} and ρ_{2s} could have been obtained by simply solving the pair of equations

$$\rho_{1s}(\mathbf{x}_1) = z + z \int \rho_{1s}(\mathbf{x}_2) f_{12} d\mathbf{x}_2,$$

$$\rho_{2s}(\mathbf{x}_1, \mathbf{x}_2) = z(1 + f_{12})\left(\rho_{1s}(\mathbf{x}_2) + \int \rho_{2s}(\mathbf{x}_3, \mathbf{x}_2) f_{13} d\mathbf{x}_3\right).$$

If in fact the procedure of (IV. 1) and (IV. 2) is continued, it is clear that the first nonzero contribution from the perturbation expansion to any of the distribution functions can be obtained by solving the approximate hierarchy:

$$\rho_{1s}(\mathbf{x}_1) = z + z \int \rho_{1s}(\mathbf{x}_2) f_{12} d\mathbf{x}_2,$$

$$\rho_{Ns}(\mathbf{x}_1 \ldots \mathbf{x}_N) = z \prod_{j=2}^{N} (1 + f_{1j}) P_N\left(\rho_{(N-1)s}(\mathbf{x}_2 \ldots \mathbf{x}_N) + \int \rho_{Ns}(\mathbf{x}_{N+1}, \mathbf{x}_2 \ldots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}\right). \tag{IV. 3}$$

We call this approximation the strip operator hierarchy. It is identical to the first covering sphere approximation of Sabry.[2]

The second point we wish to make can be illustrated by solving Eqs. (IV. 1) and (IV. 2). The solution of Eq. (IV. 2) is obtained by solving

$$\rho_{2s}(\mathbf{x}_1, \mathbf{x}_2) = z(1 + f_{12})\left(\rho_{1s}(\mathbf{x}_2) + \int \rho_{2s}(\mathbf{x}_3, \mathbf{x}_2) f_{13} d\mathbf{x}_3\right), \tag{IV. 4}$$

inserting $\rho_{2s}(\mathbf{x}_1, \mathbf{x}_2)$ in

$$\rho_{1s_1}(\bar{\mathbf{x}}_1) = z \int \rho_{2s}(\mathbf{x}_2, \mathbf{x}_3) f_{12} f_{13} d\mathbf{x}_2 d\mathbf{x}_3 + z \int \rho_{1s_1}(\mathbf{x}_2) f_{12} d\mathbf{x}_2, \tag{IV. 5}$$

and solving. Equation (IV. 5), which gives the second order peturbation expansion contribution to the single particle distribution function, is quite similar to Eq. (IV. 1) which gives the first order contribution. They are similar in that (IV. 1) and (IV. 5) are integral equations of the same form with identical kernels but different inhomogeneous terms.

In general any contribution to the Nth distribution function is obtained by solving an equation of a form identical to the Nth equation in (IV. 3) except for the inhomogeneous term.

The significance of this lies in the fact that certain properties of the solution of an integral equation depend entirely on the kernel and others are strongly influenced by it. Consequently, each term in the perturbation expansion for $\rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N)$ will have particular properties in common with contributions to $\rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N)$ of all orders and therefore with $\rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N)$

In the remaining sections of this paper we will investigate some of the properties of the solutions to the strip operator hierarchy. In this way we will obtain information about the integral equations whose solutions generate the distribution functions.

V. PRODUCT PROPERTY

The first property of the solutions to the strip operator (S-O) hierarchy that we will investigate is its behaviour when clusters of particles are separated by large distances.

The question is complicated by the fact that the three particle, and higher, S-O distribution functions are not symmetric under interchange of particles. An outline of a proof of this statement follows.

We have

$$\rho_s = z + zPK_s\rho_s \tag{V.1}$$

where ρ_s is the vector of solutions to the S-O hierarchy and K_s is the strip operator. By a method identical to that employed in Sec. II

$$\|zPK_s\| < 1$$

for

$$|z| < (\exp[\beta B' + 1]C(\beta))^{-1}.$$

This guarantees that (V.1) has a unique solution which can be written as

$$\rho_s = \sum_{n=0}^{\infty} [zPK_s]^n z.$$

Performing the indicated operations generates[7] a power series in z for each distribution function. It can be seen by inspection that the fourth iteration generates a term for $\rho_{3s}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ which is not symmetric under particle interchange. By virtue of the independence of the terms in the generated power series $\rho_{3s}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ is not symmetric under particle interchange. Further iterations indicate the same for $\rho_{4s}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4)$ and higher order functions.

This complication forces us to be more precise in the definition of

$$\rho_{Ns}(\mathbf{x}_{i1} \ldots \mathbf{x}_{iN}).$$

$\rho_{Ns}(\mathbf{x}_{i1} \ldots \mathbf{x}_{iN})$ is defined as the solution of Eq. (IV.3) with the variable dependence altered by the permutation operator

$$\prod_{1,2,\ldots N}^{i_1 \ldots i_N}.$$

We are now in a position to prove the following.

Theorem: For

$$|z| < [\exp(\beta B' + 1)C(\beta)]^{-1}, \tag{V.2}$$

$$\rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N) \to \rho_s(\mathbf{x}_1, \mathbf{x}_i \ldots \mathbf{x}_s)\rho_\phi(\mathbf{x}_\alpha, \mathbf{x}_\beta \ldots \mathbf{x}_\phi)$$

whenever

$$\min_{\substack{\forall_i \in \{x_s\} \\ \forall \beta \in \{x_\phi\}}} |\mathbf{x}_i - \mathbf{x}_\beta| = R \to \infty,$$

where

$$\{\mathbf{x}_s\} \oplus \{\mathbf{x}_\phi\} = \{\mathbf{x}_N\}.$$

Proof: It is always assumed that particle 1 is in $\{\mathbf{x}_s\}$. The proof proceeds by induction.

The function $\rho_1(\mathbf{x}_1)$ is a constant for the range of z considered and therefore trivially has the required behaviour which is called the product property. For an arbitrary N

$$\lim_{R\to\infty} (\{\mathbf{x}_s\} \oplus \{\mathbf{x}_\phi\}) = z \lim_{R\to\infty} P_N \lim_{R\to\infty} \prod_{j=2}^{N} (1 + f_{1j})$$
$$\otimes \Big(\lim_{R\to\infty} \rho_{N-1}(\mathbf{x}_2 \ldots \mathbf{x}_N)$$
$$+ \lim_{R\to\infty} \int \rho_N(\mathbf{x}_{N+1}, \mathbf{x}_2 \ldots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1} \Big).$$

$\rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N)$ is a bounded function and $\otimes$ is meant to signify simple multiplication. Therefore the integral

$$\int \rho_N(\mathbf{x}_{N+1}, \mathbf{x}_2 \ldots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}$$

is uniformly convergent. Assuming that $\rho_{N-1}(\mathbf{x}_2 \ldots \mathbf{x}_N)$ has the product property (V.2), we have

$$\lim_{R\to\infty} \rho_N(\{\mathbf{x}_s\} \oplus \{\mathbf{x}_\phi\}) = zP_sP_{\phi+1} \prod_{j\in\{x_s-1\}}^{s} (1 + f_{1j})$$
$$\otimes \Big(\rho_\phi\{\mathbf{x}_\phi\}\rho_{s-1}\{\mathbf{x}_{s-1}\}$$
$$+ \int \lim_{R\to\infty} \rho_N(\mathbf{x}_{N+1}, \mathbf{x}_2 \ldots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1} \Big) \tag{V.3}$$

where $\{\mathbf{x}_s - 1\}$ refers to the set $\{\mathbf{x}_s\}$ with particle 1 removed and $P_{\phi+1}$ will be zero if any of the particles $\{\mathbf{x}_\phi\}$ are closer together than a hard core diameter.

(V.3) can be rewritten as

$$(I - \theta) \lim_{R\to\infty} \rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N)$$
$$= zP_sP_{\phi+1} \prod_{j\in\{x_s-1\}}^{s} (1 + f_{1j})\rho_\phi(\{\mathbf{x}_\phi\})\rho_{s-1}(\{\mathbf{x}_{s-1}\})$$

where

$$\theta\psi(\mathbf{x}_1 \ldots \mathbf{x}_N) = zP_sP_{\phi+1} \prod_{j\in\{x_{s-1}\}}^{s} (1 + f_{1j})$$
$$\int f_{1,N+1}\psi(\mathbf{x}_{N+1}, \mathbf{x}_2 \ldots \mathbf{x}_N) d\mathbf{x}_{N+1}.$$

In the range of z considered

$$\|\theta\| < 1$$

so that

$$\lim_{R\to\infty} \rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N)$$
$$= zP_sP_{\phi+1}\rho_\phi\{\mathbf{x}_\phi\}\rho_{s-1}\{\mathbf{x}_{s-1}\} (1 - \theta)^{-1} \prod_{j\in\{x_{s-1}\}}^{s} (1 + f_{1j}).$$

But

$$zP_s\rho_{s-1}\{\mathbf{x}_{s-1}\} (1 - \theta)^{-1} \prod_{j\in\{x_{s-1}\}}^{s} (1 + f_{1j}) = \rho_s\{\mathbf{x}_s\}$$

and

$$\rho_{\phi+1}\rho_{\phi}\{\mathbf{x}_{\phi}\} = \rho_{\phi}\{\mathbf{x}_{\phi}\}.$$

Therefore

$$\lim_{R\to\infty} \rho_N(\mathbf{x}_1 \ldots \mathbf{x}_N) = \rho_{\phi}\{\mathbf{x}_{\phi}\}\rho_s\{\mathbf{x}_s\}.$$

VI. LONG RANGE BEHAVIOR OF S-O DISTRIBUTION FUNCTIONS

Having determined that the solutions to the S–O hierarchy have the product property, we are in a position to investigate the long range behavior of the distribution functions. To be more precise, we know that, in the limit as $R \to \infty$,

$$\lim_{R\to\infty} \rho_N(\{\mathbf{x}_s\} \oplus \{\mathbf{x}_{\phi}\}) \to \rho_s\{\mathbf{x}_s\}\rho_{\phi}\{\mathbf{x}_{\phi}\} + C_N(\{\mathbf{x}_N\}),$$

$$\lim_{R\to\infty} C_N(\{\mathbf{x}_N\}) \to 0,$$

and we are interested in the form of $C_N(\{\mathbf{x}_N\})$.

We will prove the following.

Theorem: For

$$|z| < (\exp(\beta B' + 1)C(\beta))^{-1}$$

and strictly finite range interactions

$$\lim_{R\to\infty} \rho_N(\{\mathbf{x}_s\} \oplus \{\mathbf{x}_{\phi}\}) = \rho_s\{\mathbf{x}_s\}\rho_{\phi}\{\mathbf{x}_{\phi}\} + O\left(\frac{A_{\alpha_0} e^{iK_{\alpha_0}R}}{R}\right).$$

K_{α_0} is the root with the smalles positive imaginary part of

$$1 - z\hat{f}(\mathbf{K}, \beta),$$

$$\hat{f}(\mathbf{K}, \beta) = \int e^{-i\mathbf{K}\cdot\mathbf{x}} f(\mathbf{x}) d\mathbf{x} \equiv \hat{f}(\mathbf{K}).$$

A_{α_0} is a number dependent upon $\mathbf{K}_{\alpha_0}$ but not R.

The proof proceeds by induction. Since $\rho_1(\mathbf{x}_1)$ plays no part in the analysis we start by proving $\rho_2(\mathbf{x}_1, \mathbf{x}_2)$ has the required property.

In the relevant range for $|z|$ the distribution functions depend on the distances between particles. Consequently

$$\rho_1(\mathbf{x}_1) = z/[1 - z\hat{f}(0)] = \rho.$$

Dividing both sides of

$$\rho_2(\mathbf{x}_1, \mathbf{x}_2) = z(1 + f_{12})\left(\rho + \int \rho_2(\mathbf{x}_3, \mathbf{x}_2) f_{13} d\mathbf{x}_3\right) \tag{VI. 1}$$

by $(1 + f_{12})$, we obtain

$$\rho_2'(\mathbf{x}_1, \mathbf{x}_2) = z\left(\rho + \int \rho_2(\mathbf{x}_3, \mathbf{x}_2) f_{13} d\mathbf{x}_3\right). \tag{VI. 2}$$

Since we have restricted the allowable potentials to finite range interactions, we can define

$$\begin{aligned} \rho_2'(\mathbf{x}_1, \mathbf{x}_2) &= \rho_{2I}'(\mathbf{x}_1, \mathbf{x}_2) + \rho_{20}'(\mathbf{x}_1, \mathbf{x}_2), \\ \rho_2(\mathbf{x}_1, \mathbf{x}_2) &= \rho_{2I}(\mathbf{x}_1, \mathbf{x}_2) + \rho_{20}(\mathbf{x}_1, \mathbf{x}_2), \end{aligned} \tag{VI. 3}$$

where

$$\begin{aligned} \rho_{2I}(\mathbf{x}_1, \mathbf{x}_2) = \rho_{2I}'(\mathbf{x}_1, \mathbf{x}_2) = 0, \quad |\mathbf{x}_1 - \mathbf{x}_2| \geq a, \\ \rho_{20}(\mathbf{x}_1, \mathbf{x}_2) = \rho_{20}'(\mathbf{x}_1, \mathbf{x}_2) = 0, \quad |\mathbf{x}_1 - \mathbf{x}_2| < a. \end{aligned}$$

Clearly

$$\rho_{20}(\mathbf{x}_1, \mathbf{x}_2) = \rho_{20}'(\mathbf{x}_1, \mathbf{x}_2).$$

Substituting (VI. 3) into (VI. 2), taking the Fourier transform with respect to $\mathbf{x}_1$, and employing the convolution theorem, we obtain

$$\hat{\rho}_{20}(K) = \frac{z\rho\delta(\mathbf{K})}{1 - z\hat{f}(\mathbf{K})} - \frac{\hat{\rho}_{2I}'(\mathbf{K})}{1 - z\hat{f}(\mathbf{K})} + \frac{\rho_{2I}(\mathbf{K}) z\hat{f}(\mathbf{K})}{1 - z\hat{f}(\mathbf{K})}.$$

Writing

$$1/[1 - z\hat{f}(\mathbf{K})] = 1 + z\hat{f}(\mathbf{K})/[1 - z\hat{f}(\mathbf{K})]$$

and taking the inverse Fourier transform, we have

$$\begin{aligned} \rho_{20}(\mathbf{x}_1, \mathbf{x}_2) &= \frac{z\rho}{1 - z\hat{f}(0)} \\ &\quad - \rho_{2I}'(\mathbf{x}_1, \mathbf{x}_2) + \int G(\mathbf{x}_3, \mathbf{x}_2) F(\mathbf{x}_1 - \mathbf{x}_3) d\mathbf{x}_3, \end{aligned} \tag{VI. 4}$$

$$G(\mathbf{x}_3, \mathbf{x}_2) = \rho_{2I}(\mathbf{x}_3, \mathbf{x}_2) - \rho_{2I}'(\mathbf{x}_3, \mathbf{x}_2),$$

$$\begin{aligned} F(\mathbf{x}_1 - \mathbf{x}_3) &= \int \frac{e^{i\mathbf{K}\cdot(\mathbf{x}_1 - \mathbf{x}_3)} z\hat{f}(\mathbf{K})}{1 - z\hat{f}(\mathbf{K})} d(\mathbf{K}) \\ &= zf(\mathbf{x}_1 - \mathbf{x}_3) + \int \frac{e^{i\mathbf{K}\cdot(\mathbf{x}_1 - \mathbf{x}_3)} z(\hat{f}(\mathbf{K}))^2}{1 - z\hat{f}(\mathbf{K})} d(\mathbf{K}) \\ &= zf(\mathbf{x}_1 - \mathbf{x}_3) + F'(\mathbf{x}_1 - \mathbf{x}_3). \end{aligned} \tag{VI. 5}$$

Taking the limit as $|\mathbf{x}_{12}| \to \infty$ of (VI. 4) and inverting the order of limit and integration[8] gives

$$\begin{aligned} \lim_{|\mathbf{x}_{12}|\to\infty} \rho_{20}(|\mathbf{x}_{12}|) &= \frac{z\rho}{1 - z\hat{f}(0)} \\ &\quad + \int G(|\mathbf{x}_{23}|) \lim_{|\mathbf{x}_{12}|\to\infty} f(|\mathbf{x}_{12} - \mathbf{x}_{23}|) d\mathbf{x}_{23} \\ &\quad + \int G(|\mathbf{x}_{23}|) \lim_{|\mathbf{x}_{12}|\to\infty} F'(|\mathbf{x}_{12} - \mathbf{x}_{23}|) d\mathbf{x}_{23}, \end{aligned} \tag{VI. 6}$$

where the dependence of ρ_{20}, G, f, and F' on only the distance between particles has been made explicit.

If the required integral in (VI. 5) is performed in the complex K plane on a semi-circular contour closed in the upper half-plane,[8] then

$$\lim_{|\mathbf{x}_{12}|\to\infty} F'(|\mathbf{x}_{12} - \mathbf{x}_{23}|) = \sum_{\alpha} A_{\alpha} \lim_{|\mathbf{x}_{12}|\to\infty} \frac{e^{iK_{\alpha}|\mathbf{x}_{12} - \mathbf{x}_{23}|}}{|\mathbf{x}_{12} - \mathbf{x}_{23}|}.$$

K_{α} are the roots of $1 - z\hat{f}(\mathbf{K})$ and $A_{\alpha} e^{iK_{\alpha}|\mathbf{x}_{12} - \mathbf{x}_{23}|}$ is the residue at K_{α}.

Returning to (VI. 6), $G(|\mathbf{x}_{23}|)$ demands that

$$|\mathbf{x}_{23}| < a$$

so that

$$\lim_{|\mathbf{x}_{12}|\to\infty} (|\mathbf{x}_{12} - \mathbf{x}_{23}|) \to |\mathbf{x}_{12}|,$$

$$\lim_{|\mathbf{x}_{12}|\to\infty} f(|\mathbf{x}_{12} - \mathbf{x}_{23}|) = 0.$$

Therefore

$$\begin{aligned} \lim_{|\mathbf{x}_{12}|\to\infty} \rho_{2_0}(|\mathbf{x}_{12}|) &= \frac{z\rho}{1 - z\hat{f}(0)} \\ &\quad + \sum_{\alpha_0} A_{\alpha_0} \left(\int G(|\mathbf{x}_{23}|) d\mathbf{x}_{23} \frac{e^{iK_0|\mathbf{x}_{12}|}}{|\mathbf{x}_{12}|}\right). \end{aligned}$$

K_{α_0} are those roots of

$$1 - z\hat{f}(\mathbf{K})$$

with the smallest positive imaginary parts. Since

$$\rho = z/[1 - z\hat{f}(0)],$$

$\rho_{2_s}(\mathbf{x}_1, \mathbf{x}_2)$ has the required property.

Assuming that $\rho_{(N-1)_s}(\mathbf{x}_1 \cdots \mathbf{x}_{N-1})$ also has the required property, we investigate the solution of

$$\rho_{N_s}(\mathbf{x}_1 \cdots \mathbf{x}_N) = zP_N \prod_{j=2}^{N} (1 + f_{1j}) \times \left(\rho_{(N-1)_s}(\mathbf{x}_2 \cdots \mathbf{x}_N) + \int \rho_{N_s}(\mathbf{x}_{N+1} \cdots \mathbf{x}_N) f_{1,N+1}\, d\mathbf{x}_{N+1}\right). \quad \text{(VI. 7)}$$

Before proceeding it will be useful to modify VI. 7 slightly. We define

$$\rho^P_{N_s}(\mathbf{x}_1 \cdots \mathbf{x}_N) = \frac{\rho_{N_s}(\mathbf{x}_1 \cdots \mathbf{x}_N)}{\rho_{(N-1)_s}(\mathbf{x}_2 \cdots \mathbf{x}_N)} \quad \text{(VI. 8)}$$

and divide particles 1 to N into the clusters

$$\{1, \alpha, \alpha + 1, \ldots, N\}, \quad \{2, 3, \ldots, \alpha\}.$$

(The generality of the argument is not affected by this arbitrary choice.) When the two clusters are separated by an infinite distance we know from the previous section that

$$\rho^P_{N_s}(\mathbf{x}_1 \cdots \mathbf{x}_N) \to \frac{\rho_{(\alpha-1)_s}(\mathbf{x}_2 \cdots \mathbf{x}_\alpha)\rho_{(N-\alpha+1)_s}(\mathbf{x}_1, \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N)}{\rho_{(\alpha-1)_s}(\mathbf{x}_2 \cdots \mathbf{x}_\alpha)\rho_{(N-\alpha)_s}(\mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N)} = \rho^P{}_{(N-\alpha+1)_s}(\mathbf{x}_1, \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N).$$

We can now define a function $C_N(\mathbf{x}_1 \cdots \mathbf{x}_N)$ by

$$\rho^P_{N_s}(\mathbf{x}_1 \cdots \mathbf{x}_N) = P_N \prod_{j=2}^{\alpha} (1 + f_{1j})\, \rho^p_{(N-\alpha+1)_s}(\mathbf{x}_1 \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N) + C_N(\mathbf{x}_1 \cdots \mathbf{x}_N). \quad \text{(VI. 9)}$$

Clearly if R is the minimum distance between the two clusters

$$\lim_{R\to\infty} C_N(\mathbf{x}_1 \cdots \mathbf{x}_N) \to 0.$$

From (VI. 7), (VI. 8), and (VI. 9),

$$C_N(\mathbf{x}_1 \cdots \mathbf{x}_N) + P_N \rho^P{}_{(N-\alpha+1)_s}(\mathbf{x}_1, \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N) \prod_{j=2}^{\alpha} (1 + f_{1j}) = zP_N \prod_{j=2}^{N} (1 + f_{1j}) \left(1 + \int C_N(\mathbf{x}_{N+1} \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1} + \int \prod_{j=2}^{\alpha} (1 + f_{j,N+1}) \times \rho^p_{(N-\alpha+1)_s}(\mathbf{x}_{N+1}, \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}\right).$$

Since

$$P_N \rho^p_{(N-\alpha+1)_s}(\mathbf{x}_1, \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N) = zP_N \prod_{j=\alpha+1}^{N} (1 + f_{1j}) \times (1 + \int \rho^p_{(N-\alpha+1)_s}(\mathbf{x}_{N+1}, \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}).$$

We have

$$C_N(\mathbf{x}_1 \cdots \mathbf{x}_N) = zP_N \prod_{j=2}^{N} (1 + f_{1j}) \int C_N(\mathbf{x}_{N+1} \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1} + zP_N \prod_{j=2}^{N} (1 + f_{1j}) \int \left(\prod_{j=2}^{\alpha} (1 + f_{N+1,j}) - 1\right) \times \rho^p_{(N-\alpha+1)_s}(\mathbf{x}_{N+1}, \mathbf{x}_\alpha \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}, \quad \text{(VI. 10)}$$

which is of the form

$$C = \alpha + KC.$$

The correspondence between the linear operator K, the unknown vector C, and the known inhomogeneous vector α and their counterparts in (VI. 10) is obvious.

The K operator can be written as the sum of two operators

$$K_0\psi = zP_N \prod_{j=2}^{\alpha} (1 + f_{1j}) \times \int \psi_N(\mathbf{x}_{N+1} \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}$$

$$K'\psi = zP_N \prod_{j=2}^{\alpha} (1 + f_{1j}) \left(\prod_{j=\alpha+1}^{N} (1 + f_{1j}) - 1\right) \times \int \psi_N(\mathbf{x}_{N+1} \cdots \mathbf{x}_N) f_{1,N+1} \otimes d\mathbf{x}_{N+1}. \quad \text{(VI. 11)}$$

The term $(\prod_{j=\alpha+1}^{N} (1 + f_{1j}) - 1)$ acts to restrict the range of K' so that its effect is small in comparison to that of K_0. We can, therefore, treat K' as a perturbation,

$$C = \alpha + K_0 C + \epsilon K' C.$$

With a procedure identical to that of Sec. III we find that for the indicated range of $|z|$

$$C = \sum_{n=0}^{\infty} \epsilon^n \phi_n,$$

$$\phi_0 = \alpha + K_0\phi_0, \quad \text{(VI. 12)}$$

$$\phi_N = K'\phi_{N-1} + K_0\phi_N,$$

which is uniformly convergent for $\epsilon \leqslant 1$ as long as

$$\|K'/(1 - K_0)\| < 1. \quad \text{(VI. 13)}$$

After performing the required manipulations, we find (VI. 13) to be valid as long as

$$|z| < (2 \exp(\beta B') C(\beta))^{-1} > (\exp(\beta B' + 1) C(\beta))^{-1}.$$

Since (VI. 12) is uniformly convergent, we can investigate the limit of $C_N(\mathbf{x}_1 \cdots \mathbf{x}_N)$ as $R \to \infty$ by taking the limit of each term of (VI. 12) and summing the limits.[9] In this spirit we state the following.

Theorem: For $|z| < [\exp(\beta B' + 1) C(\beta)]^{-1}$,

$$\lim_{R\to\infty} \phi_N(\mathbf{x}_1 \cdots \mathbf{x}_N) \to A^{(N)}_{\alpha} e^{iK_\alpha R}/R,$$

$A^{(N)}_{\alpha_0}$ depends on K_{α_0} and the interparticle distances of particles within the same cluster, but not on R.

Again the proof proceeds by induction:

$$\phi_0(\mathbf{x}_1 \cdots \mathbf{x}_N) = zP_N \prod_{j=2}^{\alpha} (1 + f_{1j}) \int \phi_0(\mathbf{x}_{N+1} \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1} + zP_N \prod_{j=2}^{N} (1 + f_{1j}) \int \left(\prod_{j=2}^{\alpha} (1 + f_{N+1,j}) - 1\right) \times \rho^p_{N-\alpha+1}(\mathbf{x}_{N+1}, \mathbf{x}_{\alpha+1} \cdots \mathbf{x}_N) \otimes f_{1,N+1} d\mathbf{x}_{N+1}. \quad \text{(VI. 14)}$$

Dividing by $\Pi_{j=2}^{\alpha}(1+f_{1j})$ and noting that $\phi_0(\mathbf{x}_1\ldots\mathbf{x}_N)=0$ when $\Pi_{j=2}^{\alpha}(1+f_{1j})=0$, we can write

$$\phi'_0(\mathbf{x}_1\ldots\mathbf{x}_N)=\frac{\phi_0(\mathbf{x}_1\ldots\mathbf{x}_N)}{\prod_{j=2}^{\alpha}(1+f_{1j})}. \tag{VI. 15}$$

By means of the following equations we can also define four functions $\phi_{0(0)}$, $\phi_{0(I)}$, $\phi'_{0(0)}$, $\phi'_{0(I)}$:

$$\phi'_0(\mathbf{x}_1\ldots\mathbf{x}_N)=\phi'_{0(0)}(\mathbf{x}_1\ldots\mathbf{x}_N)+\phi'_{0(I)}(\mathbf{x}_1\ldots\mathbf{x}_N),$$

$$\phi_0(\mathbf{x}_1\ldots\mathbf{x}_N)=\phi_{0(0)}(\mathbf{x}_1\ldots\mathbf{x}_N)+\phi_{0(I)}(\mathbf{x}_1\ldots\mathbf{x}_N),$$

$$\phi_{0(I)}(\mathbf{x}_1\ldots\mathbf{x}_N)=\phi'_{0(I)}(\mathbf{x}_1\ldots\mathbf{x}_N)=0, \tag{VI. 16}$$

if particle 1 is not within the potential range of at least one of the particles $\{2,3,\ldots,\alpha\}$,

$$\phi_{0(0)}(\mathbf{x}_1\ldots\mathbf{x}_N)=\phi'_0(\mathbf{x}_1\ldots\mathbf{x}_N)=0,$$

if particle 1 is within the potential range of one of the particles $\{2,3,\ldots,\alpha\}$, and

$$\phi_{0(0)}(\mathbf{x}_1\ldots\mathbf{x}_N)=\phi'_{0(0)}(\mathbf{x}_1\ldots\mathbf{x}_N).$$

Designating the inhomogeneous term in (VI. 14) by α employing definitions (VI. 15) and (VI. 16) and taking the Fourier transform of both sides with respect to $\mathbf{x}_1$ gives

$$\phi_{0(0)}(\mathbf{K},\mathbf{x}_2\ldots\mathbf{x}_N)=\frac{\hat{\alpha}zP_N\hat{f}(\mathbf{K})}{1-zP_N\hat{f}(\mathbf{K})}+\hat{\alpha}-\hat{\phi}'_{0(I)}(\mathbf{K},\mathbf{x}_2\ldots\mathbf{x}_N)$$
$$+\frac{zP_N\hat{f}(\mathbf{K})}{1-zP_N\hat{f}(\mathbf{K})}[\hat{\phi}_{0(I)}(\mathbf{K},\mathbf{x}_2\ldots\mathbf{x}_N)-\phi'_{0(I)}(\mathbf{K},\mathbf{x}_2\ldots\mathbf{x}_N)].$$

In this development $\mathbf{x}_2\ldots\mathbf{x}_N$ are variables, the value of which can be adjusted at will. Since it is clear that the solutions to the S-O equations are identically zero if any of the above set are closer together than a hard core diameter, we will exclude this possibility from consideration and set P_N equal to 1. There is no loss of generality in the argument.

Employing the identity

$$z\hat{f}(\mathbf{K})/[1-z\hat{f}(\mathbf{K})]=z\hat{f}(\mathbf{K})+z^2(\hat{f}(\mathbf{K}))^2/[1-z\hat{f}(\mathbf{K})],$$

taking the inverse Fourier transform and the limit as $R\to\infty$[8], we have

$$\lim_{R\to\infty}\phi_{0(0)}(\mathbf{x}_1\ldots\mathbf{x}_N)=\int\lim_{R\to\infty}\sum_{\alpha}\frac{B_\alpha e^{iK\alpha|\mathbf{x}_{1\nu}|}}{|\mathbf{x}_{1\nu}|}$$

Ⓐ

$$\times\Big[zP_N\prod_{j=\alpha+1}^{N}(1+f_{\nu j})\int\Big(\prod_{j=2}^{\alpha}(1+f_{N+1,j})-1\Big)\times\rho_{N-\alpha+1}(\mathbf{x}_{N+1},\mathbf{x}_{\alpha+1}\ldots\mathbf{x}_N)\int_{N+1,\nu}$$

Ⓑ (VI. 17)

$$\otimes d\mathbf{x}_{N+1}d\mathbf{x}_\nu+\int\lim_{R\to\infty}\sum_{\alpha}\frac{B_\alpha e^{iK\alpha|\mathbf{x}_{1\nu}|}}{|\mathbf{x}_{1\nu}|}\times\Big(\phi_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)-\phi'_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)\Big)d\mathbf{x}_\nu.$$

We have made use of

$$\lim_{R\to\infty}\phi'_{0(I)}(\mathbf{x}_1\ldots\mathbf{x}_N)=0,$$

$$\lim_{R\to\infty}\alpha=0,$$

$$\lim_{R\to\infty}\int f_{1,\nu}zP_N\prod_{j=\alpha+1}^{N}(1+f_{\nu j})\int\Big(\prod_{j=2}^{\alpha}(1+f_{N+1,j})-1\Big)\otimes\rho^{p}_{N-\alpha+1}(\mathbf{x}_{N+1},\mathbf{x}_{\alpha+1}\ldots\mathbf{x}_N)f_{N+1,\nu}d\mathbf{x}_{N+1}d\mathbf{x}_\nu=0,$$

$$\lim_{R\to\infty}\int f_{1,\nu}\Big(\phi_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)-\phi'_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)\Big)\otimes d\mathbf{x}_\nu=0.$$

In the limit as $R\to\infty$ of term Ⓐ of (VI. 17)

$$|\mathbf{x}_{1\nu}|\to R.$$

This is a consequence of the restrictions

$$f_{N+1,\nu}=0$$

unless ν is within the potential range of $N+1$, and

$$\prod_{j=2}^{\alpha}(1+f_{N+1,j})-1=0$$

unless $N+1$ is within the potential range of at least one of the particles of the cluster $\{2\ldots\alpha\}$. Therefore, particle ν is a finite distance from the cluster $\{2\ldots\alpha\}$ and hence a distance approximately equal to R from particle 1, for large R.

Term Ⓐ becomes

$$\lim_{R\to\infty}\sum_{\alpha_0}B_{\alpha_0}\frac{e^{iK\alpha_0R}}{R}\int zP_N\prod_{j=\alpha+1}^{N}(1+f_{\nu j})\times\int\Big(\prod_{j=2}^{\alpha}(1+f_{N+1,j})-1\Big)\otimes\rho\,\rho_{N-\alpha}(\mathbf{x}_{\alpha+1}\ldots\mathbf{x}_N)f_{N+1,\nu}d\mathbf{x}_{N+1,}d\mathbf{x}_\nu \tag{VI. 18}$$

plus terms which damp faster than $e^{iK\alpha_0R}/R$.

Since $[\phi_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)-\phi'_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)]$ restricts particle ν to the potential range of at least one of the particles in the set $\{2\ldots\alpha\}$, term B becomes

$$\lim_{R\to\infty}\sum_{\alpha_0}B_{\alpha_0}\frac{e^{iK_0R}}{R}\times\int\lim_{R\to\infty}\Big[\phi_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)-\phi'_{0(I)}(\mathbf{x}_\nu,\mathbf{x}_2\ldots\mathbf{x}_N)\Big]d\mathbf{x}_\nu$$

plus terms which damp faster than e^{iK_0R}/R.

Consequently,

$$\lim_{R\to\infty}\phi_0(\mathbf{x}_1\ldots\mathbf{x}_N)\to\sum_{\alpha_0}\lim_{R\to\infty}A^{(0)}_{\alpha_0}\frac{e^{iK\alpha_0R}}{R}.$$

$A^{(0)}_{\alpha_0}$ is a function of α_0 and distances between particles within the same cluster, but not R.

Assuming that $\phi_{(N-1)}(\mathbf{x}_1\ldots\mathbf{x}_N)$ has the required property, we investigate the large R limit of

$$\phi_N(\mathbf{x}_1\ldots\mathbf{x}_N)=zP_N\prod_{j=2}^{\alpha}(1+f_{1j})\times\int\phi_N(\mathbf{x}_{N+1}\ldots\mathbf{x}_N)f_{1,N+1}d\mathbf{x}_{N+1}$$

$$+ P_N \prod_{j=2}^{\alpha} (1 + f_{1j}) \left(\prod_{j=\alpha+1}^{N} (1 + f_{1j}) - 1 \right)$$

$$\times \int \phi_{N-1}(\mathbf{x}_{N+1} \cdots \mathbf{x}_N) f_{1,N+1} d\mathbf{x}_{N+1}.$$

With a procedure identical to that used for (VI. 14), we find

$$\lim_{R\to\infty} \phi_N(\mathbf{x}_1 \cdots \mathbf{x}_N) \to \sum_{\alpha_0} \lim_{R\to\infty} A^{(N)}_{K\alpha_0} \frac{e^{iK\alpha_0 R}}{R}$$

plus terms that damp faster than $e^{iK\alpha_0 R}/R$:

$$A^{(N)}_{K\alpha_0} = \int \lim_{R\to\infty} [\phi_{N(I)}(\mathbf{x}_{N+1}, \mathbf{x}_2 \cdots \mathbf{x}_N) - \phi'_{N(I)}(\mathbf{x}_{N+1}, \mathbf{x}_2 \cdots \mathbf{x}_N)] d\mathbf{x}_\nu + \int \left(\prod_{j=\alpha+1}^{N} (1 + f_{\nu,j}) - 1 \right) F(|\mathbf{x}_1 - \mathbf{x}_\nu|) \times \int A^{(N-1)}_{K\alpha_0} f_{\nu,N+1} d\mathbf{x}_{N+1} d\mathbf{x}_\nu.$$

As previously noted, the perturbation technique produces a uniformly convergent series.

Therefore,

$$\lim_{R\to\infty} C_N(\mathbf{x}_1 \cdots \mathbf{x}_N) \to \sum_N A^{(N)}_{K\alpha_0} \lim_{R\to\infty} \frac{e^{iK\alpha_0 R}}{R}. \quad \text{(VI. 19)}$$

Equations (VI. 19), (VI. 8), and (VI. 9) and the assumption that $\rho_{(N-1)_s}(\mathbf{x}_1 \cdots \mathbf{x}_{N-1})$ has the requisite property combine to produce the result

$$\lim_{R\to\infty} \rho_{N_s}(\{\mathbf{x}_\nu\} \oplus \{\mathbf{x}_T\}) \to \rho_{\nu_s}(\{\mathbf{x}_\nu\}) \rho_{T_s}(\{\mathbf{x}_T\}) + \sum_{\alpha_0} \lim_{R\to\infty} A_{\alpha_0} \frac{e^{iK\alpha_0 R}}{R}.$$

VII. PROPERTIES OF DERIVATIVES

In this section we investigate the properties of the derivatives of the S–O distribution function as a function of the interparticle distance R.

We restrict our considerations to hard sphere potentials, i.e.,

$$\phi(\mathbf{x}) = \infty, \quad \mathbf{x} < \sigma,$$
$$\phi(\mathbf{x}) = 0, \quad \mathbf{x} \geq \sigma.$$

Stillinger[10] has argued that the pair distribution function, in the fluid phase, is C^∞ in no interval on the real line. For the S–O pair function will prove that neither

$$\rho_{2_s}(\mathbf{x}_{12}) = z(1 + f_{12}) \left(\rho + \int \rho_{2_s}(\mathbf{x}_{23}) f_{13} d\mathbf{x}_3 \right) \quad \text{(VII. 1)}$$

or

$$\rho'_{2_s}(\mathbf{x}_{12}) = z \left[\rho + \int \rho_{2_s}(\mathbf{x}_{23}) f_{13} d\mathbf{x}_3 \right] \quad \text{(VII. 2)}$$

are C^∞ at integral multiples of the hard sphere diameter σ.

In what follows we will make use of the theory of generalized functions[11] or distributions.

If we differentiate both sides of (VII. 1) and interchange integration and differentiation,[15]

$$\frac{d\rho_{2_s}(\mathbf{x}_{12})}{d\mathbf{x}_{12}} = h\delta(\mathbf{x}_{12-1}) + z(1 + f_{12}) \int \frac{d\rho_{2_s}(\mathbf{x}_{23})}{d\mathbf{x}_{23}} \frac{d\mathbf{x}_{23}}{d\mathbf{x}_{12}} f_{13} d\mathbf{x}_{13},$$

$$h = \left[z \int \rho_{2_s}(\mathbf{x}_{23}) f_{13} d\mathbf{x}_3 + z\rho \right]_{\mathbf{x}_{12}=\sigma=1}.$$

Differentiating again

$$\frac{d^2\rho_{2s}(\mathbf{x}_{12})}{d\mathbf{x}_{12}^2} = h\delta'(\mathbf{x}_{12-1}) + zh\delta(\mathbf{x}_{12-1}) + z(1 + f_{12}) \int \frac{d\rho_{2s}(\mathbf{x}_{23})}{d\mathbf{x}_{23}} \otimes \frac{d\mathbf{x}_{23}^2}{d\mathbf{x}_{12}^2} f_{13} d\mathbf{x}_3 - z(1 + f_{12}) \times \int \frac{d\rho_{2s}(\mathbf{x}_{23})}{d\mathbf{x}_{23}} \frac{d\mathbf{x}_{23}}{d\mathbf{x}_{12}} \frac{d\mathbf{x}_{13}}{d\mathbf{x}_{12}} \delta(\mathbf{x}_{13} - 1) d\mathbf{x}_3. \quad \text{(VII. 3)}$$

If (VII. 2) is inserted in (VII. 3), it produces a term

$$-z(1 + f_{12}) \int \delta(\mathbf{x}_{23} - 1) \frac{d\mathbf{x}_{23}}{d\mathbf{x}_{12}} \frac{d\mathbf{x}_{13}}{d\mathbf{x}_{12}} \delta(\mathbf{x}_{13} - 1) d\mathbf{x}_3,$$

which has discontinuous behavior at $\mathbf{x}_{12} = 2$.

This can be proven by changing to bipolar coordinates and noting that

$$\frac{d\mathbf{x}_{23}}{d\mathbf{x}_{12}} \frac{d\mathbf{x}_{13}}{d\mathbf{x}_{12}} \frac{\mathbf{x}_{13}\mathbf{x}_{23}}{\mathbf{x}_{12}} = \left(\frac{(\mathbf{x}_{12} - (\mathbf{x}_{12}^2 + \mathbf{x}_{13}^2 - \mathbf{x}_{23}^2))(\mathbf{x}_{12} - (\mathbf{x}_{12}^2 + \mathbf{x}_{23}^2 - \mathbf{x}_{13}^2))}{\mathbf{x}_{12}^3} \right)$$

is infinitely differentiable as a function of $\mathbf{x}_{12}$ and $\mathbf{x}_{13}$ so that the integral

$$-2\pi \int \delta(\mathbf{x}_{23} - 1)\delta(\mathbf{x}_{13} - 1) \times \left(\frac{(\mathbf{x}_{12} - (\mathbf{x}_{12}^2 + \mathbf{x}_{13}^2 - \mathbf{x}_{23}^2))(\mathbf{x}_{12} - (\mathbf{x}_{12}^2 + \mathbf{x}_{23}^2 - \mathbf{x}_{13}^2))}{4\mathbf{x}_{12}^3} \right) \times d\mathbf{x}_{13} d\mathbf{x}_{23}$$

can be performed.

For $\mathbf{x}_{12} > 2$, (VII. 4) must be 0 because $\mathbf{x}_{23}$ and $\mathbf{x}_{13}$ cannot simultaneously equal 1. For $\mathbf{x}_{12} < 1$, (VII. 4) is continuous and at $\mathbf{x}_{12} = 2$, Eq. (VII. 4) equals $-\pi/4$.

Knowing that $d^2\rho_{2_s}(\mathbf{x}_{12})/d\mathbf{x}_{12}^2$ has step function behavior at $\mathbf{x}_{12} = 2$, we can continue the above process to show that $d^{2n}\rho_{2_s}(\mathbf{x}_{12})/d\mathbf{x}_{12}^{2n}$ is discontinuous at $\mathbf{x}_{12} = (n + 1)$.

Consider the equation

$$\rho'_{2_s}(\mathbf{x}_{12}) = z\left(\rho + \int \rho_2(\mathbf{x}_{23}) f_{13} d\mathbf{x}_3 \right).$$

From the above analysis the fourth derivative will contain the terms

$$\frac{d^4\rho'_{2_s}(\mathbf{x}_{12})}{d\mathbf{x}_{12}^4} = -z \int \delta(\mathbf{x}_{23-2}) \left(\frac{d\mathbf{x}_{23}}{d\mathbf{x}_{12}} \right)^3 \frac{d\mathbf{x}_{13}}{d\mathbf{x}_{12}} \delta(\mathbf{x}_{13} - 1) \otimes \frac{\mathbf{x}_{13}\mathbf{x}_{23}}{\mathbf{x}_{12}} d\mathbf{x}_{13} d\mathbf{x}_{23}, \quad \text{(VII. 4)}$$

which has discontinuous behavior at $\mathbf{x}_{12} = 3$ and $\mathbf{x}_{12} = 1$. If $\mathbf{x}_{12} < 1$, the above integral is 0 since $\mathbf{x}_{23}$ cannot equal 2 and $\mathbf{x}_{13}$ equal 1 simultaneously. Equation (VII. 4) is continuous for $\mathbf{x}_{12} > 1$, and, at $\mathbf{x}_{12} = 1$, (VII. 4) equals $-\pi/4$.

Therefore $\rho'_{2_s}(\mathbf{x}_{12})$ also shows discontinuous behavior in the fourth derivative at $\mathbf{x}_{12} = 1$. This behavior is also

exhibited by the solution to the Percus–Yevick equation for hard sphere potentials.[13]

VIII. DISCUSSION OF RESULTS

A perturbation scheme has been introduced which generates a solution to the Kirkwood–Salsburg hierarchy of integral equations. The power series in z obtained by Ruelle[3a,b] can be recovered by expanding each term in our perturbation expansion in a z series.

The advantages of this expansion are twofold. We generate an approximation scheme which can be improved step by step with a well-defined procedure.

The second advantage is the possibility of obtaining formal properties of the solutions of the Kirkwood–Salsburg equation by examining the structure of the solutions of an approximate, much simpler hierarchy.

Two properties of the approximate hierarchy were investigated, and the results are consistent with what is expected from the distribution functions.

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APPENDIX

It is the purpose of this appendix to justify three assumptions employed in Sec. VI.

(1) The assertion that

$$F(|\mathbf{x}|) = \sum_{\alpha} \frac{A_\alpha e^{iK_\alpha |\mathbf{x}|}}{|\mathbf{x}|}$$

(2) The assumed uniform convergence of this series which enabled us to take the limit of $F(|\mathbf{x}|)$ term by term.

(3) The often used assumption of commutability of limit and integral.

At the outset it should be clear that for finite range potentials

$$\int f(|\mathbf{x}|) e^{-i\mathbf{K}\cdot\mathbf{x}}\, d\mathbf{x}$$

is an analytic function of $|\mathbf{K}|$ and hence bounded. The analyticity guarantees that the singularities of

$$1/[1 - z\hat{f}(|\mathbf{K}|)]$$

are isolated poles.[12]

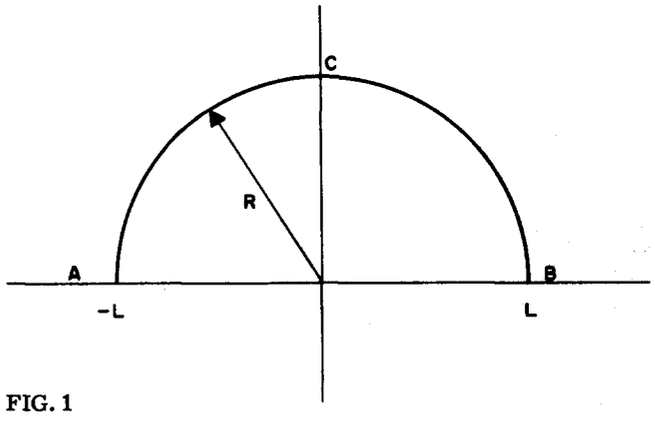

FIG. 1

Clearly for the range of $|z|$ considered

$$|z|\ |\hat{f}|(|\mathbf{K}|) < 1$$

for all real $|\mathbf{K}|$ so that for real $|\mathbf{K}|$

$$1/[1 - z\hat{f}(|\mathbf{K}|)] < M.$$

We are now in a position to prove the first assertion. By definition

$$F'(|\mathbf{x}|) = z^2 \int \frac{e^{i\mathbf{K}\cdot\mathbf{x}} (\hat{f}(|\mathbf{K}|))^2}{1 - z\hat{f}(|\mathbf{K}|)}\, d\mathbf{K}. \tag{A1}$$

Performing the integrations over the angles gives

$$F'(|\mathbf{x}|) = \frac{4\pi z^2}{|\mathbf{x}|} \int_0^\infty \frac{|\mathbf{K}| (\hat{f}(|\mathbf{K}|))^2 \sin(|\mathbf{K}|\,|\mathbf{x}|)}{1 - z\hat{f}(|\mathbf{K}|)}\, d|\mathbf{K}|. \tag{A2}$$

Recognizing that $\hat{f}(|\mathbf{K}|)$ is an even function, (A2) can be written as

$$F'(|\mathbf{x}|) = \frac{4\pi}{|\mathbf{x}|} \int_{-\infty}^{\infty} \frac{|\mathbf{K}| (z\hat{f}(|\mathbf{K}|))^2 e^{i|\mathbf{K}|\,|\mathbf{x}|}}{1 - z\hat{f}(|\mathbf{K}|)}\, d|\mathbf{K}|, \tag{A3}$$

where $|\mathbf{K}|$ now denotes a variable which can assume all values from $-\infty$ to $+\infty$. We will evaluate the integral over the contour in the complex $|\mathbf{K}|$ plane (see Fig. 1).

We have

$$|\hat{f}(|\mathbf{K}|)| = \left| \int e^{-i\mathbf{K}\cdot\mathbf{x}} f(|\mathbf{x}|) d\mathbf{x} \right|$$

$$\leq B \int_0^a \frac{4\pi}{|\mathbf{K}|} \left| \sin(|\mathbf{K}|\,|\mathbf{x}|) \right| d|\mathbf{x}|,$$

where a is the radius of the potential.

If $|\mathbf{K}|$ is complex with a modulus R, then

$$|\hat{f}(|\mathbf{K}|)| \leq B 8\pi \int_0^a e^{R|\mathbf{x}|}\, d|\mathbf{x}|$$

$$\leq aB 8\pi e^{Ra}$$

for $R > 1$. Consequently, if $|\mathbf{x}| > a$, the contribution from BCA goes to 0 as $R \to \infty$ and

$$F'(|\mathbf{x}|) = \sum_{\alpha} \frac{A_\alpha e^{iK_\alpha |\mathbf{x}|}}{|\mathbf{x}|}, \tag{A4}$$

where we have assumed that the roots $\mathbf{K}_\alpha$ of

$$1 - z\hat{f}(|\mathbf{K}|) \tag{A5}$$

are of the first order, and

$$A_\alpha e^{iK_\alpha |\mathbf{x}|}$$

is the residue of the integrand at $\mathbf{K}_\alpha$.

The roots of (A5) were assumed to be of first order. Clearly it is irrelevant what order they are for in the limit as $R \to \infty$ multiple roots will only change the factor A_α, but not the form of the large R behavior. It will also not affect any of the following analyses.

Turning to assumption (2), consider the integral

$$I_L(\mathbf{x}) = \frac{2\pi z^2}{|\mathbf{x}|} \int_{-L}^{L} \frac{|\mathbf{K}| (\hat{f}(\mathbf{K}))^2 e^{i|\mathbf{K}|\,|\mathbf{x}|}}{1 - z\hat{f}(|\mathbf{K}|)}\, d|\mathbf{K}|. \tag{A6}$$

From the above analysis

$$I_L(|\mathbf{x}|) = \sum_{\alpha=1}^{N(L)} \frac{A_\alpha e^{i\mathbf{K}_2|\mathbf{x}|}}{|\mathbf{x}|} + R_{BCA}, \tag{A7}$$

where R_{BCA} is the contribution from BCA in Fig. 1.

As the roots of (A5) are isolated clearly, either the number of terms in (A7) is finite or $N(L)$ is an increasing function of L. Since R_{BCA} becomes smaller as L gets larger, the series in (A7) becomes a better representation of $I_L(\mathbf{x})$ as L increases. The series can, in fact, be made arbitrarily close to $I_L(|\mathbf{x}|)$ for arbitrary $|\mathbf{x}|$ as long as $|\mathbf{x}|$ is larger than the range of the potential. Clearly if

$$\int_{-\infty}^{\infty} \frac{|\mathbf{K}|(\hat{f}(|\mathbf{K}|))^2 e^{i|\mathbf{K}||\mathbf{x}|}}{1 - z\hat{f}(|\mathbf{K}|)} d|\mathbf{K}| \tag{A8}$$

is uniformly convergent then (A7) is a uniformly convergent series.

Within the range of $|z|$ with which we are concerned and for real $|\mathbf{K}|$,

$$|1 - z\hat{f}(|\mathbf{K}|)| < M < \infty.$$

Clearly (A8) will be uniformly convergent if

$$\int_0^{\infty} \frac{|\mathbf{K}|(\hat{f}(|\mathbf{K}|))^2 \sin(|\mathbf{K}||\mathbf{x}|)}{1 - z\hat{f}(|\mathbf{K}|)} d|\mathbf{K}| \tag{A9}$$

is. We can guarantee the uniform convergence of the above integral by finding a function,[14] independent of $|\mathbf{x}|$ which bounds the absolute value of the integrand throughout the range of integration and whose integral over that range converges.

The function we propose is

$$H(|\mathbf{K}|) = M|\mathbf{K}|(\hat{f}(|\mathbf{K}|))^2, \quad |\mathbf{K}| < 1,$$
$$= M|\mathbf{K}|(\hat{f}(|\mathbf{K}|)^2, \quad |\mathbf{K}| \geq 1.$$

The integral of $H(|\mathbf{K}|)$ will clearly converge if

$$\int_0^{\infty} |\mathbf{K}|^2[\hat{f}(|\mathbf{K}|)]^2 d|\mathbf{K}|$$

is convergent:

$$\int_0^{\infty} |\mathbf{K}|^2(\hat{f}(|\mathbf{K}|))^2 d|\mathbf{K}| = \frac{1}{4\pi}\int (f(|\mathbf{K}|))^2 d\mathbf{K}.$$

Employing Parseval's[11] theorem, we have

$$\int (f(|\mathbf{K}|))^2 d\mathbf{K} = \int (f(\mathbf{x}))^2 d\mathbf{x},$$

which is clearly convergent. Therefore, (A4) is a uniformly convergent series.

Assumption (3) will be justified by examples. We will justify the limit integral interchange of (VI. 6).

We have

$$\lim_{|\mathbf{x}_{12}|\to\infty} \int G(|\mathbf{x}_{23}|)F'(|\mathbf{x}_{12} - \mathbf{x}_{23}|)d\mathbf{x}_{23}. \tag{A10}$$

The interchange is justified if the above integral converges uniformly.

$G(|\mathbf{x}_{23}|)$ is defined only over a finite range of $|\mathbf{x}_{23}|$ and is bounded. $F'(|\mathbf{x}_{12} - \mathbf{x}_{23}|)$ is also bounded. Therefore, a positive semidefinite function $D(|\mathbf{x}_{23}|)$ can be found[9] which bounds the integrand in (A10), is independent of $|\mathbf{x}_{12}|$, and for which

$$\int D(|\mathbf{x}_{23}|)d\mathbf{x}_{23} < \infty.$$

One choice for that function is

$$MH(|\mathbf{x}_{23}|),$$

where M is the product of the bounds of $G(|\mathbf{x}_{23}|)$ and $F'(|\mathbf{x}_{12} - \mathbf{x}_{23}|)$ and $H(|\mathbf{x}_{23}|)$ is the characteristic function of the range of integration.

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Derivation of low-temperature expansions for Ising model. II. General theory

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The enumeration problem that arises in the derivation of low-temperature and high-field expansions for the Ising model of a ferromagnet and antiferromagnet is studied. The method of partial generating functions (complete codes) is developed and a principle of complete code balance is explicitly stated. The detailed application of the method to a number of lattices is described and substitutions given that interpret the generating functions of certain lattices on the corresponding shadow lattice. It is shown that in zero-field and two dimensions some of these substitutions reduce to the well-known star triangle and magnetic-moment results.

1. INTRODUCTION

In this paper we continue our investigation of the enumerative problem that arises in the derivation of low-temperature and high-field expansions for the Ising model of a ferromagnet and antiferromagnet; a general introduction is given in the first paper[1] of this series, hereinafter referred to as I.

Following I, we write the free energy per spin (F) in the form

$$F = -\tfrac{1}{2}qJ - mH - kT\ln\Lambda(\mu, u), \tag{1.1}$$

where q is the coordination number, J the interaction energy as defined in I, m the magnetic moment per spin, H the applied magnetic field, k Boltzmann's constant, and T the absolute temperature. The expansion variables u and μ are defined by

$$\left.\begin{aligned} u = z^2 &= \exp(-4J/kT) \\ \mu &= \exp(-2mH/kT) \end{aligned}\right\}. \tag{1.2}$$

Series developments for $\ln\Lambda$ arise from a study of perturbations on the ordered state; a detailed description of their *direct* derivation is given in I. The expansion is there studied as a development in powers of μ in the form

$$\ln\Lambda = \sum_s L_s(u)\mu^s, \tag{1.3}$$

where the coefficients L_s are polynomials in u. Contributions to L_s arise from all the possible perturbations of s spins and this arrangement of the expansion we call the *μ-grouping*; alternatively it may be regarded as a *field-grouping* providing *high-field expansions* in the magnetic parameter μ ($\mu = 0$ when $H = \infty$) for fixed temperature. The expansions are valid for both the ferromagnetic and antiferromagnetic problems. We call the coefficients L_s *high-field polynomials*.

For many applications to the ferromagnetic case, for example the derivation of the spontaneous magnetization and the specific heat and susceptibility in zero field, it is more convenient to group the expansion in powers of u (or z) and we shall write

$$\ln\Lambda = \sum_s \psi_s(\mu)u^s. \tag{1.4}$$

This we call the u-grouping; alternatively, it may be regarded as a *temperature-grouping* providing expansions in the temperature parameter u, for fixed values of the field-variable μ. We call the polynomials ψ_s *ferromagnetic polynomials*. For the *honeycomb lattice* fractional powers of u occur in (1.4) and to avoid these we modify the definition of ψ_s by replacing u by z.

An important generalization is to the case of lattices which can be decomposed into two equivalent sublattices A and B. We distinguish the spins on these two sublattices by writing

$$\left.\begin{aligned} \exp(-2m_AH/kT) &= \mu \\ \exp(-2m_BH/kT) &= \nu \end{aligned}\right\}. \tag{1.5}$$

For the field grouping we define a set of *sublattice polynomials*, $L_{s,t}$

$$\ln\Lambda = \sum_{s,t} L_{s,t}(u)\mu^s\nu^t, \tag{1.6}$$

and for the temperature-grouping a corresponding set of polynomials in μ and ν

$$\ln\Lambda = \sum_s \psi_s(\mu, \nu)u^s. \tag{1.7}$$

One application of these sublattice polynomials is to the ordered region of an antiferromagnet ($H < H_c$, the critical field); J is assumed to be negative and we write $J' = -J$. We introduce new variables

$$y = \exp(-2J'/kT), \qquad w = y^2 \tag{1.8}$$

and the free energy per spin is now

$$F = -\tfrac{1}{2}qJ' - kT\ln\Lambda^a(\mu, w). \tag{1.9}$$

In the temperature-grouping μ and $1/\mu$ occur symmetrically and it is convenient to write

$$\theta_n = \mu^n + \mu^{-n}, \tag{1.10}$$

and define a new set of *antiferromagnetic polynomials*, ψ_s^a, by

$$\ln\Lambda^a = \sum_s \psi_s^a(\theta)w^s. \tag{1.11}$$

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As in the ferromagnetic case we introduce a modification for the *honeycomb lattice*; fractional powers are avoided by replacing w by y in (1.11).

To derive a useful number of terms in all the above expansions we introduced in I a method of partial generating functions. In Sec. 2 we summarise the method.

2. METHOD OF PARTIAL GENERATING FUNCTIONS

The method is to provide partial generating functions F_n for the sublattice polynomials $L_{s,t}$; each F_n corresponds to the exact solution when the number of spins overturned on one sublattice, by convention the B sublattice, is equal to n. The contributions can be set out in an array (omitting the field variable):

$$\left.\begin{aligned} F_0 &= L_{0,0} + L_{1,0} + L_{2,0} + L_{3,0} + L_{4,0} + \cdots \\ F_1 &= \quad L_{0,1} + L_{1,1} + L_{2,1} + L_{3,1} + \cdots \\ F_2 &= \quad\quad L_{0,2} + L_{1,2} + L_{2,2} + \cdots \\ F_3 &= \quad\quad\quad L_{0,3} + L_{1,3} + \cdots \\ F_4 &= \quad\quad\quad\quad L_{0,4} + \cdots \\ &\vdots \quad\quad\quad\quad\quad \vdots \end{aligned}\right\} \tag{2.1}$$

where $L_{0,0} = 0$.

An important step is to exploit the *symmetry condition*

$$L_{s,t} = L_{t,s}, \tag{2.2}$$

which holds because the two sublattices are equivalent. It follows that the first n partial generating functions are sufficient to determine the expansion of $\ln\Lambda$ correct for all $s + t \leq 2n + 1$. To take a specific example, the polynomials through L_5 can be derived from the generating functions through F_2. In the sequence of sublattice polynomials contributing to L_5

$$L_{5,0} + L_{4,1} + L_{3,2} + L_{2,3} + L_{1,4} + L_{0,5} \tag{2.3}$$

the last three follow from the symmetry condition.

The generating functions are conveniently written as sums of integer sequences, which we have called *codes*, each code being multiplied by an occurrence factor,

$$F_n = \sum(\lambda, \alpha, \beta, \gamma, \cdots), \quad \lambda = \alpha + \beta + \gamma + \cdots. \tag{2.4}$$

For example, on the honeycomb lattice

$$F_3 = 1(6,3,3) + 9(7,5,2) + 1(7,6,0,1) - 30(8,7,1) + 19\tfrac{1}{3}(9,9). \tag{2.5}$$

We shall not introduce a notation for the occurrence factors; the length of the individual integer sequences never exceeds the coordination number of the lattice by more than one, so that all honeycomb codes, for example, contain at most 4 parameters. We call F_n the *complete* nth *code*; the codes are interpreted by the substitution

$$(\lambda, \alpha, \beta, \gamma, \cdots) = Y^n(1 + bX)^\alpha(1 + b^2X)^\beta \times (1 + b^3X)^\gamma \cdots/(1 + X)^\lambda, \tag{2.6}$$

when after expansion of the right hand side the coefficient of $X^sY^nb^r$ represents the contribution of s-overturned A-spins, n overturned B-spins having r nearest neighbor links between them.

The expansion can be obtained explicitly in powers of μ, and z by making the further substitutions

$$X = \mu z^q, \quad Y = \nu z^q, \quad b = 1/z^2. \tag{2.7}$$

The zeroth code is anomalous and we must write

$$F_0 = \ln(1 + X) = \ln(1 + \mu z^q). \tag{2.8}$$

For convenience we adopt the convention that each sublattice has N sites; thus, in (2.5), and the sublattice polynomials that follow after the substitutions (2.6) and (2.7), we work on a $2N$ site lattice. When we particularize to the simple model with $\mu = \nu$, we employ the same codes and take half the resultant polynomials to obtain the $L_s(u)$.

We also assume that the sublattice equivalence or symmetry condition (2.2) is *always* exploited. For example, if we suppose the array (2.1) to be generated by the complete codes through F_4 it is immaterial whether $L_{0,3}$ is supplied by symmetry or from F_3; we assume the first method, because later we shall introduce generating functions which are not complete codes (partial codes) and the second method could then give an incorrect contribution.

An important consequence of the symmetry condition is that any complete code F_n must reproduce the sublattice polynomials $L_{m,n}$ correctly for all $m < n$. For example, F_3 must when expanded give values of $L_{0,3}, L_{1,3}, L_{2,3}$ which agree with their symmetric counterparts derived from F_0, F_1 and F_2 in the array (2.1). This *principle of complete code-balance* provides a check on the correctness of each new complete code as it is added. It implies a set of constraints on each complete code or partial generating function.

In the development of the theory we shall often require certain properties of the individual codes which contribute to a complete code; we define at this stage some concepts we shall use throughout our treatment.

If a code $(\lambda, \alpha, \beta, \gamma \cdots)$ occurs in F_s we call s the *order* of the code. The complete sth code is then the total of all codes of order s and is appropriate for the derivation of field-groupings. For temperature-groupings we shall find that an important property is the highest power of b that occurs in the coefficient of X^n in the expansion of (2.6); we call this the nth *rank* of the code. Finally, for any code $(\lambda, \alpha, \beta, \gamma, \delta, \epsilon, \cdots)$ we define the quantity

$$\gamma + 2\delta + 3\epsilon + \cdots \tag{2.9}$$

as the *class* of the code. We show later that the class of a code, and its successive ranks (for $n = 1, 2, 3 \cdots$), are of importance in a systematic treatment of the u-grouping.

The first few complete codes on a lattice can readily be derived by classifying all the possible arrangements of the appropriate shadows; the complexity of this work increases very rapidly with the order of the codes. In I we introduced a classification based on a partially isomorphic Ising problem on a related *shadow lattice*. In Sec. 3 we summarize some shadow systems and derive new substitutions which interpret the codes in a different way and provide results for the Ising problem on the shadow lattice.

3. SHADOW LATTICE TECHNIQUE

The shadow lattice is the lattice formed from the sites of the B sublattice with a bond system chosen to represent the different possible overlappings of the shadows cast on A-sites by overturned B-spins.

Honeycomb–triangular code system

As a first example we take the honeycomb lattice. The complete shadow system is illustrated in Fig. 1 (a) and

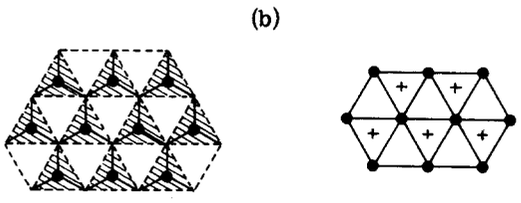


FIG. 1. (a) Honeycomb lattice and its complete shadow system; the full circles represent the B-sites. (overturned B-spins). (b) Corresponding shadow lattice. This is a triangular lattice with the original B-sites as vertices. The triangles have alternate parity; those marked with a cross are of the significant parity and correspond to three shadows that meet at one point.

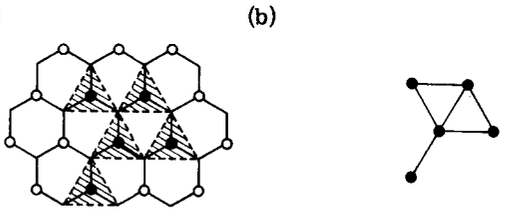


FIG. 2. ○ B-spins, ● overturned B-spins. (a) Honeycomb with 5 spins overturned on the B sub-lattice. The five shadows correspond to the code (10, 6, 3, 1). (b) Corresponding shadow graph.

the corresponding shadow lattice in Fig. 1 (b). It should be noted that the shadow lattice is not the triangular lattice delineated by the edges of the triangular shadows. Figure 2 illustrates a particular situation in which 5 B-spins are overturned; each casts a shadow on 3 A-spins, but some A-spins lie in more than one shadow. The corresponding code, (10, 6, 3, 1) simply expresses the fact that a total of 10 spins are affected; 6 lie in only one shadow, 3 in two shadows and 1 in three.

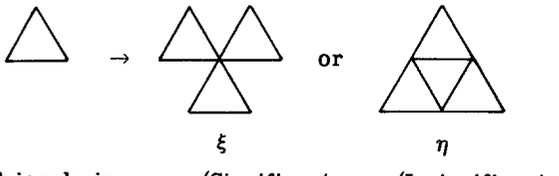
Each triangular shadow can only touch another at a vertex (and never along an edge) and no more than three shadows can meet at any point; thus, the codes involve at most four parameters. For any code $(\lambda, \alpha, \beta, \gamma)$ we have the relation

$$\lambda = \alpha + \beta + \gamma \tag{3.1}$$

which merely defines the dummy parameter λ introduced in I as a consistency check on the data. The three parameters α, β, γ are the number of A-spins which lie in 1, 2 or 3 shadows, respectively. If s is the number of B-spins, that is the *order* of the code; then, since each B-spin casts a shadow on 3 A spins,

$$3s = \alpha + 2\beta + 3\gamma. \tag{3.2}$$

The parameter β arises from pairs of triangles with a vertex in common; each of these implies a nearest neighbor bond in the corresponding graph on the shadow lattice *(shadow graph)*. The parameter γ arises from triplets of triangles with a vertex in common; these imply a nearest neighbor triangle in the shadow graph. Only alternate triangles can correspond to contacts of this type and we regard each triangle of the shadow lattice as having a parity; the parity corresponding to γ we call the *significant parity*. We have the scheme:



Triangle in shadow lattice — (Significant parity) — (Insignificant parity)

Any set of overturned spins on the honeycomb B-sublattice corresponds to a set of sites on the shadow lattice; if this set of sites is regarded as a strong embedding the total number of bonds, r, in the embedded graph (the shadow graph) is

$$r = \beta + 3\gamma, \tag{3.3}$$

because each bond will correspond to the contact of two shadows unless it lies in a triangle of significant parity; and each triangle of significant parity has three bonds but contributes only once to γ.

The last result has an important application. The complete honeycomb code F_s corresponds to the complete set of all graphs with s sites on the triangular shadow lattice; since the number of bonds in each shadow graph can be deduced from the corresponding code, F_s contains all the information required to determine the high-field polynomial L_s on the *triangular lattice*. From (3.3) we obtain the corresponding power of u for the Ising model on the triangular lattice as[2]

$$3s - r = \alpha + \beta. \tag{3.4}$$

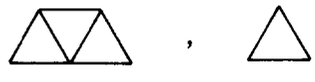
It follows that the substitution

$$(\lambda, \alpha, \beta, \gamma) = \mu^{(\alpha+2\beta+3\gamma)/3} u^{\alpha+\beta} \tag{3.5}$$

interprets the honeycomb codes in an alternative way and provides the high-field polynomials for the triangular lattice. We develop the theory of this substitution in Sec. 4.

To obtain a complete F_n for the honeycomb lattice it would suffice to find the codes corresponding to every low temperature configuration of n spins on the triangular lattice; this is a straightforward but fairly intricate operation because of the parity problem. The details of the first five complete codes are fully listed in I.

The division of triangles into the two parities is clearly symmetric, but if more than one triangle occurs in a shadow graph the distribution into parities ξ and η can be quite involved. For example the two component graph



has a total count of $12N^2 - 282N$, but divides as

$$\begin{aligned} &(3N^2 - 72N)\xi^3\eta, \\ &(6N^2 - 138N)\xi^2\eta^2, \\ &(3N^2 - 72N)\xi\eta^3, \end{aligned} \tag{3.6}$$

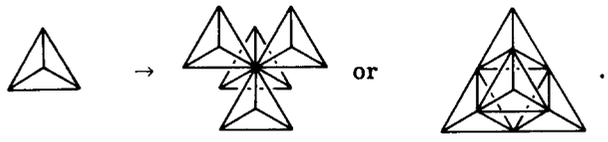
which is not quite symmetric, in the sense that the division is not the same as that for $\xi\eta(\xi + \eta)^2$.

In this particular system, once the configurational data on the shadow lattice has been *encoded* it is not possible to recover the *topology* of the shadow graph although it *is* possible, as we have seen, to recover the number of sites and bonds. Because of the substitution (3.5) the codes can be thought of either as honeycomb or triangular codes; we refer to the honeycomb-triangular code system.

For the honeycomb-triangular code system the last parameter (γ) determines the class of the code; in this system this is equivalent to the number of triangles of significant parity in the corresponding shadow graph.

Diamond-face-centered cubic code system

As a second example we take the diamond lattice. The shadows are tetrahedra and the complete shadow system is a straightforward generalization of that described for the honeycomb lattice. The shadow lattice is the face-centered cubic lattice formed by the B-sites alone, joined by first neighbor bonds. The B-sites lie at the centers of the tetrahedral shadows and the edges of these tetrahedra also delineate a face-centred cubic lattice, distinct from the shadow lattice. The only possible contacts are at a common vertex; never a common edge or common face. As in the previous example mutual contacts between two tetrahedra correspond to a bond in the shadow graph; mutual contacts between three tetrahedra (at a common vertex) correspond to half the triangles on the face-centred cubic (significant parity); mutual contacts between four tetrahedra also occurs in two ways in accordance with the following scheme:



ξ η

Tetrahedron in shadow lattice (Significant parity) (Insignificant parity)

The general code $(\lambda, \alpha, \beta, \gamma, \delta)$ now contains 5 parameters; if a shadow graph has s sites and r bonds a generalization of arguments used before establishes the results

$$4s = \alpha + 2\beta + 3\gamma + 4\delta, \tag{3.7}$$

$$r = \beta + 3\gamma + 6\delta, \tag{3.8}$$

and the corresponding substitution to (3.5)

$$(\lambda, \alpha, \beta, \gamma, \delta) = \mu^{(\alpha+2\beta+3\gamma+4\delta)/4} u^{(3\alpha+4\beta+3\gamma)/2} \tag{3.9}$$

interprets the diamond codes in an alternative way and provides the high-field polynomials on the face-centered cubic lattice.

We can now regard the codes as a diamond-face-centered cubic system. The parameter γ is the number of triangles of significant parity in the shadow graph, it being understood that none of these form part of a tetrahedron of significant parity. The parameter δ is the number of tetrahedra of significant parity. The class of each code is now $\gamma + 2\delta$ and is determined by the number of triangles and tetrahedra of significant parity.

All the results for the diamond-face-centered cubic system apply directly to the white tin-close-packed hexagonal system; these two systems are so close numerically that we have restricted our treatment to the former.

Simple quadratic code system

As a third example, we take the simple quadratic lattice. The general shadow system is composed of squares the edges of which delineate another simple quadratic lattice. The shadow lattice is formed from the B-sites of the original lattice which form a simple quadratic array. First neighbor bonds of this array correspond to two shadows touching along an edge; second neighbor bonds correspond to two shadows touching at one corner only. The shadow lattice is therefore a simple quadratic lattice with first and second neighbor bonds. We illustrate a particular situation in Fig. 3 (a) and the corresponding shadow graph in Fig. 3 (b).

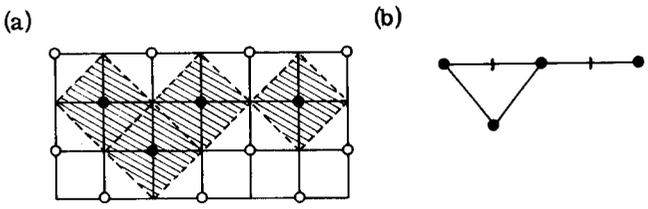


FIG. 3. ○ B-spins, ● overturned B-spins. (a) Simple quadratic with 4 spins overturned. (b) Corresponding shadow graph. ●——● , first neighbor bond. ●—+—● , second neighbor bond.

As in the previous example, the general code has 5 parameters. If r_1 and r_2 denote the number of first and second neighbor bonds in the shadow graph corresponding to $(\lambda, \alpha, \beta, \gamma, \delta)$, we have the relations

$$4s = \alpha + 2\beta + 3\gamma + 4\delta, \tag{3.10}$$

$$2r_1 + r_2 = \beta + 3\gamma + 6\delta. \tag{3.11}$$

It follows that the simple quadratic codes can be used to derive the solution for the simple quadratic lattice with second neighbor interactions if the first energy is twice the second. Unlike the two previous shadow systems, the representation requires the introduction of second neighbor bonds and this greatly complicates the treatment. All mutual contacts of three squares at a common vertex correspond to a triangle on the shadow lattice, all mutual contacts of four squares at a common vertex to a tetrahedron; the problem of parity no longer arises.

Simple and body-centered cubic code systems

The shadow systems for the simple cubic and body-centered cubic lattices may be developed along the same general lines. The codes $(\lambda, \alpha, \beta, \gamma, \cdots)$ that contribute to F_s must evidently all satisfy

$$qs = \alpha + 2\beta + 3\gamma + 4\delta + \cdots, \tag{3.12}$$

where q is the coordination number of the *original* lattice, not of the shadow lattice. A second equation can be derived which relates the codes to some special Ising problem on the shadow lattice; the body-centered cubic lattice is described in more detail in I.

4. GENERAL RESULTS: $q = 3$ SYSTEMS

In this section we investigate some general results that follow from the substitutions derived in the previous section.

We take the honeycomb-triangular system as the model of a $q = 3$ system; in general, the results of this section will apply to other $q = 3$ systems such as, for example, the hydrogen peroxide-hypertriangular system.[3] In this section we use *u for the triangular lattice variable and z for the honeycomb variable* in their usual sense; that is, we shall assume $u = \exp(-4J/kT)$ and $z = \exp(-2J^*/kT)$, where J and J^* are the interaction energies for the triangular and honeycomb lattices, respectively.

As we have shown in Sec. 2, each honeycomb code admits of two fundamental substitutions. First, from (2.6) and (2.7),

$$(\lambda, \alpha, \beta, \gamma) = (\nu z^3)^n (1 + \mu z)^\alpha (1 + \mu z^{-1})^\beta (1 + \mu z^{-3})^\gamma / (1 + \mu z^3)^{\alpha+\beta+\gamma}, \tag{4.1}$$

which yields formally, after setting $\mu = \nu$,

$$2 \ln \Lambda_{HC} = \ln(1 + \mu z^3) + \sum F_n, \tag{4.2}$$

where the 2 on the left-hand side arises because the shadow lattice has half the original number of sites; the summation $\sum$ is taken over all possible codes, interpreted by (4.1).

Second, from (3.5),

$$(\lambda, \alpha, \beta, \gamma) = \mu^n u^{\alpha+\beta}, \tag{4.3}$$

which yields

$$\ln \Lambda_T = \sum{}' F_n, \tag{4.4}$$

where again the summation $\sum'$ is taken over all possible codes but now interpreted by (4.3).

We now observe that in zero field the substitutions (4.1) and (4.3) reduce, respectively, to

$$(\lambda, \alpha, \beta, \gamma) = [z(1 + z)/(1 + z^3)]^{\alpha+\beta} = \omega^{\alpha+\beta}, \tag{4.5}$$

$$(\lambda, \alpha, \beta, \gamma) = u^{\alpha+\beta}. \tag{4.6}$$

It follows that in powers of the variable ω defined by (4.5),

$$\omega = z(1 + z)/(1 + z^3), \tag{4.7}$$

the honeycomb expansion for $\ln \Lambda$ [apart from the $\ln(1 + z^3)$ term] will be term-by-term identical with the triangular expansion. This formal equivalence corresponds to the well-known star triangle relationship[4]

$$2 \ln \Lambda_{HC}(z) = \ln(1 + z^3) + \ln \Lambda_T(\omega). \tag{4.8}$$

To extract the spontaneous magnetization, we require the quantity

$$I = \lim_{H \to 0} \left(1 - 2\mu \frac{\partial L}{\partial \mu} - 2\nu \frac{\partial L}{\partial \nu}\right), \qquad L = \ln \Lambda. \tag{4.9}$$

To evaluate this, it is convenient to exploit the sublattice symmetry; the substitution (4.1) is not symmetric in μ and ν, but the resulting full series expansion must be. It will, therefore, suffice to replace (4.9) by

$$I = \lim_{H \to 0} \left(1 - 4\nu \frac{\partial L}{\partial \nu}\right), \tag{4.10}$$

and from (4.1) and (4.3) the corresponding substitutions that correspond to this operation become for each code simply

$$\text{Honeycomb: } -2n\omega^{\alpha+\beta}, \tag{4.11}$$

$$\text{Triangular: } -2nu^{\alpha+\beta}, \tag{4.12}$$

which is equivalent to the standard result[5]

$$I_{HC}(z) = I_T(\omega). \tag{4.13}$$

The reduced susceptibility is derived from

$$\chi = \lim_{H \to 0} \left[4\left(\mu \frac{\partial}{\partial \mu} + \nu \frac{\partial}{\partial \nu}\right)^2 L\right] \tag{4.14}$$

and this reduces because of the symmetry of the resultant function *after summation* to the evaluation of

$$\lim_{H \to 0} 8\left(\frac{\partial L}{\partial \nu} + \frac{\partial^2 L}{\partial \nu^2} + \frac{\partial^2 L}{\partial \mu \partial \nu}\right). \tag{4.15}$$

Explicitly, each honeycomb code makes the contributions

$$2\frac{\partial L}{\partial \nu} = n\omega^{\alpha+\beta}, \qquad 2\frac{\partial^2 L}{\partial \nu^2} = n(n-1)\omega^{\alpha+\beta},$$

$$2\frac{\partial^2 L}{\partial \mu \partial \nu} = n\omega^{\alpha+\beta}[(\beta + \gamma)(1 - z^3) + (\alpha - \beta)z(1 - z)]/(1 + z^3). \tag{4.16}$$

It should be emphasised that these results only hold because there is an implied summation over all the codes; an individual code will generate an asymmetric function of μ and ν. We now use the result that follows using (3.2),

$$(\beta + \gamma)(1 - z^3) + (\alpha - \beta)z(1 - z) = n(1 - z^3) - \tfrac{1}{3}(\alpha - \beta)(1 - z)^3, \tag{4.17}$$

to derive the final result for the ferromagnetic susceptibility χ^f:

$$\chi^f_{HC} = 4\sum \omega^{\alpha+\beta}\{n^2 + n[n(1 - z^3) - \tfrac{1}{3}(\alpha - \beta)(1 - z)^3]/(1 + z^3)\}. \tag{4.18}$$

The corresponding antiferromagnetic susceptibility, χ^a, may be extracted in an analogous manner. The formal isomorphism between the two problems enables us to obtain the result by replacing z by $1/y$. The result is found to be

$$\chi^a_{HC} = 4\sum \tilde{\omega}^{\alpha+\beta}\{n^2 - n[n(1 - y^3) - \tfrac{1}{3}(\alpha - \beta)(1 - y)^3]/(1 + y^3)\}, \tag{4.19}$$

where $\tilde{\omega} = y(1 + y)/(1 + y^3)$. (4.20)

The ferromagnetic susceptibility of the triangular lattice is simply

$$\chi^f_T = \sum 4n^2 u^{\alpha+\beta}. \tag{4.21}$$

On taking the average of the ferromagnetic and antiferromagnetic susceptibilities of the honeycomb lattice at any temperature the numerical values of y and z are equal. The numerical values of ω and $\tilde{\omega}$ are also equal.

Thus, in (4.18) and (4.19) the second term cancels and from (4.21) we obtain

$$\tfrac{1}{2}[\chi^a_{HC}(z) + \chi^f_{HC}(z)] = \chi^f_T(u), \qquad u = z(1 + z)/(1 + z^3) \tag{4.22}$$

which is the well-known magnetic moment result of Fisher.[6]

$q = 4$ systems

The code systems that arise for $q = 4$ are more varied than those for $q = 3$; the theory becomes more complex and less generally useful. We confine our treatment to a few observations on the two systems we have already described.

Each code $(\lambda, \alpha, \beta, \gamma, \delta)$ of the diamond system, or the simple quadratic system, has a direct substitution which reduces in zero-field to the form

$$(\lambda, \alpha, \beta, \gamma, \delta) = [z(1 + z^2)/(1 + z^4)]^{\alpha+\gamma}[2z^2/(1 + z^4)]^{\beta} \tag{4.23}$$

to yield the expansion in z on the diamond or simple quadratic lattice respectively. Each diamond code can also be interpreted in zero-field on the face-centred

cubic lattice by (3.9), which reduces to

$$(\lambda, \alpha, \beta, \gamma, \delta) = z^{3\alpha+4\beta+3\gamma} = [z^3]^{\alpha+\gamma}[z^4]^{\beta} \quad (4.24)$$

and, thus, there is a formal isomorphism between the resultant expansions if sufficient detail is retained. Explicitly, if we write

$$\omega_1^3 = z(1 + z^2)/(1 + z^4), \quad \omega_2^4 = 2z^2/(1 + z^4) \quad (4.25)$$

and make the substitution

$$(\lambda, \alpha, \beta, \gamma, \delta) = [\omega_1^3]^{\alpha+\gamma}[\omega_2^4]^{\beta}, \quad (4.26)$$

we have the relationship

$$2 \ln \Lambda_D(z) = \ln (1 + z^4) + \ln \Lambda_{FCC}(\omega_1, \omega_2). \quad (4.27)$$

This is the low temperature three-dimensional star tetrahedron substitution analogous to the two-dimensional star triangle substitution. Because of the necessity of distinguishing between ω_1 and ω_2 it is apparently of little practical use. A similar formal relationship can be given for the simple quadratic lattice and its shadow lattice (when for the latter the first interaction energy is twice the second).

The results of this section are simple in form and we have developed them for application to our subsequent theoretical treatment. They are not suitable for the practical problem of obtaining series expansions since they do not exploit the sublattice symmetry and, therefore, uneconomic use is made of the codes. The objection can be countered by expanding each code in a special way, but it is just as simple to work in the presence of a field and take the zero-field limit afterwards.

In the particular instance of the honeycomb-triangular pair (or the hydrogen peroxide-hypertriangular pair) the code treatment is closely analogous to the star-triangle substitution in the presence of a field and can alternatively be treated as such; the resultant substitutions are no less cumbersome.

5. CONCLUSIONS AND SUMMARY

We have summarized the notation of I and outlined the method of partial generating functions. We have stated explicitly the principle of complete code balance; this provides a check on each new partial generating function. We show in subsequent papers how the principle may be exploited in the derivation of further codes. The shadow systems of a number of lattices have been described and substitutions given that interpret the generating functions of certain lattices on the corresponding shadow lattice. It has been shown that in zero-field and two dimensions some of these reduce to the well-known star triangle and magnetic moment results.

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Derivation of low-temperature expansions for Ising model. III. Two-dimensional lattices—field grouping

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The derivation of series expansions appropriate for low temperatures or high applied magnetic fields for the two-dimensional Ising model of a ferromagnet and antiferromagnet is studied as a field grouping. New results are given for the high field polynomials for the triangular lattice to order 10, the simple quadratic lattice to order 15, and the honeycomb lattice to order 21.

1. INTRODUCTION AND SUMMARY

In this paper we extend the series expansions of three two-dimensional lattices, the honeycomb, simple quadratic and triangular, as a field or μ-grouping. We have already introduced the problem and given the general theory in previous papers,[1,2] hereinafter referred to as I and II, respectively. It is our main object to communicate the results since these have many applications; the actual intricacies of the calculation we give only in outline. Few will wish to repeat such calculations and each lattice has to be treated on its merits, sometimes adopting one method, sometimes another. The extension of field groupings is a first logical step towards the extension of temperature groupings which we describe subsequently.

We give new results for the high-field polynomials L_9 and L_{10} on the triangular lattice, for the complete code F_7 and L_{14} and L_{15} on the simple quadratic lattice, for F_7, F_8, F_9, F_{10} and $L_{14}, L_{15}, L_{16}, L_{17}, L_{18}, L_{19}, L_{20}, L_{21}$ on the honeycomb lattice.

2. DERIVATION OF COMPLETE CODES FOR HONEYCOMB AND TRIANGULAR LATTICES

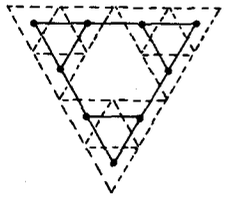
As we have shown in Paper II, Sec. 3, the partial generating functions or complete codes for the honeycomb lattice can also be regarded as codes for the triangular lattice. We begin by formalizing the concept of the honeycomb-triangular code system.

We observe that n triangular shadows that do not touch will correspond to the code $(3n, 3n)$; if any two have a common vertex, and p is the number of such pairs of contact, the code will be $(3n-p, 3n-2p, p)$; finally if t is the number of vertices common to three triangles the most general possible code will be

$$(3n-p-2t, 3n-2p-3t, p, t) \qquad (2.1)$$

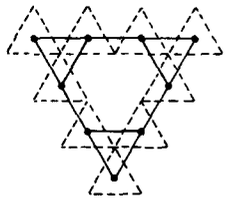
and this defines what we shall call the *algebraic* code system. The final parameter t is the number of triangles of *significant* parity in the corresponding graph on the shadow lattice; the general form of (2.1) follows from equations (3.1) and (3.2) of II.

If we set $n = 9$, $p = 12$, $t = 0$ in (2.1) we obtain the code (15, 3, 12) which corresponds to an arrangement of nine triangles with 3 free and 12 single-contact vertices. This can be realised as illustrated



and we shall say that the code is *graphical*; at least one graph can be found on the shadow lattice to correspond to it. On setting $n = 9$, $p = 13$, $t = 0$ we obtain the code (14, 1, 13) which we shall call *nongraphical* since it is not possible in practice to arrange nine triangles to correspond to it.

In the first example, the underlying shadow graph can also correspond to a second arrangement of nine triangles



with code (18, 12, 3, 3). In this latter case, the three triangles of the shadow graph are all of the significant (ξ) parity and correspond to triple contacts.

The algebraic code system is a *finite* set of codes for fixed n, since clearly limits can be placed on the parameters p and t; the graphical code system is a smaller subset, obtained by deletion of the nongraphical codes.

Since the shadow lattice is a first neighbor lattice, it is not difficult to derive the first few complete codes in a straightforward manner by enumerating all the low temperature configurations on the triangular lattice. The number of configurations increases rapidly with n; the number of distinct graphical codes in a complete code only slowly. Details of the enumeration up to $n = 5$ are given in I together with the result for F_6. We have completed F_7 and F_8 in essentially this way. Beyond $n = 8$ we proceed indirectly.

The triangular polynomial L_9 has 17 coefficients but these are not all independent; since the high temperature specific heat and susceptibility expansion are available to adequate length these coefficients must satisfy 11 constraints (I, Sec. 2) and these constraints can be used to fill in any 11 coefficients of L_9 if the

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remaining 6 are known. The method, in its simplest form, was first described by Domb,[3] and subsequently developed by other authors.[4] It is convenient to provide the lowest powers of u by direct counting since these correspond to graphs with the most bonds. We provide the first six coefficients and find

$$\begin{aligned} L_9 = {} & 27u^{11} + 160u^{12} + 483u^{13} + 228u^{14} - 4\,181u^{15} \\ & - 16\,704u^{16} - 11\,109u^{17} + 43\,868\tfrac{2}{3}\,u^{18} \\ & + 375\,483u^{19} + 408\,072u^{20} - 3\,019\,394u^{21} \\ & - 6\,438\,150u^{22} + 40\,681\,902u^{23} - 72\,302\,016u^{24} \\ & + 63\,438\,876u^{25} - 28\,314\,960u^{26} + 5\,157\,414\tfrac{4}{9}\,u^{27}. \end{aligned} \tag{2.2}$$

For the corresponding F_9 it is found by inspection that there are 47 graphical codes; in other words, there are 47 nonzero coefficients to be determined. These coefficients cannot all be independent since, by the principle of complete code balance (II, Sec. 2), F_9 must generate all the sublattice polynomials $L_{r,9}$, $r < 9$, correctly in agreement with F_0 through F_8. The determination of the number of *linearly independent* simultaneous equations that must be satisfied to ensure this consistency requires some detailed analysis and is found to be 36. The complete code must also reduce correctly, under the substitution II(3.5), to the corresponding low temperature polynomial on the triangular lattice (2.2) which we have completed by the method of Domb. This last condition yields a further set of 17 linearly independent equations, not necessarily independent of the previous set. Of the combined total of 53 constraints only 44 are found to be linearly independent; direct determination of a linearly independent set is difficult. To complete F_9 it is only necessary to supply 3 coefficients although these cannot be chosen completely at random. We have supplied the three codes

$$\left.\begin{array}{r} 6(15,4,10,1) \\ 1(15,3,12) \\ 27(16,5,11) \end{array}\right\} \tag{2.3}$$

by direct counting, and completed F_9 by solving 44 linearly independent equations.

In F_{10} we find 58 graphical codes with 45 linearly independent constraints arising from the previous 9 complete codes (principle of complete code balance). Direct calculation of the corresponding L_{10} for the triangular lattice by the method of Domb is difficult. L_{10} is a polynomial with 20 coefficients. Instead, therefore, we have exploited the fact that F_{10} must reduce correctly to L_{10} for those powers of u which are conveniently counted directly (up to u^{16} inclusive); and, furthermore, must generate correctly all those powers of z in L_{20} and L_{21} for the honeycomb lattice which are conveniently counted directly (up to z^{16} inclusive). In other words, we supply the partial information

$$\begin{aligned} L_{10} = {} & 3u^{11} + 86u^{12} + 432u^{13} + 837u^{14} + 449u^{15} \\ & - 10\,353u^{16} + \ldots \end{aligned} \tag{2.4}$$

for the triangular lattice and

$$\left.\begin{aligned} L_{20} &= 43\tfrac{1}{2}z^{12} + 5829z^{14} + 125\,336\tfrac{1}{4}z^{16} + \ldots \\ L_{21} &= 387z^{13} + 26\,111z^{15} + \ldots \end{aligned}\right\} \tag{2.5}$$

for the honeycomb lattice. These results yield a further 6 independent constraints, leaving 7 counts to be provided. In the direct procedure for obtaining L_{10} by the method of Domb 12 constraints on the coefficients would result; 10 of these from the previous polynomials through L_9 and 2 that arise from the requirement that the high temperature susceptibility and specific heat must expand correctly. The first 10 of these constraints are found to be linear combinations of the 45 constraints derived from the codes; the remaining 2 are linearly independent and reduce the number of counts to be provided to 5.

We supply the five codes

$$\left.\begin{array}{r} 6(17,4,13) \\ 259(18,6,12) \\ 96(17,5,11,1) \\ 2376(18,7,10,1) \\ -1029(19,9,9,1) \end{array}\right\} \tag{2.6}$$

and complete F_{10} by solving 53 linearly independent equations. On substitution, we obtain at the same time the polynomial (for the triangular lattice)

$$\begin{aligned} L_{10} = {} & 3u^{11} + 86u^{12} + 432u^{13} + 837u^{14} + 449u^{15} \\ & - 10\,353u^{16} - 42\,315u^{17} - 48\,618\tfrac{1}{2}u^{18} \\ & + 205\,386u^{19} + 663\,288u^{20} + 1\,680\,030u^{21} \\ & - 4\,347\,964\tfrac{1}{2}u^{22} - 22\,703\,382u^{23} + 20\,150\,487u^{24} \\ & + 236\,013\,501\tfrac{3}{5}\,u^{25} - 741\,600\,943\tfrac{1}{2}u^{26} \\ & + 1\,012\,339\,456u^{27} - 745\,686\,690u^{28} \\ & + 290\,732\,760u^{29} - 47\,346\,449\tfrac{1}{5}u^{30}. \end{aligned} \tag{2.7}$$

The above results have been obtained by sacrificing all the advantages of the powerful consistency check that follows from the principle of complete code balance. To check that our data are correct we have overcounted; that is, we have counted further codes and coefficients in every case and verified that these are consistent with those obtained by solution of the simultaneous equations.

We give the expressions for F_7 through F_{10} in the Appendix, together with the honeycomb high-field polynomials derived therefrom. The corresponding sublattice polynomials to order 21 are of course also determined by the F.

3. DERIVATION OF COMPLETE CODES FOR SIMPLE QUADRATIC LATTICE

The simple quadratic code system is more complicated than the honeycomb-triangular system. The algebraic system is based on the most general possible code which is now

$$(4n - p - 2t - 3T, 4n - 2p - 3t - 4T, p, t, T), \tag{3.1}$$

where for the shadow graph T is the number of tetrahedra, t the number of triangles which do not lie in tetrahedra, and p is the sum of twice the number of first and once the number of second neighbor bonds that do not lie in either. Again the codes that, in fact, occur are limited to the subset of graphical codes.

Because of the greater complexity of the code system (63 graphical codes in F_7 in place of 27 for the honeycomb), we have found it convenient to provide most of the codes by direct counting. To do this we have used a computer program developed by one of us (CJE). The underlying problem is to enumerate, count, and code all graphs with seven vertices on the simple quadratic lat-

tice with first and second neighbors. It would be possible to do the whole operation by computer; in practice it is more convenient to supply the contribution of many-component (separated) graphs by exploiting the principle of complete code balance.

We give in the Appendix the value of F_7 and the polynomials L_{14} and L_{15}; these, together with the known partition function[5] in zero-field, determine the first 16 coefficients of the high temperature susceptibility expansion and these are found to be in agreement with previous direct estimates.[6]

In conjunction with the 17th coefficient of the susceptibility all the field derivatives are determined to order 17 inclusive. (Likewise the results of Sec. 2 determine all the field derivatives of the honeycomb lattice to order 23, of the triangular lattice to order 12). These results will be published subsequently.

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APPENDIX: COMPLETE CODES F_n AND HIGH-FIELD POLYNOMIALS $L(u)$

Honeycomb lattice

$$F_7 = 1(12,6,3,3) + 15(12,5,5,2) + 15(13,8,2,3) + 6(12,4,7,1) + 6(14,10,1,3) + 93(13,7,4,2) + 120(13,6,6,1) - 78(14,9,3,2) - 18(15,12,0,3) + 15(14,8,5,1) + 36(13,5,8) - 615(15,11,2,2) + 396(16,13,1,2) - 3\,507(15,10,4,1) + 429(14,7,7) - 5\,536(15,9,6) + 2\,286(16,12,3,1) + 243(17,15,0,2) + 18\,789(17,14,2,1) + 2\,379(16,11,5) + 94\,851(17,13,4) - 30\,981(18,16,1,1) + 13\,167(19,18,0,1) - 320\,643(18,15,3) + 437\,997(19,17,2) - 275\,184(20,19,1) + 65\,718\tfrac{1}{7}(21,21).$$

$$F_8 = 6(13,4,7,2) + 3(13,5,5,3) + 3(14,4,10) + 48(14,5,8,1) + 123(14,6,6,2) + 57(14,7,4,3) + 3(14,8,2,4) + 255(15,6,9) + 609(15,7,7,1) + 324(15,8,5,2) + 104(15,9,3,3) + 6(15,10,1,4) + 411(16,8,8) - 2\,691(16,9,6,1) - 2\,167\tfrac{1}{2}(16,10,4,2) - 252(16,11,2,3) - 31\,143(17,10,7) - 19\,392(17,11,5,1) - 3\,117(17,12,3,2) - 267(17,13,1,3) + 101\,436\tfrac{1}{2}(18,12,6) + 62\,901(18,13,4,1) + 10\,122(18,14,2,2) + 240(18,15,0,3) + 320\,037(19,14,5) + 68\,703(19,15,3,1) - 933(19,16,1,2) - 2\,311\,238\tfrac{1}{4}(20,16,4) - 378\,705(20,17,2,1) - 4\,245(20,18,0,2) + 5\,039\,827(21,18,3) + 403\,392(21,19,1,1) - 5\,324\,130(22,20,2) - 134\,802(22,21,0,1) + 2\,778\,678(23,22,1) - 574\,205\tfrac{7}{8}(24,24).$$

$$F_9 = 3(14,4,7,3) + 1(15,3,12) + 6(15,4,10,1) + 51(15,5,8,2) + 80(15,6,6,3) + 21(15,7,4,4) + 27(16,5,11) + 384(16,6,9,1) + 774(16,7,7,2) + 444(16,8,5,3) + 80(16,9,3,4) + 3(16,10,1,5) + 1\,431(17,7,10) + 2\,055(17,8,8,1) - 628(17,9,6,2) - 426(17,10,4,3) - 12(17,11,2,4) - 8\,421\tfrac{2}{3}(18,9,9) - 29\,502(18,10,7,1) - 20\,097(18,11,5,2) - 3\,911(18,12,3,3) - 126(18,13,1,4) - 131\,952(19,11,8) - 53\,354(19,12,6,1) + 11\,022(19,13,4,2) + 1\,311(19,14,2,3) - 27(19,15,0,4) + 950\,214(20,13,7) + 621\,735(20,14,5,1) + 108\,376(20,15,3,2) + 5\,940(20,16,1,3) - 296\,232(21,15,6) - 492\,309(21,16,4,1) - 114\,300(21,17,2,2) - 2\,731\tfrac{2}{3}(21,18,0,3) - 12\,829\,824(22,17,5) - 2\,786\,429(22,18,3,1) - 49\,833(22,19,1,2) + 45\,721\,839(23,19,4) + 6\,391\,674(23,20,2,1) + 63\,267(23,21,0,2) - 73\,688\,570(24,21,3) - 5\,039\,937(24,22,1,1) + 63\,438\,876(25,23,2) + 1\,386\,554(25,24,0,1) - 28\,314\,960(26,25,1) + 5\,157\,414\tfrac{4}{5}(27,27).$$

$$F_{10} = 1(15,3,9,3) + 45(16,5,8,3) + 42(16,6,6,4) + 3(16,7,4,5) + 6(17,4,13) + 96(17,5,11,1) + 489(17,6,9,2) + 660(17,7,7,3) + 342(17,8,5,4) + 42(17,9,3,5) + 259(18,6,12) + 2\,376(18,7,10,1) + 3\,805\tfrac{1}{2}(18,8,8,2) + 1\,679(18,9,6,3) + 246(18,10,4,4) + 45(18,11,2,5) + 1(18,12,0,6) + 6\,165(19,8,11) - 1\,029(19,9,9,1) - 22\,716(19,10,7,2) - 12\,822(19,11,5,3) - 1\,719(19,12,3,4) - 69(19,13,1,5) - 93\,903(20,10,10) - 211\,086(20,11,8,1) - 115\,462\tfrac{1}{2}(20,12,6,2) - 23\,463(20,13,4,3) - 1\,432\tfrac{1}{2}(20,14,2,4) - 307\,582(21,12,9) + 291\,018(21,13,7,1) + 373\,461(21,14,5,2) + 66\,768(21,15,3,3) + 1\,482(21,16,1,4) + 6\,225\,154\tfrac{1}{2}(22,14,8) + 4\,015\,188(22,15,6,1) + 564\,444(22,16,4,2) + 36\,846(22,17,2,3) + 846(22,18,0,4) - 16\,289\,049(23,16,7) - 11\,272\,290(23,17,5,1) - 2\,054\,709(23,18,3,2) - 98\,271(23,19,1,3) - 44\,874\,801(24,18,6) - 7\,836\,459(24,19,4,1) + 699\,171(24,20,2,2) + 27\,133(24,21,0,3) + 333\,890\,820\tfrac{3}{5}(25,20,5) + 65\,891\,508(25,21,3,1) + 1\,422\,126(25,22,1,2) - 802\,927\,177\tfrac{1}{2}(26,22,4) - 97\,877\,319(26,23,2,1) - 866\,220(26,24,0,2) + 1\,026\,671\,572(27,24,3) + 61\,326\,234(27,25,1,1) - 745\,686\,690(28,26,2) - 14\,332\,116(28,27,0,1) + 290\,732\,760(29,28,1) - 47\,346\,449\tfrac{1}{5}(30,30).$$

$$L_{14} = 13\tfrac{1}{2}z^{10} + 1\,293\tfrac{1}{2}z^{12} + 10\,239z^{14} - 290\,701\tfrac{1}{2}z^{16} - 1\,106\,330\tfrac{1}{2}z^{18} + 51\,659\,587\tfrac{1}{2}z^{20} - 485\,686\,203z^{22} + 2\,531\,186\,544\tfrac{1}{2}z^{24} - 8\,650\,567\,975\tfrac{1}{2}z^{26} + 20\,696\,184\,189\tfrac{3}{14}z^{28} - 35\,683\,078\,192z^{30} + 44\,736\,756\,298\tfrac{1}{2}z^{32} - 40\,504\,406\,128\tfrac{1}{2}z^{34} + 25\,838\,073\,978z^{36} - 11\,026\,631\,670z^{38} + 2\,827\,427\,866\tfrac{1}{2}z^{40} - 329\,532\,809\tfrac{2}{7}z^{42}.$$

$$L_{15} = 99z^{11} + 4\,659z^{13} + 9\,388z^{15} - 1\,045\,935z^{17} + 589\,338z^{19} + 153\,554\,339z^{21} - 1\,800\,298\,839z^{23} + 10\,943\,966\,655\tfrac{3}{5}z^{25} - 43\,143\,273\,895\tfrac{1}{3}z^{27} + 119\,462\,312\,907z^{29} - 241\,026\,687\,060z^{31} + 359\,986\,482\,721z^{33} - 398\,673\,658\,651\tfrac{4}{5}z^{35} + 323\,656\,860\,471z^{37} - 187\,344\,453\,913z^{39} + 73\,256\,077\,056z^{41} - 17\,351\,332\,869z^{43} + 1\,880\,893\,529\tfrac{3}{5}z^{45}.$$

$$L_{16} = 1\tfrac{1}{2}z^{10} + 556\tfrac{1}{2}z^{12} + 14\,905\tfrac{1}{2}z^{14} - 53\,361\tfrac{3}{4}z^{16} - 3\,392\,069z^{18} + 15\,503\,661z^{20} + 418\,763\,238z^{22} - 6\,408\,752\,413\tfrac{1}{4}z^{24} + 45\,527\,194\,980z^{26} - 205\,702\,882\,038z^{28} + 652\,083\,122\,787z^{30} - 1\,516\,436\,885\,790\tfrac{15}{16}z^{32} + 2\,643\,388\,622\,025z^{34} - 3\,480\,793\,494\,422z^{36} + 3\,451\,237\,800\,210z^{38} - 2\,539\,062\,705\,132\tfrac{3}{4}z^{40} + 1\,345\,061\,569\,354\tfrac{1}{2}z^{42} - 485\,307\,026\,293\tfrac{1}{2}z^{44} + 106\,803\,960\,223\tfrac{1}{2}z^{46} - 10\,821\,360\,421\tfrac{3}{8}z^{48}.$$

$$L_{17} = 21z^{11} + 2\,631z^{13} + 41\,309z^{15} - 438\,600z^{17} - 9\,879\,492z^{19} + 91\,306\,307z^{21} + 992\,263\,377z^{23} - 21\,838\,264\,746z^{25} + 182\,569\,837\,122z^{27} - 941\,971\,969\,341z^{29} + 3\,391\,104\,621\,762z^{31} - 8\,985\,390\,852\,061z^{33} + 18\,000\,662\,937\,195z^{35} - 27\,608\,021\,297\,097z^{37} + 32\,496\,618\,829\,231z^{39} - 29\,161\,173\,313\,776z^{41} + 19\,612\,241\,942\,373z^{43} - 9\,576\,892\,709\,804z^{45} + 3\,207\,513\,868\,233z^{47} - 659\,192\,238\,825z^{49} + 62\,695\,314\,181\tfrac{1}{17}z^{51}.$$

$$L_{18} = 178z^{12} + 10\,809z^{14} + 91\,150\tfrac{1}{2}z^{16} - 2\,171\,765\tfrac{1}{3}z^{18} - 24\,921\,147z^{20} + 408\,173\,802z^{22} + 1\,712\,263\,896\tfrac{1}{2}z^{24} - 70\,771\,816\,570\tfrac{1}{2}z^{26} + 706\,222\,874\,728\tfrac{1}{2}z^{28} - 4\,156\,643\,653\,890z^{30} + 16\,895\,223\,554\,254\tfrac{1}{2}z^{32} - 50\,556\,121\,845\,475\tfrac{1}{2}z^{34} + 115\,018\,592\,769\,003\tfrac{1}{3}z^{36} - 202\,287\,903\,687\,066z^{38} + 276\,880\,427\,988\,466\tfrac{1}{2}z^{40} - 294\,576\,336\,961\,750\tfrac{1}{2}z^{42} + 241\,383\,297\,055\,546\tfrac{1}{2}z^{44} - 149\,496\,753\,984\,936z^{46} + 67\,703\,117\,221\,632z^{48} - 21\,157\,312\,980\,391\tfrac{1}{2}z^{50} + 4\,078\,362\,710\,029\tfrac{1}{2}z^{52} - 365\,492\,690\,504\tfrac{5}{9}z^{54}.$$

$$L_{19} = 3z^{11} + 1\,122z^{13} + 39\,217z^{15} + 103\,503z^{17} - 8\,836\,677z^{19} - 47\,879\,154z^{21} + 1\,583\,499\,405z^{23} - 146\,126\,940z^{25} - 215\,505\,807\,132z^{27} + 2\,633\,706\,637\,839z^{29} - 17\,714\,835\,415\,059z^{31} + 80\,983\,222\,780\,567z^{33} - 271\,801\,098\,256\,650z^{35} + 695\,714\,339\,542\,968z^{37} - 1\,386\,184\,993\,907\,707z^{39} + 2\,171\,920\,169\,846\,733z^{41} - 2\,683\,391\,375\,444\,535z^{43} + 2\,604\,051\,889\,539\,049z^{45} - 1\,963\,104\,873\,705\,786z^{47} + 1\,126\,607\,002\,232\,820z^{49} - 475\,676\,123\,479\,201z^{51} + 139\,322\,037\,300\,339z^{53} - 25\,287\,455\,348\,415z^{55} + 2\,142\,512\,683\,691\tfrac{1}{19}z^{57}.$$

$$L_{20} = 43\tfrac{1}{2}z^{12} + 5\,829z^{14} + 125\,336\tfrac{1}{4}z^{16} - 398\,467\tfrac{1}{2}z^{18} - 31\,663\,835\tfrac{1}{4}z^{20} - 24\,213\,138z^{22} + 5\,537\,628\,616\tfrac{1}{4}z^{24} - 20\,522\,547\,531z^{26} - 602\,189\,777\,737\tfrac{1}{2}z^{28} + 9\,449\,997\,391\,664\tfrac{2}{5}z^{30} - 73\,015\,594\,477\,080\tfrac{3}{4}z^{32} + 374\,633\,325\,888\,676\tfrac{1}{2}z^{34} - 1\,403\,030\,743\,989\,103\tfrac{3}{4}z^{36} + 4\,010\,730\,984\,549\,060z^{38} - 8\,966\,600\,232\,733\,150\tfrac{1}{2}z^{40} + 15\,886\,396\,461\,688\,887\tfrac{1}{2}z^{42} - 22\,436\,409\,786\,964\,112\tfrac{1}{4}z^{44} + 25\,255\,816\,116\,533\,859z^{46} - 22\,526\,577\,970\,085\,309\tfrac{1}{2}z^{48} + 15\,722\,693\,103\,596\,614\tfrac{1}{5}z^{50} - 8\,405\,918\,707\,839\,228z^{52} + 3\,324\,082\,711\,885\,887z^{54} - 916\,112\,238\,583\,162\tfrac{1}{2}z^{56} + 157\,101\,691\,401\,118\tfrac{1}{2}z^{58} - 12\,621\,887\,453\,735\tfrac{13}{20}z^{60}.$$

$$L_{21} = 387z^{13} + 26\,111z^{15} + 341\,706z^{17} - 3\,777\,609z^{19} - 101\,586\,109z^{21} + 390\,691\,035z^{23} + 17\,571\,739\,110z^{25} - 132\,031\,662\,576\tfrac{1}{3}z^{27} - 1\,462\,742\,482\,599z^{29} + 32\,493\,226\,019\,064z^{31} - 291\,212\,949\,840\,308z^{33} + 1\,676\,525\,162\,927\,097\tfrac{3}{7}z^{35} - 6\,979\,999\,379\,245\,722z^{37} + 22\,153\,962\,836\,019\,194z^{39} - 55\,146\,611\,831\,987\,088z^{41} + 109\,406\,684\,141\,966\,184z^{43} - 174\,460\,339\,883\,721\,134z^{45} + 224\,224\,576\,208\,023\,365z^{47} - 231\,759\,900\,926\,189\,854\tfrac{2}{7}z^{49} + 191\,225\,786\,576\,790\,611z^{51} - 124\,246\,173\,735\,835\,959z^{53} + 62\,171\,572\,759\,884\,333z^{55} - 23\,119\,019\,544\,235\,833z^{57} + 6\,016\,310\,713\,749\,579z^{59} - 977\,768\,139\,593\,331z^{61} + 74\,691\,681\,980\,346\tfrac{5}{21}z^{63}.$$

Simple quadratic lattice

$$F_7 = 16(14,5,6,1,2) + 6(14,6,4,2,2) + 4(15,5,7,3) + 8(15,5,8,1,1) + 64(15,6,6,2,1) + 8(15,6,7,0,2) + 80(15,7,4,3,1) + 16(15,8,2,4,1) + 2(16,4,12) + 20(16,5,10,1) + 108(16,6,8,2) + 8(16,6,9,0,1) + 256(16,7,6,3) + 148(16,7,7,1,1) + 188(16,8,4,4) + 168(16,8,5,2,1) - 40(16,8,6,0,2) + 40(16,9,2,5) + 28(16,9,3,3,1) + 40(17,6,11) + 340(17,7,9,1) + 1\,060(17,8,7,2) + 24(17,8,8,0,1) + 860(17,9,5,3) - 472(17,9,6,1,1) + 204(17,10,3,4) - 616(17,10,4,2,1) - 88(17,11,2,3,1) + 160(18,8,10) + 288(18,9,8,1) - 2\,040(18,10,6,2) - 536(18,10,7,0,1) - 2\,764(18,11,4,3) - 1\,368(18,11,5,1,1) - 584(18,12,2,4) - 1\,852(19,10,9) - 11\,792(19,11,7,1) - 15\,608(19,12,5,2) + 360(19,12,6,0,1) - 2\,804(19,13,3,3) + 2\,320(19,13,4,1,1) - 256(19,14,1,4) - 10\,016(20,12,8) - 8\,108(20,13,6,1) + 16\,810(20,14,4,2) + 2\,848(20,14,5,0,1) + 4\,080(20,15,2,3) + 339(20,16,0,4) + 28\,072(21,14,7) + 99\,468(21,15,5,1) + 31\,776(21,16,3,2) - 2\,992(21,16,4,0,1) + 112\,332(22,16,6) - 16\,820(22,17,4,1) - 29\,824(22,18,2,2)$$

$$- 212\,788(23,18,5) - 206\,644(23,19,3,1) - 370\,616(24,20,4) + 140\,144(24,21,2,1) + 718\,328(25,22,3)$$
$$+ 217\,696(26,24,2) - 800\,968(27,26,1) + 320\,879\tfrac{1}{7}(28,28).$$

$$L_{14} = 22u^8 + 864u^9 + 7\,372u^{10} + 11\,536u^{11} - 257\,378u^{12} - 1\,557\,816u^{13} + 1\,314\,978u^{14} + 62\,452\,942u^{15}$$
$$- 2\,072\,348u^{16} - 1\,354\,656\,284u^{17} - 785\,938\,734u^{18} + 48\,542\,073\,472u^{19} - 250\,471\,809\,911\tfrac{1}{2}u^{20}$$
$$+ 700\,726\,407\,966\tfrac{2}{7}u^{21} - 1\,278\,321\,358\,994u^{22} + 1\,613\,014\,033\,334u^{23} - 1\,429\,269\,896\,596u^{24} + 877\,614\,310\,184u^{25}$$
$$- 356\,891\,308\,190u^{26} + 86\,670\,538\,138u^{27} - 9\,532\,294\,556\tfrac{6}{7}u^{28}.$$

$$L_{15} = 6u^8 + 456u^9 + 6\,404u^{10} + 24\,436u^{11} - 94\,888u^{12} - 1\,677\,728u^{13} - 3\,997\,457u^{14} + 34\,493\,510\tfrac{2}{3}u^{15}$$
$$+ 267\,958\,908u^{16} - 885\,175\,436u^{17} - 5\,903\,060\,870\tfrac{2}{3}u^{18} + 16\,408\,972\,700u^{19} + 177\,977\,336\,689\tfrac{1}{5}u^{20}$$
$$- 1\,388\,708\,571\,629\tfrac{1}{3}u^{21} + 4\,917\,742\,574\,549u^{22} - 10\,990\,712\,090\,268u^{23} + 16\,983\,610\,970\,872\tfrac{2}{3}u^{24}$$
$$- 18\,741\,629\,318\,887\tfrac{1}{5}u^{25} + 14\,825\,042\,097\,211u^{26} - 8\,245\,969\,418\,426\tfrac{2}{3}u^{27} + 3\,071\,337\,551\,762u^{28}$$
$$- 689\,136\,584\,016u^{29} + 70\,528\,002\,102\tfrac{2}{5}u^{30}.$$

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Derivation of low-temperature expansions for Ising model. IV. Two-dimensional lattices—temperature grouping

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The derivation of series expansions appropriate for low temperatures or high applied magnetic fields for the two-dimensional Ising model of a ferromagnet and antiferromagnet is studied as a temperature grouping. New results are given for the ferromagnetic polynomials for the triangular lattice to order 16, for the ferromagnetic and antiferromagnetic polynomials for the simple quadratic lattice to order 11, and for the honeycomb lattice to order 16.

1. INTRODUCTION AND SUMMARY

In this paper we extend the series expansions of three two-dimensional lattices, the honeycomb, simple quadratic, and triangular, as a temperature or u-grouping. We refer to previous papers[1-3] as I, II and III respectively. As in III, it is our main object to communicate the results; the techniques we have used are rather specialised and are not, in general, applicable to three-dimensional lattices.

We give new results for the *ferromagnetic* polynomials ψ_{11} through ψ_{16} on the triangular lattice, ψ_8 through ψ_{11} on the simple quadratic lattice, ψ_{10} through ψ_{16} on the honeycomb lattice. We also give the corresponding *antiferromagnetic* polynomials ψ^a to the same order, and expansions for the ferromagnetic and antiferromagnetic susceptibilities χ^f and χ^a.

2. DERIVATION OF PARTIAL CODES FOR HONEYCOMB AND TRIANGULAR LATTICES

When for the honeycomb lattice the double series expansion in[4] μ and z is regrouped in powers of z, only a small part of the information in the higher codes is exploited; this is because quite low powers of z can come from higher codes. For example we can complete ψ_{11} from the μ-grouping derived from the first 9 codes since the highest power of μ that occurs is 19. But, to complete ψ_{12} requires contributions up to μ^{24} and could therefore involve F_{12}. The codes that contribute are not numerous; in the present instance, a simple *sufficient* condition can be given for finding all the codes that might contribute. It follows from the star-triangle substitution II (4.7) whereby effectively

$$u \to z(1+z)/(1+z^3) \tag{2.1}$$

that to obtain a given power of z it will suffice to encode all those triangular configurations which contribute to the corresponding power of u (or less). Thus, on the *triangular* lattice

$$\psi_{12} = 2\mu^{12} + 24\mu^{11} + 86\mu^{10} + \cdots \tag{2.2}$$

and by encoding all the graphs that contribute to these three leading terms, together with the leading term of ψ_1, we derive *partial* codes $F_{12}{}^{(12)}, F_{11}{}^{(12)}, F_{10}{}^{(12)}$ which contain sufficient information to derive ψ_{12} on the honeycomb lattice correctly. We find

$$F_{12}{}^{(12)} = (18,6,6,6) + (19,9,3,7),$$
$$F_{11}{}^{(12)} = 12(17,6,6,5) + 12(18,9,3,6),$$
$$F_{10}{}^{(12)} = 3(16,7,4,5) + (15,3,9,3) + 42(16,6,6,4) + 42(17,9,3,5) + (18,12,0,6). \tag{2.3}$$

These partial codes are based on a *sufficient* condition; not all the above codes are necessary. In fact, for $F_{10}{}^{(12)}$ the last two only contribute to z^{12} because their expansions contain X^8b^{21} and X^6b^{18}, respectively; these coefficients correspond to less than 20 overturned spins in all and, provided the *sublattice symmetry is consistently exploited*,[5] they will be correctly supplied by F_8 and F_6, respectively. We can, therefore, write

$$F_{10}{}^{(12)}\min = 3(16,7,4,5) + (15,3,9,3) + 42(16,6,6,4) \tag{2.4}$$

and, similarly,

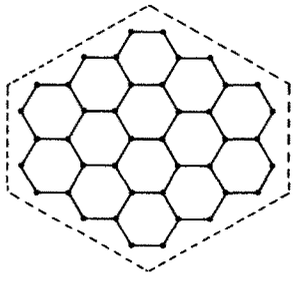
$$F_{12}{}^{(12)}\min = (18,6,6,6),$$
$$F_{11}{}^{(12)}\min = 12(17,6,6,5). \tag{2.5}$$

An elaborate detailed theory can be developed for partial codes and the relationship between the ranks of a code and the topology of the associated configuration on the shadow lattice. In practice, for the present lattice pair, it is slightly more convenient to evaluate the ψ directly.

3. TEMPERATURE GROUPING FOR HONEYCOMB AND TRIANGULAR LATTICES

To extend the z-grouping on the honeycomb lattice directly, we require an enumeration of clusters of spins with constant Ising perimeter (the power of z); in particular, we need those clusters with near the maximum number of spins since the contribution of those with a small number are supplied by the complete codes. For example, the polynomial ψ_{16} for the honeycomb lattice has two extremes: (1) a maximum of 42 overturned spins with 55 nearest neighbor bonds between them, contributing $3\mu^{42}$, and (2) a minimum of 6 overturned spins with one bond contributing $3363\mu^6$. We illustrate the actual graphs:

(1)



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(2) 

We can interpret the graphs that contribute to ψ_{16} in another way by introducing the well-known duality property[6] of the honeycomb triangular pair. The honeycomb polynomial ψ_{16} then corresponds on the *triangular* lattice to all the no-field graphs with 16 edges grouped by area (in unit triangles), each unit of area contributing one power of μ. To derive the polynomial we require an area classification of all such graphs. By reference to the figure it will be seen that the graph of highest area corresponds to a polygon of 16 sides, the graph of lowest area to five polygons with a total of 16 sides. Closer inspection reveals that all the graphs on the honeycomb lattice that contribute to μ^{30} or more correspond to polygons. An analysis of all the polygons on the triangular lattice by area is given by Hiley and Sykes[7] up to 16 sides. In terms of a dummy variable x the 1930635 polygons with 16 sides divide as

$$3x^{42} + 27x^{40} + 147x^{38} + 609x^{36} + 2079x^{34} + 6156x^{32} + 16017x^{30} + 37086x^{28} + 77040x^{26} + 142737x^{24} + 235662x^{22} + 341796x^{20} + 419913x^{18} + 406608x^{16} + 244755x^{14}. \quad (3.1)$$

The leading terms of this analysis are isomorphic with $2\psi_{16}$ on the honeycomb lattice; it suffices to replace x by μ. For areas of 28 and less more than one polygon can occur and corrections must be made; with the aid of the (unpublished) details of the 1961 calculation we have carried out these corrections down to the coefficient in μ^{22} to obtain

$$2\psi_{16} = 3\mu^{42} + 27\mu^{40} + 147\mu^{38} + 609\mu^{36} + 2079\mu^{34} + 6156\mu^{32} + 16017\mu^{30} + 36846\mu^{28} + 75462\mu^{26} + 134817\mu^{24} + 205650\mu^{22} + \cdots. \quad (3.2)$$

The polynomial can now be completed by taking the coefficients of μ^{18} down to μ^6 from the expansion of the complete codes F_0 through F_9 derived in III and determining the coefficient of μ^{20} from the known value of $\psi_{16}(1)$ derived from the exact expansion[8] for the case $H = 0$. That the resultant polynomial is correct may be verified by using the expansion for the magnetization; if this check is dispensed with, the coefficient of μ^{22} can be supplied by elimination. The coefficient of μ^{20} found in this way follows also from the expansion of F_{10}, but we have instead found it convenient to use this coefficient in the derivation of the complete F_{10}.

The calculation of the ψ for the triangular lattice proceeds in an essentially similar way. The leading terms correspond to polygons on the honeycomb lattice; by exploiting the contributions from the triangular polynomials $L_1 - L_{10}$ and the known expansions of the partition function and magnetization we have derived the corresponding polynomials to ψ_{16}. (The polygon-area distribution was not given in Ref. 7).

In the case of the honeycomb lattice, it is not especially important to obtain all the higher order partial codes, because extra coefficients are more easily obtained by direct counting on the lattice itself. A systematic theory can be developed based on the brief observations we have made. The disadvantage of the direct method is that it does not give the detailed sublattice distribution without further intricate work. In the present instance, we obtain the antiferromagnetic polynomials by first deriving the antiferromagnetic susceptibility by way of the magnetic moment result. We give the ferromagnetic polynomials ψ for the triangular and honeycomb lattices in the Appendix; from these we derive the corresponding ferromagnetic susceptibilities as

$$\chi_T^f = 4u^3 + 48u^5 + 16u^6 + 516u^7 + 288u^8 + 5328u^9 + 3840u^{10} + 53\,676u^{11} + 45\,488u^{12} + 531\,600u^{13} + 505\,584u^{14} + 5\,199\,404u^{15} + 5\,399\,136u^{16} + \cdots, \quad (3.3)$$

$$\chi_{HC}^f = 4z^3 + 24z^4 + 108z^5 + 488z^6 + 2064z^7 + 8592z^8 + 35\,168z^9 + 142\,488z^{10} + 572\,316z^{11} + 2\,283\,320z^{12} + 9\,058\,596z^{13} + 35\,769\,744z^{14} + 140\,678\,464z^{15} + 551\,357\,232z^{16} + \cdots, \quad (3.4)$$

and from these by II (4.22),

$$\chi_{HC}^a = 4y^3 + 12y^5 + 8y^6 + 48y^7 + 96y^8 + 320y^9 + 888y^{10} + 2748y^{11} + 8384y^{12} + 26\,340y^{13} + 83\,568y^{14} + 268\,864y^{15} + 873\,648y^{16} + \cdots. \quad (3.5)$$

We give the ferromagnetic susceptibilities in full as they are not given in I. From the expansion (3.5) and a study of the contributions of some special codes, it is now possible to calculate three new antiferromagnetic polynomials in the presence of a field. By solving the resultant simultaneous equations, these are found to be

$$\begin{aligned} 2\psi_{14}^a &= 13\,890 + 4\,779\theta_2 + 111\theta_4, \\ 2\psi_{15}^a &= 31\,558\theta_1 + 3\,917\theta_3 + 16\tfrac{1}{5}\theta_5, \\ 2\psi_{16}^a &= 118\,857\tfrac{3}{4} + 46\,635\theta_2 + 1\,992\theta_4. \end{aligned} \quad (3.6)$$

4. TEMPERATURE GROUPING FOR SIMPLE QUADRATIC LATTICE

For the simple quadratic lattice each complete code F_n corresponds to an analysis of all the possible contacts of n squares. As before, rearrangement as a temperature grouping only uses a part of the last few complete codes available. The general code $(\lambda, \alpha, \beta, \gamma, \delta)$ contains 5 parameters and we have shown (II, Sec. 4) that in zero-field the general substitution reduces to

$$(\lambda, \alpha, \beta, \gamma, \delta) = [z(1 + z^2)/(1 + z^4)]^{\alpha+\gamma}\,[2z^2/(1 + z^4)]^{\beta}. \quad (4.1)$$

We deduce that the lowest power of z that derives from any particular code is

$$\alpha + 2\beta + \gamma = 4n - 2(\gamma + 2\delta). \quad (4.2)$$

For the z grouping the codes required at any fixed power of z could be characterised by their having their maximum possible values of $\gamma + 2\delta$, which we have defined as the *class* of the code (II, Sec. 2), large enough to yield the chosen power, or less, through (4.2). The condition is sufficient but not necessary. In general, every configuration on the simple quadratic lattice is accounted for in the direct expansion of F_n by two contributions; one corresponds to fixed spins on the A sublattice, the other to fixed spins on the B sublattice. The corresponding codes we call conjugate with respect to the graph generated. If both conjugate codes are of the same order the above condition is necessary; if the conjugate codes are of different order then the condition is necessary only for the code of *lower* order.

For example, there are found to be only two 8th order codes which could contribute to z^{20} and, therefore, by (4.2) must have $\gamma + 2\delta = 6$. They are

$$(18, 10, 4, 2, 2),$$
$$(19, 12, 2, 4, 1),$$

but in fact the first code is its own conjugate while the second has a 7th order conjugate

$$(15, 8, 2, 4, 1),$$

which will provide the total contribution if the sublattice symmetry is exploited.

Again, we have found it convenient to extend the ferromagnetic polynomials by the method of the previous section. The simple quadratic lattice is self-dual and an analysis by area of the polygons up to 18 sides is given by Hiley and Sykes; we have extended the relevant part of this analysis to 20 and 22 sides and derived the polynomials $\psi_8, \psi_9, \psi_{10}, \psi_{11}$ by applying the necessary corrections. We have verified that these polynomials are consistent with the known values[9] of $\ln\Lambda$ and the magnetization in zero-field. Since no useful relation has been found between the ferromagnetic and antiferromagnetic susceptibility, we have derived the corresponding antiferromagnetic polynomials by direct enumeration; as a check we have employed the partial codes. The values of ψ_2^a through ψ_9^a were given in I; for the next two, we find

$$\begin{aligned} 2\psi_{10}^a &= -23\,316 + 25\,704\theta_1 - 8\,556\theta_2 + 2\,929\theta_3 \\ &\quad - 252\theta_4 + 7\tfrac{1}{5}\theta_5 \\ 2\psi_{11}^a &= 150\,572 - 88\,060\theta_1 + 58\,632\theta_2 - 12\,856\theta_3 \\ &\quad + 2\,400\theta_4 - 100\theta_5 \end{aligned} \tag{4.3}$$

and these provide two further coefficients for the antiferromagnetic susceptibility χ^a given in I:

$$\cdots + 55\,956w^{10} + 266\,656w^{11}, \quad (w = y^2). \tag{4.4}$$

From the ferromagnetic polynomials we extract the ferromagnetic susceptibility as

$$\begin{aligned} \chi^f &= 4u^2 + 32u^3 + 240u^4 + 1664u^5 + 11\,164u^6 \\ &\quad + 73\,184u^7 + 472\,064u^8 + 3\,008032\mu^9 \\ &\quad + 18\,985\,364u^{10} + 118\,909\,888u^{11}. \end{aligned} \tag{4.5}$$

We give the ferromagnetic polynomials in the Appendix.

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APPENDIX. FERROMAGNETIC POLYNOMIALS $\psi(\mu)$

Honeycomb lattice

$\psi_3 = \mu, \quad \psi_4 = 1\tfrac{1}{2}\mu^2, \quad \psi_5 = 3\mu^3,$

$\psi_6 = \tfrac{1}{2}\mu^6 + 7\mu^4 - 2\mu^2, \quad \psi_7 = 3\mu^7 + 18\mu^5 - 9\mu^3,$

$\psi_8 = 1\tfrac{1}{2}\mu^{10} + 13\tfrac{1}{2}\mu^8 + 46\tfrac{1}{2}\mu^6 - 33\tfrac{3}{4}\mu^4,$

$\psi_9 = \mu^{13} + 12\mu^{11} + 55\mu^9 + 116\mu^7 - 121\mu^5 + 6\tfrac{1}{5}\mu^3,$

$\psi_{10} = 1\tfrac{1}{2}\mu^{16} + 13\tfrac{1}{2}\mu^{14} + 67\tfrac{1}{2}\mu^{12} + 199\tfrac{1}{2}\mu^{10} + 270\mu^8 - 421\tfrac{1}{2}\mu^6 + 51\mu^4,$

$\psi_{11} = 3\mu^{19} + 21\mu^{17} + 99\mu^{15} + 318\mu^{13} + 654\mu^{11} + 534\mu^9 - 1\,422\mu^7 + 288\mu^5,$

$\psi_{12} = \tfrac{1}{2}\mu^{24} + 7\mu^{22} + 43\tfrac{1}{2}\mu^{20} + 178\mu^{18} + 556\tfrac{1}{2}\mu^{16} + 1\,293\tfrac{1}{2}\mu^{14} + 1\,938\tfrac{1}{4}\mu^{12} + 639\tfrac{1}{2}\mu^{10} - 4\,640\tfrac{1}{2}\mu^8 + 1\,400\tfrac{1}{2}\mu^6 - 24\tfrac{1}{2}\mu^4,$

$\psi_{13} = 3\mu^{27} + 21\mu^{25} + 105\mu^{23} + 387\mu^{21} + 1\,122\mu^{19} + 2\,631\mu^{17} + 4\,659\mu^{15} + 5\,013\mu^{13} - 1\,275\mu^{11} - 14\,583\mu^9 + 6\,225\mu^7 - 291\mu^5,$

$\psi_{14} = 1\tfrac{1}{2}\mu^{32} + 13\tfrac{1}{2}\mu^{30} + 73\tfrac{1}{2}\mu^{28} + 292\tfrac{1}{2}\mu^{26} + 958\tfrac{1}{2}\mu^{24} + 2\,593\tfrac{1}{2}\mu^{22} + 5\,829\mu^{20} + 10\,809\mu^{18} + 14\,905\tfrac{1}{2}\mu^{16} + 10\,239\mu^{14} - 13\,866\mu^{12} - 43\,740\mu^{10} + 25\,938\mu^8 - 2\,212\tfrac{1}{2}\mu^6,$

$\psi_{15} = \mu^{37} + 12\mu^{35} + 64\mu^{33} + 269\mu^{31} + 918\mu^{29} + 2\,645\mu^{27} + 6\,630\mu^{25} + 14\,264\mu^{23} + 26\,111\mu^{21} + 39\,217\mu^{19} + 41\,309\mu^{17} + 9\,388\mu^{15} - 70\,989\mu^{13} - 123\,466\mu^{11} + 102\,659\mu^9 - 13\,647\mu^7 + 106\tfrac{1}{5}\mu^5,$

$\psi_{16} = 1\tfrac{1}{2}\mu^{42} + 13\tfrac{1}{2}\mu^{40} + 73\tfrac{1}{2}\mu^{38} + 304\tfrac{1}{2}\mu^{36} + 1\,039\tfrac{1}{2}\mu^{34} + 3\,078\mu^{32} + 8\,008\tfrac{1}{2}\mu^{30} + 18\,423\mu^{28} + 37\,731\mu^{26} + 67\,408\tfrac{1}{2}\mu^{24} + 102\,825\mu^{22} + 125\,336\tfrac{1}{4}\mu^{20} + 91\,150\tfrac{1}{2}\mu^{18} - 53\,361\tfrac{3}{4}\mu^{16} - 290\,701\tfrac{1}{2}\mu^{14} - 319\,373\tfrac{1}{4}\mu^{12} + 388\,501\tfrac{1}{2}\mu^{10} + 74\,083\tfrac{7}{8}\mu^8 + 1\,681\tfrac{1}{2}\mu^6.$

Triangular lattice

$\psi_3 = \mu, \quad \psi_4 = 0, \quad \psi_5 = 3\mu^2,$

$\psi_6 = 2\mu^3 - 3\tfrac{1}{2}\mu^2, \quad \psi_7 = 3\mu^4 + 9\mu^3,$

$\psi_8 = 6\mu^5 + 12\mu^4 - 30\mu^3,$

$$\psi_9 = \mu^7 + 14\mu^6 + 21\mu^5 + 5\mu^4 + 19\tfrac{1}{3}\mu^3,$$

$$\psi_{10} = 6\mu^8 + 30\mu^7 + 42\mu^6 + 18\mu^5 - 178\tfrac{1}{2}\mu^4,$$

$$\psi_{11} = 3\mu^{10} + 27\mu^9 + 69\mu^8 + 105\mu^7 + 33\mu^6 - 177\mu^5 + 288\mu^4,$$

$$\psi_{12} = 2\mu^{12} + 24\mu^{11} + 86\mu^{10} + 160\mu^9 + 227\mu^8 + 24\mu^7 - 278\mu^6 - 680\mu^5 - 129\tfrac{3}{4}\mu^4,$$

$$\psi_{13} = 3\mu^{14} + 27\mu^{13} + 117\mu^{12} + 249\mu^{11} + 432\mu^{10} + 483\mu^9 + 120\mu^8 - 564\mu^7 - 1\,320\mu^6 + 2\,637\mu^5,$$

$$\psi_{14} = 6\mu^{16} + 42\mu^{15} + 168\mu^{14} + 414\mu^{13} + 702\mu^{12} + 1\,092\mu^{11} + 837\mu^{10} + 228\mu^9 - 1\,822\tfrac{1}{2}\mu^8 - 2\,682\mu^7 - 136\tfrac{1}{2}\mu^6 - 2\,796\mu^5,$$

$$\psi_{15} = \mu^{19} + 14\mu^{18} + 87\mu^{17} + 290\mu^{16} + 729\mu^{15} + 1\,320\mu^{14} + 2\,072\mu^{13} + 2\,539\mu^{12} + 1\,726\mu^{11} + 449\mu^{10} - 4\,181\mu^9 - 5\,313\mu^8 - 3\,007\mu^7 + 16\,807\mu^6 + 971\tfrac{1}{5}\mu^5,$$

$$\psi_{16} = 6\mu^{21} + 42\mu^{20} + 198\mu^{19} + 606\mu^{18} + 1\,368\mu^{17} + 2\,622\mu^{16} + 4\,044\mu^{15} + 5\,553\mu^{14} + 5\,142\mu^{13} + 3\,567\mu^{12} - 1\,734\mu^{11} - 10\,353\mu^{10} - 16\,704\mu^9 - 8\,859\mu^8 + 21\,168\mu^7 - 34\,920\mu^6.$$

Simple quadratic lattice

$$\psi_2 = \mu, \quad \psi_3 = 2\mu^2, \quad \psi_4 = \mu^4 + 6\mu^3 - 2\tfrac{1}{2}\mu^2,$$

$$\psi_5 = 2\mu^6 + 8\mu^5 + 18\mu^4 - 16\mu^3,$$

$$\psi_6 = \mu^9 + 6\mu^8 + 22\mu^7 + 40\mu^6 + 43\mu^5 - 85\mu^4 + 10\tfrac{1}{3}\mu^3,$$

$$\psi_7 = 2\mu^{12} + 8\mu^{11} + 30\mu^{10} + 72\mu^9 + 134\mu^8 + 136\mu^7 + 30\mu^6 - 400\mu^5 + 118\mu^4,$$

$$\psi_8 = \mu^{16} + 6\mu^{15} + 22\mu^{14} + 68\mu^{13} + 151\mu^{12} + 310\mu^{11} + 461\mu^{10} + 540\mu^9 + 194\tfrac{1}{2}\mu^8 - 486\mu^7 - 1\,651\mu^6 + 926\mu^5 - 52\tfrac{1}{4}\mu^4,$$

$$\psi_9 = 2\mu^{20} + 8\mu^{19} + 30\mu^{18} + 88\mu^{17} + 218\mu^{16} + 456\mu^{15} + 864\mu^{14} + 1\,340\mu^{13} + 1\,894\mu^{12} + 1\,864\mu^{11} + 1\,144\mu^{10} - 1\,420\mu^9 - 3\,986\mu^8 - 5\,664\mu^7 + 5\,992\tfrac{2}{3}\mu^6 - 872\mu^5,$$

$$\psi_{10} = \mu^{25} + 6\mu^{24} + 22\mu^{23} + 68\mu^{22} + 187\mu^{21} + 426\mu^{20} + 914\mu^{19} + 1\,728\mu^{18} + 2\,978\mu^{17} + 4\,566\mu^{16} + 6\,404\mu^{15} + 7\,372\mu^{14} + 7\,389\mu^{13} + 3\,315\mu^{12} - 3\,373\mu^{11} - 15\,480\mu^{10} - 19\,786\mu^9 - 13\,323\mu^8 + 33\,609\mu^7 - 9\,144\mu^6 + 295\tfrac{1}{5}\mu^5,$$

$$\psi_{11} = 2\mu^{30} + 8\mu^{29} + 30\mu^{28} + 88\mu^{27} + 238\mu^{26} + 560\mu^{25} + 1\,208\mu^{24} + 2\,408\mu^{23} + 4\,472\mu^{22} + 7\,572\mu^{21} + 12\,168\mu^{20} + 17\,716\mu^{19} + 23\,910\mu^{18} + 28\,744\mu^{17} + 30\,892\mu^{16} + 24\,436\mu^{15} + 11\,536\mu^{14} - 20\,332\mu^{13} - 53\,428\mu^{12} - 91\,688\mu^{11} - 66\,020\mu^{10} + 5\,112\mu^9 + 164\,790\mu^8 - 75\,640\mu^7 + 6\,520\mu^6.$$

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The density of a nonuniform system in the thermodynamic limit

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We discuss the existence, continuity, and other properties of the canonical and grand canonical density distributions in the thermodynamic limit for nonuniform classical mechanical systems. For an external potential ϕ defined on a domain Λ the free energy per unit volume for fixed temperature is given by $F(\rho_0,\phi) = \min \int_\Lambda [\rho(x)\phi(x) + f(\rho(x))]dx/V(\Lambda)$ where the minimum is over all density distributions satisfying the restriction of fixed average density ρ_0, and $f(\rho_0,\beta)$ is the free energy per unit volume in the thermodynamic limit when $\phi = 0$. We prove that if ϕ is not constant over any region of finite volume then the density distribution which minimizes is unique, and also that the density is the functional derivative of $F(\rho_0,\phi)$ with respect to ϕ. We also show that the density distribution of an infinite nonuniform system is the limit of density distributions associated with finite systems of increasing size.

1. INTRODUCTION

Recently a number of authors have treated the problem of definition and existence of the thermodynamic limit for a classical system of interacting particles influenced by an external potential.[1,2,3,4] For such a nonuniform system, the free energy and average pressure in the thermodynamic limit are determined by an extremum problem defined over all possible macroscopic density distributions. In this paper we shall be concerned with demonstrating that the macroscopic density distribution which solves the extremum problem is the limit of the density distribution sequence obtained from the partition functions associated with finite systems of increasing size. Further, we shall show that those situations in which the macroscopic density distribution solving the extremum problem is not unique are associated with thermodynamic phase transitions.

2. CANONICAL DENSITY DISTRIBUTION

We shall consider a classical system of n particles with Hamiltonian of the form

$$H_n = \frac{1}{2m}\sum_{i=1}^{n} p_i^2 + W_n(x_1,\ldots,x_n), \tag{2.1}$$

where

$$W_n(x_1,\ldots,x_n) = \sum_{i=1}^{n}\phi(x_i) + U_n(x_1,\ldots,x_n). \tag{2.2}$$

The interaction potential $U_n(x_1,\ldots,x_n)$ is translationally invariant and defined for $x_i \in R^K$ (K-dimensional Euclidean space). The external potential ϕ is defined on Λ which is a bounded subset of R^K. We shall consider a sequence of external potentials $\{(\Lambda,\phi)\}$ obtained from an initial pair (Λ_0,ϕ_0) by

$$\phi(x) = \phi_0(x/\alpha) \quad \text{and} \quad \Lambda = \alpha\Lambda_0 \tag{2.3}$$

for $\alpha = (n/n_0)^{1/K}$, $n \geq n_0$.

The free energy per unit volume is

$$-\beta\mathfrak{F}(\Lambda,n,\beta,\phi) = V(\Lambda)^{-1}\ln Z(\Lambda,n,\beta,\phi), \tag{2.4}$$

where

$$Z(\Lambda,n,\beta,\phi) = \frac{1}{n!}\int_{R^{nK}}\int_{\Lambda^n} e^{-\beta H_n}\,dp_1\cdots dp_n dx_1\cdots dx_n \tag{2.5}$$

is the canonical partition function for the nonuniform system (2.1). For each $n \geq n_0$, the canonical density distribution is given by

$$\bar{\rho}_n(x) = \frac{1}{(n-1)!}\int_{\Lambda^{n-1}} e^{-\beta W_n(x,x_2,\cdots,x_n)}dx_2\cdots dx_n \Big/ Q(\Lambda,n,\beta,\phi), \tag{2.6}$$

where $Q(\Lambda,n,\beta,\phi)$ is the configurational partition function of (2.2). The density distributions (2.6) satisfy the normalization

$$V(\Lambda)^{-1}\int_\Lambda \bar{\rho}_n(x)dx = \rho_0, \tag{2.7}$$

where $n_0 V(\Lambda_0)^{-1} = \rho_0$.

We can obtain the densities (2.6) from the free energy (2.4) by means of a functional derivative with respect to the external potential. Let $\{(\Lambda,\psi)\}$ be defined from an initial pair (Λ_0,ψ_0) as in (2.3). For convenience, let

$$q(t) = Q(\Lambda,n,\beta,\phi + t\psi), \tag{2.8}$$

where t is a real parameter. The external potentials ϕ and ψ are bounded measurable functions so that we have for the derivative with respect to t

$$q'(0) = -\frac{\beta}{n!}\int_{\Lambda^n}\sum_{i=1}^{n}\psi(x_i)e^{-\beta W_n(x_1,\cdots,x_n)}dx_1\cdots dx_n. \tag{2.9}$$

Now

$$-\beta\frac{d}{dt}\mathfrak{F}(\Lambda,n,\beta,\phi + t\psi) = V(\Lambda)^{-1}q'(t)/q(t) \tag{2.10}$$

and (2.9) give that

$$\frac{d}{dt}\mathfrak{F}(\Lambda,n,\beta,\phi + t\psi)\big|_{t=0} = V(\Lambda)^{-1}\int_\Lambda \psi(x)\bar{\rho}_n(x)dx. \tag{2.11}$$

In terms of definitions which will be given in Sec. 4, the density (2.6) is the Gateaux gradient of $\mathfrak{F}$ at ϕ. The mapping associating $\bar{\rho}_n$ with ϕ is called a gradient mapping. Interesting results related to gradient mapping are to be found in the references.

We can study the convergence of $\{\bar{\rho}_n\}$ by its behavior on the reference domain Λ_0. Define

$$\rho_{0,n}(y) = n_0\int_{\Lambda^{n-1}} e^{-\beta W_n(\alpha y,x_2,\cdots,x_n)}dx_2\cdots dx_n \Big/ \int_{\Lambda_0}\int_{\Lambda^{n-1}} e^{-\beta W_n(\alpha y,x_2,\cdots,x_n)}dy\,dx_2\cdots dx_n \tag{2.12}$$

for $y \in \Lambda_0$. Then

$$V(\Lambda)^{-1}\int_\Lambda \psi(x)\bar{\rho}_n(x)dx = V(\Lambda_0)^{-1}\int_{\Lambda_0}\psi_0(y)\rho_{0,n}(y)dy. \tag{2.13}$$

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Now if the sequence $\{\rho_{0,n}\}$ is weakly convergent for every essentially bounded measurable function ψ_0, then the weak limit provides a macroscopic density in the thermodynamic limit. We shall demonstrate in Sec. 7 that density distributions related to the thermodynamic limit of the free energy (2.4) provide the limits of the canonical density distributions (2.6). The objective of this paper is to show that the thermodynamic limit operation and differentiation with respect to the external potential can be interchanged. A similar program to find the correlation functions of a uniform system in the thermodynamic limit has been carried out by Fisher.[5] First we must consider the density distributions associated with the thermodynamic limit operation.

3. THERMODYNAMIC LIMIT

It has previously been shown that the thermodynamic limit for a nonuniform system can be defined and that a limit exists which describes macroscopic systems. If $\mathcal{F}(\Lambda, n, \beta, \phi)$ is the sequence of free energy per unit volume, then we have that

$$\lim_{\Lambda\to\infty} \mathcal{F}(\Lambda, n, \beta, \phi) = F_0(\rho_0, \phi) \tag{3.1}$$

when $nV(\Lambda)^{-1} \to \rho_0$ for $0 \le \rho_0 < \rho_{cp}$ where F_0 is the free energy per volume of a macroscopic system. The free energy per volume is defined by

$$F_0(\rho_0, \phi) = \inf\{(\rho, \phi) + F(\rho) \mid \|\rho\|_1 = \rho_0\}, \tag{3.2}$$

where

$$(\rho, \phi) = \int_\Lambda \rho(x)\phi(x)d\nu(x) \tag{3.3}$$

and

$$F(\rho) = \int_\Lambda f(\rho(x))d\nu(x) \tag{3.4}$$

with $d\nu(x) = dx/V(\Lambda)$ the normalized Lebesque measure on the domain Λ (Λ is a compact subset of K-dimensional Euclidean space and has a connected interior). The density $\rho(x)$ and external potential $\phi(x)$ are elements of the real Banach space of functions bounded and measurable with supremum norm $\|\cdot\|$. The function f which defines the functional (3.4) is the free energy per volume obtained from the uniform thermodynamic limit, and it is a continuous convex function on the interval $[0, \rho_{cp})$. We shall assume that f is lower semi-continuous on the closed interval $[0, \rho_{cp}]$. Further, the free energy function f used in this paper will include the contribution due to momentum. The result expressed by (3.1) is valid if the external potential is a step potential of the form

$$\phi_r(x) = \sum_{i=1}^{r} a_i \chi_{\Lambda_i} \tag{3.5}$$

for $\{\Lambda_i\}_{i=1}^r$ a disjoint partition of Λ or if ϕ is the uniform limit of step potentials (3.5).[6]

An important problem related to the existence of the thermodynamic limit for nonuniform systems depends on the demonstration that a density distribution which solves the minimization problem posed in (3.2) is actually the density of a macroscopic nonuniform system. The existence and uniqueness of densities which solve the minimization problem (3.2) will then be related to the phase transitions of a system influenced by external forces.

We begin with a demonstration that a density distribution which solves (3.2) for some continuous potential ϕ is related to the sequences of step potentials which approximate ϕ.

We let L denote the real Banach space of bounded measurable functions on Λ with supremum norm $\|\cdot\|$. We shall also use the real Banach space $L_1(\Lambda)$ with norm $\|\cdot\|_1$ and the Banach space $L_\infty(\Lambda)$ of essentially bounded functions. The infimum of (3.2) can be taken over all $\rho \in L_1(\Lambda)$ [notice that L is dense in $L_1(\Lambda)$].

Now let $\phi_r \to \phi$ uniformly on Λ. A step density distribution ρ_r defined over the same disjoint partition $\{\Lambda_i\}_{i=1}^r$ which defines ϕ_r is of the form

$$\rho_r(x) = \sum_{i=1}^{r} \eta_i \chi_{\Lambda_i} \tag{3.6}$$

for real numbers η_i. It was shown that there exists a sequence of step densities $\{\bar{\rho}_r\}$ where

$$\{\bar{\rho}_r\} \subset \{\rho \in L \mid \rho \ge 0, \quad \|\rho\| < \rho_{cp}, \|\rho\|_1 = \rho_0\} \tag{3.7}$$

such that

$$F_0(\rho_0, \phi_r) = (\bar{\rho}_r, \phi_r) + F(\bar{\rho}_r) \tag{3.8}$$

for all r, and

$$\lim_r F_0(\rho_0, \phi_r) = F_0(\rho_0, \phi). \tag{3.9}$$

The existence of $\{\bar{\rho}_r\}$ followed from the fact that the minimization problem (3.2) reduces to a lower semi-continuous function on a compact subset of r-dimensional Euclidean space for each ϕ_r. We extend the definition of the convex functional (3.4) by setting $f(\eta) = +\infty$ if $\eta < 0$. Observe that f now defined on $(-\infty, \infty)$ remains a lower semicontinuous convex function. This defines (3.4) on all of $L_1(\Lambda)$ with an effective domain

$$\text{dom } F = \{\rho \in L_1(\Lambda) \mid F(\rho) < +\infty\} \tag{3.10}$$

(write f as the limit of a monotonic increasing sequence of functions continuous on $[0, \infty]$ and apply Lebesque's monotone convergence theorem). The range of F is contained in $(-\infty, +\infty]$.

It has been suggested that the minimizing sequence $\{\bar{\rho}_r\}$ may be found by application of the usual Lagrange multiplier technique.[7] However, this method fails to be general enough since the required derivative of the convex function $f(\eta)$ may not exist at a countable set of points. While it has been shown that $\partial f/\partial\eta$ exists and is continuous for the case of pair interactions which include a hard core, the question of whether $\partial f/\partial\eta$ exists for more general interactions in continuous systems is not completely answered.[8] We shall give a method for determining $\{\bar{\rho}_r\}$ which does not require that the above derivative exist everywhere. If the graph of $f(\eta)$ contains linear segments then the minimizing density is not a unique function for certain external potentials.

Our next section applies some new methods of convex analysis developed by R. T. Rockafellar. See references for a complete list of further references to convex analysis.

4. A LAGRANGE MULTIPLIER METHOD

We begin with some definitions required for the subsequent discussion. Let E be a locally convex Hausdorff topological vector space over the real numbers. The Banach spaces L, $L_\infty(\Lambda)$, and $L_1(\Lambda)$ with which we shall be concerned are examples of E. E^*, the dual of E, is the set of all continuous linear functionals defined on E. If E is a Banach space then E^* can be organized as a Banach space in the usual way.[9] Let F be a proper con-

vex function defined on E with range in the real numbers. A subgradient of F at a point $u \in E$ is a $u^* \in E^*$ such that

$$F(w) \geq F(u) + u^*(w - u) \tag{4.1}$$

holds for all $w \in E$.

The set of subgradients of F at u is denoted by $\partial F(u)$. The function F is said to be Gateaux differentiable at $u \in E$ if there exists a $u^* \in E^*$ such that

$$\frac{d}{dt} F(u + tw)\,|_{t=0} = u^*(w) \tag{4.2}$$

for all $w \in E$. The unique u^* satisfying (4.2) is denoted by $\nabla F(u)$ and is called the Gateaux gradient of F at u. The Gateaux gradient and subgradient are related in that if F has a gradient $\nabla F(u)$, then $\partial F(u)$ is the singleton set $\{\nabla F(u)\}$. Let F be a proper convex function on E. The conjugate of F is defined by

$$F^*(u^*) = \sup \{u^*(u) - F(u) \mid u \in E\} \tag{4.3}$$

for each $u^* \in E^*$. The conjugate F^* is again a convex function defined on E^* organized in the usual way as a vector space over R. From the definitions (4.1) and (4.3) we obtain the relationships

$$u^* \in \partial F(u) \quad \text{if and only if} \quad F(u) + F^*(u^*) = u^*(u) \tag{4.4}$$

and

$$u \in \partial F^*(u^*) \quad \text{if and only if} \quad F^{**}(u) + F^*(u^*) = u^*(u), \tag{4.5}$$

where the second conjugate F^{**} is defined by

$$F^{**}(u) = \sup \{u^*(u) - F^*(u^*) \mid u^* \in E^*\}, \tag{4.6}$$

and the set $\partial F^*(u^*)$ of subgradients of F^* at $u^* \in E^*$ is defined by

$$F^*(w^*) \geq F^*(u^*) + (w^* - u^*)(u) \tag{4.7}$$

holding for all $w^* \in E^*$.

Now let E^* also be a locally convex Hausdorff topological vector space over the reals and let E^{**} be the dual. The space E is reflexive if every $u^{**} \in E^{**}$ is of the form

$$u^{**}(u^*) = u^*(u) \tag{4.8}$$

for some $u \in E$. If E is reflexive, then E and E^* are duals of each other. If E^*, the dual space of E, can be given a locally convex Hausdorff topology so that E becomes the dual space of E^* according to (4.8), then the topologies of E and E^* are admissible to the theory of conjugate convex functions. For the application we consider, the Banach space $L_1(\Lambda)$ as E and $L_\infty(\Lambda)$ as E^* are duals if each has the weak topology induced on it by the other under the bilinear form

$$(u, u^*) = \int_\Lambda u(x)u^*(x)d\nu(x) \tag{4.9}$$

for $u \in L_1(\Lambda)$, $u^* \in L_\infty(\Lambda)$.[10] We can also allow $L_1(\Lambda)$ to have its $\|\cdot\|_1$ topology so that $L_\infty(\Lambda)$ is its dual, and let $L_\infty(\Lambda)$ have the weak* topology so that $L_1(\Lambda)$ is its dual.[11] Let E be admissible then we have the following remarkable theorem.[12]

Theorem 4.1: If F is a lower semicontinuous proper convex function on E, then

$$F^{**}(u) = F(u) \quad \text{for all } u \in E. \tag{4.10}$$

This theorem is also an if and only if statement in that if (4.10) holds, then the proper convex function F is lower semicontinuous in the topology which makes E admissible. Further, the conjugate F^* is always lower semicontinuous in the topology of E^* even if F is not lower semicontinuous.

Rockafellar has derived the following Lagrange multiplier method.[13] Suppose we wish to minimize the proper convex function $h(u)$ subject to the constraints

$$w_i^*(u) - c_i \geq 0, \quad c_i \in R (i = 1, \ldots, K). \tag{4.11}$$

Then this problem is the same as minimizing $h + g$ on E where g is 0 at all solutions of (4.11) and $+\infty$ elsewhere. Let h be finite and continuous at some solution of (4.11). Then h attains its minimum subject to (4.11) at $\bar{u}$ if and only if $-u^* \in \partial h(\bar{u})$ for some $u^* \in \partial g(\bar{u})$. Now $u^* \in \partial g(\bar{u})$ if and only if the linear functional u^* attains its maximum on (4.11) at $\bar{u}$. These statements are equivalent to the existence of real numbers $\lambda_1, \ldots, \lambda_K$ and a $\bar{u}$ satisfying

$$\lambda_i \geq 0, \quad w_i^*(\bar{u}) - c_i \geq 0, \quad \lambda_i[w_i^*(\bar{u}) - c_i] = 0,$$

and

$$u^* = -(\lambda_1 w_1^* + \cdots + \lambda_K w_K^*). \tag{4.12}$$

The above method can be applied to solving (3.2) by letting

$$h(\rho) = (\rho, \phi) + F(\rho) \tag{4.13}$$

and replacing the restriction $\|\rho\|_1 = \rho_0$ by the pair of inequalities

$$(\rho, I) - \rho_0 \geq 0 \quad \text{and} \quad (\rho, -I) + \rho_0 \geq 0 \tag{4.14}$$

where $I = \chi_\Lambda$. Since $F(\rho)$ is continuous in the interior of its effective domain with respect to the supremum norm, we let $\rho \in L$. The Banach space L is not reflexive in its supremum norm, but this property is not needed here. Notice that every $\phi \in L_1(\Lambda)$ provides a continuous linear functional $\phi^* \in L^*$ defined by

$$\phi^*(\rho) = (\rho, \phi) \quad \text{on } L. \tag{4.15}$$

However, not every $\phi^* \in L^*$ is of the form (4.15). This means that $L_1(\Lambda)$ is identified with a subspace of L^*. From (4.11) and (4.12) we find that $h(\rho)$ takes a minimum at $\bar{\rho} \in L$ with $\|\bar{\rho}\|_1 = \rho_0$ if and only if there exists a real number λ such that

$$\lambda[\|\bar{\rho}\|_1 - \rho_0] = 0 \quad \text{and} \quad \lambda I^* \in \partial h(\bar{\rho}) \tag{4.16}$$

where $I^* = (\cdot, I)$. Rockafellar has shown that if F_1 and F_2 are proper convex functions on E such that there exists a point where both functions are continuous then for all $u \in E$

$$\partial(F_1 + F_2)(u) = \partial F_1(u) + \partial F_2(u). \tag{4.17}$$

Since $\nabla\phi^*(\rho)$ exists for (4.15) and equals ϕ^*, we have that the second part of (4.16) becomes

$$\lambda I^* \in \partial h(\bar{\rho}) = \phi^* + \partial F(\bar{\rho}). \tag{4.18}$$

Proposition 4.1: Suppose that λ and $\bar{\rho} \in L$ satisfy (4.16). Further, suppose that the Gateaux gradient $\nabla F(\bar{\rho})$ exists and has the form $(\cdot, \nabla F(\bar{\rho}))$ on L. Then the problem (3.2) is solved by $\bar{\rho}$ where $\bar{\rho}$ satisfies

$$\lambda I = \phi + \nabla F(\bar{\rho}) \tag{4.19}$$

almost everywhere on Λ.

It is to be expected that if $\bar{\rho}$ equals the points in $[0, \rho_{cp}]$ at which the derivative $f'(\eta)$ does not exist only on a subset of Λ with measure zero then

$$\nabla F(\bar{\rho}) = f'(\bar{\rho}). \tag{4.20}$$

When ϕ is a step potential (3.5), then the minimization problem (3.2) can be solved in the finite dimensional space $E = R^r$. For this case $E^* = R^r$ and there is no difficulty with the representation of subgradients of F since they are elements of R^r. It is tempting to consider (4.18) for $\rho \in E = L_1(\Lambda)$ since then every continuous linear functional on E is representable by an element of $L_\infty(\Lambda)$, i.e., $E^* = L_\infty(\Lambda)$. However, some of the most important F are not continuous in their domain as a subset of $L_1(\Lambda)$. The continuity required in (4.16) and (4.17) would not be obtained. To demonstrate an F discontinuous in the $\|\cdot\|_1$ topology let $\rho_{cp} < +\infty$ for f where

$$\lim_{\eta \to \rho_{cp}} f(\eta) = +\infty \quad (\eta < \rho_{cp}). \tag{4.21}$$

Consider dom F as a subset of $L_1(\Lambda)$. Now $\rho \in$ dom F cannot be an interior point for the $\|\cdot\|_1$ topology, and F cannot be continuous in this topology. If $\rho_{cp} = +\infty$, then the convex function $f(\eta)$ continuous on $[0, \infty)$ satisfies

$$f(\eta) \geq \eta[\ln\eta - 1 - \beta B + \tfrac{K}{2}\ln(\beta/2\pi m)]/\beta \tag{4.22}$$

with B from the stability property.

Again the functional F is not bounded in any $L_1(\Lambda)$ neighborhood, however small. Now if the convex function f is bounded on $[0, \rho_{cp}]$ for ρ_{cp} finite then F satisfies a Lipschitz condition on its effective domain as a subset of $L_1(\Lambda)$ and so F is continuous in this case.

Although different f as defined above seem to yield functionals F with different properties when defined on $L_1(\Lambda)$, they do have the following common property.

Theorem 4.2: The proper convex functional $F(\rho)$ defined on $L_1(\Lambda)$ is lower semicontinuous on its convex effective domain. The proof of Theorem 4.2 is obtained as a consequence of Theorem 5.1 which was proven by Rockafellar. A direct proof can be obtained by using the fact that f satisfies a Lipschitz condition over every closed interval contained in $[0, \rho_{cp})$. Observe that Theorem 4.2 also shows that F is lower semicontinuous on $L_\infty(\Lambda)$. Just apply the norm $\|\cdot\|_1$ to $L_\infty(\Lambda)$ as a subspace of $L_1(\Lambda)$ and use $\|\rho - \rho'\|_1 \leq \|\rho - \rho'\|_\infty$ for $\nu(\Lambda) = 1$. Applying convexity along with semicontinuity, we have that

$$\liminf_{\rho' \to \rho} F(\rho') = F(\rho) \tag{4.23}$$

for $\rho', \rho \in$ dom F, where convergence of ρ' to ρ can be in $L_1(\Lambda)$ or $L_\infty(\Lambda)$. The application of (4.22) is immediate since $F(\rho) + (\rho, \phi)$ is also lower semicontinuous on dom F and therefore will take its minimum on compact subsets of dom F. Since compactness and sequential compactness are equivalent concepts in metric spaces, the limit in dom F of any convergent subsequence of $\{\bar{\rho}_r\}$ defined by (3.8) provides a density distribution which solves (3.2). Note that the set $\|\rho\|_1 = \rho_0$ is not compact in $L_1(\Lambda)$ so that we cannot apply lower semicontinuity directly here.

In the next section with the use of a theorem by R. T. Rockafellar we shall see that F is also lower semicontinuous in the weak topology of $L_1(\Lambda)$ and lower semicontinuous in the weak* topology of $L_\infty(\Lambda)$. First we shall give a description of some of the subgradients of F required in solving the Lagrange multiplier characterization of (3.2).

5. SUBGRADIENTS AND EQUIVALENCE OF ENSEMBLES

It has been proven that the average pressure associated with the thermodynamic limit of the grand canonical ensemble is given by

$$P(\mu, \beta, \phi) = \sup\{(\rho, \mu - \phi) - F(\rho) \,|\, \rho \in L_1(\Lambda)\}, \tag{5.1}$$

where μ is the chemical potential.[14] Here the contribution of the momentum to the free energy is included in F which also depends on β. In terms of conjugates for $\rho \in L_1(\Lambda)$ and $\phi \in L_\infty(\Lambda)$, we have

$$P(\mu, \beta, \phi)\ ) = F^*(\mu - \phi). \tag{5.2}$$

In case that $F(\rho)$ is a lower semicontinuous proper convex functional (Theorem 4.1), we also have

$$F(\rho) = \sup\{(\rho, \phi) - F^*(\phi) \,|\, \phi \in L_\infty(\Lambda)\} \tag{5.3}$$

for $\rho \in L_1(\Lambda)$.

Now a remarkable demonstration by Rockafellar directly applicable to our problem is the following: Let E and E^* be any pair of the three Banach spaces L, L_∞, L_1; and let each of E and E^* as real vector spaces have the weak topology induced on it by the other so that they are duals under the bilinear form (3.3).

Then we have

Theorem 5.1: (Rockafellar): Let f be a lower semicontinuous closed proper convex function on R. Let f^* be the conjugate of f defined by

$$f^*(\xi) = \sup\{\eta\xi - f(\eta) \,|\, \eta \in R\} \tag{5.4}$$

for $\xi \in R$. (f^* has automatically the same properties as assumed for f.) Then

$$F^*(\phi) = \int_\Lambda f^*(\phi(x))d\nu(x) \tag{5.5}$$

for $\phi \in E^*$ and $F(\rho)$ for $\rho \in E$ are convex conjugates of each other. [A lower semicontinuous function is closed if $\{\eta \,|\, f(\eta) \leq \lambda\} \cap$ dom f is a closed subset of R for every real number λ. This is the case for our f[15].]

Hence the conjugate integrands f and f^* provide conjugate convex functionals. Furthermore, F and F^* are automatically lower semicontinuous by Theorem 4.1. For uniform thermodynamic systems it has been shown that

$$p(\mu, \beta) = \sup_{0 \leq \eta \leq \rho_{cp}} [\mu\eta - f(\eta, \beta)], \tag{5.6}$$

where $p(\mu, \beta)$ is the average pressure.[16] Now if f and p are convex conjugates of each other, then

$$P(\mu, \beta, \phi) = \int_\Lambda p(\mu - \phi(x), \beta)d\nu(x) \tag{5.7}$$

and (5.3) holds. With these results in mind we shall say that the canonical and grand canonical ensembles for a nonuniform system are equivalent for $\mu, \phi, \bar{\rho}$ if the following thermodynamic relation holds:

$$F^*(\mu - \phi) = (\bar{\rho}, \mu - \phi) - F(\bar{\rho}). \tag{5.8}$$

This relation holds if and only if

$$\mu I - \phi \in \partial F(\bar{\rho}) \tag{5.9}$$

or, equivalently,

$$\bar{\rho} \in \partial F^*(\mu - \phi). \tag{5.10}$$

These statements are clearly the same as those which describe the Lagrange multiplier solution of the minimization problem (3.2). The only difference appearing to be the function spaces used. Returning to the original derivation of (5.1), we find that $L_1(\Lambda)$ in (5.1) can be replaced by L since our ϕ is bounded and measurable. Then $\rho \in L$ and $\phi^* \in L^*$ where ϕ^* has the representation (4.15), and L^* takes the weak* topology induced on it by L. Therefore, the Lagrange multiplier in (4.18) and the chemical potential play the same role. In order to study the existence and uniqueness of $\bar{\rho}$ we shall need more specific information about the subgradients involved.

Let E be any of the three Banach spaces L, L_∞, L_1 and $t \in R$. Define the right-hand Gateaux derivative (directional derivative) by

$$F'_R(\rho_1;\rho) = \lim_{t \downarrow 0} [F(\rho_1 + t\rho) - F(\rho_1)]/t \tag{5.11}$$

for $\rho_1, \rho \in E$. If $\rho_1 \in \text{dom } F$ and $\rho_1 + t'\rho \in \text{dom } F$ some $t' > 0$, then the derivative (5.11) exists since the function $F(\rho_1 + t\rho)$ is finite and convex in t for some interval $[0, t']$. Furthermore, $F'_R(\rho_1; \cdot)$ is a proper convex functional on E since it is bounded below. For $\rho_1 \in \text{dom } F$, according to Rockafellar, we have that

$$\phi^* \in \partial F(\rho_1) \quad \text{if and only if} \quad F'_R(\rho_1;\rho) \geq \phi^*(\rho) \tag{5.12}$$

all $\rho \in E$.[17] Now the left-hand derivative $f'_L(\eta)$ and the right-hand derivative $f'_R(\eta)$ of f exist on $[0, \rho_{cp})$ and are monotone increasing functions satisfying $f'_L(\eta) \leq f'_R(\eta)$. They are equal, and their common value is the derivative of f except on at most a countable set $\{\xi\}$. We can extend the definition of the derivative of f to all of R by taking $f'(\eta) = +\infty$ if $\eta \geq \rho_{cp}$ and $f'(\eta) = -\infty$ if $\eta < 0$. Here the condition (4.21) is assumed. Furthermore,

$$f(\eta) \geq f(\eta_1) + b_1(\eta - \eta_1) \quad \text{for } \eta \in R \tag{5.13}$$

and any $b_1 \in [f'_L(\eta_1), f'_R(\eta_1)]$. If η_1 is not equal to one of the points $\{\xi\}$, then the interval indicated is a single point equal to the derivative of f at η_1. We shall demonstrate that $f'_R(\rho_1(x))$ and $f'_L(\rho_1(x))$ often yield subgradients of F for $\rho_1 \in \text{dom } F$.

Let $\rho_1 \in \text{dom } F$ and suppose that $\rho_1 + t \in \text{dom } F$ for some sufficiently small $t > 0$. Then it follows by the Lebesque convergence theorems that $f'_R(\rho_1) \in L_1(\Lambda)$. Now suppose that $\rho_1 - t \in \text{dom } F$ for some sufficiently small $t > 0$. Then we find that $f'_L(\rho_1) \in L_1(\Lambda)$. Furthermore, if ρ_1 is a $\|\cdot\|_\infty$ interior point of dom F then $f'_L(\rho_1)$, $f'_R(\rho_1) \in L_\infty(\Lambda)$. Note that the $\|\cdot\|_\infty$ interior of dom F is nonempty. Now for $\rho_1 \in \text{dom } F$, inequality (5.13) gives

$$F(\rho_1 + t\rho) \geq F(\rho_1) + (\rho, \psi)t \tag{5.14}$$

for $\rho \in E$ and $t \in R$, where ψ is any ν-measurable function defined on Λ such that

$$f'_L(\rho_1) \leq \psi \leq f'_R(\rho_1) \tag{5.15}$$

holds a.e. on Λ. Hence

$$F'_R(\rho_1;\rho) \geq (\rho, \psi) \tag{5.16}$$

for $\rho \in E$. Now if E is $L_\infty(\Lambda)$ and $\rho_1 \pm t \in \text{dom } F$ for some sufficiently small $t > 0$, then $\psi \in L_1(\Lambda)$ and both sides of inequality (5.16) are finite. We evidently have a stronger result regarding the existence of the Gateaux gradient.

The left-hand Gateaux derivative is defined by

$$F'_L(\rho_1;\rho) = -F'_R(\rho_1; -\rho) \tag{5.17}$$

for $\rho_1 \in \text{dom } F$ and $\rho \in E$. Now consider F defined on $L_\infty(\Lambda)$ and suppose that ρ_1 is an interior point of dom F such that $f'(\rho_1)$ exists on Λ except perhaps for a set of measure zero. Since f satisfies a Lipschitz condition on every closed interval contained in $[0, \rho_{cp})$ and $f'(\rho_1) \in L_\infty(\Lambda)$, the Lebesque dominated convergence theorem can be applied to show that

$$F'_L(\rho_1;\rho) = (\rho, f'(\rho_1)) = F'_R(\rho_1;\rho) \tag{5.18}$$

for $\rho \in L_\infty(\Lambda)$. This verifies the validity of (4.20), and $f'(\rho_1)$ is the Gateaux gradient of F at ρ_1. The inequality (5.15) can be used to solve (5.8) or (4.16).

Proposition 5.1: Let F be defined on $L_\infty(\Lambda)$. Suppose that there exist $\bar{\rho} \in \text{dom } F$ and μ such that

$$f'_L(\bar{\rho}) \leq \mu - \phi \leq f'_R(\bar{\rho}) \tag{5.19}$$

holds a.e. on Λ. Then (5.8) holds and the ensembles are equivalent for μ, ϕ, and $\bar{\rho}$.

Proof: apply (5.16) and (5.12).

This completes our investigation of the condition (5.9) and the subgradients of F. In the next section we consider the equivalent condition (5.10) and relate it to equivalence of ensembles.

6. THE EXISTENCE AND UNIQUENESS OF DENSITY DISTRIBUTIONS

In previous sections we described the relationship between the chemical potential μ and a minimizing density $\bar{\rho}$. However, we have not proven the existence of $\bar{\rho}$ which solves (3.2). We shall investigate requirements for existence. From Proposition 5.1, we observe that it is not difficult to have situations where $\bar{\rho}$ is not unique. In this section we shall also describe conditions on the potential ϕ which make $\bar{\rho}$ unique when it exists. The study of uniqueness amounts to a study of the linear sections of the graph of $f(\eta)$ which in turn are responsible for the multivaluedness of the subgradients $\partial F^*(\mu - \phi)$.

In the next proposition we consider the situation $\rho \in L_\infty(\Lambda)$ and $\phi \in L_1(\Lambda)$. Let $L_1(\Lambda)$ have the weak topology induced by $L_\infty(\Lambda)$ and let $L_\infty(\Lambda)$ have the weak* topology induced by $L_1(\Lambda)$. In these topologies, the spaces $L_1(\Lambda)$ and $L_\infty(\Lambda)$ are duals with respect to (3.3).

Proposition 6.1: Suppose that f is lower semicontinuous and has a finite hard core packing density ρ_{cp}. Let the external potential ϕ be the uniform limit of a sequence of step potentials (3.5). Then there exists a minimizing density for (3.2). Furthermore, the weak* limits of the sequence (3.7) provide densities at which (3.2) takes a minimum.

Proof: Corresponding to the sequence of step potentials (3.5), we define sets of step densities.

$$D_r = \{\rho \geq 0 \mid \rho = \sum_{i=1}^{r} \eta_i \chi_{\Lambda_i}, \|\rho\|_1 = \rho_0\} \tag{6.1}$$

for $0 \leq \rho_0 < \rho_{cp}$. Now let $D = \overline{\bigcup_r D_r}$ be the weak* closure

of the union. Note that D is the intersection of all weak* closed sets containing $UD_\gamma \subset L_\infty(\Lambda)$, and D contains all limits of weakly convergent sequences in D. Define

$$S = \{\rho \in L_\infty(\Lambda) \mid \|\rho\|_\infty \leq \rho_{cp} < \infty\}. \tag{6.2}$$

According to the theorem of Alaoglu, the sphere S is closed and compact in the weak* topology of $L_\infty(\Lambda)$. This makes $D \cap S$ a weak* closed and compact subset. Now in view of what has been proven, we have

$$F_0(\rho_0, \phi) = \inf\{(\rho, \phi) + F(\rho) \mid \rho \in D \cap S\}. \tag{6.3}$$

We originally demonstrated (6.3) where D was the closure in L of UD_γ. The weak* closure of UD_γ contains the closure of UD_γ in L. Notice that if $\rho \geq 0$ a.e. on Λ is a weak* accumulation point of UD_γ then $\|\rho\|_1 = \rho_0$ since there exists a sequence $\rho_s \in D_s$ such that $(\rho_s, I) \to (\rho, I)$. The weak* closed set D will not include points which do not satisfy $\|\rho\|_1 = \rho_0$.

These facts justify the restatement of (3.2) in form (6.3). Now by Rockafellar's results, the functional F is lower semicontinuous in the weak* topology of $L_\infty(\Lambda)$ so that $(\rho, \phi) + F(\rho)$ is also lower semicontinuous. Since a lower semicontinuous function defined on a compact set always assumes its minimum, there exists a $\bar{\rho}$ in the weak* compact set $D \cap S$ such that[18]

$$F_0(\rho_0, \phi) = (\bar{\rho}, \phi) + F(\bar{\rho}). \tag{6.4}$$

Further suppose that $\{\bar{\rho}_s\}$ is a weakly convergent subsequence of $\{\bar{\rho}_\gamma\}$ defined in (3.8). That is, $(\bar{\rho}_s, \psi) \to (\bar{\rho}, \psi)$ for every $\psi \in L_1(\Lambda)$. Then $\bar{\rho} \in D$ since $\bar{\rho}_s \in D_s$. Now lower semicontinuity of F in the weak* topology gives

$$\liminf_s F(\bar{\rho}_s) \geq \liminf_{\rho' \to \bar{\rho}} F(\rho') = F(\bar{\rho}). \tag{6.5}$$

Therefore,

$$F_0(\rho_0, \phi) = \liminf_s [(\bar{\rho}_s, \phi) + F(\bar{\rho}_s)]$$

$$\geq \liminf_s (\bar{\rho}_s, \phi) + \liminf_s F(\bar{\rho}_s) \geq (\bar{\rho}, \phi) + F(\bar{\rho}). \tag{6.6}$$

Observe that $\bar{\rho} \in S$, otherwise the finiteness of $F_0(\rho_0, \phi)$ is contradicted.

Hence, also,

$$(\bar{\rho}, \phi) + F(\bar{\rho}) \geq F_0(\rho_0, \phi). \tag{6.7}$$

Finally, the assumption that $\{\bar{\rho}_\gamma\}$ actually has a weakly convergent subsequence is valid for the following reason. Since Λ is a compact subset of R^K the space $L_1(\Lambda)$ is separable, and the closed sphere S considered as a topological subspace of $L_\infty(\Lambda)$ in the weak* topology is a compact metric space.[19] Then $D \cap S$ is a compact subset of a metric space S. Hence $D \cap S$ is a closed and sequentially compact subset of S. Since $\{\bar{\rho}_\gamma\}$ is contained in $D \cap S$, this sequence must have a weakly convergent subsequence with some limit $\bar{\rho}$ in $D \cap S$. This completes the proof of the proposition.

In case $\rho_{cp} = +\infty$, the above method can be applied if $\{\bar{\rho}_\gamma\}$ has a subsequence bounded in $L_\infty(\Lambda)$. We can then take a sphere S which contains the bounded subsequence and apply the above argument to $D \cap S$. For the case $\rho_{cp} = +\infty$ it appears useful to consider the problem (3.2) for $\rho \in L_1(\Lambda)$ and $\phi \in L_\infty(\Lambda)$ with each space having the weak topology. A prerequisite that $\{\bar{\rho}_\gamma\}$ be weakly sequentially compact in $L_1(\Lambda)$ is that it be bounded in norm. This is automatic since $\|\bar{\rho}_\gamma\|_1 = \rho_0$. If we take the weak closure of $\{\bar{\rho}_\gamma\}$, then the weak closure of $\{\bar{\rho}_\gamma\}$ is a weak compact subset of $L_1(\Lambda)$ if and only if $\{\bar{\rho}_\gamma\}$ is weakly sequentially compact (see p. 430, Dunford–Schwartz). We most likely cannot expect $\{\bar{\rho}_\gamma\}$ to yield a $\bar{\rho} \in L_1(\Lambda)$ satisfying (6.4) unless this sequence has at least one weakly convergent subsequence. We shall consider this problem along with the uniqueness problem.

We shall now consider the minimization problem (3.2) from the viewpoint of the pressure (5.1). For convenience we write $\psi = \mu - \phi$. We are interested in the case $\|\psi\| < +\infty$. We consider densities at which the following assumes its minimum:

$$F^*(\psi) = -\inf\{F(\rho) - (\rho, \psi) \mid \rho \in L_1(\Lambda)\}. \tag{6.8}$$

In the case ρ_{cp} finite, the space $L_1(\Lambda)$ can obviously be replaced by $\rho \in L_\infty(\Lambda)$ satisfying $\|\rho\|_\infty \leq \rho_{cp}$, and minimizing densities exist since F is weak* lower semicontinuous on the weak* compact sphere (6.2). For $\rho_{cp} = +\infty$, in view of the bound (4.22), there exists an $a < \rho_{cp}$ such that

$$f(a) - a\|\psi\| = \delta > 0 \tag{6.9}$$

and such that

$$f(\eta') - \eta'\psi(x) \geq f(\eta) - \eta\psi(x) \geq \delta > 0 \tag{6.10}$$

holds for $\eta' \geq \eta \geq a$ and all $x \in \Lambda$. Inequality (6.10) also follows from convexity of f.

Let $\rho \in L_1(\Lambda) \cap \text{dom } F$ and define $\Lambda_a = \{x \mid \rho > a\}$. If $\nu(\Lambda_a) \neq 0$ then $\|\rho\|_\infty > a$ and conversely. Using inequality (6.10) we have

$$\int_{\Lambda_a} [f(\rho) - \rho\psi] d\nu \geq \delta\nu(\Lambda_a) > 0. \tag{6.11}$$

Let $\rho_a = \rho\chi_{\Lambda - \Lambda_a} + a\chi_{\Lambda_a}$ on Λ, then

$$F(\rho_a) - (\rho_a, \psi) \leq F(\rho) - (\rho, \psi). \tag{6.12}$$

We conclude that

$$F^*(\psi) = -\inf\{F(\rho) - (\rho, \psi) \mid \|\rho\|_\infty \leq a\} \tag{6.13}$$

and that there exists a $\bar{\rho} \in L_\infty(\Lambda)$ such that

$$F^*(\psi) = (\bar{\rho}, \psi) - F(\bar{\rho}). \tag{6.14}$$

We can at least solve (3.2) for $\rho_0 = \|\bar{\rho}\|_1$ associated with μ and satisfying (6.14).

We now investigate the uniqueness of $\bar{\rho}$ satisfying (6.14) by using the condition $\bar{\rho} \in \partial F^*(\psi)$. This is the condition (5.10) given previously. Our approach will be to construct $\partial F^*(\psi)$ from f which is defined as a lower semicontinuous proper convex function on the real numbers R. It will be demonstrated that linear sections of the graph of f are responsible for the multivalued nature of the subgradients of F^*. We have the following interesting chain of equivalent statements:

$$\eta_1 \in \partial f^*(\xi_1) \iff f^*(\xi) \geq f^*(\xi_1) + \eta_1(\xi - \xi_1) \tag{6.15}$$

$$\iff \eta_1 \in [f_L^{*\prime}(\xi_1), f_R^{*\prime}(\xi_1)] \tag{6.16}$$

$$\iff f(\eta_1) + f^*(\xi_1) = \eta_1\xi_1 \tag{6.17}$$

$$\iff \xi_1 \in [f_L'(\eta_1), f_R'(\eta_1)], \tag{6.18}$$

$$\xi_1 \in \partial f(\eta_1) \iff f(\eta) \geq f(\eta_1) + (\eta - \eta_1)\xi_1 \tag{6.19}$$

for $\xi, \eta \in R$. The proper convex functions f and f^* are conjugates. The convex conjugate f^*, being lower semicontinuous in R and finite in every bounded open interval, is therefore continuous in every bounded open interval. Let $\psi \in L_\infty(\Lambda)$. Rockafellar has shown that $f^*(\psi)$ is a measurable function.[20] Let $\rho_1 \in L_1(\Lambda)$ and suppose that $\rho_1 \in \partial f^*(\psi_1)$ for every $x \in \Lambda$. If ψ_1 is bounded then ρ_1 is also bounded. Using (6.15) and Theorem 5.1 gives

$$F^*(\psi) \geq F^*(\psi_1) + (\rho_1, \psi - \psi_1) \tag{6.20}$$

and $\rho_1 \in \partial F^*(\psi_1)$ follows.

The graph of f has a linear section over the interval $[\eta_1, \eta_2] \subset [0, \rho_{cp})$ if

$$f(\eta) = f(\eta_1) + \xi_1(\eta - \eta_1) \tag{6.21}$$

for all $\eta \in [\eta_1, \eta_2]$ and some $\xi_1 \in R$. If f has a linear section of slope ξ_1, we denote by $I(f, \xi_1)$ the largest closed interval $[\eta_1, \eta_2]$ over which f is linear with slope ξ_1. Since $f_L'(\eta)$ is left-continuous and $f_R'(\eta)$ is right-continuous, the interval $I(f, \xi_1)$ can be found from

$$\eta_1 = \inf\{\eta \mid f_R'(\eta) = \xi_1\} \quad \text{and} \quad \eta_2 = \sup\{\eta \mid f_L'(\eta) = \xi_1\} \tag{6.22}$$

using the facts that $f_L'(\eta) \leq f_R'(\eta)$ on R and $f_L'(\eta_2) \geq f_R'(\eta_1)$ if $\eta_2 > \eta_1$. Notice that η_1 and η_2 defined in (6.22) satisfy $\eta_2 \geq \eta_1$; and if $\eta_2 > \eta_1$, then $[\eta_1, \eta_2]$ must be an interval over which f is linear with slope ξ_1. The fact that f_L' and f_R' are increasing is also used. Then

$$I(f, \xi_1) = [\eta_1, \eta_2] \tag{6.23}$$

for the interval of (6.22). Notice that (6.22) gives either a point or a closed interval for every ξ_1. With this definition we have the following useful fact.

Lemma 6.1: Suppose that f has a linear section over $I(f, \xi_1)$. Then

$$f(\eta) + f^*(\xi_1) = \eta\xi_1 \tag{6.24}$$

for all $\eta \in I(f, \xi_1)$.

Proof: Let $I(f, \xi_1) = [\eta_1, \eta_2]$. The line $f(\eta_1) + \xi_1(\eta - \eta_1)$ is a supporting line for f and, since the interval $[\eta_1, \eta_2]$ is maximal, $f(\eta) > f(\eta_1) + \xi_1(\eta - \eta_1)$ if $\eta \notin [\eta_1, \eta_2]$. Thus

$$\inf_\eta [f(\eta) - \eta\xi_1] = f(\eta_1) - \eta_1\xi_1 = f(\eta) - \eta\xi_1$$

for $\eta \in [\eta_1, \eta_2]$ which completes the proof.

According to Lemma 6.1 and (6.17) it must be true that

$$I(f, \xi_1) \subset \partial f^*(\xi_1). \tag{6.25}$$

With (6.24) in mind, if there is only one $\eta_1 \in \partial f^*(\xi_1)$ we define $I(f, \xi_1) = \{\eta_1\}$.

Now let $\partial f^*(\xi_1) = [\eta_L, \eta_R]$ as in (5.16). Then

$$f(\eta) = f(\eta_L) + (\eta - \eta_L)\xi_1 \tag{6.26}$$

for all $\eta \in [\eta_L, \eta_R]$ and this implies

$$\partial f^*(\xi_1) \subset I(f, \xi_1). \tag{6.27}$$

We conclude that the relationship between linear sections and subgradients must be

$$\partial f^*(\xi) = I(f, \xi) \quad \text{and} \quad \partial f(\eta) = I(f^*, \eta). \tag{6.28}$$

Next consider what (6.28) has to do with uniqueness of the $\bar{\rho}$ which minimize, i.e., densities at which the ensembles are equivalent. Define the measurable sets

$$\Lambda_\xi = \{x \in \Lambda \mid \psi(x) = \xi\}. \tag{6.29}$$

Assume $I(f, \xi)$ is an interval and $\nu(\Lambda_\xi) > 0$. For η_1, η_2 in $I(f, \xi)$ and $\eta_1 < \eta_2$ let

$$\bar{\rho}_1 = \bar{\rho}\chi_{\Lambda - \Lambda_\xi} + \eta_1\chi_{\Lambda_\xi} \quad \text{and} \quad \bar{\rho}_2 = \bar{\rho}\chi_{\Lambda - \Lambda_\xi} + \eta_2\chi_{\Lambda_\xi}. \tag{6.30}$$

Now $\|\bar{\rho}_1 - \bar{\rho}_2\|_1 = |\eta_1 - \eta_2|\,\nu(\Lambda_\xi) > 0$ and

$$F^*(\psi) = (\bar{\rho}_1, \psi) - F(\bar{\rho}_1) = (\bar{\rho}_2, \psi) - F(\bar{\rho}_2). \tag{6.31}$$

This makes it clear that two different densities can yield the same average pressure and even the same pressure distribution. In this example, the free energy distributions are different; however, it is possible to introduce more linear sections and sets (6.29) of nonzero measure so that average pressure and free energy are the same for distinctly different densities. These ideas motivate the following definitions on the behaviour of external potentials.

Definition 6.1: We say that the ν-measurable function ψ on Λ is of continuous measure at $\xi \in R$ if $\nu(\Lambda_\xi) = 0$, and ψ is of continuous measure on R if $\nu(\Lambda_\xi) = 0$ for all $\xi \in R$.

Notice that if ξ is a measure discontinuity of ψ [i.e., $\nu(\Lambda_\xi) > 0$] then $\mu - \xi$ is a measure discontinuity of ϕ.

We shall want to find $\bar{\rho}$ pointwise so that

$$f(\bar{\rho}) + f^*(\psi) = \bar{\rho}\psi \quad \text{on } \Lambda. \tag{6.32}$$

Since ψ is bounded and $f(\eta) - \eta\psi$ is lower semicontinuous on R for each $x \in \Lambda$, a bounded $\bar{\rho}$ does exist satisfying (6.32). The difficulty is that we cannot always be sure that $\bar{\rho}$ found in this way is ν-measurable.

Now $\psi_\tau \to \psi$ uniformly on Λ, and for each ψ_τ there exists a measurable step density $\bar{\rho}_\tau$ satisfying (6.32) with ψ_τ. Let $\bar{\rho}$ be either of the measurable limit functions

$$\lim_\tau \inf\, \bar{\rho}_\tau(x) \quad \text{or} \quad \lim_\tau \sup\, \bar{\rho}_\tau(x). \tag{6.33}$$

These functions are bounded above by ρ_{cp}. For fixed $x \in \Lambda$ there is a subsequence $\{\bar{\rho}_K\}$ such that $\bar{\rho}_K \to \bar{\rho}$. Then by continuity

$$\lim_K f(\bar{\rho}_K) = f(\bar{\rho}) \quad \text{and} \quad \lim_K f^*(\psi_K) = f^*(\psi)$$

for this $x \in \Lambda$. The limits (6.33) evidently are measurable $\bar{\rho}$ conforming to (6.32).

Lemma 6.2: Suppose that $f(\eta)$ has no linear sections or that if $f(\eta)$ has linear sections then $\xi_1 \in R$ is not the slope of f on any linear section. Then η_1 such that $f(\eta_1) + f^*(\xi_1) = \eta_1\xi_1$ is unique.

Proof: Now obvious from $\eta_1 \in \partial f^*(\xi_1) = I(f, \xi_1)$ and the set $\partial f^*(\xi_1)$ being a singleton set.

Theorem 6.1: Suppose that f has no linear sections or that ψ on Λ does not equal (except for a set of measure zero) the slope of f on any linear sections. Then $\bar{\rho}$ is unique.

Proof: A measurable $\bar{\rho}$ satisfying

$$f(\bar{\rho}) + f^*(\psi) = \bar{\rho}\psi$$

at each point $x \in \Lambda$ is unique by Lemma 6.2. The next theorem is more general.

Theorem 6.2: Suppose that the slopes of linear sections of f and points where ψ is of discontinuous measure do not coincide. Then $\bar{\rho}$ satisfying (6.14) is unique.

Proof: The proper convex function f can have at most a countable set of distinct linear sections. Let $\{\xi\}$ be the countable set of slopes associated with linear sections of f. Now $\nu(\Lambda_\xi) = 0$ for each ξ by assumption. If ρ_1 and ρ_2 are two density distributions satisfying

$$f(\rho_i) + f^*(\psi) = \rho_i\psi \quad (i = 1, 2)$$

for each $x \in \Lambda$ then they can only differ on the set $U\Lambda_\xi$. But we have

$$\nu(\cup_\xi \Lambda_\xi) = \sum_\xi \nu(\Lambda_\xi) = 0,$$

which implies $\|\rho_1 - \rho_2\|_\infty = 0$. This proves that $\bar{\rho} \in L_\infty(\Lambda)$ satisfying (6.14) is unique.

As a corollary, if ψ on Λ is of continuous measure, then the minimizing $\bar{\rho}$ is unique. If $\bar{\rho}$ is unique, then it must be the limit of $\{\bar{\rho}_\nu\}$ since the limits (6.33) satisfy (6.32).

7. CONVERGENCE OF CANONICAL DENSITY

In this section we shall discuss the relationship between a density distribution which satisfies (6.14) and the canonical density sequence (2.6). Now the initial domain Λ_0 is not special in that we can define for any fixed Λ a density sequence (2.12) corresponding to (2.6). Thus we denote by $\{\rho_n(x)\}$ the sequence (2.12) referred to any fixed domain Λ. Notice that $\{\bar{\rho}_n(x)\}$ of (2.6) satisfies the condition $nV(\Lambda)^{-1} = \rho_0$ but $\{\rho_n\}$ does not. The domain Λ is the same for all ρ_n. We define

$$g_n(t) = -\mathfrak{F}(\Lambda, n, \beta, \phi + t\psi) \tag{7.1}$$

for $\phi, \psi \in L_\infty(\Lambda)$. The sequence (7.1) is a sequence of convex functions for $t \in R$.[21] Furthermore, each g_n is differentiable with respect to t. Further define

$$g(t) = -F_0(\rho_0, \phi + t\psi). \tag{7.2}$$

The function F_0 is concave in $\phi \in L_\infty(\Lambda)$. Also F_0 has the property of being continuous in ϕ for the norm topology of $L_\infty(\Lambda)$ and upper semicontinuous in ϕ for the weak* topology of $L_\infty(\Lambda)$. Evidently there is no weak* neighborhood on which F_0 is bounded below and therefore F_0 cannot be continuous in $\phi \in L_\infty(\Lambda)$ for the weak* topology. The free energy $F_0(\rho_0, \phi)$ is also convex in ρ_0. For these properties, $g(t)$ is a continuous convex function for $t \in [-1, 1]$ The functions (7.1) are continuous convex on $[-1, 1]$ also. Now for $\|\phi_1 - \phi_2\|_\infty < \epsilon$ we have that

$$|\mathfrak{F}(\Lambda, n, \beta, \phi_1) - \mathfrak{F}(\Lambda, n, \beta, \phi_2)| \le \rho_0\epsilon \tag{7.3}$$

holds for all n such that $nV(\Lambda)^{-1} = \rho_0$. Let $t_1, t_2 \in [-1, 1]$ such that $|t_1 - t_2| < \epsilon/M$ and let $\phi_i = \phi + t_i\psi$ for $\|\psi\|_\infty \le M$. Then (7.3) says that

$$|g_n(t_1) - g_n(t_2)| \le \rho_0\epsilon \tag{7.4}$$

for all n. Inequality (7.4) indicates that the sequence (7.1) is equicontinuous on $[-1, 1]$. When ϕ and ψ are step potentials or uniform limits of step potentials, i.e., limits in the $\|\cdot\|_\infty$ norm, then

$$\lim_n g_n(t) = g(t). \tag{7.5}$$

By the Ascoli theorem, the sequence (7.1) converges uniformly on $[-1, 1]$ whenever it converges pointwise. Pointwise convergence of the sequence (7.1) occurs whenever the thermodynamic limit exists. Let $T(\Lambda)$ denote the closure in $L_\infty(\Lambda)$ of the set of all step potentials of form (3.5). Then $T(\Lambda)$ is a subspace of $L_\infty(\Lambda)$, and (7.5) holds if $\phi, \psi \in T(\Lambda)$. Observe that $T(\Lambda)$ contains the Banach space $C(\Lambda)$ of all continuous functions defined on the compact set Λ. For the sequence (7.1) and the canonical densities $\{\rho_n\}$ defined for a fixed Λ, we have

$$-g_n'(0) = (\rho_n, \psi) \tag{7.6}$$

and

$$|g_n'(0)| \le \|\rho_n\|_1 \|\psi\|_\infty = \rho_0\|\psi\|_\infty. \tag{7.7}$$

By convexity

$$g_n(t) \ge g_n(0) + g_n'(0)t \tag{7.8}$$

holds on $[-1, 1]$ for all n. Given $\epsilon > 0$, by the uniformity of convergence,

$$g(t) \ge g(0) - \epsilon + g_n'(0)t \tag{7.9}$$

holds for $t \in [-1, 1]$ and all n sufficiently large. Inequality (7.9) indicates that the $g_n'(0)$ for n sufficiently large are approximate subgradients of $g(t)$.[22] In fact, every convergent subsequence of $\{g_n'(0)\}$ provides the slope of a supporting line of $g(t)$ at $t = 0$. The sequence (7.6) has convergent subsequences since it is bounded according to (7.7). Because $g(t)$ is convex the left-hand derivative $g_L'(t)$ and the right-hand derivative $g_R'(t)$ exist in $(-1, 1)$, and by (7.9) we have

$$g_R'(0) \ge \lim\sup_n g_n'(0) \ge \lim\inf_n g_n'(0) \ge g_L'(0). \tag{7.10}$$

Let C^* be the dual space of the Banach space $C(\Lambda)$ of continuous functions on Λ. Then application of inequality (7.10) gives the following.

Proposition 7.1: Suppose that $F_0(\rho_0, \phi)$ is Gateaux differentiable at ϕ for ψ in $C(\Lambda)$, and suppose that the Gateaux gradient $\rho^* \in C^*$ exists at ϕ. Then

$$\lim_n (\rho_n, \psi) = \frac{d}{dt} F_0(\rho_0, \phi + t\psi)|_{t=0} = \rho^*(\psi) \tag{7.11}$$

for $\psi \in C(\Lambda)$.

If (7.11) holds on $C(\Lambda)$, then ρ^* must be a positive functional since each ρ_n is positive. We know that according to the Riesz representation theorem every positive continuous linear functional defined on $C(\Lambda)$ is expressible as

$$\rho^*(\psi) = \int_\Lambda \psi(x)d\nu^*(x), \tag{7.12}$$

where ν^* is a unique positive Borel measure on Λ. If ν^* is absolutely continuous with respect to ν then the Radon–Nikodym derivative exists and

$$\rho^*(\psi) = (\bar{\rho}, \psi) \tag{7.13}$$

for a unique $\bar{\rho} \in L_1(\Lambda)$. That is, $\bar{\rho} = d\nu^*/d\nu$ is the Radon–Nikodym derivative when it exists as an element of $L_1(\Lambda)$. Of course, a similar result can be stated for Proposition 7.1 with $T(\Lambda)$ replacing $C(\Lambda)$. The continuous linear functionals on $T(\Lambda)$ are extensions of the continuous linear functionals on $C(\Lambda)$. According to Rockafellar's results, since $-F_0(\rho_0, \phi)$ is finite and continuous for $\phi \in L_\infty(\Lambda)$ (norm topology), the free energy func-

tional does have subgradients.[23] Because $\mathfrak{F}(\Lambda,n,\beta,\phi)$ converges uniformly to $F_0(\rho_0,\phi)$ on compact subsets of $L_\infty(\Lambda)$ (Ascoli theorem) the subgradients of $-\mathfrak{F}(\Lambda,n,\beta,\phi)$ provide approximate subgradients of $-F_0(\rho_0,\phi)$ over compact subsets of $L_\infty(\Lambda)$. In fact, the weakly convergent subsequences of $\{\rho_n\}$ yield subgradients of $-F_0(\rho_0,\phi)$.

Proposition 7.2: Suppose that $\rho \in L_1(\Lambda)$ is the weak limit over $C(\Lambda)$ of some subsequence of $\{\rho_n\}$. Then $-\rho$ is a subgradient of $-F_0(\rho_0,\phi)$ over $C(\Lambda)$.

Proof: Let $\{\rho_J\}$ be a subsequence of $\{\rho_n\}$ such that $(\rho_J,\psi)\to(\rho,\psi)$ for each $\psi \in C(\Lambda)$ as $J\to\infty$. Now $g_J(t) \geq g_J(0) + g_J'(0)t$ for $t \in [-1,1]$. Hence

$$F_0(\rho_0,\phi+t\psi) \leq F_0(\rho_0,\phi) + (\rho,\psi)t \tag{7.14}$$

for all $\psi \in C(\Lambda)$, and this completes the proof.

A corresponding result can be stated for the Banach space $T(\Lambda)$ or for any subspace of this space.

Suppose that in addition to the hypothesis of Proposition 7.1 there exists a $\bar\rho \in L_1(\Lambda)$ such that

$$F_0(\rho_0,\phi) = (\bar\rho,\phi) + F(\bar\rho). \tag{7.15}$$

We now know that if $f(\eta)$ has the property (4.21) for finite ρ_{cp} then $\bar\rho$ exists. Also, $\bar\rho$ exists if ρ_0 is associated with a chemical potential μ as in (6.14). If (7.15) holds, then $-\bar\rho \in \partial(-F_0(\rho_0,\phi))$ since

$$F_0(\rho_0,\phi+\psi) \leq (\bar\rho,\phi+\psi) + F(\bar\rho) = F_0(\rho_0,\phi) + (\bar\rho,\psi). \tag{7.16}$$

Then $\bar\rho$ is the unique Gateaux gradient of Proposition 7.1 satisfying (7.13). In view of Proposition 7.1, we shall want to investigate conditions under which $F_0(\rho_0,\phi)$ is differentiable.

It has been shown that

$$P(\mu,\phi) = \sup\{\mu\eta - F_0(\eta,\phi) \mid \eta \in R\} \tag{7.17}$$

for the pressure (5.1). We find $F_0(\eta,\phi) = +\infty$ if $\eta < 0$ or if $\eta > \rho_{cp}$, and $F_0(\eta,\phi)$ is a proper convex function in η.

Theorem 7.1: Let f have the property that

$$\lim_{\eta\to\rho_{cp}} f(\eta) = +\infty. \tag{7.18}$$

Then $F_0(\eta,\phi)$ is a lower semicontinuous closed proper convex function for $\eta \in R$ and

$$F_0(\eta,\phi) = \sup\{\mu\eta - P(\mu,\phi) \mid \mu \in R\}. \tag{7.19}$$

That is, $F_0(\eta,\phi)$ and $P(\mu,\phi)$ are convex conjugates for $\eta,\mu \in R$.

Proof: Let $\phi \in L_\infty(\Lambda)$. Using Jensen's inequality we have that

$$-\|\rho\|_1\|\phi\|_\infty + F(\|\rho\|_1) \leq (\rho,\phi) + F(\rho) \tag{7.20}$$

and

$$-\eta\|\phi\|_\infty + f(\eta) \leq F_0(\eta,\phi). \tag{7.21}$$

Now [apply (4.22) if $\rho_{cp} = +\infty$]

$$\lim_{\eta\to\rho_{cp}} (f(\eta) - \eta\|\phi\|_\infty) = +\infty \tag{7.22}$$

and dom $F_0(\eta,\phi) = \{\eta \in R \mid F_0(\eta,\phi) < +\infty\} = [0,\rho_{cp})$.

Hence $F_0(\eta,\phi)$ is continuous convex for $\eta \in [0,a] \subset [0,\rho_{cp})$ and is closed and lower semicontinuous on R. As in Theorem 4.1 this implies (7.19) and completes the proof.

From Theorem 7.1 we obtain that

$$\mu_0 \in \partial F_0(\rho_0,\phi) \quad \text{if and only if } \rho_0 \in \partial P(\mu_0,\phi) \tag{7.23}$$

or if and only if

$$F_0(\rho_0,\phi) + P(\mu_0,\phi) = \mu_0\rho_0. \tag{7.24}$$

If $\rho_0 \in \partial P(\mu_0,\phi)$ then (7.15) holds if and only if

$$F^*(\mu_0-\phi) = (\bar\rho,\mu_0-\phi) - F(\bar\rho). \tag{7.25}$$

For the property (7.18) there always exists a $\bar\rho$ which satisfies (7.25) if ϕ is bounded.

Let ϵ_t be a sequence of positive numbers such that $\epsilon_t/t \to 0$ as $t\to 0$. There exists a sequence $\{\rho_t\}$ with $\|\rho_t\|_1 = \rho_0$, in general depending ψ, such that

$$F_0(\rho_0,\phi+t\psi) \geq (\rho_t,\phi+t\psi) + F(\rho_t) - \epsilon_t \tag{7.26}$$

for $t \geq 0$. For the sequence $\{\rho_t\}$ satisfying (7.26), we have that

$$\lim_{t\to 0} (\rho_t,\phi) + F(\rho_t) = F_0(\rho_0,\phi) \tag{7.27}$$

since $|(\rho_t,\psi)| \leq \rho_0\|\psi\|_\infty$ and

$$\lim_{t\to 0} F_0(\rho_0,\phi+t\psi) = F_0(\rho_0,\phi). \tag{7.28}$$

The right-hand derivative $F_0'(\phi;\psi)$ exists and is defined by

$$F_0'(\phi;\psi) = \lim_{t\downarrow 0} [F_0(\rho_0,\phi+t\psi) - F_0(\rho_0,\phi)]/t. \tag{7.29}$$

Inequality (7.26) implies that

$$F_0'(\phi;\psi) \geq \limsup_{t\to 0} (\rho_t,\psi). \tag{7.30}$$

Suppose that $F_0'(\phi;\psi) = (\bar\rho,\psi)$ for all ψ where $\bar\rho$ is the Gateaux gradient.[24] Choose $\{\rho_t\}$ so that (independent of ψ)

$$F_0(\rho_0,\phi) \geq (\rho_t,\phi) + F(\rho_t) - \epsilon_t. \tag{7.31}$$

Then

$$\liminf_{t\to 0} (\rho_t,\psi) \geq F_0'(\phi;\psi) \tag{7.32}$$

and $\rho_t \to \bar\rho$ weakly. Since $\{\rho_t\}$ is weakly convergent, we have

$$\begin{aligned} F_0(\rho_0,\phi) &\geq \liminf_{t\to 0} (\rho_t,\phi) + \liminf_{t\to 0} F(\rho_t) \\ &\geq (\bar\rho,\phi) + F(\bar\rho). \end{aligned} \tag{7.33}$$

Now $\bar\rho$ is in dom F and $\|\bar\rho\|_1 = \rho_0$. This demonstrates that the Gateaux gradient $\bar\rho$ is the unique density at which (3.2) assumes its infimum.

We shall say that the infimum $F_0(\rho_0,\phi)$ is attained strongly if every sequence $\{\rho_t\}$ with $\|\rho_t\|_1 = \rho_0$ satisfying (7.27) has a weakly convergent subsequence. In particular, the weak limit of a weakly convergent subsequence is a point at which the infimum of (3.2) is attained.

Proposition 7.3: Suppose that the infimum $F_0(\rho_0,\phi)$ is attained strongly and that $\bar\rho$ satisfying (7.15) is unique.

Then $F_0(\rho_0, \phi)$ is Gateaux differentiable at ϕ with gradient $\bar{\rho}$.

Proof: For each ψ, the sequence $\{\rho_t\}$ satisfying (7.26) has a subsequence which converges weakly to $\bar{\rho}$. In view of (7.16) and (7.30), $\bar{\rho}$ is the Gateaux gradient of $F_0(\rho_0, \phi)$ at ϕ.

The sphere $S = \{\rho \mid \|\rho\|_\infty \leq a\}$ has an important topological property. Since the linear spaces $C(\Lambda)$, $T(\Lambda)$, and $L_\infty(\Lambda)$ are dense subsets of $L_1(\Lambda)$ ($\|\cdot\|_1$-dense), the weak topology induced on S by any of these linear spaces coincides with the weak* topology [$L_1(\Lambda$-topology] on S. Furthermore, the sphere S as a topological space with the $L_1(\Lambda)$-topology is sequentially compact since it is compact and $L_1(\Lambda)$ is separable. Now if for each ψ there is a sphere S which contains the sequence $\{\rho_t\}$ of (7.26), then $\{\rho_t\}$ has a weakly convergent subsequence. This implies that $F_0(\rho_0, \phi)$ is attained strongly. We have

Theorem 7.2: If $\rho_{cp} < +\infty$ and $\bar{\rho}$ satisfying (7.15) is unique, then

$$\frac{d}{dt} F_0(\rho_0, \phi + t\psi)\big|_{t=0} = (\bar{\rho}, \psi) = \lim_n (\rho_n, \psi) \tag{7.34}$$

for $\psi \in T(\Lambda)$ and $0 \leq \rho_0 < \rho_{cp}$.

Proof: An application of Propositions 7.1 and 7.3. The next theorem will allow us to show that unique $\bar{\rho}$ satisfying (7.25) are Gateaux gradients.

Theorem 7.3: The supremum $F^*(\psi)$ is attained strongly.

Proof: Let $\{\rho_t\}$ be a sequence in $L_1(\Lambda)$ such that

$$\lim_t F(\rho_t) - (\rho_t, \psi) = -F^*(\psi) \tag{7.35}$$

for $\psi \in L_\infty(\Lambda)$. We shall show that $\{\rho_t\}$ has a weakly convergent subsequence, and the limit of a convergent subsequence provides a $\bar{\rho}$ satisfying (7.25) for $\psi = \mu_0 - \phi$. If ρ_{cp} is finite, then $\{\rho_t\}$ is contained in a sphere S with $a = \rho_{cp}$, and there is a weakly convergent subsequence. Now consider the case $\rho_{cp} = +\infty$. By convexity of f and property (4.22), for $\delta > 0$ there exists an $a > 0$ such that

$$f(\eta) - \eta\psi(x) \geq f(\eta) - \eta\|\psi\|_\infty \geq \delta\eta \tag{7.36}$$

holds for almost all $x \in \Lambda$ when $\eta \geq a$. Inequality (7.36) follows from

$$f(\eta) \geq m_a \eta \quad (\eta \geq a) \tag{7.37}$$

for

$$m_a = (f(a) - f(0))/a, \tag{7.38}$$

where $m_a \to \infty$ as $a \to \rho_{cp}$ by (4.22). We also pick a to be as in (6.12) and (6.13). Since $f(0) = 0$, F has the following important property. Let $\rho_1 = \rho\chi_{\Lambda_1}$ and $\rho_2 = \rho\chi_{\Lambda_2}$, where Λ_1 and Λ_2 constitute a disjoint partition of Λ. Then

$$F(\rho) = \int_{\Lambda_1} f(\rho) d\nu + \int_{\Lambda_2} f(\rho) d\nu = F(\rho_1) + F(\rho_2), \tag{7.39}$$

since $f(\rho)\chi_{\Lambda_i} = f(\rho\chi_{\Lambda_i})$. Define

$$\Lambda_t = \{x \in \Lambda \mid \rho_t > a\} \tag{7.40}$$

and

$$\bar{\rho}_t = \rho_t \chi_{\Lambda - \Lambda_t} + a\chi_{\Lambda_t}. \tag{7.41}$$

Observe that the sequence $\{\bar{\rho}_t\}$ is contained in the sphere S of radius a. Then

$$-F^*(\psi) \leq F(\bar{\rho}_t) - (\bar{\rho}_t, \psi) \leq F(\rho_t) - (\rho_t, \psi). \tag{7.42}$$

Let $\rho'_t = \rho_t \chi_{\Lambda - \Lambda_t}$. The sequences $\{\bar{\rho}_t\}$ and $\{\rho'_t\}$ have subsequences $\{\rho'_\alpha\}$ and $\{\bar{\rho}_\alpha\}$ which are weakly convergent. This implies that $\{a\chi_{\Lambda_\alpha}\}$ is also weakly convergent, and the sequence $\nu(\Lambda_\alpha)$ converges. Let $\bar{\rho}$ be the weak limit of $\{\rho'_\alpha\}$, then

$$\lim_\alpha F(\rho'_\alpha) - (\rho'_\alpha, \psi) = F(\bar{\rho}) - (\bar{\rho}, \psi) = -F^*(\psi), \tag{7.43}$$

since

$$F(\bar{\rho}_\alpha) = F(\rho'_\alpha) + F(a\chi_{\Lambda_\alpha}) \tag{7.44}$$

and

$$F(a\chi_{\Lambda_\alpha}) - (a\chi_{\Lambda_\alpha}, \psi) \geq 0 \tag{7.45}$$

converges. Let $\rho''_\alpha = \rho_\alpha \chi_{\Lambda_\alpha}$ so that $\rho_\alpha = \rho'_\alpha + \rho''_\alpha$. Then using (7.39, we see that

$$\lim_\alpha F(\rho''_\alpha) - (\rho''_\alpha, \psi) = 0. \tag{7.46}$$

Inequality (7.36) shows that

$$F(\rho''_\alpha) - (\rho''_\alpha, \psi) \geq \delta \int_{\Lambda_\alpha} \rho_\alpha d\nu \geq 0. \tag{7.47}$$

Hence, for any $\psi \in L_\infty(\Lambda)$

$$\left|\int_{\Lambda_\alpha} \rho_\alpha \psi d\nu\right| \leq \|\psi\|_\infty \int_{\Lambda_\alpha} \rho_\alpha d\nu, \tag{7.48}$$

and the sequence (7.48) converges to zero. Because $(\rho''_\alpha, \psi) \to 0$ for every $\psi \in L_\infty(\Lambda)$ and $(\rho'_\alpha, \psi) \to (\bar{\rho}, \psi)$, this proves that $\{\rho_\alpha\}$ converges weakly to $\bar{\rho}$. This completes the proof.

We can apply Theorem 7.3 to the Gateaux differentiability of $F_0(\rho_0, \phi)$ in the case ρ_{cp} is not finite. Let $\{\rho_t\}$ be as in (7.26) and let ρ_0 correspond to μ_0 as in (7.24). Then

$$\lim_t (\rho_t, \mu_0 - \phi) - F(\rho_t) = F^*(\mu_0 - \phi) \tag{7.49}$$

and by Theorem 7.3 there exists a subsequence of $\{\rho_t\}$ which is weakly convergent to some $\bar{\rho}$. If this $\bar{\rho}$ which satisfies (7.25) is unique, then it is the gradient of F_0 at ϕ. Theorem 7.3 gives just the property needed to consider the differentiability of the pressure $P(\mu, \phi)$ with respect to the external potential ϕ. Let $\bar{\psi} = \mu - \phi$ and suppose that $\bar{\rho}$ satisfying

$$F^*(\bar{\psi}) = (\bar{\rho}, \bar{\psi}) - F(\bar{\rho}) \tag{7.50}$$

is unique.

Let

$$\lim_\alpha (\rho_\alpha, \bar{\psi}) - F(\rho_\alpha) = F^*(\bar{\psi}). \tag{7.51}$$

Then $\rho \to \bar{\rho}$ weakly according to Theorem 7.3, and the supremum ($\bar{\psi}$) of $(\cdot, \bar{\psi}) - F$ is attained strongly at $\bar{\rho}$. Assuming that F and F^* are conjugates, a direct application of a theorem by Rockafellar gives (see the proof of Theorem 8.1)

Theorem 7.4: The density $\bar{\rho}$ satisfies (7.50) and is unique if and only if $\bar{\rho}$ is the Gateaux gradient of F^* at $\bar{\psi}$. That is, $\bar{\rho} = \nabla F^*(\bar{\psi})$.

We have a stronger result.[25] The pressure F^* is Fréchet differentiable at $\bar{\psi}$ if and only if the function

$(\cdot, \bar{\psi}) - F$ attains its supremum strongly with respect to the norm topology of $L_1(\Lambda)$. This means that the sequence $\{\rho_\alpha\}$ must converge (in $\|\cdot\|_1$ norm) to $\bar{\rho}$ in order that $\bar{\rho}$ be the Fréchet gradient.

We complete the study of the equivalence of canonical and grand canonical ensembles with a discussion of the grand canonical density.

8. GRAND CANONICAL DENSITY DISTRIBUTION

The grand canonical partition function is defined by

$$\Xi(\Lambda, \mu, \beta, \phi) = \sum_{n=0}^{\infty} Z(\Lambda, n, \beta, \phi - \mu) \tag{8.1}$$

and the average pressure is given by

$$\beta P(\Lambda, \mu, \beta, \phi) = V(\Lambda)^{-1} \ln \Xi(\Lambda, \mu, \beta, \phi). \tag{8.2}$$

For $\phi \in T(\Lambda)$, the sequence $P(\Lambda, \mu, \beta, \phi)$ is convergent to $F^*(\mu - \phi)$ [also called $P(\mu, \phi)$]. The grand canonical density distribution (or one body correlation function) is defined as

$$\bar{\rho}_\Lambda(x) = \sum_{n=1}^{\infty} \frac{e^{\beta\mu n}}{(n-1)!} \int_{R^{Kn}\Lambda^{n-1}} e^{-\beta H_n(x, x_2, \ldots, x_n)} \times dp_1 \cdots dp_n dx_2 \cdots dx_n / \Xi(\Lambda, \mu, \beta, \phi) \tag{8.3}$$

for each Λ and $x \in \Lambda$. Using the definition (2.6) of the canonical density distribution, (8.3) becomes

$$\bar{\rho}_\Lambda(x) = \sum_{n=1}^{\infty} Z(\Lambda, n, \beta, \phi - \mu) \bar{\rho}_n(x) / \Xi(\Lambda, \mu, \beta, \phi). \tag{8.4}$$

For any divergent sequence $\{\alpha\}$ of positive numbers, let $\Lambda = \alpha\Lambda_0$ and let $\{\rho_\alpha\}$ denote the sequence of functions obtained by referring each $\bar{\rho}_\Lambda$ to the initial domain Λ_0. That is, define

$$\rho_\alpha(x) = \bar{\rho}_\Lambda(\alpha x) \tag{8.5}$$

for all $x \in \Lambda_0$. In this section we shall show that $\bar{\rho}$ satisfying (5.8) over Λ_0 is usually the weak limit of $\{\rho_\alpha\}$. We know that the pressure $P(\mu, \beta, \phi + t\psi)$ is a convex function in t, and in conjunction with this we have the following:

Lemma 8.1: The functions $P(\Lambda, \mu, \beta, \phi + t\psi)$ are convex in t, and

$$\frac{d}{dt} P(\Lambda, \mu, \beta, \phi - t\psi)\,|_{t=0} = V(\Lambda)^{-1} \int_\Lambda \psi(x) \bar{\rho}_\Lambda(x) dx. \tag{8.6}$$

Proof: Let $\phi, \psi \in L_\infty(\Lambda)$ and consider $t \in (-1, 1)$. First, since the interaction U_n is stable, we have an inequality which gives uniform convergence of the series defining $\Xi(\Lambda, \mu, \beta, \phi + t\psi)$ and its derivatives:

$$\left| \frac{\beta^J}{n!} \left(\sum \psi \right)^J e^{-\beta(W_n + t\sum\psi)} \right| \leq \frac{\beta^J}{n!} (n \|\psi\|_\infty)^J e^{\beta M n} \tag{8.7}$$

for $M = B + \|\phi\|_\infty + \|\psi\|_\infty$, $x_i \in \Lambda$ $(i = 1, \ldots, n)$, and $t \in (-1, 1)$. Here $U_n(x_1, \ldots, x_n) \geq -nB$ for all n is the usual stability condition. Let $z_n(t) = Z(\Lambda, n, \beta, \phi + t\psi)$ and

$$\lambda_n(t) = \sum_{i=0}^{n} e^{\beta\mu i} z_i(t). \tag{8.8}$$

Now derivatives of $z_n(t)$ exist and

$$z_n^{(J)}(t) = \frac{(-\beta)^J}{n!} \int_{R^{Kn}\Lambda^n} \left(\sum_{i=1}^{n} \psi(x_i) \right)^J e^{-\beta(H_n + t\sum_{i=1}^{n}\psi(x_i))} \times dp_1 \ldots dp_n dx_1 \ldots dx_n, \tag{8.9}$$

since

$$\lim_{t' \downarrow t} \frac{e^{-\beta t' \Sigma\psi} - e^{-\beta t \Sigma\psi}}{t' - t} = -\beta \sum \psi e^{-\beta t \Sigma\psi} \tag{8.10}$$

for each $(x_1, \ldots, x_n) \in \Lambda^n$. Using the convexity of $\exp(-\beta t \sum\psi)$ in t and the Lebesque dominated convergence theorem, we obtain (8.9) from (8.10). We define $\lambda(t) = \Xi(\Lambda, \mu, \beta, \phi + t\psi)$. Then for each Λ the sequence of derivatives $\{\lambda_n^{(J)}(t)\}$ converges uniformly on $(-1, 1)$ to $\lambda^{(J)}(t)$ [an application of the Weierstrass test with bound (7.7)]. Furthermore, the sum (8.4) converges uniformly to $\bar{\rho}_\Lambda(x)$ a.e. on Λ. These results verify (8.6), since

$$\beta \frac{d}{dt} P(\Lambda, \mu, \beta, \phi + t\psi)\Big|_{t=0} = V(\Lambda)^{-1} \frac{\lambda'(0)}{\lambda(0)}. \tag{8.11}$$

It remains to show that $\ln \lambda(t)$ is a convex function for $t \in (-1, 1)$. Convexity is verified if

$$(\ln \lambda_n)'' = (\lambda_n \lambda_n'' - \lambda_n'^2)/\lambda_n^2 \geq 0 \tag{8.12}$$

holds for $t \in (-1, 1)$ and all n, since then

$$(\ln \lambda(t))'' \geq 0 \tag{8.13}$$

for $t \in (-1, 1)$. Hölder's inequality gives that

$$z_n'' z_n - z_n'^2 \geq 0 \tag{8.14}$$

and this demonstrates convexity for the functions (7.1). Then

$$\begin{aligned} z_n'' z_J - z_n' z_J' + z_J'' z_n - z_J' z_n' &\geq z_n' \left(\frac{z_n'}{z_n} z_J - z_J' \right) + z_J' \left(\frac{z_J'}{z_J} z_n - z_n' \right) \\ &= (z_n' z_J - z_n z_J')^2 / z_n z_J \geq 0. \end{aligned} \tag{8.15}$$

Hence

$$\sum_{J=0}^{n} z_J'' \sum_{J=0}^{n} z_J - \left(\sum_{J=0}^{n} z_J' \right)^2 \geq 0 \tag{8.16}$$

for $t \in (-1, 1)$ and all n. Notice that it is sufficient to consider (8.8) for $\mu \equiv 0$. This completes the proof. Applying Lemma 8.1, we have that

$$P_\alpha(t) \geq P_\alpha(0) + (\rho_\alpha, \psi)t \tag{8.17}$$

holds for $t \in (-1, 1)$, where $P_\alpha(t) = P(\Lambda, \mu, \beta, \phi - t\psi)$. Now for $\phi, \psi \in T(\Lambda)$, $P_\alpha(t) \to P(\mu, \beta, \phi - t\psi)$ and we have

Theorem 8.1: If $\bar{\rho}$ is a unique density satisfying (7.50), then

$$\frac{d}{dt} P(\mu, \beta, \phi - t\psi)\,|_{t=0} = (\bar{\rho}, \psi) = \lim_\alpha (\rho_\alpha, \psi) \tag{8.18}$$

for $\phi, \psi \in T(\Lambda)$.

Proof: A direct application of Theorem 7.4 and Lemma 8.1 and the following applicable theorem proven by Rockafellar: Let f and g be proper convex functions conjugate to each other on X and Y, respectively. Then f is Gateaux differentiable at x with $y = \nabla f(x)$ if and only if the infimum of the function $g - (x, \cdot)$ over Y is finite and attained at y strongly with respect to $W(Y, X)$. Here $W(Y, X)$ denotes the weak topology induced on Y by X.[26]

On the continuity of density distributions we have the following: Let $\psi \in L_1(\Lambda)$ and $\rho \in L_\infty(\Lambda)$ so that $L_\infty(\Lambda) =$

$L_1(\Lambda)^*$. Suppose that V is a nonempty $\|\cdot\|_1$-open subset of $L_1(\Lambda)$ such that F^* is Gateaux differentiable throughout V. Then the density distribution $\bar{\rho} = \nabla F^*(\psi)$, which is a gradient mapping from V to $L_\infty(\Lambda)$, is continuous from the norm topology to the weak* topology on $L_\infty(\Lambda)$. This fact follows from another of Rockafellar's theorems since F^* is a weak lower semicontinuous proper convex function on $L_1(\Lambda)$.[27] That is, we have that if

$$\bar{\rho}(\psi) = \nabla F^*(\psi) \quad \text{on } V, \tag{8.19}$$

then for $\psi \in V$

$$(\bar{\rho}(\psi_\alpha), \phi) \to (\bar{\rho}(\psi), \phi) \tag{8.20}$$

as $\|\psi_\alpha - \psi\|_1 \to 0$ for all $\phi \in L_1(\Lambda)$.

Apparently the continuity of the pressure as a function of the density distribution ρ is determined by the behavior of the interaction. In the case of pair interaction with positive or hard core pair potential, the derivative $f'(\eta)$ exists in $(0, \rho_{cp})$ since the graph of $p(\mu)$ has no linear segments. Then the Gateaux gradient of F at ρ equals $f'(\rho)$ and is continuous on dom F from the norm topology of $L_\infty(\Lambda)$ to the norm topology of $L_1(\Lambda)$, since f' is uniformly continuous on closed subintervals of $[0, \rho_{cp})$. The canonical pressure distribution is given by

$$p_0(\rho, \beta) = \rho f'(\rho, \beta) - f(\rho, \beta) \tag{8.21}$$

and corresponds to $p(\mu - \phi, \beta)$ if $\mu - \phi = f'(\rho, \beta)$. The pressure distribution $p_0(\rho)$ is continuous on dom F from the $L_\infty(\Lambda)$ norm topology to the $L_1(\Lambda)$ norm topology since $f(\rho)$ is continuous in this way and

$$\|\rho f'(\rho) - \rho_1 f'(\rho_1)\|_1 \le \|\rho - \rho_1\|_\infty \|f'(\rho_1)\|_1 + \|\rho\|_\infty \|f'(\rho) - f'(\rho_1)\|_1 \tag{8.22}$$

for $\rho, \rho_1 \in$ dom F. Therefore, we have

$$\|p_0(\rho, \beta) - p_0(\rho_1, \beta)\|_1 \to 0 \tag{8.23}$$

as $\|\rho - \rho_1\|_\infty \to 0$.

9. PHASE TRANSITIONS

Next we consider the phase transitions of a nonuniform system at fixed temperature. Such phase transition behavior is exhibited by nonuniqueness of the density distribution.[28] Consider the situation in which the density distribution $\bar{\rho}$ satisfying

$$P(\mu_0, \phi) = (\bar{\rho}, \mu_0 - \phi) - F(\bar{\rho}) \tag{9.1}$$

is not unique. Thus, suppose that ϕ is of discontinuous measure at ξ_0 and that $f(\eta)$ has a linear segment over the interval $[\eta_1, \eta_2] \subset [0, \rho_{cp})$ with slope $(\mu_0 - \xi_0)$. Then $\bar{\rho}$ can be expressed as

$$\bar{\rho} = \bar{\rho}\chi_{\Lambda - \Lambda_{\xi_0}} + \bar{\rho}\chi_{\Lambda_{\xi_0}}, \tag{9.2}$$

where $\Lambda_{\xi_0} = \{x \in \Lambda \mid \phi(x) = \xi_0\}$ and

$$\eta_1 \chi_{\Lambda_{\xi_0}} \le \bar{\rho}\chi_{\Lambda_{\xi_0}} \le \eta_2 \chi_{\Lambda_{\xi_0}} \tag{9.3}$$

holds according to Lemma 6.1. Now let ρ be any density distribution on Λ such that

$$\eta_1 \chi_{\Lambda_{\xi_0}} \le \rho\chi_{\Lambda_{\xi_0}} \le \eta_2 \chi_{\Lambda_{\xi_0}}. \tag{9.4}$$

Then (9.1) also holds if $\bar{\rho}$ is replaced by

$$\rho' = \bar{\rho}\chi_{\Lambda - \Lambda_{\xi_0}} + \rho\chi_{\Lambda_{\xi_0}}. \tag{9.5}$$

Furthermore, if ρ satisfies the condition

$$\|\rho\chi_{\Lambda_{\xi_0}}\|_1 = \|\bar{\rho}\chi_{\Lambda_{\xi_0}}\|_1, \tag{9.6}$$

as well as (9.4) for $\|\bar{\rho}\|_1 = \rho_0$, then the density distribution (9.5) satisfies

$$F_0(\rho_0, \phi) = (\rho', \phi) + F(\rho'). \tag{9.7}$$

We conclude that a density distribution which is not unique for one ensemble is then not unique for the other. In fact, suppose that $\bar{\rho}$ corresponds to minimizing the free energy and satisfies (9.3) on a region Λ_{ξ_0} of constant potential, where

$$f(\eta) = (\mu_0 - \xi_0)\eta + f_0 \tag{9.8}$$

for $\eta \in [\eta_1, \eta_2]$. Now we have

$$(\bar{\rho}\chi_{\Lambda_{\xi_0}}, \phi) + F(\bar{\rho}\chi_{\Lambda_{\xi_0}}) = \int_{\Lambda_{\xi_0}} (\mu_0\bar{\rho} + f_0)\,d\nu, \tag{9.9}$$

so that (9.7) holds for a ρ' satisfying (9.5) and (9.6). Let $y(x)$ denote a one-to-one transformation of Λ_{ξ_0} onto itself such that $y(x)$ has a Jacobian equal one. Then

$$\rho\chi_{\Lambda_{\xi_0}}(x) = \bar{\rho}\chi_{\Lambda_{\xi_0}}(y(x)) \tag{9.10}$$

satisfies (9.4) and (9.6) and yields another ρ' according to (9.5) where (9.7) holds.

We shall now show that if the density distribution $\bar{\rho}$ is not unique then the pressure is constant over the convex set of all $\bar{\rho}$ satisfying (9.1). Consider the situation where the density is not unique and let $\bar{\rho}_1$ and $\bar{\rho}_2$ be two different densities satisfying (9.1). Then

$$\bar{\rho} = \lambda\bar{\rho}_1 + (1 - \lambda)\bar{\rho}_2, \tag{9.11}$$

where $\rho_0 = \lambda\eta_1 + (1 - \lambda)\eta_2$ $(0 \le \lambda \le 1)$ for $\|\bar{\rho}\|_1 = \rho_0$ and $\|\bar{\rho}_i\|_1 = \eta_i$ is also a density distribution satisfying (9.1). Note that η_1 and η_2 need not be different. For this situation, we find that

$$F(\bar{\rho}) = \lambda F(\bar{\rho}_1) + (1 - \lambda)F(\bar{\rho}_2) \tag{9.12}$$

and

$$F_0(\rho_0, \phi) = \lambda F_0(\eta_1, \phi) + (1 - \lambda)F_0(\eta_2, \phi). \tag{9.13}$$

The average canonical pressure is defined as

$$P_0(\eta, \phi) = \eta \frac{\partial}{\partial \eta} F_0(\eta, \phi) - F_0(\eta, \phi) \tag{9.14}$$

and is also a function of β. Now if $P_0(\eta, \phi)$ is constant over an interval $[\eta_1, \eta_2]$, then the free energy is linear in the average density ρ_0 as in (9.13) for $\rho_0 = \lambda\eta_1 + (1 - \lambda)\eta_2$, and conversely.

Furthermore, if the free energy $F_0(\rho_0, \phi)$ is linear in the average density ρ_0 over an interval $[\eta_1, \eta_2]$, then $\bar{\rho}$ is linear in ρ_0 as in (9.11). We shall demonstrate this last statement. Suppose that $F_0(\rho_0, \phi)$ satisfies (9.13) and let

$$F_0(\eta_i, \phi) = (\bar{\rho}_i, \phi) + F(\bar{\rho}_i) \quad (i = 1, 2) \tag{9.15}$$

for $\|\rho_i\|_1 = \eta_i$. Then $\bar{\rho}$ determined as in (9.11) satisfies

$$F(\bar{\rho}) \leq \lambda F(\bar{\rho}_1) + (1-\lambda)F(\bar{\rho}_2) \tag{9.16}$$

and

$$F_0(\rho_0, \phi) \leq (\bar{\rho}, \phi) + F(\bar{\rho}) \leq \lambda F_0(\eta_1, \phi) + (1-\lambda)F_0(\eta_2, \phi). \tag{9.17}$$

Hence

$$F_0(\rho_0, \phi) = (\bar{\rho}, \phi) + F(\bar{\rho}) \tag{9.18}$$

follows, proving that $\bar{\rho}$ corresponds to minimizing the free energy. The linearity of F as in (9.12) also follows.

The canonical pressure distribution $p_0(\rho(x), \beta)$ is defined by (8.21) so that the ensembles are equivalent if

$$p_0(\bar{\rho}(x), \beta) = p(\mu_0 - \phi(x), \beta) \tag{9.19}$$

when $\bar{\rho}$ corresponds to $\mu_0 - \phi$ as in (9.1), and if

$$P_0(\rho_0, \phi) = P(\mu_0, \phi). \tag{9.20}$$

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Rigorous results for Ising ferromagnets of general spin with degeneracy or symmetric potentials

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The circle theorem of Lee and Yang is proved for Ising ferromagnets of general spin with degeneracy or symmetric potentials $\phi_j(-S_j) = \phi_j(S_j)$; i.e., all the zeros of the partition function $\Xi = \mathrm{Tr}\exp(\Sigma K_{ij}S_iS_j + \beta\lambda\Sigma_j\phi_j(S_j) + h\Sigma_jS_j)$ lie on the unit circle of the complex fugacity plane ($z = e^{-h}$) for $K_{ij} \geq 0$, $\lambda \geq 0$, and for "nondecreasing functions" $\phi_j(S_j)$; $\phi_j(S) \geq \phi_j(S-1) \geq \cdots \geq \phi_j(1/2)$ [or $\phi_j(0)$], including the proof by Griffiths for the usual Ising model of arbitrary spin. The analyticity of the limiting free energy of such a generalized Ising ferromagnet and the absence of a phase transition are thereby established for all (real) nonzero magnetic field. Griffiths-Kelly-Sherman inequalities on spin correlations and Baker's inequalities on critical exponents are discussed in connection with the above model and also in a more general case.

1. INTRODUCTION

Since Lee and Yang[1] discovered a remarkable circle theorem on the distribution of zeros of the partition function for Ising ferromagnets with spin $\frac{1}{2}$, this circle theorem has been extended to other several cases such as Ising ferromagnets of *higher spin*,[2-5] the monomer-dimer problem,[6] Heisenberg ferromagnets,[7-9] and ferroelectric models.[9,10] This theorem has application[11-13] to discussions of scaling behaviors in above ferromagnets.

In a previous paper,[4] the present author discussed the circle theorem for an extended Ising model with applications to dilute ferromagnetism. Unfortunately, there was given only a partial proof for the circle theorem. The present paper gives a quite general proof for it by using Griffiths' reduction technique[5] of higher spin and in terms of affine transformations.

Now, the model we discuss here is given by the Hamiltonian

$$\mathcal{H} = -\sum J_{ij}S_iS_j - H\sum S_j, \quad J_{ij} \geq 0, \tag{1.1}$$

with degenerate states for S_j:

$$S_j = \underbrace{p,\ldots,p}_{n_1},\underbrace{p-2,\ldots,p-2}_{n_2},\cdots \underbrace{-p+2,\ldots,-p+2}_{n_2},\underbrace{-p,\ldots,-p}_{n_1}, \tag{1.2}$$

where n_k ($= 0, 1, 2, \cdots; n_1 \neq 0$) indicates the degeneracy of the state $S_j = \pm[p - 2(k-1)]$. The set $\{n_k\}$ may depend on the lattice site j (i.e., $n_k = n_k^{(j)}$). This model is equivalent to a special case of the following Hamiltonian:

$$\mathcal{H} = -\sum J_{ij}S_iS_j - \lambda\sum\phi(S_j) - H\sum S_j, \quad J_{ij} \geq 0, \tag{1.3}$$

where S_j assumes nondegenerate discrete values p, $p-2, \cdots, 2-p, -p$, and $\phi(S_j)$ satisfies the symmetric property

$$\phi(-S_j) = \phi(S_j). \tag{1.4}$$

[The function $\phi(S_j)$ may depend on the lattice site j; $\phi = \phi_j(S_j)$]. The equivalence is assured by the relation

$$n_k \propto y_{k-1} \equiv \exp\{\beta\lambda\phi[p-2(k-1)]\}, \tag{1.5}$$

with the same proportionality coefficient for all $k \geq 1$.

The main results in the present investigations are summarized as follows.

1. The Lee–Yang circle theorem is valid in the following "triangular" region (A):

(A) $n_1 \geq n_2 \geq n_3 \geq \cdots$

for the Hamiltonian (1.1) and

$$\phi(p) \geq \phi(p-2) \geq \phi(p-4) \geq \cdots \tag{1.6}$$

for the Hamiltonian (1.3).

2. In particular, the Lee–Yang theorem holds when $\phi(S_j)$ is expressed as[4]

$$\phi(S) = \sum_k c_k S^{2k}, \quad c_0 \gtrless 0 \quad \text{and} \quad c_k \geq 0. \tag{1.7}$$

This yields a sufficient extension of conditions for the circle theorem discussed in a previous paper.[4]

3. There occurs a phase transition in the generalized Ising ferromagnet described by the Hamiltonian (1.3) under condition (A) and in particular with the potential (1.7).

In the above Hamiltonian (1.3) and in particular (1.1), Griffiths–Kelly–Sherman inequalities on spin correlations are easily shown to hold as a special case of the general results obtained by Ginibre.[14]

In Sec. 2, following Griffiths,[5] we investigate a representation of an Ising particle of spin $p/2$ in terms of a cluster of p spin-$\frac{1}{2}$ particles interacting among themselves through ferromagnetic pair interactions. Main results derived there are Theorems 1 and 2. Applications of the theorems and some related problems are discussed in Sec. 3. In the last section, discussions are given on further extensions of the present results.

2. REPRESENTATION IN TERMS OF SPIN–½ PARTICLES AND FERROMAGNETIC PAIR WEIGHT FUNCTIONS (FPWF)

A. Recurrence formulas and affine transformations

Following Griffiths,[5] we shall write the spin variable S as a sum

$$S = \sigma_1 + \sigma_2 + \cdots + \sigma_p, \tag{2.1}$$

where the σ_j are "ordinary" Ising variables which

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assume the values + 1 and − 1. Provided the weight function $W_p(\sigma_1, \ldots, \sigma_p)$ is properly chosen, we may write

$$\sum f(S)_{S(\text{degenerate})} = \sum_{q=-p}^{p} W_p(q) f(q)$$

$$= \sum_{\{\sigma_j\}} W_p(\sigma_1, \ldots, \sigma_p) f(\sigma_1 + \sigma_2 + \cdots + \sigma_p), \quad (2.2)$$

for any function $f(S)$, where $W_p(q)$ denotes the degeneracy of state $S = q$ or plays a role of a partial Boltzmann factor $\exp[\beta\lambda\phi(q)]$ in the Hamiltonian (1.3) except an irrelevant constant factor. We shall require that the weight function $W_p(\{\sigma_j\})$ be nonnegative, and it must obviously have the property

$$\sum_{\{\sigma_j\}} W_p(\{\sigma_j\}) \delta\left(\sum_{j=1}^{p} \sigma_j ; q\right) = W_p(q), \quad (2.3)$$

for any q which assumes descrete values $p, p-2, \ldots, -(p-2), -p$, where

$$\delta(a;b) = 1, \quad \text{if } a = b,$$
$$= 0, \quad \text{if } a \neq b. \quad (2.4)$$

The present Hamiltonian (1.3) [or (1.1) with (1.2)] is reduced to the usual Ising model of general spin (and consequently the statements 1 to 3 in Sec. 1 result immediately from the work by Yang and Lee,[1] Griffiths,[5,15] and Kelly and Sherman,[16] provided one can find a *ferromagnetic pair* weight function of the form

$$W_p(\sigma_1, \ldots, \sigma_p) = \prod_{i<j} [\tfrac{1}{2}(1 + \sigma_i\sigma_j) + \tfrac{1}{2}(1 - \sigma_i\sigma_j) X_{ij}]$$

$$= \exp[\tfrac{1}{2} \sum_{ij} K_{ij}(\sigma_i\sigma_j - 1)] \quad (2.5)$$

with

$$0 \leq X_{ij} = \exp(-K_{ij}) \leq 1 \quad \text{or} \quad 0 \leq K_{ij} \leq \infty. \quad (2.6)$$

The problem is to find a region $\mathfrak{W}^*$ in which a set of FPWF exists. This is, in general, a very complicated problem of solving non-linear equations with respect to the variables $\{X_{ij}\}$. Then, it is convenient to deal with a special set of $\{K_{ij}\}$ which may be expected to cover a wide region of $\mathfrak{W}^*$. That is, all X_{ij} in Eq. (2.5) shall be set equal to 1, except for the following:

$$X_{j,j+1} = \begin{cases} X_j & \text{for } 1 \leq j \leq r \\ 0 & \text{for } r+1 \leq j \leq p-1, \end{cases} \quad (2.7)$$

where r is defined by $p = 2r$ for p even and $p = 2r + 1$ for p odd, and $\{X_j\}$ are parameters in the range $0 \leq X_j \leq 1$. Thus, weight functions $W_p(\{\sigma_j\})$ are expressed as

$$W_p(\{\sigma_j\}) = \begin{cases} W_p(\sigma_1, \ldots, \sigma_r, 1, 1, \ldots, 1) \\ \qquad \equiv w_r(\sigma_1, \sigma_2, \ldots, \sigma_r) \\ W_p(\sigma_1, \ldots, \sigma_r, -1, -1, \ldots, -1) \\ \qquad = w_r(-\sigma_1, -\sigma_2, \ldots, -\sigma_r) \\ 0 \quad \text{for other configurations.} \end{cases} \quad (2.8)$$

Now, the relevant problem is to study the properties of $\{W_p(q)\}$ as functions of parameters $\{X_j\}$. From (2.3) and (2.8), we have

$$W_p(q) = \sum_{\{\sigma_j\}} w_r(\{\sigma_j\}) \left[\delta\left(\sum_{j=1}^{r} \sigma_j ; r - p + q\right) + \delta\left(\sum \sigma_j ; r - p - q\right)\right]. \quad (2.9)$$

Clearly, $W_p(q)$ has the symmetry property $W_p(-q) = W_p(q)$. For $q > 0$, it can be written as

$$W_p(q) = \sum_{\{\sigma_j\}} w_r(\{\sigma_j\}) \delta\left(\sum_{j=1}^{r} \sigma_j ; r - p + q\right). \quad (2.10)$$

In particular one obtains that $W_p(p) = 1$, and

$$W_p(0) = 2X_r \quad \text{for} \quad p = 2r, \quad (2.11a)$$
$$W_p(1) = X_r \quad \text{for} \quad p = 2r + 1. \quad (2.11b)$$

It is convenient to introduce the following functions:

$$f_j^{(r)} = \sum_{\{\sigma_k\}} w_r(\{\sigma_k\}) \delta\left(\sum_{k=1}^{r} \sigma_k ; r - 2j\right)$$

$$= \sum_{\{\sigma_k\}} \prod_{k=1}^{r} X_k^{(1-\sigma_k\sigma_{k+1})/2} \delta\left(\sum_{k=1}^{r} \sigma_k ; r - 2j\right) \delta(\sigma_{r+1}; 1), \quad (2.12)$$

for $j = 1, 2, \ldots, r$. The functions $\{f_j^{(r)}\}$ are related to the set $W_p(q)$ as follows. When $q > 0$, we have $W_p(q) = f_{(p-q)/2}^{(r)}$ both for $p = 2r$ and for $p = 2r + 1$. For $p = 2r$, we have $W_p(0) = 2f_r^{(r)}$. The first key-point of the present argument is to notice the following recurrence relations for $f_j^{(r)}$:

$$f_j^{(r)} = f_j^{(r-1)} + X_r f_{r-j}^{(r-1)} \quad (2.13)$$

for $j = 1, 2, \ldots, r-1$, and $f_r^{(r)} = X_r$ for $j = r$. For convenience, we use new notations

$$\mathbf{x}, \quad x_j = f_j^{(r)}, \quad (2.14)$$
$$\mathbf{y}, \quad y_j = f_j^{(r+1)} \quad (j = 1, 2, \ldots r).$$

Then, the recurrence relations (2.13) can be written as

$$\mathbf{y} = A_r(X_{r+1})\mathbf{x}, \quad (2.15)$$

where $A_r(X_{r+1})$ is a linear transformation defined by

$$A_k(a) = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ 0 & & & (1+a) & \\ & & a & & \\ & \iddots & & & \\ a & & & & 1 \end{pmatrix} \quad (2.16)$$

with $a = X_{r+1}$. The determinant of this matrix is given by

$$\det A_r(a) = \begin{cases} (1-a^2)^{r/2} & \text{for } r \text{ even}, \\ (1+a)(1-a^2)^{(r-1)/2} & \text{for } r \text{ odd}. \end{cases} \quad (2.17)$$

Thus, for $0 \leq a < 1$ (i.e., $0 \leq X_{r+1} < 1$), we have

$$\det A_r(a) \neq 0. \quad (2.18)$$

This implies that the matrix $A_r(a)$ is an *affine* transformation φ, which has the following properties.

1. One-to-one mapping: If $\mathbf{P} \neq \mathbf{Q}$, then $\varphi(\mathbf{P}) \neq \varphi(\mathbf{Q})$, and the converse is also true.

2. A hyperplane is projected to a hyperplane, and parallel ones to parallel. These properties may be of use to visualize proofs given below.

Definition 1: Domain $\mathfrak{D}_r$ is defined by

$$\mathfrak{D}_r = \{x_1, \ldots, x_r \,;\, x_j = f_j^{(r)} \ (j = 1, 2, \ldots, r) \text{ and } 0 \leq X_j \leq 1\}, \quad (2.19)$$

where $f_j^{(r)}$ is given by Eq. (2.12)

Recurrence relation on $\mathfrak{D}_r$: From the recurrence relations (2.13), we have

$$\mathfrak{D}_{r+1} = \alpha_r \mathfrak{D}_r, \tag{2.20}$$

where α_r is a transformation operator defined by

$$\alpha_r \mathcal{T}_r \equiv \{y_1, \ldots, y_{r+1}; \mathbf{y} = A_r(y_{r+1})\mathbf{x}, \mathbf{x} \in \mathcal{T}_r \text{ and } 0 \le y_{r+1} \le 1\}. \tag{2.21}$$

That is α_r transforms a r-dimensional domain $\mathcal{T}_r$ to a $(r+1)$-dimensional region, whose cut perpendicular to the y_{r+1} axis is mapped from $\mathcal{T}_r$ by the affine transformation $A_r(a)$ with $a = y_{r+1}$.

Thus, one arrives at the following result.

Theorem 1: The domain $\mathfrak{D}_r$ is given by

$$\mathfrak{D}_r = \alpha_{r-1}\alpha_{r-2}\cdots\alpha_1\mathfrak{D}_1 \tag{2.22}$$

and

$$\mathfrak{D}_1 = \{x_1; 0 \le x_1 \le 1\}. \tag{2.23}$$

This yields the statement 3 in Sec. 1. The transformation α_r is expressed more explicitly in terms of the inverse matrix of $A_r(a)$:

$$A_r^{-1}(a) = (1-a^2)^{-1}\begin{pmatrix} 1 & & & & -a \\ & \ddots & & & \\ & & 1 & & \\ 0 & & & (1+a)^{-1}(1-a^2) & 0 \\ & & & & 1 \\ & & & & \ddots \\ -a & & & 0 & & 1 \end{pmatrix} \tag{2.24}$$

where the central matrix element $(1+a)^{-1}(1-a^2)$ appears only for r odd. Thus, one may write as

$$\mathfrak{D}_{r+1} = \alpha_r\mathfrak{D}_r = \{y_1, \ldots, y_r, y_{r+1}; A_r^{-1}(y_{r+1})\mathbf{y} \in \mathfrak{D}_r \text{ for } 0 \le y_{r+1} < 1, \text{ or } y_{r+1} = 1, y_j = y_{r+1-j} = x_j + x_{r+1-j}, \mathbf{x} \in \mathfrak{D}_r\}. \tag{2.25}$$

Thus, for any value of spin, one can obtain explicitly sufficient conditions in which ferromagnetic pair weight functions exist and consequently in which the Lee–Yang circle theorem is valid.

For example, we have

$$\begin{aligned} &\mathfrak{D}_1 = \{y_1; 0 \le y_1 \le 1\}, \\ &\mathfrak{D}_2 = \alpha_1\mathfrak{D}_1 = \{y_1, y_2; 0 \le y_1 \le 1 + y_2 \le 2 \text{ and } 0 \le y_2\}, \\ &\mathfrak{D}_3 = \alpha_2\mathfrak{D}_2 = \{y_1, y_2, y_3; 0 \le y_1 - y_2y_3 \le 1 \\ &\quad + y_2 - y_1y_3 - y_3^2 \le 2 - 2y_3^2, 0 \le y_3 < 1, \\ &\quad \text{or } 0 \le y_1 = y_2 \le 3, y_3 = 1\}. \end{aligned} \tag{2.26}$$

B. Lemmas on r-dimensional triangular cone and affine transformations

In this subsection, we prove lemmas necessary for discussing the statement 1 in Sec. 1 (or Theorem 2 in the succeeding subsection).

Definition 2: We define the following domains:

$$\begin{aligned} &T^{(r)} = \{x_1, \ldots, x_r; 1 \ge x_1 \ge x_2 \ge \cdots \ge x_r \ge 0\}, \\ &\hat{T}_a^{(r)} = \{y_1, \ldots, y_r; \mathbf{y} = A_r(a)\mathbf{x}, \mathbf{x} \in T^{(r)}\}, \\ &\hat{S}_a^{(r)} = \{y_1, \ldots, y_r; 1 \ge y_1 \ge y_2 \ge \ldots \ge y_r \ge a\}, \end{aligned} \tag{2.27}$$

and

$$S_a^{(r)} = \{x_1, \ldots, x_r; A_r(a)\mathbf{x} \in \hat{S}_a^{(r)}\},$$

where $A_r(a)$ is given by (2.16) with a in the range $1 \ge a \ge 0$.

Lemma 1: For $0 \le a < 1$, one has the relation

$$S_a^{(r)} \subset T_a^{(r)}. \tag{2.28}$$

Proof: The condition that $A_r(a)\mathbf{x} \in \hat{S}_a^{(r)}$ leads to the inequality

$$x_j + ax_{r+1-j} \ge x_{j+1} + ax_{r-j}. \tag{2.29}$$

That is,

$$x_j - x_{j+1} \ge a(x_{r-j} - x_{r+1-j}), \tag{2.30}$$

for any j. Similarly, one has

$$x_{r-j} - x_{r+1-j} \ge a(x_j - x_{j+1}). \tag{2.31}$$

For $0 \le a < 1$, the above inequalities (2.30) and (2.31) yield the relation

$$x_j \ge x_{j+1}. \tag{2.32}$$

In the same way, one can derive

$$1 \ge x_1 \quad \text{and} \quad x_r \ge 0, \tag{2.33}$$

from the inequalities

$$1 \ge x_1 + ax_r \quad \text{and} \quad x_r + ax_1 \ge a, \tag{2.34}$$

which come from the condition that $A_r(a)\mathbf{x} \in \hat{S}_a^{(r)}$. Thus, we arrive finally at the inequalities

$$1 \ge x_1 \ge x_2 \ge \cdots \ge x_r \ge 0. \tag{2.35}$$

This implies that $S_a^{(r)} \subset T_a^{(r)}$.

Lemma 2: For $0 \le a \le 1$,

$$\hat{S}_a^{(r)} \subset \hat{T}_a^{(r)}. \tag{2.36}$$

Proof: The case $0 \le a < 1$ is an immediate consequence of Lemma 1, and the special case $a = 1$ can be checked easily, because the domain $\hat{S}_a^{(r)}$ shrinks to the single point $y_1 = y_2 = \cdots = y_r = 1$ for $a = 1$.

Lemma 3:

$$T^{(r+1)} \subset \alpha_r T^{(r)}, \tag{2.37}$$

where the mapping α_r is defined by Eq. (2.21).

Proof: First, note that the cut of $(r+1)$-dimensional triangular cone $T^{(r+1)}$ at $y_{r+1} = a$ is $\hat{S}_a^{(r)}$:

$$T^{(r+1)} = (\hat{S}_a^{(r)}, a; 0 \le a \le 1). \tag{2.38}$$

Similarly, we have

$$\alpha_r T^{(r)} = (\hat{T}_a^{(r)}, a; 0 \le a \le 1). \tag{2.39}$$

Since $\hat{S}_a^{(r)} \subset \hat{T}_a^{(r)}$ (Lemma 2), it follows from (2.38) and (2.39) that $T^{(r+1)} \subset \alpha_r T^{(r)}$.

C. Sufficient conditions for existence of ferromagnetic pair weight functions

Our aim in this subsection is to prove the following theorem.

Theorem 2: For $r = 1, 2, \ldots$, we have

$$T^{(r)} \subset \mathfrak{D}_r. \tag{2.40}$$

This implies the statements 1 and 2 in Sec. 1.

Proof: Clearly, we have

$$T^{(1)} \subset \mathfrak{D}_1 (T^{(1)} = \mathfrak{D}_1) \quad \text{and} \quad T^{(2)} \subset \mathfrak{D}_2. \tag{2.41}$$

Now assume that Theorem 2 is true for $r = n$. Then, we find

$$\alpha_n T^{(n)} \subset \alpha_n \mathfrak{D}_n. \tag{2.42}$$

Since $\alpha_n \mathfrak{D}_n = \mathfrak{D}_{n+1}$, we are led to

$$\alpha_n T^{(n)} \subset \mathfrak{D}_{n+1}. \tag{2.43}$$

Combining the above relation (2.43) with Lemma 3, we obtain

$$T^{(n+1)} \subset \mathfrak{D}_{n+1}. \tag{2.44}$$

This completes the proof of Theorem 2 by mathematical induction.

Corollary: We have $\alpha_r T^{(r)} \subset \mathfrak{D}_{r+1}$.

The above results are summarized in the following statement. The Lee–Yang theorem holds in the domain $\mathfrak{W}$:

$$\mathfrak{W} = \{y_0, y_1, y_2, \ldots y_r; \mathbf{y} \in \mathfrak{D}_r\} \text{ for } p = 2S = 2r + 1,$$

and

$$\mathfrak{W} = \{y_0, y_1, \ldots y_{r-1}, 2y_r; \mathbf{y} \in \mathfrak{D}_r\} \text{ for } p = 2S = 2r, \tag{2.45}$$

where without loss of generality $y_0 = 1$ has been assumed. The domain $\mathfrak{D}_r$ is expressed in terms of successive operations α_j:

$$\mathfrak{D}_r = \alpha_{r-1}\alpha_{r-2}\cdots\alpha_1 \mathfrak{D}_1, \tag{2.46}$$

and

$$\mathfrak{D}_1 = \{y_1; 0 \le y_1 \le 1\}, \tag{2.47}$$

Here the transformation α_k is defined by Eq. (2.21), and $A_k(a)$ is given by (2.16).

3. APPLICATIONS AND RELATED PROBLEMS

A. The circle theorem of Lee and Yang

In §2, for the region $\mathfrak{W}$ given by (2.45), the Hamiltonian (1.3) has been reduced to the Ising model with ferromagnetic pair interactions in which Lee and Yang[1] proved that all the zeros of the partition function lie on the unit circle of the complex fugacity plane. Then, we arrive at the statements 1 and 2 in §1.

B. Baker's inequalities

Using the Lee–Yang theorem and the analyticity of the free energy proven from it for the usual Ising–Heisenberg model, Baker[17] has derived the following inequalities on critical exponents[18]:

$$\delta \ge \Delta/(\Delta - \gamma), \quad \delta \ge \Delta'/(\Delta' - \gamma'), \quad \Delta \le \Delta', \quad \gamma \le \gamma'. \tag{3.1}$$

Quite in the same way, the above Baker's inequalities are shown to hold for the Ising model with degeneracy (1.2) or symmetric potentials in the region $\mathfrak{W} = \{1, y_1, \ldots, y_r; \mathbf{y} \in \mathfrak{D}_r\}$ for $p = 2S = 2r + 1$, and $\mathfrak{W} = \{1, y_1, \ldots, y_{r-1}, 2y_r; \mathbf{y} \in \mathfrak{D}_r\}$ for $p = 2S = 2r$ with the definition (1.5) for y_j. In particular, Baker's inequalities are valid for the triangular region

$$n_1 \ge n_2 \ge n_3 \ge \cdots. \tag{3.2}$$

C. Griffiths-Kelly-Sherman inequalities

The validity of GKS inequalities for the present system is clear from our observation that our system is reduced to the usual Ising model with ferromagnetic pair interactions, in which Kelly and Sherman[16] proved the inequalities of the forms

$$\langle \sigma^A \rangle \ge 0 \quad \text{and} \quad \langle \sigma^A \sigma^B \rangle \ge \langle \sigma^A \rangle \langle \sigma^B \rangle \tag{3.3}$$

for $H \ge 0$. In fact, our system is included in Ginibre's ones,[14] in which he has developed a general formulation of Griffiths' inequalities.

D. Correlation inequalities for antiferromagnets

Griffiths–Kelly–Sherman inequalities can be easily extended to the following Hamiltonian with antiferromagnetic interactions between two sublattices A and B:

$$\mathcal{H} = + \sum_{\substack{i\in A \\ j\in B}} J_{ij}^{AB} S_i^A S_j^B - \sum_{i,j\in A} J_{ij}^A S_i^A S_j^A - \sum_{i,j\in B} J_{ij}^B S_i^B S_j^B$$
$$- \lambda \sum_{j\in A} \phi_j(S_j^A) - \lambda \sum_{j\in B} \phi_j(S_j^B) + \sum_{j\in A} H_j S_j^A + \sum_{j\in B} H_j S_j^B, \tag{3.4}$$

where

$$J_{ij}^A, J_{ij}^B, \text{ and } J_{ij}^{AB} \ge 0, \tag{3.5}$$

and symmetric potentials ϕ_j satisfy condition $\mathfrak{W}$, and in particular condition (A).

By using the result pointed out for antiferromagnets of spin-$\frac{1}{2}$ by Lebowitz[19] from the general inequality of Fortuin, Ginibre, and Kasteleyn,[20] we obtain the following propositions: (i) For zero magnetic field, we have $\langle S^A \rangle \ge 0$, and $\langle S^B \rangle \ge 0$ if S^B is a product of even number of spins, and $\langle S^A S^B \rangle \le 0$ if S^B is "odd"; (ii) for all values of the external magnetic field at the different lattice sites, we get

$$\langle S_i^A S_j^A \rangle \ge \langle S_i^A \rangle \langle S_j^A \rangle \quad \text{and} \quad \langle S_j^B S_j^B \rangle \ge \langle S_j^B \rangle \langle S_j^B \rangle; \tag{3.6}$$

and (iii) for all values of $\{H_j\}$, we have

$$\langle S^A S^B \rangle \ge \langle S^A \rangle \langle S^B \rangle, \quad \text{or} \quad \langle S^A S^B \rangle \le \langle S^A \rangle \langle S^B \rangle \tag{3.7}$$

if S^B is "even", or "odd", respectively, for the Hamiltonian (3.4) under condition $\mathfrak{W}$, and in particular condition (A). Applications of these inequalities to phase transitions of antiferromagnets will be discussed in the next subsection E.

E. Existence of phase transition

In the Hamiltonian (1.3), there occur phase transitions in two and three dimensions, because the magnetization $\langle S_j \rangle$ is a nondecreasing function of λ in the Hamiltonian

(1. 3) for $H \geq 0$, and because Griffiths[5] has proved the existence of the spontaneous magnetization for $\lambda = 0$ and $H = 0$. The critical point $T_c(\lambda)$ is also a nondecreasing function of λ:

$$\frac{\partial}{\partial\lambda} T_c(\lambda) \geq 0. \tag{3.8}$$

Similar arguments are valid even in antiferromagnets described by the Hamiltonian (3. 4) under condition (A) and in particular (1. 7), because there occurs a phase transition in the two-dimensional Ising antiferromagnets with nearest neighbor interactions and because spin correlations $|\langle S_i S_j\rangle|$ are nondecreasing functions of interactions $\{J_{kl}\}$ as shown in the previous subsection D. (Note that the spontaneous sublattice magnetization M_s is defined by $M_s^2 = \lim_{|i-j|\to\infty} \langle S_i^A S_j^A\rangle$.)

4. DISCUSSIONS

The present paper has discussed the Ising model of general spin with degeneracy or symmetric potentials. The statements 1 to 3 in Sec. 1 have been proved. In particular, our explicit condition (A) for degeneracy or symmetric potentials has the simple physical meaning that a spin system described by the Hamiltonian (1. 3) with restriction (A) is *more ferromagnetic* than the usual Ising model of general spin (i.e., with degeneracy $n_1 = n_2 = n_3 = \ldots$ or a constant potential $\phi(p) = \phi(p-2) = \ldots$). Thus, our statements 1 and 2 are physically quite natural results.

Our explicit condition (A) contains the usual Ising model as a special case, for which Griffiths[5] has obtained more explicit ferromagnetic weight functions. For p *even*, he has found a *unique* solution in the representation (2. 7). However, for p *odd*, he pointed out that the solution is *not unique* even if one confines oneselves in the representation (2. 7). These situations are clearly understood from our present arguments as follows. The usual Ising model corresponds to the special point $(1, 1, \ldots, 1)$ in $\mathfrak{W}$, which is expressed in (2. 45) by the following set of $\{y_j\}$ in the domain $\mathfrak{D}_r$:

$$y_1 = y_2 = \ldots = y_{r-1} = 1 \quad \text{and} \quad y_r = \tfrac{1}{2} \quad \text{for } p \text{ even}, \tag{4.1}$$

and

$$y_1 = y_2 = \ldots = y_{r-1} = y_r = 1 \quad \text{for } p \text{ odd}. \tag{4.2}$$

Here recall that the domain $\mathfrak{D}_r$ is expressed again in terms of successive operations α_j:

$$\mathfrak{D}_r = \alpha_{r-1}\alpha_{r-2}\ldots\alpha_1\mathfrak{D}_1. \tag{4.3}$$

The operation α_{r-1} is essentially the linear transformation $A_{r-1}(a)$ defined by (2. 16) with $a = y_r$. From the expression (2. 17) for the determinant of the matrix $A_{r-1}(a)$, it is an affine transformation for p *even* (i.e., for $a = y_r = \frac{1}{2}$), hence *one-to-one mapping*. For p *odd* (i.e., $a = y_r = 1$), the determinant of the matrix is *vanishing*, hence there exists no inverse matrix; i.e., its mapping is not unique.

In connection with the present model with degeneracy, it may be of use to introduce the following Ising model of general spin variable S_j assumes the value

$$S_j = a_1, a_2, a_3, \ldots, (0), \ldots, -a_3, -a_2, -a_1, \tag{4.4}$$

where

$$a_1 \geq a_2 \geq a_3 \geq \ldots \geq a_r \geq 0. \tag{4.5}$$

The Hamiltonian has the usual form (1. 1). We may have the following theorem.

Conjectured Theorem A: The Lee–Yang circle theorem is valid for the above model under condition (B):

$$\text{(B)} \qquad 0 \leq \delta_1 \leq \delta_2 \leq \delta_3 \leq \cdots, \quad \delta_n = a_n - a_{n+1}. \tag{4.6}$$

In more general, we may have the following theorem.

Conjectured Theorem B: The Lee–Yang circle theorem is valid for the Hamiltonian:

$$\mathcal{H} = -\sum J_{ij}\psi(S_i)\psi(S_j) - \lambda\sum\phi(S_j) - H\sum h(S_j), \quad J_{ij} \geq 0, \tag{4.7}$$

where S_j takes discrete values $p, p-2, \ldots, 2-p, -p$, and $\psi(S)$, $\phi(S)$, and $h(S)$ satisfy the conditions (C):

(C)
1. $\psi(-S) = -\psi(S), h(-S) = -h(S)$ and $\phi(-S) = \phi(S)$,
2. $\delta\psi(S) = \psi(S) - \psi(S-1)$ and $\delta h(S) = h(S) - h(S-1)$ are nonincreasing functions of S for $S \geq 0$,

(4.8)

and

3. $\phi(S)$ is such an appropriate symmetric function as is defined in the region $\mathfrak{W}$.

The following several remarks may be useful to discussions on the above conjectured theorems.

(a) The model (4. 4) may be equivalent to some class of the Ising model in which S_j assumes descrete values $p, p-2, p-4, \ldots$, and their corresponding weights are given by

$$1, \underbrace{0, \ldots, 0}_{d_1}, 1, \underbrace{0, \ldots, 0}_{d_2}, 1, 0, \cdots, \tag{4.9}$$

respectively [where $d_1, d_2, \ldots$ denote numbers of zeros in the above string (4. 9)], under the relation

$$\delta_1 : \delta_2 : \delta_3 : \ldots = d_1 : d_2 : d_3 : \cdots \tag{4.10}$$

with $\delta_n = a_n - a_{n+1}$.

(b) Condition (B) implies that this system is *more ferromagnetic* than the usual Ising model of general spin (i.e., $\delta_1 = \delta_2 = \delta_3 = \ldots = 0$).

(c) For "spin $S = \frac{3}{2}$" in the sense (4. 4) (the cases $S = \frac{1}{2}$ and $S = 1$ are trivial), Conjectured Theorem A is easily confirmed in more general condition by using the representation

$$S_j = c_1\sigma_{j1} + c_2\sigma_{j2}, \quad \sigma_{jk} = \pm 1, \tag{4.11}$$

with $c_1 = \frac{1}{2}(a_1 + a_2)$ and $c_2 = \frac{1}{2}(a_1 - a_2)$. For $a_1 \geq a_2 \geq 0$, the coefficients c_1 and c_2 are nonnegative. Thus, the Hamiltonian has the form

$$\mathcal{H} = -\sum_{ij}\sum_{k,l=1}^{2} J_{ij,kl}\sigma_{jk}\sigma_{jl} - H\sum_j\sum_{k=1}^{2} c_k\sigma_{jk}, \tag{4.12}$$

with

$$J_{ij,kl} = J_{ij}c_k c_l \geq 0. \tag{4.13}$$

This yields that the Lee–Yang theorem is valid for the Hamiltonian (1. 1) with $a_1 \geq a_2 \geq 0$, and in particular under condition (B).

For "general spin S" in the sense (4.4), one may use a representation

$$S_j = \sum_{k=1}^{m} c_k \sigma_{jk} \quad , \quad c_k \geq 0 \tag{4.14}$$

when $r = 2^{m-1}$, and also $r = 2^{m-1} - n$, if one uses ferromagnetic weight functions which give zero weight to some $2n$ states of $S_j = \pm a_{j_1}, \ldots,$ and $\pm a_{j_n}$. [However, allowed values of the set $a_1, a_2, \ldots, a_r$ are rather restricted except for $r = 2$, and they do not cover condition (B).] That is, obviously the Lee–Yang theorem holds for such values of the set $\{a_j\}$ as make the representation (4.14) possible.

(d) Condition (B) is equivalent to the inequality

$$\text{(C)} \quad d_1 \leq d_2 \leq d_3 \cdots \tag{4.15}$$

under the equivalence relation (4.10). It is not yet clear whether or not this condition (C) is included in the domain $\mathfrak{W}$ discussed in the present paper. Perhaps we may have to handle more complex representations in order to obtain ferromagnetic weight functions for condition (B), or equivalently condition (C).

(e) The model with unequal separations (4.4) discussed above becomes equivalent to a special case of (4.7) with $\lambda = 0$ and

$$\psi(q) = h(q) = a_{(p-q+2)/2}. \tag{4.16}$$

The present result on the Lee–Yang theorem or its generalized proposition that all the zeros of the partition function lie on the imaginary H axis may be also true *(Conjectured Theorem C)* for the following anisotropic Heisenberg model of general spin with symmetric potentials $\phi(S_j^z)$ satisfying condition (A):

$$\mathcal{H} = -\sum (J_{ij}^x S_i^x S_j^x + J_{ij}^y S_i^y S_j^y + J_{ij}^z S_i^z S_j^z) - \lambda \sum \phi(S_j^z) - H \sum S_j^z, \tag{4.17}$$

with $J_{ij}^z \geq |J_{ij}^x|$, $J^z \geq |J_{ij}^y|$, and $\lambda \geq 0$. It is clear for $\phi(S_j^z) = (S_j^z)^2$ from the arguments by Suzuki and Fisher.[9]

It should be also remarked that correlation inequalities have been extended to several other systems.[20,21]

Applications of the present results to alloy problems will be discussed in a separate paper.[22]

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Equivalent variational functionals in potential scattering

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The equivalence is established between dual pairs of variational functionals (Kohn type) derived from the differential equation description of potential scattering and other dual pairs of variational functions (Schwinger type) derived from the integral equation description. Apparent differences are resolved by suitable choice of trial vector. The Kohn functional and minus the Schwinger functional are shown to be duals of each other.

1. INTRODUCTION

A not uncommon view[1] is that differential and integral equation descriptions lead to essentially different variational functionals for scattering processes. Dual pairs of variational functionals have been derived[2-5] which provide (under favorable circumstances) upper and lower bounds on phase shifts and scattering lengths; the pairs of functionals from the differential and integral equation approaches are apparently quite different. In this paper actual equivalence of functionals derived from the two approaches is demonstrated, apparent differences being resolved by choice of trial vector. Further the dual role of Kohn- and Schwinger-type functionals is revealed. Relationships between functionals from the two approaches are not new,[6-10] but these particular equivalence and duality properties may not previously have been realised. For simplicity only potential scattering is considered, but extensions are possible.

2. SCATTERING EQUATIONS

Scattering at wavenumber k by a short-range potential proportional to $q(r)$ gives rise to an lth partial wave $\phi(r)$ with the differential equation description

$$\left\{-\frac{d^2}{dr^2} - k^2 + \frac{l(l+1)}{r^2} + q(r)\right\}\phi(r) = 0, \quad 0 \leq r < \infty, \tag{1}$$

$$\phi(0) = 0, \tag{2}$$

$$\phi(r) \sim \alpha\{\tan\eta_l \cos(kr - \tfrac{1}{2}l\pi) + \sin(kr - \tfrac{1}{2}l\pi)\} \quad \text{as } r \to \infty. \tag{3}$$

If $q(r)$ is absent, the solution with proper behavior is

$$\phi_0(r) = \alpha k r j_l(kr) \sim \alpha \sin(kr - \tfrac{1}{2}l\pi). \tag{4}$$

Popular choices for the normalization constant α are 1 and $1/k$, but zero-energy scattering is described by the choice k^{-l-1} and procedure to the zero-k limit.

The equivalent integral equation description of $\phi(r)$ is

$$\phi(r) + \int_0^\infty [-krr' j_l(kr_<) n_l(kr_>)]\, q(r')\phi(r')dr' = \phi_0(r), \tag{5}$$

in which j_l, n_l are spherical Bessel functions and $r_<, r_>$ denote the lesser and greater of r, r'.

We think of (1) and (5) as operator equations. Let X play the role of the differential operator $\{-d^2/dr^2 - k^2 + l(l+1)/r^2\}$ and let Q denote multiplication by $q(r)$. Then the differential equation (1) takes the form

$$(X + Q)\phi = 0, \quad \phi \in D_\Phi, \tag{6}$$

where

$$X\phi_0 = 0 \tag{7}$$

and ϕ goes to ϕ_0 if Q disappears. Likewise if Y plays the role of the integral operator with symmetric kernel $-krr' j_l(kr_<) n_l(kr_>)$, the integral equation (5) becomes

$$\phi + YQ\phi = \phi_0, \quad \phi \in D_\Phi, \tag{8}$$

or in symmetrized form

$$(QYQ + Q)\phi = Q\phi_0. \tag{9}$$

Here

$$XY = \text{unit operator} \tag{10}$$

and

$$YX\phi = \phi - \phi_0, \tag{11}$$

so that Y is only a one-sided inverse of X.

The real vector space D_Φ on which X, Q, and Y are defined does not admit the scalar product

$$\langle \Phi_1, \Phi_2 \rangle = \int_0^\infty \Phi_1(r)\Phi_2(r)dr \tag{12}$$

because this integral diverges for vectors Φ behaving as in (3). However, we are only concerned with scalar products of type

$$\langle \Phi_1, A\Phi_2 \rangle = \int_0^\infty \Phi_1(r) A\Phi_2(r)dr, \tag{13}$$

where A is an operator like X or Q and the integral in (13) exists. Let us define

$$\tilde{A}(\Phi_1, \Phi_2) = \langle \Phi_1, A\Phi_2 \rangle - \langle A\Phi_1, \Phi_2 \rangle, \tag{14}$$

which is a quantity which vanishes when A is self-adjoint, as when $A = Q$ or $A = QYQ$. The operator X is *not* self-adjoint, since

$$\tilde{X}(\Phi_1, \Phi_2) = \left[-\Phi_1 \frac{d\Phi_2}{dr} + \Phi_2 \frac{d\Phi_1}{dr}\right]_0^\infty \tag{15}$$

is a nonvanishing boundary term.

The variational functionals discussed below are stationary around the quantity

$$-\tilde{X}(\phi, \phi_0) = \langle X\phi, \phi_0 \rangle = -\langle Q\phi, \phi_0 \rangle = -\langle \phi, Q\phi_0 \rangle = k\alpha^2 \tan\eta_l, \tag{16}$$

which is of physical interest, being proportional to the phase-shift tangent (or generalized scattering length at zero k).

3. VARIATIONAL FUNCTIONALS FOR $(Z + Q)\phi = f$ (Z SELF-ADJOINT)

A. Basic dual functionals

Equation (9) is of the standard type

$$(Z + Q)\phi = f, \tag{17}$$

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where Z and Q are self-adjoint operators and Q has an inverse Q^{-1}. Associated with (17) are dual variational functionals

$$J(\Phi) = \langle\Phi, (Z + Q)\Phi\rangle - 2\langle\Phi, f\rangle \tag{18}$$

$$= J(\phi) + \langle\delta\phi, (Z + Q)\delta\phi\rangle \tag{19}$$

and

$$G(\Phi) = -\langle\Phi, Z\Phi\rangle - \langle(Z\Phi - f), Q^{-1}(Z\Phi - f)\rangle \tag{20}$$

$$= G(\phi) - \langle\delta\phi, Z\delta\phi\rangle - \langle Z\delta\phi, Q^{-1}Z\delta\phi\rangle, \tag{21}$$

each of which is stationary around the common value

$$J(\phi) = G(\phi) = -\langle\phi, f\rangle \tag{22}$$

for variations in $\Phi = \phi + \delta\phi$ around ϕ, the solution of Eq. (17). The functional $J(\Phi)$ is just a Rayleigh-Ritz functional, and $G(\Phi)$ can be derived from the Rayleigh-Ritz functional for a new equation obtained by operating on (17) with ZQ^{-1}.

The basic functionals J and G are called dual, or complementary, for two reasons. Firstly they provide upper and lower bounds

$$J(\Phi) \geq -\langle\phi, f\rangle \geq G(\Phi) \tag{23}$$

under favorable circumstances, as, for example, when Z and Q are each positive operators. Secondly (and more fundamentally) they can be derived in a dual manner when Eq. (17) is decomposed into a pair of canonical Euler-Hamilton equations.[2-5]

B. Schwinger-type functionals

The J and G functionals for equation (9) are respectively the Schwinger[11,12] functional and its dual. Calling them $\mathcal{J}$ and $\mathcal{G}$, and setting $Z = QYQ, f = Q\phi_0$, we obtain for a trial vector Ψ

$$\mathcal{J}(\Psi) = \langle\Psi, (QYQ + Q)\Psi\rangle - 2\langle\Psi, Q\phi_0\rangle \quad \text{(Schwinger)}, \tag{24}$$

$$\mathcal{G}(\Psi) = -\langle\Psi, QYQ\Psi\rangle - \langle(YQ\Psi - \phi_0), Q(YQ\Psi - \phi_0)\rangle \quad \text{(dual Schwinger)}. \tag{25}$$

These functionals are stationary around the quantity

$$\mathcal{J}(\phi) = \mathcal{G}(\phi) = -\langle\phi, Q\phi_0\rangle = k\alpha^2 \tan\eta_l. \tag{26}$$

[Schwinger's name is often attached to the stationary-amplitude form of (24), i.e. to $\mathcal{J}(t\Psi)$ with $\partial\mathcal{J}/\partial t = 0$, which is $-\langle\Psi, Q\phi_0\rangle^2\langle\Psi, (QYQ + Q)\Psi\rangle^{-1}$. But here we are not concerned with special cases of the functionals.]

4. VARIATIONAL FUNCTIONALS FOR $(X + Q)\phi = 0$ (X NON-SELF-ADJOINT)

A. Preliminaries

The scattering differential equation in its operator form (6) is not an example of the standard type (17) because X is not self-adjoint. However, there is the compensation of zero f, and we may still consider the J and G functionals which are simply

$$J(\Phi) = \langle\Phi, (X + Q)\Phi\rangle, \tag{27}$$

$$G(\Phi) = -\langle\Phi, X\Phi\rangle - \langle X\Phi, Q^{-1}X\Phi\rangle \tag{28}$$

with the property that

$$J(\phi) = G(\phi) = 0. \tag{29}$$

Instead of the variational principles (19) and (21) we have now

$$J(\Phi) - J(\phi) - \tilde{X}(\phi, \Phi) = \langle\delta\phi, (X + Q)\delta\phi\rangle, \tag{30}$$

$$G(\Phi) - G(\phi) - \tilde{X}(\phi, \Phi) = -\langle\delta\phi, X\delta\phi\rangle - \langle X\delta\phi, Q^{-1}X\delta\phi\rangle. \tag{31}$$

As they stand, Eqs. (30) and (31) are not true variational principles of the type

$$\delta F = F(\Phi) - F(\phi) = O(\langle\delta\phi, \delta\phi\rangle), \tag{32}$$

since there is insufficient knowledge of the boundary term $\tilde{X}(\phi, \Phi)$ which arises because X is not self-adjoint.

B. Kohn-type variational principles

To make progress the class of trial vectors is restricted so that, for arbitrary Ψ,

$$\Phi = \phi_0 - YQ\Psi. \tag{33}$$

Then, like ϕ, Φ goes to ϕ_0 if Q disappears. Further, if Ψ is an iterative approximate solution of Eq. (8), then Φ is the next iterate. This sensible choice of trial vector leads to a favorable expression for $\tilde{X}(\phi, \Phi)$. From (7), (10), and (33) it follows that

$$X\Phi = -Q\Psi \tag{34}$$

so that

$$\Phi = \phi_0 + YX\Phi. \tag{35}$$

Thus

$$\begin{aligned}\tilde{X}(\phi, \Phi) &= \langle\phi, X\Phi\rangle - \langle X\phi, \Phi\rangle \\ &= \langle\phi_0 + YX\phi, X\Phi\rangle - \langle X\phi, \phi_0 + YX\Phi\rangle \\ &= \langle X\Phi, \phi_0\rangle - \langle X\phi, \phi_0\rangle + \tilde{Y}(X\Phi, X\phi).\end{aligned} \tag{36}$$

Since Y is self-adjoint, the last term in (36) is zero. We are left with

$$\tilde{X}(\phi, \Phi) = S(\Phi) - S(\phi) = \delta S, \tag{37}$$

where

$$S(\Phi) = \langle X\Phi, \phi_0\rangle. \tag{38}$$

The left-hand sides of Eqs. (30) and (31) are now $\delta(J - S)$ and $\delta(G - S)$, so we have recovered true variational principles, namely the Kohn principle (or Spruch-Rosenberg[12,13] at zero k) and its dual. The dual variational functionals

$$J(\Phi) - S(\Phi) = \langle\Phi, (X + Q)\Phi\rangle - \langle X\Phi, \phi_0\rangle \quad \text{(Kohn)} \tag{39}$$

and

$$G(\Phi) - S(\Phi) = -\langle\Phi, X\Phi\rangle - \langle X\Phi, Q^{-1}X\Phi\rangle - \langle X\Phi, \phi_0\rangle \quad \text{(dual Kohn)} \tag{40}$$

are each stationary around the common value (cf. (26)]

$$-S(\phi) = -\langle X\phi, \phi_0\rangle = \langle\phi, Q\phi_0\rangle = -k\alpha^2 \tan\eta_l = -\mathcal{J}(\phi) = -\mathcal{G}(\phi). \tag{41}$$

Since from (4) and (33) we have

$$\Phi \sim \alpha[B\cos(kr - \tfrac{1}{2}l\pi) + \sin(kr - \tfrac{1}{2}l\pi)], \tag{42}$$

where

$$-\alpha B = \int_0^\infty r j_l(kr) q(r) \Psi(r) dr = \langle Q\Psi, \phi_0/k\alpha \rangle, \tag{43}$$

it follows that we may substitute

$$\langle X\Phi, \phi_0 \rangle = k\alpha^2 B \tag{44}$$

in the Kohn-type functionals if desired.

C. Equivalence

It appears that there are two different pairs of dual variational functionals for the quantity $-k\alpha^2 \tan\eta_l$, namely the Kohn pair involving the differential operator X, and minus the Schwinger pair involving the integral operator Y (a one-sided inverse of X). But the difference is illusory. Substitution for Φ in terms of Ψ from (33) and (34) into (39) and (40) shows that

$$\begin{aligned}\text{(Kohn)}\quad J(\Phi) - S(\Phi) &= \langle \Phi, Q\Phi \rangle + \langle X\Phi, \Phi - \phi_0 \rangle \\ &= \langle (\phi_0 - YQ\Psi), Q(\phi_0 - YQ\Psi) \rangle \\ &\quad + \langle Q\Psi, YQ\Psi \rangle = -\mathcal{G}(\Psi) \\ &\qquad (-\text{ dual Schwinger}),\end{aligned} \tag{45}$$

and also

$$\begin{aligned}\text{(dual Kohn)}\quad C(\Phi) - S(\Phi) &= \langle \phi_0 - YQ\Psi, Q\Psi \rangle \\ &\quad - \langle Q\Psi, \Psi \rangle + \langle Q\Psi, \phi_0 \rangle \\ &= -\langle \Psi, QYQ\Psi \rangle - \langle \Psi, Q\Psi \rangle \\ &\quad + 2\langle \Psi, Q\phi_0 \rangle = -\mathcal{J}(\Psi) \\ &\qquad (-\text{ Schwinger}).\end{aligned} \tag{46}$$

5. DISCUSSION

We see that when the trial vectors Φ and Ψ are related by Eq. (33), the Kohn variational functional is equivalent to minus the dual of the Schwinger variational functional, and the dual of the Kohn is equivalent to minus the Schwinger. The Kohn functional and minus the Schwinger functional can therefore be regarded as duals of each other. Note that although the trial vector Ψ is arbitrary, Eq. (33) places a restriction on Φ. This restriction does not mar the equivalence as it is necessary anyway for the existence of the Kohn-type variational functionals.

Conditions under which Kohn-type and Schwinger-type variational functionals provide upper and lower bounds on phase-shift tangents and scattering lengths have been investigated elsewhere.[2-5,9,14] Often it is easier[4,14] to establish these bounding properties for Schwinger-type than for Kohn-type functionals. The equivalence proved here means that whenever Schwinger-type functionals provide upper and lower bounds, so also do the Kohn-type (always provided that the respective trial vectors are appropriately related). Further in such circumstances the Kohn functional and minus the Schwinger functional will provide dual bounds.

In conclusion it is perhaps relevant to remark that the equivalence properties established above were suggested to the writer by somewhat similar results which are available for the standard equation (17) when the self-adjoint operator Z has a two-sided inverse Z^{-1} and no boundary terms are involved. Operating on (17) with QZ^{-1}, we have

$$(QZ^{-1}Q + Q)\phi = QZ^{-1}f, \tag{47}$$

which is again of standard type. Thus, by analogy with (17)-(22), the dual variational functionals

$$\bar{J}(\Psi) = \langle \Psi, (QZ^{-1}Q + Q)\Psi \rangle - 2\langle \Psi, QZ^{-1}f \rangle, \tag{48}$$

$$\bar{G}(\Psi) = -\langle \Psi, QZ^{-1}Q\Psi \rangle - \langle Z^{-1}(Q\Psi - f), QZ^{-1}(Q\Psi - f) \rangle \tag{49}$$

have common stationary value

$$\begin{aligned}\bar{J}(\phi) = \bar{G}(\phi) &= -\langle \phi, QZ^{-1}f \rangle \\ &= -\langle Z^{-1}Q\phi, f \rangle = \langle \phi, f \rangle - \langle fZ^{-1}f \rangle\end{aligned} \tag{50}$$

and lead to the pair of variational functionals $-[\bar{J}(\Psi) + \langle f, Z^{-1}f \rangle]$ and $-[\bar{G}(\Psi) + \langle f, Z^{-1}f \rangle]$ for the quantity $-\langle \phi, f \rangle$. These apparently new functionals involving Z^{-1} in fact satisfy the relations

$$\bar{J}(\Psi) + \langle f, Z^{-1}f \rangle = -C(\Phi), \tag{51}$$

$$\bar{G}(\Psi) + \langle f, Z^{-1}f \rangle = -J(\Phi), \tag{52}$$

where

$$Z\Phi + Q\Psi = f. \tag{53}$$

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Finite and infinitesimal canonical transformations. II*

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Linear differential equations generating finite canonical transformations are obtained for cases where the infinitesimal generator $\omega(q,p)$ is a homogeneous function of degree α in either one or both canonical variables.

1. INTRODUCTION

In a previous article,[1] the author discussed the relationship between the finite and infinitesimal representations of a one-parameter subgroup of canonical transformations given by

$$Q = Q(q,p,\tau), \qquad P = P(q,p,\tau), \tag{1}$$

with q and p denoting canonical variable n-tuples, τ a real 1-tuple parameter, and where $\tau = 0$ corresponds to the identity transformation. By using Lie representation theory together with the infinitesimal generator $\omega(q,p)$, canonical transformations of the form (1) are obtained through the formula[2]

$$\begin{pmatrix} Q \\ P \end{pmatrix} = T(\tau)\begin{pmatrix} q \\ p \end{pmatrix}, \tag{2}$$

with

$$T(\tau) \equiv \exp\left[\tau\left(\frac{\partial\omega}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial\omega}{\partial q_i}\frac{\partial}{\partial p_i}\right)\right], \tag{3}$$

and where the summation convention is employed over repeated indices. In addition, the operator $T(\tau)$ satisfies the function theorem for Lie representations given by

$$T(\tau)f(q,p) = f(T(\tau)q, T(\tau)p) \tag{4}$$

for an arbitrary observable $f(q,p)$. Although the more lucid Lie representation is convenient from the point of view of infinitesimal transformations, the generation of finite transformations is not generally straightforward since this requires the evaluation of the formal operator $T(\tau)$ in closed form.

An alternative method[3] for constructing canonical transformations of the form (1) makes use of finite generating functions $\mathfrak{F}_k$, explicit in one old and one new canonical variable n-tuple. Because the transformations (1) require connectivity to the identity, only the functions $\mathfrak{F}_2(q,P,\tau)$ and $\mathfrak{F}_3(Q,p,\tau)$ are of interest, generating canonical transformations through the relations

$$p(q,P,\tau) = \frac{\partial\mathfrak{F}_2}{\partial q}, \qquad Q(q,P,\tau) = \frac{\partial\mathfrak{F}_2}{\partial P}, \tag{5}$$

$$q(Q,p,\tau) = -\frac{\partial\mathfrak{F}_3}{\partial p}, \qquad P(Q,p,\tau) = -\frac{\partial\mathfrak{F}_3}{\partial Q}, \tag{6}$$

where free indices are suppressed for notational convenience. The general relation between the above finite and infinitesimal representations of the one-parameter subgroup of canonical transformations (1) was found[1] to be simply a generalization of the Hamilton–Jacobi equation subject to certain boundary conditions. These relations for the functions $\mathfrak{F}_2$ and $\mathfrak{F}_3$ are given by

$$\frac{\partial\mathfrak{F}_2}{\partial\tau} = \omega\left(q, \frac{\partial\mathfrak{F}_2}{\partial q}\right) = \omega\left(\frac{\partial\mathfrak{F}_2}{\partial P}, P\right), \tag{7}$$

$$\mathfrak{F}_2(q,P,0) = q_iP_i = q_ip_i, \tag{8}$$

$$\frac{\partial\mathfrak{F}_3}{\partial\tau} = \omega\left(-\frac{\partial\mathfrak{F}_3}{\partial p}, p\right) = \omega\left(Q, -\frac{\partial\mathfrak{F}_3}{\partial Q}\right), \tag{9}$$

$$\mathfrak{F}_3(Q,p,0) = -Q_ip_i = -q_ip_i. \tag{10}$$

Formal integral representations of solutions to the above equations for $\mathfrak{F}_2$ and $\mathfrak{F}_3$, analogous to the action integral of Hamiltonian dynamics, assume the form

$$\mathfrak{F}_2[Q,P] = \int_0^\tau \left(Q_i\frac{dP_i}{d\tau} + \omega(Q,P)\right)d\tau + q_ip_i, \tag{11}$$

$$\mathfrak{F}_3[Q,P] = \int_0^\tau \left(-P_i\frac{dQ_i}{d\tau} + \omega(Q,P)\right)d\tau - Q_iP_i. \tag{12}$$

The differential equations (7) and (9) together with (5) and (6) provide general prescriptions for obtaining closed form evaluations of (2) for a given infinitesimal generator $\omega(q,p)$. However, this procedure can itself be difficult because of the generally nonlinear character of (7) and (9).

In the present paper, we note that for cases where $\omega(q,p)$ is a homogeneous function of degree α in either one or both canonical variables, additional linear differential equations are obtained for the transformation (1), resulting in a procedure possibly preferred over both direct evaluation of $T(\tau)$ and the Hamilton–Jacobi method.

2. PRELIMINARY ANALYSIS

By treating $\mathfrak{F}_2$ and $\mathfrak{F}_3$ as functions of the original canonical variables q and p, direct application of (5) and (6) yields the conditions

$$\begin{aligned}\left(\frac{\partial\mathfrak{F}_2}{\partial q}\right)_{p,\tau} &= p + Q_i\left(\frac{\partial P_i}{\partial q}\right)_{p,\tau},\\ \left(\frac{\partial\mathfrak{F}_2}{\partial p}\right)_{q,\tau} &= Q_i\left(\frac{\partial P_i}{\partial p}\right)_{q,\tau},\end{aligned} \tag{13}$$

$$\begin{aligned}\left(\frac{\partial\mathfrak{F}_3}{\partial q}\right)_{p,\tau} &= -P_i\left(\frac{\partial Q_i}{\partial q}\right)_{p,\tau},\\ \left(\frac{\partial\mathfrak{F}_3}{\partial p}\right)_{q,\tau} &= -q - P_i\left(\frac{\partial Q_i}{\partial p}\right)_{q,\tau}.\end{aligned} \tag{14}$$

Using Poisson bracket notation defined by

$$[f,g] \equiv \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}, \tag{15}$$

we see that suitable linear combinations of (13) and (14) give the general differential equations

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$$[P, \mathfrak{F}_2] + p_i \left(\frac{\partial P}{\partial p_i}\right)_{q,\tau} = 0, \tag{16}$$

$$[Q, \mathfrak{F}_3] + q_i \left(\frac{\partial Q}{\partial q_i}\right)_{p,\tau} = 0, \tag{17}$$

$$[X, \mathfrak{F}_5] + q_i \left(\frac{\partial X}{\partial q_i}\right)_{p,\tau} + p_i \left(\frac{\partial X}{\partial p_i}\right)_{q,\tau} = X, \tag{18}$$

$$X \equiv \begin{pmatrix} Q \\ P \end{pmatrix},$$

where we have introduced the convenient definition

$$\mathfrak{F}_5 \equiv \mathfrak{F}_2 + \mathfrak{F}_3. \tag{19}$$

Although valid in general, these relations are not useful unless one of the finite generating functions $\mathfrak{F}_k$ is known in terms of the original canonical variables q and p. However, it is shown in what follows that explicit expressions for $\mathfrak{F}_2$ and $\mathfrak{F}_3$ in terms of q and p are easily obtained for cases where $\omega(q,p)$ is a homogeneous function of degree α in either one or both canonical variable n-tuples.

3. HOMOGENEOUS INFINITESIMAL GENERATORS

We first consider the special case defined by

$$\omega(\lambda q, p) = \lambda^\alpha \omega(q,p). \tag{20}$$

By applying (2), the function theorem (4) and (20) to (11), we obtain

$$\mathfrak{F}_2 = \int_0^\tau T(\tau) \left(-q_i \frac{\partial \omega}{\partial q_i} + \omega(q,p)\right) d\tau + q_i p_i$$
$$= \tau(1-\alpha)\omega(q,p) + q_i p_i. \tag{21}$$

Substitution of (21) into (13) and (16) then yields the system of linear equations

$$\tau(1-\alpha)[P,\omega] + q_i \left(\frac{\partial P}{\partial q_i}\right)_{p,\tau} = 0, \tag{22}$$

$$Q_i \left(\frac{\partial P_i}{\partial q}\right)_{p,\tau} = \tau(1-\alpha)\frac{\partial \omega}{\partial q}. \tag{23}$$

Similarly, for the case given by

$$\omega(q, \lambda p) = \lambda^\alpha \omega(q,p), \tag{24}$$

we find that

$$\mathfrak{F}_3 = \tau(1-\alpha)\omega(q,p) - q_i p_i. \tag{25}$$

This result together with (14) and (17) gives the equations

$$\tau(1-\alpha)[Q,\omega] + p_i \left(\frac{\partial Q}{\partial p_i}\right)_{q,\tau} = 0, \tag{26}$$

$$P_i \left(\frac{\partial Q_i}{\partial p}\right) = \tau(\alpha - 1)\frac{\partial \omega}{\partial p}. \tag{27}$$

Finally, for the case defined by

$$\omega(\lambda q, \lambda p) = \lambda^\alpha \omega(q,p) \tag{28}$$

it follows that

$$\mathfrak{F}_5 = \tau(2-\alpha)\omega(q,p), \tag{29}$$

which when substituted into (18) yields

$$\tau(2-\alpha)[X,\omega] + q_i \left(\frac{\partial X}{\partial q_i}\right)_{p,\tau} + p_i \left(\frac{\partial X}{\partial p_i}\right)_{q,\tau} = X. \tag{30}$$

Solutions to each of the above differential equations must satisfy the conditions

$$Q(q,p,0) = q, \qquad P(q,p,0) = p. \tag{31}$$

It is important to note that for certain singular values of α, $\alpha = 1$ in (20) or (24), and $\alpha = 2$ in (28), the content of the corresponding differential equations is minimal and the solution method breaks down.

To illustrate our procedure for obtaining finite canonical transformations of the form (1) from a homogeneous infinitesimal generator $\omega(q,p)$, we consider the special case given by

$$\omega(q,p) = p^k q^l, \qquad n = 1. \tag{32}$$

Since (32) satisfies (20) with $\alpha = l$, substitution into (22) and (23) yields the equations

$$[q + \tau(1-l)kp^{k-1}q^l]\frac{\partial P}{\partial q} - [\tau(1-l)lp^k q^{l-1}]\frac{\partial P}{\partial p} = 0, \tag{33}$$

$$Q\frac{\partial P}{\partial q} = \tau(1-l)lp^k q^{l-1}. \tag{34}$$

Integration of (33) subject to (31) using the method of Lagrange,[4] together with (34) yields the relations

$$Q(q,p,\tau) = \begin{cases} q[(k-l)p^{k-1}q^{l-1}\tau + 1]^{k/(k-l)}, & k \neq l, \\ q\exp(l\tau p^{l-1}q^{l-1}), & k = l, \end{cases} \tag{35}$$

$$P(q,p,\tau) = \begin{cases} p[(k-l)p^{k-1}q^{l-1}\tau + 1]^{l/(l-k)}, & k \neq l, \\ p\exp(-l\tau p^{l-1}q^{l-1}), & k = l. \end{cases} \tag{36}$$

That the expressions (35) and (36) constitute a canonical transformation can be easily shown by verifying that they satisfy the fundamental Poisson bracket relation

$$[Q,P] = 1.$$

Furthermore, since (32) also satisfies (24) and (28), the above transformations can be obtained from one of the other systems of differential equations. Consequently, as can be verified by explicit calculation, the relations (35) and (36) also satisfy (26) and (27) with $\alpha = k$ and (30) with $\alpha = k + l$.

The above procedure for obtaining finite canonical transformations of the form (1) from a homogeneous infinitesimal generator $\omega(q,p)$ is amenable to linear methods, and therefore may be preferred over both closed form evaluation of $T(\tau)$ and the Hamilton–Jacobi method.

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Static gravitational fields. II. Ricci rotation coefficients

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Investigations of static gravitational fields in paper I are continued further. Instead of the system of second order partial differential equations in I, the equivalent first order system involving the Ricci rotation coefficients is dealt with here. The algebraic and the differential dependences among the equations have been sorted out to prove that the system is determinate. Then an attempt towards classifying this system of partial differential equations has been made. Except for "the potential equation" which is obviously elliptic, the remaining system is hyperbolic for which the characteristic surfaces have been determined. To obtain some exact solutions the lead of Newman–Penrose is followed in constructing the complex linear combinations of the equations. The class of static universes where "gravitational lines of force" are geodesics have been found. In this class one subclass is transformable to the conformastat metric and the remaining one reduces to a new metric involving the gravitational field of an arbitrary number of parallel infinite plates clamped at infinity. The source at infinity corresponds to that of the Newtonian potential $\varphi = (1/2)[(m + 1/2)(x^1)^2 - (1/2)\{m + 1/2 - (m^2 - 1/4)^{1/2}\}(x^2)^2 - (1/2)\{m + 1/2 + (m^2 - 1/4)^{1/2}\}(x^3)^2]$. This metric belongs to the nondegenerate Type I of Petrov's classification scheme. Next the class of static universes with "shearfree lines of force" is obtained. Here too one subclass goes over to the conformastat metric and the remaining one reduces to a Weyl-type universe.

1. INTRODUCTION

In the study of gravitational radiation, Newman and Penrose[1] have used successfully the method of complex Ricci rotation coefficients. Perjes[2] has recently applied the Ricci rotation coefficients to the stationary fields. It is pertinent to ask then what a similar method can offer in the more limited area of static gravitation which has been partly explored in paper I.[3] Here the static gravitational equations have been expressed as first order partial differential equations involving the Ricci rotation coefficients. But unlike the previous authors who used $R_{ABCD} = C_{ABCD}$ as field equations and treated the right-hand sides as inhomogeneities compatible with Petrov classification, here the field equations $R_{AB} = 0$ have been used. Furthermore, in the complex combinations of the field equations the spinor considerations have been discarded in favor of an alternative combination, more suited to the static situation.

The number of real first order equations derived exceeds that of the unknown functions. But when all the algebraic and differential identities are taken into account the system turns out to be determinate.

In the next theorem the system of quasilinear first order partial differential equations which are equivalent to the static field equations has been classified. The system turns out to be hyperbolic when the single 'potential equation' is excluded. Characteristic surfaces for the hyperbolic equations are found together with the constraining condition on the Cauchy data prescribed on a characteristic surface.

One of the motivations behind the derivation of the first order system is to obtain some exact solution representing a special class of static gravitational universes. For that purpose certain complex linear combinations have been taken which are not a consequence of spinor considerations. Besides that two of the coordinates have been chosen to be the complex conjugate coordinates.

In Newtonian physics the class of gravitational fields with lines of force being straight lines is generated by a sphere or an infinite rod or an infinite plate or some suitable superposition of these sources. The Einsteinian analog of this problem is the class of static universes with 'lines of force' being geodesics. This class is found by solving the first order system involving complex Ricci rotation coefficients. It turns out that the universe due to a sphere or a rod or a plate (but not any superposition) is still in this class and any one of these is reducible to the conformastat form. In addition there exists another class without Newtonian analog which is transformable to a new metric. This metric physically represents the gravitational universe generated by an arbitrary number of parallel infinite plates held together at infinity. The mass at infinity corresponds to that of the Newtonian potential

$$\varphi = (1/2)[(m + 1/2)(x^1)^2 - (1/2)\{m + 1/2 - (m^2 - 1/4)^{1/2}\}(x^2)^2 - (1/2)\{m + 1/2 + (m^2 - 1/4)^{1/2}\}(x^3)^2].$$

This new metric belongs to the nondegenerate class $[1^2, 1^2, 1^2]$ of Petrov's classification scheme. All these results are concisely stated in Theorem 3.

The next theorem deals with the class of static universes with 'shearfree lines of force'. One subcase turns out to be of the conformastat form and the other reduces to a Weyl-type metric.

2. DEFINITIONS AND NOTATIONS

V_4 denotes a Riemannian universe of events. A point $x \in V_4$ has coordinates x^i (i and other Latin indices take 1, 2, 3, 4). A x^4-constant spatial universe of V_4 is denoted by V_3 and a point $\mathbf{x} \in V_3$ has co-ordinates x^α (α and other Greek indices take 1, 2, 3).

$$\Phi = -e^{-w(\underline{x})}\bar{g}_{\alpha\beta}(\underline{x})dx^\alpha dx^\beta + e^{w(\underline{x})}(dx^4)^2.$$

The metric form $\overline{\Phi} = \bar{g}_{\alpha\beta}(\underline{x})dx^\alpha dx^\beta$ defines a positive definite $\overline{V}_3$.

A domain of V_4 is purely gravitational provided the Ricci tensor $R_{ij} = 0$ there. It follows[3] then in the spatial domain of $\overline{V}_3$ for a static gravitational V_4,

$$\text{(F)} \quad \begin{aligned} &\tilde{\sigma}_{\alpha\beta} \equiv \overline{R}_{\alpha\beta} + \tfrac{1}{2}w_{,\alpha}w_{,\beta} = 0, \\ &\rho \equiv \overline{\Delta}_2 w = 0, \end{aligned}$$

where comma denotes partial derivatives, $\overline{R}_{\alpha\beta}$ is the Ricci subtensor of $\overline{V}_3$, and $\overline{\Delta}_2$ is the invariant Laplacian in $\overline{V}_3$.

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In addition to this summary of the definitions and notations in the paper[3] denoted by I, the following will be needed.

Definition 1: An orthonormal triad field $\lambda_A{}^\alpha(\underset{\sim}{x})$ in $\overline{V}_3$ satisfies

$$\lambda_A{}^\alpha\lambda_{B\alpha} = \delta_{AB}, \qquad \lambda_{A\alpha}\lambda_{A\beta} = \tilde{g}_{\alpha\beta}(\underset{\sim}{x}), \tag{2.1}$$

where δ_{AB} is the Kronecker delta and the summation convention is followed on the capital Latin labels that take 1, 2, 3 except when otherwise mentioned.

Definition 2: The set of invariants of a tensor field $T^{\alpha\beta\cdots}_{\gamma\delta\cdots}(\underset{\sim}{x})$ in $\overline{V}_3$ relative to $\lambda_A{}^\alpha$, are defined to be

$$T_{AB\cdots CD\cdots} \equiv \lambda_{A\alpha}\lambda_{B\beta}\cdots\lambda_C{}^\gamma\lambda_D{}^\delta\cdots T^{\alpha\beta\cdots}_{\gamma\delta\cdots}. \tag{2.2}$$

Remark: Because of the bisymmetry of the correspondence between tensor components and its invariants any tensorial relationship not involving derivatives will be preserved in invariants.

Definition 3: The intrinsic derivative of an invariant is defined as follows:

$$T_{AB\cdots|S} \equiv T_{AB\cdots,\alpha}\lambda_S{}^\alpha. \tag{2.3}$$

Definition 4: The Ricci rotation coefficients are defined as

$$\gamma_{ABC} \equiv \lambda_{A\mu\|\nu}\lambda_B{}^\mu\lambda_C{}^\nu, \tag{2.4}$$

where the double stroke denotes covariant derivative in $\overline{V}_3$.

Definition 5: The set of invariants corresponding to the Riemann and Ricci tensors in $\overline{V}_3$ are denoted by $\overline{R}_{ABCD}$ and $\overline{R}_{AB}$, respectively.

3. STATIC GRAVITATIONAL EQUATIONS IN TERMS OF THE INVARIANTS

For the sake of subsequent use, condensed results of six known results[4] will be displayed below.

(i) $$\gamma_{ABC} = -\gamma_{BAC}, \tag{3.1}$$

(ii) $$T\cdots_{|[AB]} + \gamma_{C[AB]}T\cdots_{|C} = 0, \tag{3.2}$$

where the square bracket around two indices denotes antisymmetrization.[1] (The present notation differs from that of Schouten by a factor 2.) Choosing $T\cdots = x^\alpha$ one obtains

(*M*): $$\lambda_A{}^\alpha{}_{,\nu}\lambda_B{}^\nu - \lambda_B{}^\alpha{}_{,\nu}\lambda_A{}^\nu + \gamma_{C[AB]}\lambda_C{}^\alpha = 0, \tag{3.2′}$$

(iii) $$\overline{R}_{ABCD} = \gamma_{AB[C|D]} + \gamma_{ABM}\gamma_{M[CD]} + \gamma_{MAD}\gamma_{MBC} - \gamma_{MAC}\gamma_{MBD}. \tag{3.3}$$

(iv) $$\overline{R}_{ABCD} = -\overline{R}_{BACD} = \overline{R}_{CDAB}, \quad \overline{R}_{A[BCD]} = 0, \quad \overline{R}_{CABC} = \overline{R}_{AB} = \overline{R}_{BA}, \tag{3.4}$$

where the square bracket around three indices denotes the cyclic permutation.[1]

(v) $$\overline{R}_{ABCD} = \delta_{AD}\overline{R}_{BC} - \delta_{AC}\overline{R}_{BD} + \delta_{BC}\overline{R}_{AD} - \delta_{BD}\overline{R}_{AC} + \frac{\overline{R}}{2}(\delta_{AC}\delta_{BD} - \delta_{AD}\delta_{BC}), \tag{3.5}$$

(vi) (*B*): $$\overline{R}_{AB[CD|E]} = \gamma_{AM[E}\overline{R}_{CD]MB} - \gamma_{BM[E}\overline{R}_{CD]MA} + \overline{R}_{ABM[D}\gamma^M_{\cdot EC]} - \overline{R}_{ABM[D}\gamma^M_{\cdot CE]}, \tag{3.6}$$

where $\gamma^M_{\cdot EC} \equiv \gamma_{MEC}$.

Static gravitational field equations in terms of the invariants are the following:

(*F*): $$\tilde{\sigma}_{AB} = \overline{R}_{AB} + \tfrac{1}{2}w_{|A}w_{|B} = 0, \qquad \rho = w_{|AA} + \gamma_{CAA}w_{|C} = 0. \tag{3.7}$$

These follow from (*F*). But for the present purpose equivalent equations which follow from (4.6) of I, will be written below:

(*F″*): $$\sigma_{ABCD} = \overline{R}_{ABCD} + \tfrac{1}{2}(\delta_{AD}w_{|B}w_{|C} - \delta_{AC}w_{|B}w_{|D} + \delta_{BC}w_{|A}w_{|D} - \delta_{BD}w_{|A}w_{|C}) + \tfrac{1}{4}(w_{|E}w_{|E})(\delta_{AC}\delta_{BD} - \delta_{AD}\delta_{BC}) = 0, \quad \rho = 0. \tag{3.8}$$

Results (3.1)–(3.8) followed from well-known tensor equations in Riemannian geometry together with static gravitational equations (*F*) or (*F″*) in I. To simplify the field equations the congruence of $\lambda_{A\alpha}$ will be chosen to be normal. In a $\overline{V}_3$ this choice can be made without loss of generality. This assumption brings in the following simplifications:

$$\lambda_{A\alpha} = U_{(A)}f_{A,\alpha} \quad (A \text{ not summed}), \tag{3.9}$$

$$\gamma_{ABC} = 0, \quad (A,B,C \neq), \tag{3.10}$$

(*N*): $$\gamma_{LPP|R} - \gamma_{RPP|L} + \gamma_{RLL}\gamma_{LPP} - \gamma_{LRR}\gamma_{RPP} = 0, \quad \text{(no summation and } L,P,R \neq). \tag{3.11}$$

Making the coordinate transformation $x'^1 = f_1(\underset{\sim}{x})$, $x'^2 = f_2(\underset{\sim}{x})$, $x'^3 = f_3(\underset{\sim}{x})$ and dropping primes subsequently, (3.9) goes over to

$$\lambda_{A\alpha} = U_{(A)}\delta_{A\alpha}. \tag{3.12}$$

A more convenient nomenclature will be introduced in the following:

$$U = U_{(1)}, \quad V = U_{(2)}, \quad W = U_{(3)}, \tag{3.13}$$

$$a = \gamma_{121}, \quad b = \gamma_{122}, \quad l = \gamma_{131}, \quad n = \gamma_{133}, \quad s = \gamma_{232}, \quad t = \gamma_{233}. \tag{3.14}$$

From definitions one obtains

$$(\tilde{g}_{\mu\nu}) = \begin{pmatrix} U^2 & 0 & 0 \\ 0 & V^2 & 0 \\ 0 & 0 & W^2 \end{pmatrix}, \quad UVW > 0, \tag{3.15}$$

$$T\cdots_{|1} = U^{-1}T\cdots_{,1}, \quad T\cdots_{|2} = V^{-1}T\cdots_{,2}, \quad T\cdots_{|3} = W^{-1}T\cdots_{,3}.$$

Putting (3.12)–(3.15) into (3.8), (3.2′), (3.11) one gets, respectively,

$$(\underset{\sim}{F}''): \quad U^{-1}b_{,1} - V^{-1}a_{,2} + a^2 + b^2 + ls + \tfrac{1}{4}(U^{-2}w^2_{,1} + V^{-2}w^2_{,2} - W^{-2}w^2_{,3}) = 0, \tag{3.16a}$$

$$U^{-1}n_{,1} - W^{-1}l_{,3} + l^2 + n^2 - at + \tfrac{1}{4}(U^{-2}w^2_{,1} - V^{-2}w^2_{,2} + W^{-2}w^2_{,3}) = 0, \tag{3.16b}$$

$$V^{-1}t_{,2} - W^{-1}s_{,3} + s^2 + t^2 + bn + \tfrac{1}{4}(-U^{-2}w^2_{,1} + V^{-2}w^2_{,2} + W^{-2}w^2_{,3}) = 0, \tag{3.16c}$$

$$V^{-1}n_{,2} + t(n-b) + \tfrac{1}{2}U^{-1}V^{-1}w_{,1}w_{,2} = 0, \tag{3.16d}$$

$$U^{-1}t_{,1} + n(a+t) + \tfrac{1}{2}U^{-1}V^{-1}w_{,1}w_{,2} = 0, \tag{3.16e}$$

$$W^{-1}a_{,3} - l(a+t) - \tfrac{1}{2}V^{-1}W^{-1}w_{,2}w_{,3} = 0, \tag{3.16f}$$

$$V^{-1}l_{,2} - a(l-s) - \tfrac{1}{2}V^{-1}W^{-1}w_{,2}w_{,1} = 0, \tag{3.16g}$$

$$U^{-1}s_{,1} - b(l-s) - \tfrac{1}{2}W^{-1}U^{-1}w_{,3}w_{,1} = 0, \tag{3.16h}$$

$$W^{-1}b_{,3} + s(n-b) + \tfrac{1}{2}W^{-1}U^{-1}w_{,3}w_{,1} = 0, \tag{3.16i}$$

$$\begin{aligned}\rho = {} & U^{-2}w_{,11} + V^{-2}w_{,22} + W^{-2}w_{,33} \\ & + w_{,1}(U^{-1}(U^{-1})_{,1} + b + n) \\ & + w_{,2}(V^{-1}(V^{-1})_{,2} + t - a) \\ & + w_{,3}(W^{-1}(W^{-1})_{,3} - l - s) = 0,\end{aligned} \tag{3.16j}$$

(M):
$$(\ln U)_{,2} = -aV, \tag{3.17a}$$

$$(\ln U)_{,3} = -lW, \tag{3.17b}$$

$$(\ln V)_{,1} = bU, \tag{3.17c}$$

$$(\ln V)_{,3} = -sW, \tag{3.17d}$$

$$(\ln W)_{,2} = tV, \tag{3.17e}$$

$$(\ln W)_{,1} = nU, \tag{3.17f}$$

(N):
$$W^{-1}a_{,3} - V^{-1}l_{,2} - tl - sa = 0, \tag{3.18a}$$

$$W^{-1}b_{,3} + U^{-1}s_{,1} - lb + ns = 0, \tag{3.18b}$$

$$U^{-1}t_{,1} - V^{-1}n_{,2} + bt + an = 0. \tag{3.18c}$$

The system of partial differential equations (3.16a)–(3.18c) has 19 equations in 10 unknown functions. But there exist 9 identities (algebraic and differential) which make the system determinate. (N) is satisfied identically by algebraic combinations of (3.16d)–(3.16i). (M) and the 3 integrability conditions of (M) imply 3 equations obtainable by the algebraic combinations of (3.16d)–(3.16i). In $(\underline{\mathfrak{F}}'')$ there exist three differential identities which are related to the Eqs. (3.5). This accounts for 9 identities. Therefore, the system is determinate.

Now an attempt towards the classification[3] of the system of quasilinear partial differential equations (3.16a)–(3.18c) will be made. In this discussion the potential equation (3.16j) which is obviously elliptic, will be excluded. The remaining first order system is equivalent to the usual second order field equations in orthogonal coordinates. Remembering this fact,[5] independent equations that have to be chosen from the system (3.16a)–(3.18c) are (3.16a)–(3.16c) and (N). Now the theorem regarding the classification can be stated below:

Theorem 1: Let the Ricci rotation coefficients a, b, l, n, s, t be of C^1 and U, V, W of C^2 with $UVW > 0$ in $\underline{D} \subset \underline{V}_3$.

(i) Then the system of first order quasilinear partial differential equations (3.16a)–(3.16c), (3.18a)–(3.18c) is hyperbolic.

(ii) If a surface $\varphi(x^1, x^2, x^3) = 0$ is such that $\varphi_{,\alpha} \neq 0$ $(\alpha = 1, 2, 3)$, then from arbitrarily prescribed Cauchy data on the surface the derivatives $a_{,\alpha}, \ldots, t_{,\alpha}$ can be uniquely determined.

(iii) If a surface $\varphi = 0$ is such that any one or two (not three) of $\varphi_{,\alpha}$ is zero than it is a characteristic surface of the system of partial differential equations. Moreover, $\exists$ is a differential relation which restricts the Cauchy data on such a surface.

Proof: Defining $[u^1, u^2, \ldots, u^6] = [a, b, \ldots, t]$ the system of differential equations can be written as

$$\begin{aligned} & L_j(u^i) = a^{ij,\nu}u^i_{,\nu} + b^j = 0, i, j = (1, \ldots, 6) \\ \text{or} \quad & L(\mathbf{u}) = A^\nu \mathbf{u}_{,\nu} + \mathbf{b} = \mathbf{0}, \end{aligned} \tag{3.19}$$

where the matrix $A^\nu = (a^{ij,\nu})$ and the vector $\mathbf{b} = [b^i]$ do not depend on the derivatives $u^i_{,\alpha}$.

For a surface S: $\varphi(x^1, x^2, x^3) = 0$, $\varphi_{,\alpha}\varphi_{,\alpha} > 0$, the characteristic matrix is[5]

$$A \equiv A^\nu \varphi_{,\nu} = \begin{bmatrix} -V^{-1}\phi_{,2} & 0 & 0 & 0 & W^{-1}\phi_{,3} & 0 \\ U^{-1}\phi_{,1} & 0 & 0 & 0 & 0 & W^{-1}\phi_{,3} \\ 0 & -W^{-1}\phi_{,3} & 0 & 0 & -V^{-1}\phi_{,2} & 0 \\ 0 & U^{-1}\phi_{,1} & 0 & V^{-1}\phi_{,2} & 0 & 0 \\ 0 & 0 & -W^{-1}\phi_{,3} & 0 & 0 & U^{-1}\phi_{,1} \\ 0 & 0 & V^{-1}\phi_{,2} & -U^{-1}\phi_{,1} & 0 & 0 \end{bmatrix}. \tag{3.20}$$

Now the characteristic determinant

$$\det(A) = 0 \Rightarrow \varphi_{,1}\varphi_{,2}\varphi_{,3} = 0. \tag{3.21}$$

The above condition shows that the system is hyperbolic.

From (3.21) one concludes that for a surface S: $\varphi = 0 \ni \varphi_{,\alpha} \neq 0 (\alpha = 1, 2, 3)$, $\det(A) \neq 0$. On S however $u^i_{,\alpha}\varphi_{,\beta} - u^i_{,\beta}\varphi_{,\alpha}$ is an interior derivative. Hence $u_{,\alpha}$ is known in S from the data if $u_{,\beta}$ is known. Multiplying (3.19) by $\varphi_{,\alpha}$ one has

$$\varphi_{,\alpha}L(\mathbf{u}) = A^\beta \varphi_{,\beta}\mathbf{u}_{,\alpha} + \mathbf{s}_\alpha = A\mathbf{u}_{,\alpha} + \mathbf{s}_\alpha = \mathbf{0}, \tag{3.22}$$

where $\mathbf{s}_\alpha$ is an interior derivative on $\mathbf{u}$ in S. Hence under the condition $\det(A) \neq 0$ the system (3.22) of linear equations for the vector $\mathbf{u}_{,\alpha}$ determines it uniquely.

The condition (3.21) under the restriction $\varphi_{,\alpha}\varphi_{,\alpha} > 0$ gives a characteristic surface S_0. Now the condition $\det(A) = 0 \Rightarrow \exists\ \mathbf{v}(x^1, x^2, x^3) \ni A\mathbf{v} = \mathbf{0}$. Multiplying (3.22) by v^i yields an equation

$$v^i\varphi_{,\alpha}L_i(\mathbf{u}) = v^i g_{i\alpha} = 0,$$

expressed by an interior differential operator on the data along S_0; this operator $v^i g_{i\alpha}$ does not contain $u^i_{,\alpha}$. Thus $v^i g_{i\alpha} = 0$ is a differential relation which restricts the initial values of u^i on S_0.

4. COMPLEX CONJUGATE COORDINATES AND COMPLEX ROTATION COEFFICIENTS

For the purposes of obtaining a solution, the system of partial differential equations (3.16a)–(3.17f), one introduces complex conjugate coordinates, complex Ricci

rotation coefficients, a suitable triad and three suitable coordinate conditions.

The triad field will be chosen such that the congruence of $\lambda_{1\alpha}$ is normal to the surface $w(\underline{x})$. This would imply that

$$\lambda_{1\alpha} = Uw_{,\alpha}, \tag{4.1}$$

$$\gamma_{123} = \gamma_{132}. \tag{4.2}$$

Congruences $\lambda_2^\alpha, \lambda_3^\alpha$ are chosen to be the first and second normal respectively to the congruence λ_1^α ("lines of force"). This choice introduces the simplification

$$\gamma_{131} = 0. \tag{4.3}$$

The three coordinate conditions to be imposed are

$$\begin{aligned} w &= x^1, \\ \bar{g}_{23} &= 0, \\ \bar{g}_{22} &= \bar{g}_{33}. \end{aligned} \tag{4.4}$$

The first choice implies that $\lambda_{1\alpha} = U\delta_{1\alpha}$ and the two other choices are made to simplify the Eqs. (3.8).

The following linear combinations of γ_{ABC} in the complex field will be made:

$$A \equiv (1/2)^{1/2}\gamma_{121}, \tag{4.5}$$

$$\beta \equiv (1/2)(\gamma_{122} - \gamma_{133}) + i\gamma_{123}, \tag{4.6}$$

$$H \equiv (1/2)(\gamma_{122} + \gamma_{133}), \tag{4.7}$$

$$\sigma \equiv (1/2)^{1/2}(\gamma_{233} - i\gamma_{232}), \tag{4.8}$$

$$\rho \equiv -i\gamma_{231}. \tag{4.9}$$

Here and subsequently capital Latin letters will indicate real valued and Greek letters indicate complex valued functions. Geometrically, $(2A)^{1/2}i\rho, \beta, H$ indicate respectively first, second curvature, complex shear, and divergence of the "lines of force".

Furthermore, a formal transformation to complex conjugate coordinates[4] will be made by

$$\begin{aligned} z^2 &= x^2 + ix^3, \\ z^{\dot{2}} &= x^2 - ix^3. \end{aligned} \tag{4.10}$$

It should be mentioned that a coordinate transformation of the type

$$\begin{aligned} x'^1 &= x^1, \\ z'^2 &= f(x^1, z^2), \\ z'^{\dot{2}} &= \overline{f(x^1, z^2)}, \end{aligned} \tag{4.10'}$$

where $f(x^1, z^2)$ is analytic with respect to z^2 and the bar denotes complex conjugation, does not disturb the coordinate conditions implied in (4.4).

Because of (4.4), (4.10) the complex triad field in complex coordinates must be of the following form:

$$\lambda_{1\alpha} = U(x^1, z^2, z^{\dot{2}})\delta_{1\alpha}, \tag{4.11}$$

$$\Lambda_1^\alpha \equiv \lambda_{1\dot{}}^{\ \alpha} = U^{-1}\delta_{1\dot{}}^{\ \alpha} + \eta(x^1, z^2, z^{\dot{2}})\delta_{2\dot{}}^{\ \alpha} + \bar{\eta}\delta_{2\dot{}}^{\ \alpha}, \tag{4.12}$$

$$\Lambda_2^\alpha \equiv (1/2)^{1/2}(\lambda_{2\dot{}}^{\ \alpha} + i\lambda_{3\dot{}}^{\ \alpha}) = \Sigma(x^1, z^2, z^{\dot{2}})\delta_{2\dot{}}^{\ \alpha}, \tag{4.13}$$

$$\Lambda_{\dot{2}}^\alpha \equiv (1/2)^{1/2}(\lambda_{2\dot{}}^{\ \alpha} - i\lambda_{3\dot{}}^{\ \alpha}) = \bar{\Sigma}\delta_{\dot{2}\dot{}}^{\ \alpha}, \tag{4.14}$$

where Greek indices now take $1, 2, \dot{2}$.

Remembering (4.2), (4.3), $w = x^1$, and plugging (4.5)–(4.9), (4.11)–(4.14) into (3.8), (3.2') and taking certain complex linear combinations of the resulting equations one obtains the following system:

$$(\mathfrak{F}): \quad \Sigma A_{,2} - U^{-1}\beta_{,1} - \eta\beta_{,2} - \bar{\eta}\beta_{,\dot{2}} + 2\beta(\rho - H) - A(A + \sigma) = 0, \tag{4.15a}$$

$$\Sigma\rho_{,2} - U^{-1}\sigma_{,1} - \eta\sigma_{,2} - \bar{\eta}\sigma_{,\dot{2}} - H(A + \sigma) + \rho(\sigma - A) + \beta(A + \bar{\sigma}) = 0, \tag{4.15b}$$

$$U^{-1}H_{,1} + \eta H_{,2} + \bar{\eta}H_{,\dot{2}} - \Sigma A_{,2} + H^2 + |\beta|^2 + A(A - \sigma) + U^{-2}/4 = 0, \tag{4.15c}$$

$$\bar{\Sigma}\beta_{,\dot{2}} - \Sigma H_{,2} + 2\beta\bar{\sigma} = 0, \tag{4.15d}$$

$$\Sigma\bar{\sigma}_{,2} + \bar{\Sigma}\sigma_{,\dot{2}} + 2|\sigma|^2 + H^2 - |\beta|^2 - U^{-2}/4 = 0, \tag{4.15e}$$

$$U^{-1}(\ln U)_{,1} + \eta(\ln U)_{,2} + \bar{\eta}(\ln U)_{,\dot{2}} - 2H = 0, \tag{4.15f}$$

$$(M): \quad \Sigma(\ln U)_{,2} + A = 0, \tag{4.16a}$$

$$U^{-1}\Sigma_{,1} + \eta\Sigma_{,2} + \bar{\eta}\Sigma_{,\dot{2}} - \Sigma\eta_{,2} + A\eta + (H - \rho)\Sigma = 0, \tag{4.16b}$$

$$\Sigma\bar{\eta}_{,2} - A\bar{\eta} - \beta\bar{\Sigma} = 0, \tag{4.16c}$$

$$\bar{\Sigma}\Sigma_{,\dot{2}} + \bar{\sigma}\Sigma = 0. \tag{4.16d}$$

Besides these isothermic conditions[4] should have been considered which are fortunately satisfied by (4.15f), (4.16a).

5. THE CLASS OF STATIC GRAVITATIONAL UNIVERSES WHERE 'LINES OF FORCE' ARE GEODESICS

In case that $\lambda_{1\alpha}$ defines a geodesic congruence (meaning "lines of force" are geodesics), the choice of $\lambda_{2\alpha}, \lambda_{3\alpha}$ as the first and second normal [cf. after (4.2)] becomes meaningless. In such a case, it would be convenient to fix the real triad field by parallely propagating $\lambda_{2\alpha}, \lambda_{3\alpha}$ along geodesics generated by $\lambda_{1\alpha}$. This choice would imply that $\gamma_{121} = \gamma_{131} = \gamma_{231} = 0 \Rightarrow A = \rho = 0$, the Eqs. (4.15a)–(4.16d) would yield the following system:

$$(\mathfrak{F}_0): \quad U^{-1}\beta_{,1} + \eta\beta_{,2} + \bar{\eta}\beta_{,\dot{2}} + 2H\beta = 0, \tag{5.1a}$$

$$U^{-1}\sigma_{,1} + \eta\sigma_{,2} + \bar{\eta}\sigma_{,\dot{2}} + H\sigma - \beta\bar{\sigma} = 0, \tag{5.1b}$$

$$U^{-1}H_{,1} + \eta H_{,2} + \bar{\eta}H_{,\dot{2}} + H^2 + |\beta|^2 + U^{-2}/4 = 0, \tag{5.1c}$$

$$\bar{\Sigma}\beta_{,\dot{2}} - \Sigma H_{,2} + 2\beta\bar{\sigma} = 0, \tag{5.1d}$$

$$\bar{\Sigma}\sigma_{,\dot{2}} + \Sigma\bar{\sigma}_{,2} + 2|\sigma|^2 + H^2 - |\beta|^2 - U^{-2}/4 = 0, \tag{5.1e}$$

$$(\ln U)_{,1} - 2HU = 0, \tag{5.1f}$$

$$(M_0): \quad (\ln U)_{,2} = 0, \tag{5.2a}$$

$$U^{-1}\Sigma_{,1} + \eta\Sigma_{,2} + \bar{\eta}\Sigma_{,\dot{2}} - \Sigma\eta_{,2} + H\Sigma = 0, \tag{5.2b}$$

$$\Sigma\bar{\eta}_{,2} - \beta\bar{\Sigma} = 0, \tag{5.2c}$$

$$\bar{\Sigma}\Sigma_{,\dot{2}} + \bar{\sigma}\Sigma = 0. \tag{5.2d}$$

The general solution of the above system of the partial differential equations will be obtained presently.

Theorem 2: Let static field equations $(\mathfrak{F})$ be valid in $\underline{D} \subset \overline{V}_3$. Let the vector field $\omega_{,\alpha}/(\Delta_1\omega)^{1/2}$ be defined and generate a geodesic congruence in $\underline{D}$. If, moreover, (i) $\beta \neq 0$ (nonvanishing shear) then in the corresponding open cylinder of V_4 the metric form must be transformable to

$$\Phi = -a^{-2}e^{-(2m+1)x^1}\{a^{-2}e^{-2mx^1}(dx)^1{}^2 + |dz - [(m^2 - 1/4)^{1/2}\bar{z} + \Omega(x^1)]dx^1|^2\} + e^{x^1}dx^4{}^2,$$

where $a \neq 0, m^2 > (1/4)$ are real constants and $z = x^2 + ix^3$ and $\Omega(x^1)$ is an arbitrary complex valued function of x^1.

In the case (ii) corresponding to $\beta = 0$ the metric forms go over to conformastat cases.[3]

Proof: From the discussions of previous sections, it is clear that in the domain D the Eqs. (5.1a)–(5.2d) have to be satisfied. Therefore, firstly, the general solution of this system has to be obtained for the case (i) corresponding to $\beta \neq 0$.

By (5.2a), (5.1f), (5.1c) one obtains

$$U = U(x^1), \tag{5.3}$$

$$H = H(x^1), \tag{5.4}$$

$$|\beta| = B^2(x^1). \tag{5.5}$$

From (5.1f) and the real part of (5.1a) it follows that

$$B^2 = kU^{-1}, \tag{5.6}$$

where $k > 0$ is a real constant.

By (5.6) the Eq. (5.1c) becomes

$$U^{-1}H' + H^2 + (k^2 + \tfrac{1}{4})U^{-2} = 0, \tag{5.7}$$

where the prime denotes the differentiation with respect to the argument x^1. The general solution of the coupled equations (5.1f) and (5.7) is the following:

$$\begin{aligned} U^{-1} &= (ae^{mx^1} - be^{-mx^1})^2 > 0, \\ H &= -m(a^2e^{2mx^1} - b^2e^{-2mx^1}), \\ m^2 &\equiv k^2 + (1/4) > (1/4), \end{aligned} \tag{5.8}$$

where a, b are real constants of integration. From (5.6) it follows that

$$B^2 = (m^2 - 1/4)^{1/2}(ae^{mx^1} - be^{-mx^1})^2. \tag{5.9}$$

Eliminating σ by (5.2d) and noting $\Sigma \neq 0$, $\beta \neq 0$, $H_{,2} = 0$ the Eq. (5.1d) yields

$$[\ln(\beta\Sigma^{-2})]_{,\dot{2}} = 0. \tag{5.10}$$

This can be readily integrated to obtain

$$\beta\Sigma^{-2} = \chi^2(x^1, z^2). \tag{5.11}$$

Here $\chi(x^1, z^2) \neq 0$ is otherwise an arbitrary analytic function of z^2 and sufficiently differentiable in x^1.

Now making a coordinate transformation of the type (4.10a)

$$\begin{aligned} x'^1 &= x^1, \\ z'^2 &= \chi(x^1, z^2), \\ z'^{\dot{2}} &= \overline{\chi(x^1, z^2)}, \end{aligned}$$

and dropping primes subsequently one has

$$\beta\Sigma^{-2} = (z^2)^2, \tag{5.11'}$$

$$\beta = B^2(z^2/z^{\dot{2}})e^{2is(x^1, z^2, z^{\dot{2}})}, \tag{5.12}$$

$$\Sigma^2 = B^2|z^2|^{-2}e^{2is}, \tag{5.13}$$

where $s = \arg\Sigma$. With (5.12), (5.13), (5.2d) the Eq. (5.1e) boils down to the simple condition

$$abm^2 = 0. \tag{5.14}$$

Because $m^2 > (1/4)$ one has to choose either $a = 0$ or else $b = 0$ (the case $a = b = 0$ makes U singular). Both of these cases can be simultaneously taken care of by putting

$$\begin{aligned} U^{-1} &= a^2e^{2mx^1}, \\ H &= -ma^2e^{2mx^1}, \\ \beta &= (m^2 - (1/4))^{1/2}a^2e^{2mx^1}(z^2/z^{\dot{2}})e^{2is}, \\ \Sigma^2 &= (m^2 - (1/4))^{1/2}a^2e^{2mx^1}|z^2|^{-2}e^{2is} \end{aligned} \tag{5.15}$$

where $a \neq 0$ is a real constant.

Now writing

$$\eta = (m^2 - (1/4))^{1/2}a^2e^{2mx^1}\xi(x^1, z^2, z^{\dot{2}}), \tag{5.16}$$

and plugging in (5.17), one can solve (5.2c) to obtain

$$\xi = (z^{\dot{2}})^2/2z^2 + \Gamma(x^1, z^2)/z^2, \tag{5.17}$$

$\Gamma(x^1, z^2)$ being arbitrary analytic function of z^2.

Inserting the imaginary part of (5.1a)

$$\begin{aligned} 2a^2e^{2mx^1}[s_{,1} + k\xi(s_{,2} - i(z^2)^{-1}/2) \\ + k\bar{\xi}(s_{,\dot{2}} + i(z^{\dot{2}})^{-2}/2)] = 0 \end{aligned} \tag{5.18}$$

into (5.2b) one gets

$$(z^2\xi)_{,2} = 0. \tag{5.19}$$

From (5.17) and (5.18) it follows that

$$\Gamma = \Omega(x^1), \tag{5.20}$$

where $\Omega(x^1)$ is an arbitrary function of x^1 and thus

$$\eta = (m^2 - (1/4))^{1/2}a^2e^{2mx^1}(z^2)^{-1}[(z^{\dot{2}})^2/2 + \Omega(x^1)]. \tag{5.21}$$

One need not solve (5.18) because s does not contribute in the metric form. The eq. (5.16) is identically satisfied by (5.15), (5.21).

Substituting (5.15), (5.21) into (4.12)–(4.14) and obtaining $\bar{g}^{\alpha\beta} = \Lambda_1^{\alpha}\Lambda_1^{\beta} + \Lambda_2^{\alpha}\Lambda_2^{\beta} + \Lambda_{\dot{2}}^{\alpha}\Lambda_{\dot{2}}^{\beta}$ the metric form comes out to be

$$\begin{aligned} \Phi = &-a^{-2}e^{-(2m+1)x^1}[a^{-2}e^{-2mx^1}dx^{1\,2} \\ &+ (m^2 - \tfrac{1}{4})^{-1/2}|z^2|^2|dz^2 - (m^2 - \tfrac{1}{4})^{1/2} \\ &\times (z^2)^{-1}\{(z^{\dot{2}})^2/2 + \Omega\}dx^1|^2] + e^{x^1}(dx^4)^2. \end{aligned} \tag{5.22}$$

Making a coordinate transformation

$$\begin{aligned} x'^1 &= x^1, \\ z'^2 &= (z^2)^2/2(m^2 - 1/4)^{1/4} \\ z'^{\dot{2}} &= (z^{\dot{2}})^2/2(m^2 - 1/4)^{1/4} \\ \Omega' &\equiv \Omega/(m^2 - 1/4)^{1/4}, \end{aligned}$$

and dropping prime the case (i) of the theorem follows.

In case (ii) corresponding to $\beta = 0$ the Eqs. (5.1a)–(5.2d) reduce to the following:

$$U^{-1}\sigma_{,1} + \eta\sigma_{,2} + \bar{\eta}\sigma_{,\dot{2}} + H\sigma = 0, \tag{5.23a}$$

$$U^{-1}H_{,1} + \eta H_{,2} + \bar{\eta}H_{,\dot{2}} + H^2 + U^{-2}/4 = 0, \tag{5.23b}$$

$$\Sigma H_{,2} = 0, \tag{5.23c}$$

$$\bar{\Sigma}\sigma_{,2} + \Sigma\bar{\sigma}_{,2} + 2|\sigma|^2 + H^2 - U^{-2}/4 = 0, \quad (5.23d)$$

$$(\ln U)_{,1} - 2HU = 0, \quad (5.23e)$$

$$(\ln U)_{,2} = 0, \quad (5.23f)$$

$$U^{-1}\Sigma_{,1} + \eta\Sigma_{,2} + \bar{\eta}\Sigma_{,\dot{2}} - \Sigma\eta_{,2} + H\Sigma = 0, \quad (5.23g)$$

$$\bar{\eta}_{,2} = 0, \quad (5.23h)$$

$$\bar{\Sigma}\Sigma_{,\dot{2}} + \bar{\sigma}\Sigma = 0. \quad (5.23i)$$

The general solutions of (5.23b), (5.23c), (5.23e), (5.23f) are

$$U^{-1} = (ae^{x^1/2} - be^{-x^1/2})^2, \quad (5.24)$$
$$H = -(1/2)(a^2e^{x^1} - b^2e^{-x^1}),$$

where a, b are real constants and it is assumed that $U^{-1} > 0$ in the domain of consideration.

The Eq. (5.23h) can be solved to obtain

$$\bar{\eta} = U^{-1}\overline{f(x^1, z^2)}. \quad (5.25)$$

Making a transformation

$$x'^1 = x^1,$$
$$z'^2 = f(x^1, z^2),$$
$$z'^{\dot{2}} = \overline{f(x^1, z^2)},$$

and dropping primes subsequently one gets

$$\eta = U^{-1}z^2. \quad (5.26)$$

Without any loss of generality one is permitted to put

$$\Sigma = (ae^{x^1/2} - be^{-x^1/2})e^{S+is}, \quad (5.27)$$

where S, s are real valued functions of $x^1, z^2, z^{\dot{2}}$,

By (5.26), (5.27) the real and imaginary parts of (5.23g) yield, respectively,

$$S + z^2S_{,2} + z^{\dot{2}}S_{,\dot{2}} = 1, \quad (5.28)$$

$$s + z^2z_{,2} + z^{\dot{2}}s_{,\dot{2}} = 0. \quad (5.29)$$

The general solutions of these first order, linear, partial differential equations obtainable by the method of characteristic curves[5] are

$$T[S - x, z^2e^{-x}, z^{\dot{2}}e^{-x}] = c, \quad (5.30)$$

$$s = t(z^2e^{-x}, z^{\dot{2}}e^{-x}). \quad (5.31)$$

Here c is any real constant and T, t are arbitrary C^2-functions of its arguments.

Now using (5.24) and (5.27), the Eq. (5.23d) gives

$$S_{,2\dot{2}} = (ab/2)e^{-2S}. \quad (5.32)$$

Here three separate cases (i) $ab > 0$, (ii) $ab < 0$, (iii) $ab = 0$ have to be considered. In case $ab > 0$ the general solution of (5.32) is[6]

$$S = \ln[(1 + |\psi(x^1, \zeta)|^2)/|\psi_{,\zeta}|],$$
$$\zeta = (ab/2)^{1/2}z^2, \quad (5.33)$$

where $\psi(x^1, \zeta)$ is an arbitrary analytic function of ζ such that $\psi_{,\zeta} \neq 0$ in the domain of consideration.

The solutions (5.30), (5.33) are compatible provided

$$\psi(x^1, (ab/2)^{1/2}z^2) = \psi((ab/2)^{1/2}z^2e^{-x^1}). \quad (5.34)$$

Equation (5.23a) is identically satisfied by (5.24)–(5.34). Therefore, in this case the metric form of V_4 becomes

$$\Phi = -e^{-x^1}[U^2(dx^1)^2 + 2U|\psi_{,\zeta}|^2(1 + |\psi|^2)^{-2}|dz^2|^2] + e^{x^1}(dx^4)^2, \quad (5.35)$$
$$U^{-1} = (ae^{x^1/2} - be^{-x^1/2})^2.$$

Making a coordinate transformation

$$x'^1 = x^1,$$
$$z' = 2(ab)^{-1/2}\psi((ab/2)^{1/2}z^2e^{-x^1}),$$
$$\bar{z}' = 2(ab)^{-1/2}\psi,$$

and dropping primes subsequently (5.47) goes to

$$\Phi = -e^{-x^1}[U^2(dx^1)^2 + U(1 + (ab/4)|z|^2)^{-2}|dz|^2] + e^{x^1}(dx^4)^2. \quad (5.36)$$

Comparing the above metric with the case (B) of Theorem 8 in paper I it is obvious that (5.36) is transformable to the Schwarzschild's case. Similarly, for the cases $ab < 0, ab = 0$ the metric can be reduced to the other two conformastat forms. Thus part (ii) of the theorem is proved.

Remarks: The metric form exhibited in the preceding theorem is a new solution and therefore requires closer examination. The metric is singular at $x^1 = \pm\infty, x^2 = \pm\infty, x^3 = \pm\infty$ and at the singularities of the arbitrary function $\Omega(x^1)$. Physically this metric can be regarded as being generated by "arbitrary number of plates parallel to $x^2 - x^3$ plane which are clamped at infinity" But more information about 'sources at infinity' can be obtained by putting $\Omega(x^1) = 0, a = 1$. The resulting metric then is nonsingular at every finite point and reduces to the Minkowskian form at the origin. There the three surviving components of Riemann tensor are given by

$$(R_{1441})_0 = m + 1/2,$$
$$(R_{2442})_0 = -(1/2)[m + 1/2 - (m^2 - 1/4)^{1/2}],$$
$$(R_{3443})_0 = -(1/2)[m + 1/2 + (m^2 - 1/4)^{1/2}].$$

Now Synge[7] has arrived at a relation between the Riemann tensor and the corresponding Newtonian potential φ by the following prescription

$$\varphi_{,\alpha\beta} = R_{ijkl}\lambda^i_{(\alpha)}\lambda^j_{(4)}\lambda^k_{(4)}\lambda^l_{(\beta)},$$

where $\lambda^i_{(A)}$ is an orthonormal tetrad. Comparing the above relation with the Riemann tensor of the universe under consideration one can conclude that the corresponding Newtonian potential is

$$\varphi = (1/2)\{(m + 1/2)(x^1)^2 - (1/2)[m + 1/2 - (m^2 - 1/4)^{1/2}](x^2)^2 - (1/2)[m + 1/2 + (m^2 - 1/4)^{1/2}](x^3)^2\},$$

and this provides some insight into the "sources at infinity." From the well-known inversion theorems of the classical potential theory it can be deduced that this field can also be regarded as being generated by a quadrupole at the origin with the moment tensor

$$Q = [Q_{\alpha\beta}] = \begin{bmatrix} (1/2)(m + 1/2) & 0 & 0 \\ 0 & -(1/4)[m + 1/2 - (m^2 - 1/4)^{1/2}] & 0 \\ 0 & 0 & -(1/4)[m + 1/2 + (m^2 - 1/4)^{1/2}] \end{bmatrix}$$

The original Petrov classification of the gravitational universes hinged on two symmetric, traceless matrices M, N each of size (3×3). In any static case $N = 0$ and in the present situation $M = Q$. Therefore, the universe under consideration falls under the class $[1^2, 1^2, 1^2]$ of the type I.

In this universe there are no finite boundaries along x^2, x^3, x^4-coordinate lines. Assuming $m > 1/2$, along negative x^1 line it is open but on the positive x^1 line there is a boundary at a finite distance.

Another special class of solutions will be exhibited in the following theorem.

Theorem 3: Let static field equations $(\mathfrak{F})$ prevail in $D \subset \overline{V}_3$. Let the congruence ω^{α} be shearfree $[\beta = (1/2)(\gamma_{122} - \gamma_{133}) + i\gamma_{123} = 0]$. (i) If, moreover, the congruence has nonvanishing first curvature $(A \neq 0)$ then in the corresponding open cylinder of a nonflat V_4 the metric form can be reduced to the Weyl-type solution

$$\Phi = -e^{-x^1}[e^{(k-(x^2)^2)/4}((dx^1)^2 + (dx^2)^2) + (x^2)^2(dx^3)^2] + e^{x^1}(dx^4)^2,$$

k being any real constant.

(ii) In case $A = 0$ besides $\beta = 0$ the metric forms go over to conformastat cases.

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Constants of motion and degeneration in Hamiltonian systems

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A rigorous formulation of the connection between nonergodicity (degeneration) of the motion of a Hamiltonian system and existence of global constants of motion (isolating integrals) is proposed. Necessary and sufficient conditions for the occurrence of a properly defined kind of complete degeneration are given. Finally, a wide-spread opinion is criticized about the mutual implications between complete degeneration and separability of the Hamilton-Jacobi equation in more than one coordinate systems.

1. INTRODUCTION

The purpose of this paper is to give a unified presentation of the concept of *isolating integral* (see Ref. 1 Chap. II, Sec. 119) for a Hamiltonian System.

It is well known in general dynamics that while a dynamical system with n degrees of freedom always admits $2n - 1$ local constants of motion, a distinguishing role is played by those time-independent first integrals $f(qp)$ which are global constants of motion, defined throughout the phase space. It is essential, roughly speaking, that the equation $f(qp) = \text{const}$ does define a true hypersurface in the phase space of the system Ω_{2n}, so that it can be used to decrease the dimension of the submanifold of Ω_{2n} where the phase trajectory is situated. However, little is known of how many global integrals of motion an arbitrary system possesses. Since Bruns and Poincaré,[2] a number of negative theorems can be found in the literature about the existence of "algebraic" or "uniform" integrals of motion for a generic Hamiltonian system; but, as Wintner[1] stresses, all these elegant negative results of arithmetical type do not have any dynamical significance since the "algebraic" or else "single-valued" nature of an integral $f(qp)$ cannot provide an exhaustive characterization of the very meaning of "isolatingness." Important theorems (Kolmogorov–Arnol'd[3]) have been proved recently about the existence of global constants of motion for analytic Hamiltonians which are close to "integrable systems", i.e., systems admitting action-angle variables. However, strangely enough, there seems to be no generally accepted and detailed definition of what an isolating integral actually is. No matter how familiar this concept may be to the specialists in general dynamics and statistical mechanics, we have not yet seen it explicitly characterized. As a matter of fact it appears that this notion enters the discussions mainly at an operative level.

The motivations of our attempt for an explicit definition of isolating integrals lie in our particular point of view about this matter. It is clear that, independently of any rigorous definition, the lack of existence of isolcating integrals beside the energy and the usual "external" integrals, such as linear momentum and angular momentum, should be considered not as an "exceptional" but rather as the "general" case. Thus, statistical mechanics deals in general with systems which do not possess isolating integrals other than those above, corresponding to the relevant kinematical symmetry group (Galilei or Poincaré). Instead, we will be concerned with just the opposite situation, namely with the cases in which there exist sufficiently many isolating integrals to cause what is known as a degeneration of the motion. This is why we are especially interested in questions of dynamical symmetry and in the problems of intrinsic quantization[4,5] via dynamical symmetries. It is well known that the degenerate multiperiodic motions played a relevant role in the ancient Quantum Theory[6] and yet the great majority of the first quantized Hamiltonian solvable models have classical counterparts which are degenerate systems. It is very likely, also at a heuristic level, that an intrinsic, coordinate-independent, quantization procedure can be established in general only for highly symmetrical systems, admitting a maximal dynamical symmetry group or even a "noninvariance" dynamical group. Such systems have the remarkable property that all the orbits on a given energy surface are diffeomorphic one to another; in particular, every orbit is closed, as a submanifold, if a single one is; in such a case the system is everywhere *completely degenerate*. For this reason we will not discuss a generic partial degeneration but we will focus our attention on the extreme situation of maximal or complete degeneration. This means also that the present paper should be read as a preliminary technical step in view of a more general program of investigation. Anyway, the definitions we propose are valid in themselves and a number of theorems about partial degeneration could easily be derived as well. In particular, we give here a definition of degeneracy which is more general than the usual one in that it is not confined to "bounded" systems; this also is in view of group-theoretical considerations.

This paper is intended for physicists. However, the exposition of the matter necessarily requires the language of modern differential geometry and the reader is supposed to be familiar with the fundamentals of this discipline. (A brief introduction to the mathematical concepts involved in this paper can be found in the Appendix.) As already pointed out by Wintner,[1] the approaches based on classical "arithmetical" methods, which are coordinate dependent, seem rather limited in generality and power of insight; moreover, they are usually developed starting from assumptions of analyticity[7] which are not strictly necessary and which severely restrict the range of physical considerations; yet the matter itself fits naturally with the more general domain of $C^{(\infty)}$ differential geometry. Questions of analyticity will possibly become relevant in the sequel when dealing with the quantum side of these problems.

The main points of the paper are the following:

(a) preliminary definition of *local* and *global* degeneration (with particular emphasis on *complete* degeneration): Defs. 2.1. and 2.2; (b) definition of *isolating functions* and *isolating set* of functions: Defs. 2.3. and 2.4; (c) *sufficient* criteria for complete degeneration: Theorem 2.1; (d) characterization of isolating

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functions and sets: Theorem 2.2; (e) formulation of the problem in terms of a new, more refined, definition of *regular* degeneration and a generalized concept of isolating integrals: Defs. 3.1., 3.2., and 3.3., Theorems 3.1., 3.2., and 3.3; (f) mutual implication between regular degeneration and isolating integrals (in the generalized sense): Theorem 3.4; (g) criticism of a widespread opinion about the connection between degeneration and multiseparability of the Hamilton–Jacobi equation: Sec. 4. (h) a list of the symbols, definitions and theorems in differential geometry used throughout the paper (see Appendix). For an introduction to the subject the reader is referred to the books by Sternberg[8] and Abraham.[9]

2. ISOLATING INTEGRALS AND DEGENERATION

Our first definition of complete degeneration is the following:

Definition 2.1: A dynamical system (Ω_{2n}, X_H) (see Appendix, § 40) will be called *locally completely degenerate in U*, and U will be called a *domain of local complete degeration* if

(1) U is an open connected subset of Ω_{2n};

(2) $X_H \restriction U$ is complete (§17);

(3) every orbit of $X_H \restriction U$ is a *closed submanifold* in Ω_{2n}.

(From here on, § denotes a paragraph of the Appendix.)

In particular, if there exists a domain of degeneration U which is *bounded* in Ω_{2n} (since Ω_{2n} is not a metric space we shall use "bounded" for "contained in a compact set"), then every orbit of $X_H \restriction U$ is compact and diffeomorphic to S^1, i.e., the motion is simply periodic for an open set of initial conditions and then it is stable. Note that this is just what is usually meant by "complete degeneration." Our definition is more general in that it can also include the case of noncompact orbits such as the "scattering states."

By replacing the following requirement for condition (3), we can define a *local k-fold partial degeneration:*

(3′) Every orbit of $X_H \restriction U$ is dense over a $(2n-k)$-dimensional closed submanifold in Ω_{2n} $(1 \leq k \leq 2n-2)$. Note that the usual definition of degeneration in terms of action variables starts from $k = n+1$. However, in the following, we will be interested only in Def. 2.1.

Now, we "globalize" our definition.

Definition 2.2: A dynamical system (Ω_{2n}, X_H) will be called *globally* completely degenerate if it is *locally completely degenerate* in the domain $U \equiv \Omega_{2n}$. Particularly interesting is the case of local degeneration in a domain of the form $U = \cup_E H^{-1}(E) = H^{-1}(I)$, where $H: \Omega_{2n} \to R$ is the Hamiltonian function and $E \in I \subset R$ (I open and connected). A degeneration corresponding to a domain U of this kind will be called a *uniform local degeneration.* This will be the case in presence of a "dynamical symmetry" group of H, transitive on the energy surface. A classical example is the (regularized) three-dimensional hydrogen atom problem, where for $H < 0$ a global canonical action of $SO(4)$ is defined. Actually, according to our definition, this system is *globally completely* degenerate and it is not surprising that also for $H = 0$, $H > 0$, a global canonical action exists for $E(3)$ and $SO(3,1)$, respectively,[10] which are analytic continuations of $SO(4)$. Problems of this kind will be dealt with in a future paper.

We propose now a definition of isolating integral which will prove suitable for the connection with degeneration.

Definition 2.3: Let M be an n-dimensional differentiable manifold. A function $f: M \to R$ will be called *isolating* in M if

(1) $f(M)$ is an open connected subset $I \subset R$;

(2) for every $c \in I$, $f^{-1}(c)$ is a $(n-1)$-dimensional closed submanifold of M.

Definition 2.4: Let M be an n-dimensional differentiable manifold. A set of k functions $(1 \leq k \leq n-1)$ $f_i: M \to R$ will be called a *k-dimensional isolating set* in M if each f_i is isolating in M and $\cap_{i=1}^{k} f_i^{-1}(c_i)$ $(\forall c_i \in I_i)$ is a $(n-k)$-dimensional closed submanifold of M.

Then we have

Theorem 2.1: A dynamical system (Ω_{2n}, X_H) is *locally completely* degenerate in $U \subset \Omega_{2n}$ if

(i) There exists an open submanifold M of Ω_{2n}, including $\overline{U}$, which does not contain critical points of X_H (§8);

(ii) there is a $(2n-1)$-dimensional isolating set in $M\{f_i\}$ such that $((df_i)^{\#}, X_H) = 0$ for every i (§41);

(iii) $X_H \restriction U$ is complete.

Proof: $((df_i)^{\#}, X_H) = 0$ and the absence of critical points of X_H imply that the orbit Σ of X_H through $x \in U$ is a connected component of $\cap_{i=1}^{2n-1} f_i^{-1}(f_i(x))$, which is a closed submanifold in M; by (iii) $\Sigma \subset U$ so that it is a closed submanifold in Ω_{2n} too. The condition $M \supset \overline{U}$ is introduced to prevent the existence of curves in U which are closed submanifolds in U without being closed in Ω_{2n} (limit points on $\partial\overline{U}$); see Def. 2.1, Condition (3).

Note that the condition (iii) can be eliminated in the case of compact $\overline{U}$, $\partial\overline{U}$ submanifold of Ω_{2n}, and $X_H \restriction \partial\overline{U} \in \mathfrak{X}(\partial\overline{U})$, that is X_H is tangent to $\partial\overline{U}$. Theorem 2.1 still holds true if condition (iii) is replaced by the following one:

(iii) there exist an integer $k < 2n-1$ and a choice of indices $i_1 \cdots i_k$ such that

$$f_{i_1}^{-1}(c_1) \cap f_{i_2}^{-1}(c_2) \cap \cdots \cap f_{i_k}^{-1}(c_k), \quad \forall c_m \in f_{i_m}(U)$$

is bounded and contained in U.

In fact if condition (iii) is satisfied for a certain choice $(i_1 \cdots i_k)$ and $i_{k+1} \neq i_m$, $1 \leq m \leq k$, then also $\cap_{i=1}^{k+1} f_i^{-1}(c_i)$ is bounded and contained in U. Thus, by induction, the same is true for $\cap_{i=1}^{2n-1} f_i^{-1}(c_i)$ which by condition (ii) is then compact. Now, being X_H tangent to a compact manifold, it is necessarily complete (§18). Note that this is a more sophisticated version of the usual statement: If a dynamical system admits $2n-1$ isolating integrals, all its bounded orbits are simply periodic.

We come now to the characterization of *isolating sets.*

Theorem 2.2. Consider k $C^{(\infty)}$ functions $f_1 \cdots f_k$, $f_i: M \subset \Omega_{2n} \to R$, such that $f_i(M)$ is an open connected set $I_i \subset R$, and for every $x \in M$ there exist a neighborhood $O(x) \subset M$ and a local chart $(q_1 \cdots q_{2n}; O(x))$, such that the matrix

$$J = \left\| \frac{\partial f_i}{\partial q_k} \right\|_{q = q(x)}$$

is of maximum rank. Then $f_1 \cdots f_k$ is a *k-dimensional isolating set* in M.

Proof: The k functions f_i define a mapping $f: M \to R^k$ which is a submersion (§12), be the condition on J; for the same reason, each f_i defines a submersion $M \to R$. Therefore, the conclusions follows by Theorem 16.8.8. of Ref. (11), as a particular case; see also Ref. (9), Proposition 5.18. ■

Note that the essential part of the condition on the matrix J is the requirement that it be satisfied for open connected sets I_i. Actually the fact that the condition is satisfied almost everywhere is guaranteed by Sard's theorem:

Theorem 2.3. (Sard): Let M and N be differentiable manifolds of dimensions m and n, respectively, with $m \geq n$ and $\varphi: M \to N$ be a $C^{(\infty)}$ mapping. If S is the subset of points $x \in M$, such that $\text{rank}(T_x\varphi) < n$, then $\varphi(S)$ is of measure zero in N, and $N - \varphi(S)$ is everywhere dense in N. For the proof see Ref. (11), Theorem 16.23.1 or Ref. (8), Theorem 3.1.

An important remark is in order at this point. We stress that Theorem 2.1. is concerned with sufficient conditions for *local degeneration* only. It would be desirable to extend the theorem in two directions: (a) to give *necessary* conditions for local degeneration; (b) to extend the theorem to *global* degeneration. An answer to point (a) is given by Theorem 3.3.: given a dynamical system (Ω_{2n}, X_H) locally degenerate in U, for every trajectory $\mathcal{O} \subset U$ there exist a neighborhood $U(\mathcal{O})$ included in U and $(2n-1)$ $C^{(\infty)}$ functions f_i which constitute an isolating set in $U(\mathcal{O})$; (see Sec. 3). We observe that this is *not* the inverse to Theorem 2.1., since, in general, $U(\mathcal{O})$ cannot be extended to all of U. For point (b), it is actually possible to extend the theorem to global degeneration; but this is rather trivial since in this case the existence of an isolating set is such a strong condition that it is usually not verified; for instance, on *compact* manifolds (a function on a compact manifold has always critical points).

Example 2.1: Let $\Omega_2 = T^2 = S^1 \times S^1$; q, p be the angles on T^2. Two charts are sufficient to form an atlas: Choose two overlapping intervals I_1, I_2 of length 2π; $\{q, p \in I_1\}, \{q, p \in I_2\}$ are the domains of the charts. Let $\omega = dp \wedge dq$ be the fundamental 2-form; consider the locally Hamiltonian vector field $X = (dq)^{\#}$ (§39); it is complete and globally degenerate. The most general constant of motion is $f(q)$ being f a $C^{(\infty)}$ function periodic in q. However, it must be $f'(q) = 0$ somewhere so that an isolating set in Ω_2 does not exist.

Summarizing, the definition of isolating set given in this chapter provides results well-suited to treating local degeneration only. A generalization of this definition seems to be in order to deal with the global problem. This is just what we want to do in the next section. To this aim we shall introduce another definition of complete degeneration (called *regular* degeneration). This is slightly more restrictive than the previous one, but very naturally leads to a new definition of isolating set and allows to state necessary and sufficient conditions for global degeneration. We shall make use of notations and results given by Palais.[12]

3. GENERALIZED ISOLATING INTEGRALS AND REGULAR DEGENERATION

Consider an n-dimensional differentiable manifold, M, with complete atlas $\mathfrak{A} = \{(\psi_i, U_i)\}$. We quote from Palais the following definitions:

Definitions 3.1: (a) A p-dimensional *differential system* on M is a mapping $x \to \Theta_x \subset T_xM$, $x \in M$, which assigns at every $x \in M$ a p-dimensional subspace Θ_x of the tangent space T_xM (§4). (b) The differential system Θ is called *differentiable* if, for every $x \in M$, there exists a neighborhood $O(x)$ and p differentiable vector fields in $O(x)$, $L_1 \cdots L_p$, such that $(L_1)_y \cdots (L_p)_y$ is a base for Θ_y for $y \in O(x)$. (From now on, differential system will mean differentiable differential system). (c) The differential system Θ is called *involutive* if any pair L_i, L_j of vector fields belonging to Θ have a Lie Bracket $[L_i, L_j]$ also belonging to Θ (§5). (d) Given a p-dimensional differential system Θ, a connected submanifold $\mathcal{L}$ of M is called a *leaf* of Θ if for every $x \in \mathcal{L}$, $T_x\mathcal{L} = \Theta_x$. There exist a leaf of Θ through every point of M. A leaf is *maximal* if it is not contained in another leaf of Θ. The set of maximal leaves is called the *foliation* of M determined by Θ and is denoted by M/Θ. The mapping Π_Θ which assigns to every $x \in M$ the maximal leaf through x is called the *canonical projection*. An open subset $U \subset M$ is said to be *saturated* with respect to Θ if $\Pi_\Theta^{-1}(\Pi_\Theta U) = U$. A local chart $(x_1 \cdots x_n, U)$ is called *flat* with respect to Θ if $\partial/\partial x_1 \cdots \partial/\partial x_p$ is a base of Θ for every $x \in U$. A *slice* of $(x_1 \cdots x_n, U)$ is a subset of U given by $(x_1 \cdots x_p \bar{x}_{p+1} \cdots \bar{x}_n)$. ($\bar{x}_k$ denotes a fixed value of x_k.) (e) If Θ is an involutive p-dimensional differential system on M, a coordinate system $(x_1 \cdots x_n, U)$ in M is called *regular* with respect to Θ if it is cubical and flat with respect to Θ, and if each leaf of Θ intersects U in at most one p-dimensional slice of $(x_1 \cdots x_n, U)$. [A local chart (ψ, U) is called *cubical* if $\psi(U)$ is an open cube in R_n.] A leaf of Θ is called a *regular leaf* of Θ if it intersects the domain of a coordinate system regular with respect to Θ. Finally, Θ is called *regular* if every leaf of Θ is a regular leaf of Θ.

Regular differential systems have the following distinguishing properties:

(1) If Θ is a regular differential system on the differentiable manifold M, then every leaf of Θ is a closed submanifold of M (see Palais, Theorem 1–VII).

(2) If Θ is a regular differential system on the differentiable manifold M, then the quotient set M/Θ can be equipped with a unique differentiable structure such that the projection

$$\Pi_\Theta: M \to M/\Theta$$

is a *submersion* of M onto M/Θ (see Palais Theorem 1-VIII, X). Another relevant result is the following:

Theorem 3.1: Let φ be a submersion of an m-dimensional differentiable manifold M into a $(m-p)$-dimensional differentiable manifold N, with $0 < p < m$. Then, the differential system defined by

$$\Theta: x \in M \to \ker(T_x\varphi) \subset T_xM \quad (\S 15)$$

is a regular involutive differential system of dimension p. The proof can be found in Ref. (12) Chap. I, Theorem 13 and Ref. (13), Proposition 11.4.1.

We propose now the following definition:

Definition 3.2: A dynamical system (Ω_{2n}, X_H) will be called *locally regularly degenerate in* U, and U will be called a *domain of local regular degeneration* if

(1) U is an open connected subset of Ω_{2n} such that $X_H \restriction U$ is complete;

(2) There exists an open subset $M \subset \Omega_{2n}$ including $\bar{U}$ such that $X_H \restriction M$ forms a base for a one-dimensional

regular differential system Θ_H. (Note that this implies that X_H has no critical points in M.)

As before, global regular degeneration means $U = \Omega_{2n}$.

Theorem 3.2: A dynamical system (Ω_{2n}, X_H) is *locally completely degenerate* in U if it is *locally regularly degenerate* in U.

Proof: The proof is similar to that of Theorem 2.1, since requirements (i) and (ii) are satisfied and (iii) is replaced by the regularity of the differential system Θ_H which implies that the leaves of Θ_H are closed submanifolds of M. ∎

The converse is not true, in general; this means that the new definition of degeneration is somewhat more restrictive, as anticipated in Sec. 2. (See, for instance, Ex. 4.2.) The main interest in giving Def. 3.2 lies in that it renders more clearly the connection between degeneration and the existence of isolating integrals. We have seen that the existence of $2n-1$ $C^{(\infty)}$ functions satisfying Theorem 2.2 is not necessary for a system to be *completely degenerate*. But now we can say that a *regularly degenerate* system in U is such that there exist a $M \supset \overline{U}$ and a mapping $\Pi_{\Theta_H} : M \to M/\Theta_H$, which is a submersion, i.e., something very close to a $(2n-1)$-dimensional isolating set, the only difference being that M/Θ_H need not be an open connected submanifold of R^{2n-1}. Certainly, if we introduce a local chart (ψ, V) in M/Θ_H with $\psi(V)$ cubical in R^{2n-1}, then $\psi \circ \Pi_{\Theta_H}$ will be an isolating set of $C^{(\infty)}$ functions in $\Pi^{-1}_{\Theta_H}(V)$. As a matter of fact we have

Theorem 3.3: If (Ω_{2n}, X_H) is *locally regularly degenerate* in U and $x \in U$, then there is a neighborhood $O(x) \subset U$ saturated with respect to X_H, and $2n-1$ $C^{(\infty)}$ functions $f_i : O(x) \to R$, such that $((df_i)^{\#}, X_H) = 0$ which define a $(2n-1)$-dimensional *isolating set* in $O(x)$.

Proof: Let $\Pi_{\Theta_H} x = y$; take a local cubical chart $(y_1 \cdots y_{2n-1}; V)$ in U/Θ_H; then $O(x) = \Pi^{-1}_{\Theta_H}(V)$ and $f_i = y_i \circ \Pi_{\Theta_H}$. ∎

But we can do more than this. Actually, with reference to Def. 3.2, we can state an *iff* theorem. First of all, looking at Example 2.1, we realize that the essential point is to generalize the definition of isolating integral or isolating set by considering "functions" in a generic differentiable manifold rather than simply in R. This is done by means of the following definition.

Definition 3.3: Given differentiable manifolds M and N of dimensions m and n, respectively, with M symplectic, and an open connected subset $U \subset M$, a differentiable mapping $\varphi : U \subset M \to N$ is said to be "in involution" with a closed 1-form α if, for every local chart (ψ, V) in N and coordinates $y_1 \cdots y_n$ of (ψ, V),

$$((d(y_i \circ \varphi))^{\#}, \alpha^{\#}) = 0$$

holds. We do not follow Abraham's definition (16.28) in that we do not require $d(y_i \circ \varphi)$ and α to be linearly independent. Then we have

Theorem 3.4: Let (Ω_{2n}, X_H) be a dynamical system and U an open connected subset in Ω_{2n}; then the following two statements are equivalent:

(i) X_H is *locally regularly degenerate* in U;

(ii) $X_H \restriction U$ is complete and there is a $M \supset \overline{U}$, a $(2n-1)$-dimensional differentiable manifold N and a submersion $\Pi : M \to N$, such that (a) Π is in involution with X_H^p, (b) X_H has no critical points in M.

Proof: (i) $\Rightarrow$ (ii) follows by considering $\Pi = \Pi_{\Theta_H}$. The converse (ii) $\Rightarrow$ (i) follows at once from Theorem 3.1 with $\varphi = \Pi$, $m = 2n$, and $p = 1$. ∎

A final remark on this last theorem. Let us suppose that statement (ii) holds true. Then we can construct a regular system Θ_H and a quotient manifold M/Θ_H. N and M/Θ_H will not be, in general, diffeomorphic. It may happen that $\Pi^{-1}(c)$, $c \in N$ is not connected, and its connected components are distinct elements in M/Θ_H; also $\Pi \neq \Pi_{\Theta_H} \cdot \Pi_{\Theta_H}$ can be regarded as an *isolating set of functions* over the manifold M/Θ_H with the remarkable property that its "values" are in one-to-one correspondence with the orbits of X_H. The price to be paid for this is that M/Θ_H could possible be non-Hausdorff even if N is Hausdorff. As a simple example consider the following

Example 3.1: Let $\Omega_2 = R^2 - \{(0,0), (a,0), (-a,0)\}$; $\omega = dp \wedge dq$ and $H(q,p) = (q^2 + p^2)^2 - 2a^2(q^2 - p^2)$, ($a$ positive real constant); $H(\Omega_2) = (-a^4 \cdots + \infty)$. The two connected components of $H^{-1}(0)$ are distinct elements in Ω_2/Θ_H which are not separated by open sets. In a certain sense we can regard Ω_2/Θ_H as the "Riemann surface" of H^{-1} and the point 0 as a "branch point." (See Ref. 12, Chap. I: corollary to Theorem 13). Yet, X_H is *globally regularly degenerate*. This shows that we cannot hope to get rid of non-Hausdorff manifolds in the general case. However, if we restrict ourselves to the set K of *compact* orbits, then K is a Hausdorff open subspace of Ω_{2n}/Θ_H (see Ref. 12, Theorem 1-VI).

4. DEGENERATION AND SEPARABILITY OF THE HAMILTON-JACOBI EQUATION

As it is well known, a very useful technique to find constants of motion of a dynamical system in practical applications is provided, whenever possible, by the process of coordinate separation in the Hamilton-Jacobi equation. In this connection it is generally accepted in the physical literature[6,7,14,15] that there is mutual implication between the separability in more than one independent systems of coordinates and the degeneration of the motion. The first part of this implication is usually justified by the existence of $2N-2$ independent separation constants, besides the energy, which are tacitly assumed to be isolating. This belief has even originated a classification of completely degenerate systems and related dynamical symmetries (Ref. 15). However, what is generally overlooked in this connection is the local character of any coordinate system (except for the Cartesian ones), so that this kind of approach has mainly a heuristic value. As a matter of fact, a direct consequence of the local nature of coordinate charts is that a separation constant λ may fail to be a function in Ω_{2n}; then Theorem 2.2. applies only if, for an open set of initial conditions, the motion takes place entirely within the domain of the separation chart. This fact is not true in general, of course. To illustrate this point, consider the two-dimensional system:

Example 4.1: $H(r, \varphi, p_r, p_\varphi) = (1/2m)(p_r^2 + p_\varphi^2/r^2) - k/r + \beta \cdot \sin\frac{1}{2}\varphi/\sqrt{r}$. This Hamiltonian has been classified by Fris et al.[15] as being completely degenerate and $O(3)$ symmetrical essentially in force of the fact that the corresponding Hamilton-Jacobi

equation separates in the following two systems of parabolic coordinates:

$$\text{(a)}\ \begin{cases} x = \frac{1}{2}(\mu^2 - \nu^2) \\ y = \mu\nu \end{cases}, \qquad \text{(a')}\ \begin{cases} x = \mu'\nu' \\ y = \frac{1}{2}(\nu'^2 - \mu'^2) \end{cases}.$$

Actually we have found, using techniques introduced in a previous work,[16] that separability occurs in the one-parameter continuous family of parabolic charts rotated by an arbitrary angle δ:

$$\begin{cases} x = \frac{1}{2}(\mu^2 - \nu^2)\cos\delta + \mu\nu\sin\delta \\ y = -\frac{1}{2}(\mu^2 - \nu^2)\sin\delta + \mu\nu\cos\delta \end{cases},$$

$$\nu\cos\tfrac{1}{2}\delta + \mu\sin\tfrac{1}{2}\delta > 0.$$

However, any separation constant $\lambda[\delta]$ corresponding to $\delta \neq 0$ is discontinuous along the positive x-axis and, what is worse, the discontinuity is not a constant but a function of x: This means that $\lambda[\delta]$ ($\delta \neq 0$) has not even a regular differential and it does not define closed submanifolds in phase space. As a consequence only the orbits which do not cross the positive x-axis are closed, i.e., orbits which lie entirely within the domain of the chart $\delta = 0$. Such orbits exist only for a suitable interval of values of $\lambda[0]$ if $\beta < 0$, while for $\beta > 0$ all the orbits go off the domain. Thus we have only a local degeneration if $\beta < 0$; yet separability is independent of the sign of β.

The fact that a separation constant may fail to be a function (or even a closed 1-form) on Ω_{2n} is certainly due, in the example above, to the $C^{(\omega)}$ nature of the Hamiltonian; for $C^{(\infty)}$ functions such phenomena should not happen. However, there is an obvious way to get rid of this possibility, namely to properly define separability in an atlas of local charts. On the other hand, this is indeed necessary if we want to deal with general phase spaces, in which it is not possible to introduce a single chart *regular almost everywhere*. We are thus led to give the following definition.

Definition 4.1: The Hamilton–Jacobi equation for a dynamical system $(\Omega_{2n}, X_H = (dH)^{\#})$, will be called *globally separable* in a sympletic atlas $\mathfrak{A} = \{(\psi_i, U_i)\}$ if

(1) it is separable in every local chart (ψ_i, U_i) with $n-1$ separation constants $\lambda_k^{(i)}: U_i \to R$, $(k = 1, \ldots, n-1)$;

(2) for every pair (i,j) it holds:

$$\lambda_k^{(i)} = \lambda_k^{(j)} \quad \text{when restricted to } U_i \cap U_j .$$

Also a 1-form, under certain conditions (see Appendix §45), can determine closed submanifolds. Therefore the definition can be generalized as follows, for locally Hamiltonian vector fields: Condition (2) is changed to (2'): $\lambda_k^{(i)} - \lambda_k^{(j)} = c_k^{ij}$ in $U_i \cap U_j$ and the constants c_k^{ij} are all commensurable (for k fixed).

This definition is such that global separation entails the existence of $n-1$ integrals of motion in involution (besides the energy) defined over the whole Ω_{2n}. To deal with local degeneration we can also consider separation in an atlas restricted to an open submanifold U. The separation constants λ_k have global implications on the Hamiltonian flow only if $X_H \restriction U$ is complete. In terms of separability in an atlas, we can now understand the usual occurrence of degeneration for Hamiltonians which admit separation in two different "independent" systems of coordinates A and B. Since "independent" means that $H, \lambda_{Ak}, \lambda_{Bk}$ are functionally independent, i.e., that the condition of linear independence of their differentials is already verified almost everywhere, one is left to find a domain for which the remaining conditions of Theorems 2.1. and 2.2. are satisfied. Let us observe that our definition of global separability provides the correct starting point for the definition of action-angle variables (Arnold's theorem[9,17]). On the other hand, as well known, Arnold's theorem, which assumes the existence of an n-dimensional isolating set, provides a very simple technique for finding, if any, further isolating integrals (algebraic conditions on the fundamental frequencies).

We give two simple examples of globally Hamiltonian vector fields to illustrate our definitions; In the first case two atlases are introduced in which separation takes place in a domain U saturated with respect to X_H; local degeneration follows in U since the separation constants are functionally independent. In the second example, two atlases are introduced in which separation takes place in a domain U which is not saturated with respect to X_H; the motion in this case is not degenerate.

Example 4.2: $\Omega_4 = T^*R^2$; $H = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + \Lambda$; Λ is a $C^{(\infty)}$ function of $r = (q_1^2 + q_2^2)^{1/2}$, such that

$$\Lambda(r) = \begin{cases} 0, & r \leq r_0 \\ \text{nonincreasing and} \\ r + \dfrac{d\Lambda}{dr}(r) \neq 0, & r > r_0 \end{cases}$$

Choose $U_{\pm} = \{x \in \Omega_4; q_1p_2 - q_2p_1 \gtrless 0; 0 < H < \frac{1}{2}r_0^2\}$; $U_{\pm}$ are both saturated with respect to $(dH)^{\#}$; moreover, separability of the Hamilton–Jacobi equation takes place in the two atlases:

$$\mathfrak{A}_1 = \{(r, 0 < \varphi < 2\pi, p_r, p_\varphi), (r, -\pi < \varphi < \pi, p_r, p_\varphi)\}$$
(polar coordinates);

$$\mathfrak{A}_2 = \{(q_1, q_2, p_1, p_2)\} \text{ (a single Cartesian chart).}$$

Separation is also possible, as is well known, in a one-parameter continuous family of elliptical atlases (Ref. 16).

The corresponding constants of motion $\lambda_1 = q_1p_2 - q_2p_1, \lambda_2 = p_1^2 - p_2^2 + q_1^2 - q_2^2$, together with their Poisson bracket $\lambda_3 = p_1p_2 + q_1q_2$ form an isolating set since the $d\lambda_i$ are linearly independent. This implies that the system is locally degenerate in every domain $0 < H < c < \frac{1}{2}r_0^2$, $\lambda_1 \neq 0$. Actually the system is locally degenerate in the whole domain $0 < H < r_0^2/2$; note, however, that it is not regularly degenerate there.

Example 4.3: Consider the Hamiltonian

$$H = \frac{1}{2}\left(p_r^2 + \frac{p_\varphi^2}{r^2}\right) - \frac{k}{r} + \frac{U(\varphi)}{2r^2},$$

$$U(\varphi)\ C^{(\infty)} \text{ and } \neq 0 \text{ only in } |\varphi| < \varphi_0,$$

in the phase space $\Omega_4 = \{T^*(R^2 - \{(0,0)\}); H < 0\}$. X_H is *not* complete for $p_\varphi = 0$; thus we restrict to a domain with $p_\varphi \neq 0$. Let $\mathfrak{A}_1$ be as in Ex. 4.2 and $\mathfrak{A}_2$ be a local chart of parabolic coordinates as in Ex. 4.1 with $\delta = 0$. Hamilton–Jacobi equation is separable in both $\mathfrak{A}_1$ and $\mathfrak{A}_2$ only in a domain U which excludes the region $|\varphi| < \varphi_0$. (Here also there is a one-parameter continuous family of elliptical coordinates.[16]) Such a domain is never saturated with respect to X_H (the orbits are arcs of Kepler ellipses which cross

$|\varphi| = \varphi_0$ somewhere), so that λ_2 has only a local validity.

The converse implication, namely the assertion that from degeneration multiseparability will necessarily follow, is also generally accepted in the literature (see for instance Ref. 14: Landau–Lifshitz, Chap. VII, Sec. 50). The explicit terms of this assertion appear to be the following: "If a dynamical system with structure ($\Omega_{2n} = T^*M_n X_H$) (§35) is completely degenerate, then there exist more than one independent coordinate systems $(q_1 \cdots q_n)$ in M, such that the Hamilton–Jacobi equation separates in the "extended charts" $(q_1 \cdots q_n, p_1 \cdots p_n)$. Now, this proposition is false. It suffices to consider the elementary example of the two-dimensional anisotropic harmonic oscillator with $m : n$ frequency ratio. This system is *globally and regularly degenerate*; however, with the exception of the case $(m,n) = (1,1)$ or $(1,2)$, its Hamilton–Jacobi equation separates only in the atlas given by the Cartesian canonical coordinates. This follows from the fact that, for a Hamiltonian of the form $H(q,p) = \frac{1}{2}p^2 + V(q)$, separation is possible in systems of confocal conics only, due to the Eisenhart theorem (see Ref. 16, 18). This implies in turn that the separation constants must be quadratic at most in the "momenta" p; then the conclusion follows since only one independent quadratic constant of motion exist for the anisotropic oscillator (except for $m/n = 1$ or 2). On the other hand, it may be that a proposition similar to the above is valid if we enlarge the class of coordinate systems, e.g., to general canonical coordinates in Ω_{2n}. Such a proposition, however, if true, would be of very little interest because the search for separation systems of this kind is not less difficult than the search for integrals of motion in general, which is the true actual problem.

Let us add some final remarks. As the reader will have realized, the concepts of isolating integrals discussed in the present paper go far beyond the standard ideas of "uniform" or "algebraic" constants of motion. This is true firstly because $C^{(\infty)}$ functions include algebraic or else analytic functions as particular cases; then, because we have seen that the naive approach is in general inadequate in dealing with non-Euclidean manifolds. One could argue, at this point, that these generalizations, suitable for classical dynamics, are of a rather academic value from the point of view of quantum theory. Actually, the restriction to algebraic or at least to analytic functions appears to be a necessary sacrifice in view of the standard correspondential procedure of quantization. Our attitude in this connection, however, is to consider the correspondential process of quantization itself as suffering from shortcomings analogous to those of the naive approach to classical dynamics. As a matter of fact, within the framework of an intrinsic quantization procedure such as the canonical[4] or dynamical[5] quantization, the above difficulties are by-passed and $C^{(\infty)}$ functions result quantizable objects. Admittedly, there are still many open problems in these approaches and the above considerations do not prevent the possibility that questions of analyticity turn out to be important in the final stages of quantization.

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APPENDIX

§1. A *topological n-dimensional manifold* M is a topological space such that every point of it has an open neighborhood homeomorphic to an open subset in R^n.

§2. A *differentiable structure* S on a topological manifold M is a finite or countable number of homeomorphisms $\psi_i: U_i \subset M \to R^n$ with the following properties:

$$\text{(i)} \quad \bigcup_i U_i = M, \qquad \text{(ii)} \quad \psi_i \circ \psi_j^{-1}: \psi_j(U_i \cap U_j) \to R^n, \quad C^{(\infty)} \text{ and nonsingular.} \tag{A1}$$

Each (ψ_i, U_i) is called a *local chart*, U_i is the *domain*, and the Cartesian coordinates $\psi_i(x)$ are the *local* coordinates of the point x. The collection $(\psi_i, U_i)_{i=1,2,\cdots}$ is called an *atlas* $\mathfrak{A}$. It is obvious that an atlas can consist of a single chart only if M is homeomorphic to an open subset of R^n. A topological n-dimensional manifold M together with a differentiable structure S is called an *n-dimensional differentiable manifold.*

§3. A function $f: M \to R$ is called $C^{(\infty)}$ [notation $f \in \mathfrak{F}(M)$] if its expression in terms of local coordinates, i.e.,

$$f_i = f \circ \psi_i^{-1} \tag{A2}$$

is $C^{(\infty)}$.

§4. Given a point $x \in M$, the *tangent space* to M at x is defined as follows: a *tangent vector to M at x* is a linear map $L: \mathfrak{F}(M) \to R$ such that

$$\text{(i)} \quad L(f+g) = L(f) + L(g), \qquad \text{(ii)} \quad L(fg) = f(x)L(g) + L(f)g(x). \tag{A3}$$

The tangent space to M at x is the linear space whose elements are the tangent vectors; it is denoted by T_xM.

§5. *T_xM is an n-dimensional vector space.* A base in $T_{\bar{x}}M$ is given by $\partial/\partial x_1, \ldots, \partial/\partial x_n$ if $x_1 \cdots x_n$ are local coordinates in a domain including $\bar{x}$, i.e.,

$$L(f) = \sum_{i=1}^{n} a_i \left(\frac{\partial}{\partial x_i} (f \circ \psi^{-1}) \right), \quad x = \bar{x}, \quad a_i \text{ real numbers.} \tag{A4}$$

The union $\cup_x T_xM \equiv TM$ (called the *tangent bundle*) is a differentiable manifold whose points are couples $(x, L_x \in T_xM)$.

§6. A *vector field* is a $C^{(\infty)}$ section of TM, which means that for every $x \in M$ a vector $L_x \in T_xM$ is selected in such a way that $L_x(f)$ is a $C^{(\infty)}$ function on M for every $f \in \mathfrak{F}(M)$. The set of vector fields is denoted by $\mathfrak{X}(M)$.

§7. Given a vector field $X \in \mathfrak{X}(M)$ and a local chart (ψ, U) it is possible to express X as a linear combination

$$X = \sum_{i=1}^{n} a_i(x) \frac{\partial}{\partial x_i}, \quad \text{where } a_i(x) = X(x_i) \text{ is } C^{(\infty)} \text{ in } U.$$

§8. A point x is called a *critical point* of X if $X_x = 0$, i.e., if $X(f)(x) = 0$ for every $f \in \mathfrak{F}(M)$.

§9. The *Lie Bracket* of two vector fields X_1, X_2 is defined as follows:

$$[X_1, X_2](f) = X_1(X_2(f)) - X_2(X_1(f)).$$

A generalization of the concept of vector field is given by the concept of *differential system* (see Chap. 3 and §15).

§10. Given two differentiable manifolds M_1, M_2 (n_1, n_2-dimensional, respectively) a mapping $\varphi: M_1 \to M_2$ is called *differentiable* if for every couple of local charts $(\psi_i^{(1)}, U_i^{(1)})(\psi_j^{(2)}, U_j^{(2)})$, the mapping

$$F = \psi_j^{(2)} \circ \varphi \circ (\psi_i^{(1)})^{-1} \tag{A5}$$

is $C^{(\infty)}$ where it is defined, namely for every $y \in \psi_i^{(1)}(U_i^{(1)})$ such that $(\psi_i^{(1)})^{-1}(y) \in U_i^{(1)} \cap \varphi^{-1}(U_j^{(2)})$. The *differentiable mapping* φ is called a *diffeomorphism* if it is a homeomorphism *and* φ^{-1} is differentiable.

§11. A differentiable mapping φ defines a linear mapping of the tangent space $T_x M_1$ into $T_{\varphi x} M_2$, denoted by $T_x\varphi$ and given by

$$\forall\, L \in T_x M_1,\ T_x\varphi(L) = L' \in T_{\varphi x} M_2; \quad L'(f) = L(f \circ \varphi),\ f \in \mathfrak{F}(M_2).$$

In given reference frames $(\partial/\partial x_i)^{(1)}$, $(\partial/\partial y_j)^{(2)}$ the mapping $T_x\varphi$ is represented by an $n_1 \times n_2$ matrix which is a differentiable function of the point x. The rank of the matrix $(T_x\varphi)_{ij}$ is also a function (possibly discontinuous) of x and is denoted by $\operatorname{rank}(T_x\varphi)$.

§12. A differentiable mapping $\varphi: M_1 \to M_2$ is called *a submersion* if $\operatorname{rank}(T_x\varphi) = n_2$ everywhere; it is called an *immersion* if $\operatorname{rank}(T_x\varphi) = n_1$ everywhere.

§13. A subset $M' \subset M$ is called a *submanifold* of M if the *inclusion map* ι, namely $\iota: M' \to M: x \in M' \to x \in M$, is an immersion and it is one-to-one. Consider for instance

$$\varphi: R \to R^2: \quad t \to \begin{cases} x(t) = t - a\sin t \\ y(t) = 1 - a\cos t \end{cases},$$

then $(T_t\varphi)_{ij} = \| 1 - a\cos t, a\sin t \|$; $\operatorname{rank}(T_t\varphi) = 1$ everywhere if $|a| \neq 1$. We find that for $|a| < 1$, φ is a one-to-one immersion, for $|a| = 1$ it is not an immersion and for $|a| > 1$, φ is an immersion which is not one-to-one.

§14. Let $\varphi: M_1 \to M_2$ be a submersion; let $y \in \varphi(M_1) \subseteq M_2$; then $\varphi^{-1}(y)$ *is a closed submanifold* in M_1, i.e., it is a submanifold of M_1 and it is closed as a subset.

§15. Given a differentiable mapping $\varphi: M_1 \to M_2$ and a point $x \in M_1$, the kernel of $T_x\varphi$ is defined as follows:

$$\ker(T_x\varphi) = \{L \in T_x M_1 \mid T_x\varphi(L) = 0\}.$$

If φ is a submersion, $\ker(T\varphi)$ is a *regular differentiable system* (see Theorem 3.1).

Note: For the sake of simplicity, we shall always think of an n-dimensional differentiable manifold as a submanifold of R^{n+1}. (Actually this becomes completely rigorous if one considers R^{n+p} with sufficiently large p.) This gives an intuitive flavor to all abstract concepts introduced up to now. If M is an n-dimensional submanifold in R^{n+1}, a tangent vector at a point can actually be written as $\mathbf{a}\cdot\operatorname{grad}$ with $\operatorname{grad} = [(\partial/\partial x_1)\cdots(\partial/\partial x_{n+1})]$ and a tangent to M in the usual geometrical sense. Of course, the $(n+1)$ vectors $\partial/\partial x_i$ are *not* linearly independent on the surface since they are linked by the equation of the surface. However it is always possible to choose locally an n-tuple $x_1 \cdots \hat{x}_k \cdots x_{n+1}$ ($\hat{x}_k$ deleted) which constitute a local chart.

§16. A *curve* γ in M is a differentiable mapping $\gamma: I \subset R \to M$, where I is an open connected subset of R. At every point $x = \gamma(\lambda), \lambda \in I$, a *tangent vector to* γ is defined by

$$L_x = (T_\lambda\gamma)\left(\frac{d}{d\lambda}\right). \tag{A6}$$

§17. Given a vector field $X \in \mathfrak{X}(M)$ and a point $x \in M$, there exists a curve γ with $\gamma(0) = x$, such that X is the tangent vector to γ in a neighborhood of $\lambda = 0$. γ is called the *integral curve* of X at x. If I can be extended to $-\infty < \lambda < \infty$, then X is *complete at* x; X is *complete* if it is complete at every point of M.

§18. A vector field on a *compact manifold* is always complete. As an example of a *noncomplete* vector field, take the following: Let $M = R^2 - \{(0,0)\}$ and $X = a\partial/\partial r + b\partial/\partial\varphi$, where r, φ are the usual polar coordinates and a, b are real positive constants. Then the integral curves of X are given by

$$\lambda \in I \xrightarrow{\gamma} \begin{cases} r = a\lambda + r(0) \\ \varphi = b\lambda + \varphi(0) \end{cases},$$

so that the interval I can be extended at most to $-r(0)/a < \lambda < +\infty$. The vector field $Y = ar\partial/\partial r + b\partial/\partial\varphi$ is complete, since its integral curves are given by

$$\lambda \in (-\infty \cdots +\infty) \xrightarrow{\gamma} \begin{cases} r = r(0)\, e^{a\lambda} \\ \varphi = b\lambda + \varphi(0) \end{cases}.$$

§19. The *Lie derivative* $L_X f$ of a function f with respect to the vector field X is defined by $(L_X f)(x) = (d/d\lambda)(f \circ \gamma)|_{\lambda=0}$, λ being the integral curve of X at x. It holds: $L_X f = X(f)$, which means that $X(f) = 0$ everywhere implies that f is constant along the integral curves of X.

§20. The dual space of $T_x M$, i.e., the space of linear functionals on $T_x M$, is a linear space of the same dimension and is called the *cotangent space to* M *at* x and denoted by $T_x^* M$. The union $\cup_x T_x^* M$ is called the *cotangent bundle* and denoted by T^*M. *A* $C^{(\infty)}$ section of T^*M is a map $\tau_\omega: M \to T^*M$ which assigns to every $x \in M$ a linear functional $\omega_x \in T_x^* M$ in such a way that ω_x depend differentiably on x, i.e., $\{\omega_x(X_x)\} \in \mathfrak{F}(M)$. Such a $C^{(\infty)}$ section is called a 1-form [notation $\omega \in \mathfrak{X}^*(M)$].

§21. Locally in M it is possible to introduce a base in $T_x^* M$ $\omega_1 \cdots \omega_n$ defined by $\omega_i(\partial/\partial x_j) = \delta_{ij}$; every 1-form is locally expressed as $\omega = \sum_1^n \bar{b}_i(x)\omega_i$ with $\bar{b}_i \in \mathfrak{F}(M)$. An essential point is that the value of $\omega(X)$ at x depends only on ω_x and X_x and *not* on their values in a neighborhood; this is evident since

$$X = \sum a_i(x)\frac{\partial}{\partial x_i} \Rightarrow \omega(X) = \sum_1^n a_i(x)\bar{b}_i(x).$$

§22. To every function $f \in \mathfrak{F}(M)$ there is associated a 1-form denoted by df and defined by $df(X) = X(f)$. In particular we can write for the base convectors ω_i:

$$\delta_{ij} = \frac{\partial}{\partial x_i}(x_j) = dx_j\left(\frac{\partial}{\partial x_i}\right), \quad \omega_i = dx_i.$$

A 1-form ω is called *exact* if there exists a function f such that $\omega = df$.

§23. An m-form is defined as follows. Consider the space of multilinear functionals on T_xM: $T_xM \times T_xM \times \cdots \times T_xM \to R$ and restrict to the subspace of completely antisymmetric multilinear functionals, i.e., such that

$$\omega(X_1,\ldots,X_m) = (-1)^{\delta_P}\omega(X_{P1},\ldots,X_{Pm}), \tag{A7}$$

δ_P is the parity of the permutation P. Then we can define the *bundle* $T^{(m)*}M$; a $C^{(\infty)}$ section of it is called an *m-form*; the set of m-forms is denoted by $\Omega^m(M)$. As an example, consider $m = 2$: $(dx_1 dx_2)(X, Y) = dx_1(X)dx_2(Y)$ is the local expression of a bilinear functional; we obtain a 2-form from it by antisymmetrizing: $\omega(X, Y) = \frac{1}{2}[dx_1(X)dx_2(Y) - dx_1(Y)dx_2(X)]$. The notation usually employed is $\omega = dx_1 \wedge dx_2$ (called exterior product of dx_1, dx_2).

§24. The *exterior product* of a k-form α and an m-form β is a $(k+m)$-form $\alpha \wedge \beta$ defined by

$$\begin{aligned}(\alpha \wedge \beta)(X_1,\ldots,X_{k+m}) &= \frac{1}{(k+m)!}\sum_P (-1)^{\delta_P} \mathcal{P}\alpha(X_1,\ldots,X_k) \\ &\quad \times \beta(X_{k+1}\cdots X_{k+m}) \\ &= \frac{1}{(k+m)!}\sum_P (-1)^{\delta_P}\alpha(X_{P1}\cdots X_{Pk}) \\ &\quad \times \beta(X_{P(k+1)}\cdots X_{P(k+m)}).\end{aligned} \tag{A8}$$

§25. A base for the m-forms is locally given by

$$\omega_{i_1\ldots i_m} = dx_{i_1} \wedge \cdots \wedge dx_{i_m},$$

so that the most general expression for an m-form is

$$\omega = \sum_{i_1\ldots i_m} a_{i_1\ldots i_m}(x)dx_{i_1} \wedge \cdots \wedge dx_{i_m}.$$

§26. Given an m-form ω, we obtain an $(m+1)$-form $\mathbf{d}\omega$ by application of the *exterior derivative operator* $\mathbf{d}$ defined through the following properties:

(i) $\mathbf{d}(\alpha \wedge \beta) = (\mathbf{d}\alpha) \wedge \beta + (-1)^k \alpha \wedge (\mathbf{d}\beta)$, α, β as in §(24),

(ii) $\mathbf{d}f(X) = X(f) = df$, (A9)

(iii) $\mathbf{dd} = 0$.

Relation (i) makes sense also if $k = 0$, i.e., $\mathbf{d}(f\omega) = \mathbf{d}f \wedge \omega + f\mathbf{d}\omega$.

§27.

$$\begin{aligned}(\mathbf{d}\omega)(X_0X_1\cdots X_m) &= \frac{1}{m+1}\Big\{\sum_{k=0}^{m}(-1)^k X_k(\omega(X_0\cdots\hat{X}_k\cdots X_m)) \\ &\quad + \sum_{i<j}(-1)^{i+j}\omega([X_i,X_j],X_0,\ldots,\hat{X}_i, \\ &\quad \ldots,\hat{X}_j,\ldots,X_m)\Big\}\end{aligned} \tag{A10}$$

holds.

($\hat{X}_k$ means that X_k is deleted). As the simplest example, take a 1-form ω, then $(\mathbf{d}\omega)(X_0,X_1) = \frac{1}{2}\{X_0(\omega(X_1)) - X_1(\omega(X_0)) - \omega([X_0,X_1])\}$. It is to be noted that the two sums in formula (A10) individually depend on the values of ω and $X_0,\ldots X_m$ in a neighborhood of the point, while the sum, i.e., $\mathbf{d}\omega$, is a true $(m+1)$-form.

§28. An m-form ω is called *closed* if $\mathbf{d}\omega = 0$; it is called exact if there exists an $(m-1)$-form α such that $\omega = \mathbf{d}\alpha$. Due to $\mathbf{dd} = 0$, an exact form is also closed, but the converse is not true in general, depending on the topology of the manifold.

§29. Given a mapping $\varphi: M_1 \to M_2$, a mapping between $\Omega^m(M_1)$ and $\Omega^m(M_2)$ is defined, namely

$$\begin{aligned}\omega \in \Omega^m(M_2),\ (\varphi_*\omega)(X_1^{(1)}\cdots X_m^{(1)}) \\ = \omega(T\varphi(X_1^{(1)})\cdots T\varphi(X_m^{(1)})).\end{aligned}$$

In particular $\varphi_*(df)(X) = (df)(T\varphi(X)) = T\varphi(X)(f) = X(f\circ\varphi) = d(f\circ\varphi)(X) \Rightarrow \varphi_*(df) = d(f\circ\varphi)$ ("naturality" of $\mathbf{d}$ with respect to mappings).

§30. The "pullback" φ_* allows the definition of the *Lie derivative* of an m-form with respect to a given vector field; let γ be the integral curve at x; $\varphi(\lambda)$ the mapping $\varphi(\lambda)x = \gamma(\lambda)$. Then the Lie derivative L_X is given by

$$L_X\omega = \frac{d}{d\lambda}\varphi_*(\lambda)\omega\,|_{\lambda=0}.$$

§31. The *inner product* of a vector field X and an m-form ω is the $(m-1)$-form $\mathbf{i}_X\omega$ defined by

$$(\mathbf{i}_X\omega)(X_1\ldots X_{m-1}) = m\omega(X,X_1\ldots X_{m-1}).$$

It holds:

(i) $L_X\omega = \mathbf{d}(\mathbf{i}_X\omega) + \mathbf{i}_X(\mathbf{d}\omega)$,

(ii) $(L_X\omega)(X_1,\ldots,X_k) = X(\omega(X_1,\ldots,X_k)) - \sum_{i=1}^{k}\omega(X_1,\ldots,[X,X_i],\ldots,X_k)$.

§32. A differentiable manifold M is called a *symplectic manifold* if there is defined a 2-form ω on it, called the *fundamental 2-form*, with the following properties:

(i) $\mathbf{d}\omega = 0$, i.e., ω is closed

(ii) $\omega(X_1,X_2) = 0$ for every X_2 implies $X_1 = 0$, i.e., ω is nondegenerate. M is necessarily even-dimensional.

§33. It is possible to introduce local charts (called *symplectic charts* or canonical coordinates) such that ω has the following expression:

$$\omega = \sum_1^{n/2} dx_i \wedge dx_{i+n/2} = \sum_1^{n/2} dp_i \wedge dq_i. \tag{A11}$$

§34. A simple example of a natural way in which symplectic manifolds arise in mechanics is the following. Consider a point particle on an n-dimensional surface M immersed in R^{n+1} and subjected to stationary conservative forces; the Lagrangian function is supposed to belong to $\mathfrak{F}(TM)$; in particular we assume that in any local chart,

$$\mathcal{L} = \tfrac{1}{2}\sum_{i,j} a_{ij}(x)v^i v^j - U(x)$$

being $a_{ij}(x)$, the metric tensor induced on M by the Euclidean metric in R_{n+1}. The kinetic energy $\mathcal{T} = \mathcal{L} + U$ defines a bilinear nondegenerate functional $\mathcal{T}: \mathfrak{X}(M) \times \mathfrak{X}(M) \to R$ which induces a one-to-one onto mapping $\tau: \mathfrak{X}(M) \to \mathfrak{X}^*(M)$, namely $(\tau v)(v') = \mathcal{T}(v,v')$. In local charts $v = \sum v^i(\partial/\partial x^i)$; $\tau v = \sum a_{ij}v^j dx^i \equiv \sum p_i dx^i$. The "coordinate transformation" $p_i = \sum a_{ij}v^j \equiv (\partial\mathcal{L}/\partial v^i)$ coincide with the usual definition of

"conjugate momenta." The state of the particle can now be described by a point on T^*M. It is then easy to show that the Lagrange second order equations in M transform into a first order systems of $2n$ differential equations of the form

$$\frac{dq^i}{dt} = X_H(q^i),$$

$$\frac{dp_i}{dt} = X_H(p_i) \text{ with } X_H \in \mathfrak{X}(\Omega_{2n}) .$$

But the important fact to be noted is that T^*M has given the structure of a symplectic manifold in a very natural way (see next paragraph).

§35. T^*M can be given a symplectic structure. Let us define a 1-form $\vartheta \in \mathfrak{X}^*(T^*M)$ as follows: $x \in M$, $\vartheta_0 \in T_x^*M$, $(x, \vartheta_0) \in T^*M$, $X \in \mathfrak{X}(T^*M)$; denote by π the projection $T^*M \to M$: $\pi(x, \vartheta_0) = x$. Then $\vartheta(X) \equiv \vartheta_0(T\pi(X))$, or $\vartheta = \pi_* \vartheta_0$. The 2-form $\omega = \mathbf{d}\vartheta$ is nondegenerate. This is easily seen in each local chart:

$$x = \{q^i\}, \quad \vartheta_0 = \sum p_i dq^i,$$

$$X = \sum_i \left(a^i(qp) \frac{\partial}{\partial q^i} + \bar{b}_i(qp) \frac{\partial}{\partial p_i}\right),$$

$$T\pi(X) = \sum a_i \frac{\partial}{\partial q^i}, \quad \vartheta_0(T\pi(X)) = \sum p_i a^i,$$

$$\vartheta\left(\frac{\partial}{\partial q^i}\right) = p_i, \quad \vartheta\left(\frac{\partial}{\partial p_i}\right) \equiv 0 \Rightarrow \vartheta = \sum_1^n p_i dq^i,$$

$$\mathbf{d}\vartheta = \sum_1^m dp_i \wedge dq^i.$$

§36. A $2n$-dimensional symplectic manifold is denoted by Ω_{2n}.

§37. The nondegenerate closed 2-form ω induces an isomorphism between $\mathfrak{X}^*(\Omega_{2n})$ and $\mathfrak{X}(\Omega_{2n})$; to every vector field X there corresponds the 1-form $X^\flat$ defined by

$$X^\flat = \mathrm{i}_X \omega. \tag{A12}$$

Conversely, to every 1-form α, there is associated a vector field $X = \alpha^\#$ such that $(\alpha^\#)^\flat = \alpha$. In local canonical coordinates, we have

$$\begin{aligned} X &= \sum_i \left(a^i \frac{\partial}{\partial p^i} + \bar{b}^i \frac{\partial}{\partial q^i}\right), \\ \mathrm{i}_X \omega &= \sum_i (dp_i(X) dq^i - dq^i(X) dp_i) \\ &= \sum_i (a_i dq^i - b^i dp_i) \\ &\equiv X^\flat, \text{ i.e., } \left(\frac{\partial}{\partial p_i}\right)^\flat = dq_i, \left(\frac{\partial}{\partial q_i}\right)^\flat = -dp_i. \end{aligned} \tag{A13}$$

§38. A differentiable mapping φ is called symplectic if $\varphi_* \omega = \omega$. Recalling the definition of Lie derivative § 30, the condition that X generates a continuous one-parameter local group of symplectic transformations is simply given by $L_X \omega = 0$. By §31, Eq. (i),

$$0 = L_X \omega = \mathbf{d}(\mathrm{i}_X \omega) + \mathrm{i}_X(\mathbf{d}\omega) = \mathbf{d}(\mathrm{i}_X \omega) \equiv \mathbf{d}X^\flat \tag{A14}$$

i.e., $X^\flat$ is closed.

§39. A vector field X is called *locally Hamiltonian* if $X^\flat$ is closed; it is called *globally Hamiltonian* if $X^\flat$ is exact, i.e., there exist a function $H \in \mathfrak{F}(\Omega_{2n})$ such that $X = (dH)^\#$ or $X^\flat = dH$. H is usually called the *generating function* of the "infinitesimal canonical transformation"

$$\frac{dq^i}{dt} = X(q^i), \quad \frac{dp_i}{dt} = X(p_i). \tag{A15}$$

Since in R^n every closed form is also exact, for every $x \in \Omega_{2n}$ there exist a neighborhood $O(x)$ and a function $H \in \mathfrak{F}(\Omega_{2n})$ such that $dH = X^\flat$ when restricted to $O(x)$, i.e., every locally Hamiltonian vector field can be described by *local Hamiltonians*.

§40. A *dynamical system* is a couple (Ω_{2n}, X_H) where Ω_{2n} is a $2n$-dimensional symplectic manifold and X_H is a locally or globally Hamiltonian vector field.

§41. Through the fundamental 2-form ω the *Lagrange bracket* of two vector fields X, Y is defined as

$$(X, Y) = 2\omega(X, Y) = X^\flat(Y) = -Y^\flat(X). \tag{A16}$$

In local symplectic charts this looks like

$$(X, Y) = \sum_1^n \{X(p_i) Y(q^i) - X(q^i) Y(p_i)\} \tag{A17}$$

and

$$\mathbf{d}(X, Y) = [X, Y]^\flat - L_X Y^\flat + L_Y X^\flat$$

holds. In particular, if X, Y are locally Hamiltonian vector fields,

$$\mathbf{d}(X, Y) = -[X, Y]^\flat. \tag{A18}$$

§42. If we put $\alpha = X^\flat, \beta = Y^\flat$, we can define the *Poisson bracket* of the two closed forms α, β by

$$\{\alpha, \beta\} = \mathbf{d}(\alpha^\#, \beta^\#) = -[\alpha^\#, \beta^\#]^\flat. \tag{A19}$$

The *Poisson bracket* is usually extended also to nonclosed 1-forms by $\{\alpha, \beta\} = -[\alpha^\#, \beta^\#]^\flat$. The *Poisson bracket of functions* f, g is defined by $\{f, g\} = ((df)^\#: (dg)^\#)$, so that $\{df, dg\} = d\{f, g\}$. Equation (A19) shows that the P.B. of two closed 1-forms is exact. We leave to the reader to rederive the customary expressions of P.B. in local coordinates.

§43. To illustrate the geometric meaning of (X, Y), some concepts from the theory of integration over differentiable manifolds are needed; in particular, the "Stokes theorem"

$$\int_{\partial c} \vartheta = \int_c \mathbf{d}\vartheta,$$

where c is a p-chain and ϑ is a $(p-1)$-form (see Ref. 8, Chap. III). Now, let X_1, X_2 be two vector fields in Ω_{2n} and let γ_1, γ_2 be their (local) integral curves. We consider an infinitesimal circuit made up with arcs of γ_1, γ_2 with a vertex in (q, p) and with sides equal to $(\lambda_1 X_1(q^i), \lambda_1 X_1(p_i))$ and $(1 \to 2)$. Let $\Delta\Gamma$ be the algebraic sum of the areas of the projections of the circuit onto the coordinate planes $q^1 p_1, \ldots, q^n p_n$; then to first order in $\lambda_1 \lambda_2$ $\Delta\Gamma$ is given by $\lambda_1 \lambda_2 (X_1, X_2)$.

§44. The relations

$$\{\alpha, \beta\} = L_{\beta^\#} \alpha = -L_{\alpha^\#} \beta = \mathbf{d}(\alpha^\#, \beta^\#), \quad \mathbf{d}\alpha = \mathbf{d}\beta = 0, \tag{A20}$$

$$\{f,g\} = L_{(dg)^\#} f = -L_{(df)^\#} g = ((df)^\#, (dg)) \qquad \text{(A21)}$$

motivate our choice of Lagrange brackets as fundamental objects when dealing with locally Hamiltonian vector fields; in fact, the relation $(X_1, X_2) = 0$ is a necessary and sufficient condition for the local Hamiltonians of X_1 (of X_2) to be constant along the integral curves of X_2 (of X_1). The same condition state in terms of Poisson brackets would require the explicit introduction of local Hamiltonians and would look like $\{H_i^1, H_j^2\} = 0$ in $U_i^1 \cap U_j^2$ being H_i^1 (respectively H_j^2) the local Hamiltonian of $X_1(X_2)$ in $U_i^1(U_j^2)$. Example $\Omega_2 = T^2 = S^1 \times S^1$; w_1, w_2 angles on T^2; $\omega = dw_1 \wedge dw_2$; let $X = \partial/\partial w_1$, $Y = \partial/\partial w_2$; $-w_1$ and w_2 are local Hamiltonians for X, Y and within a local chart we have $\{w_1, w_2\} = -1$. This is shared by the global statement $(X, Y) = 1$. Note that $\{dw_1, dw_2\} = 0$ tells nothing about the "conservation" of w_2 "under" $(dw_1)^\#$

§45. Finally, we want to discuss the conditions under which a locally Hamiltonian vector field has a regular "energy surface." A 1-cycle is a differentiable map $\gamma: S^1 \to M$. Cycles can be added and multiplied by integers. A cycle γ is said to be homologous to zero ($\gamma \sim 0$) if it can be continuously contracted to a point. r 1-cycles $\gamma_1 \ldots \gamma_r$ are independent if $n_1\gamma_1 + \cdots + n_r\gamma_r \sim 0$ implies $n_1 = \cdots = n_r = 0$. Now, suppose that M is of rank k, i.e., that there are k independent irreducible 1-cycles γ_i; then $T_i = \oint_{\gamma_i} \vartheta$ are called the periods of the closed 1-form ϑ. There are only two cases in which ϑ leads to the definition of a submersion, that is, in conclusion, to closed submanifolds. These two cases are

(i) $T_i = 0$ (trivial), this means that $f = \int_{x_0}^{x} \vartheta \in \mathfrak{F}(M)$ i.e., ϑ is actually exact, $\vartheta = df$.

(ii) $T_i = n_i T$; in this case the integral $\varphi = (2\pi/T)\int_{x_0}^{x} \vartheta$ defines a differentiable mapping $M \to S^1$. In both cases the condition $\vartheta \neq 0$ everywhere is sufficient for f and φ to be submersions. If at least two periods are incommensurable, $\int_{x_0}^{x} \vartheta$ cannot define a mapping either in R or in S^1, which are the only possibilities. We always suppose that the locally Hamiltonian vector field X_H is such that $X_H^\flat$ satisfy (i) or (ii). The usual requirement of absence of critical points is precisely $X_H^\flat \neq 0$.

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On the noniterative solution of integral equations for scattering of electromagnetic waves*

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The scattering of electromagnetic waves is considered using the integral equation form of Maxwell's equations for the electric field. These equations are analogous to but not identical to the Lippmann–Schwinger equation in quantum mechanical scattering theory. A transformation procedure discovered by Drukarev (and independently by Sams and Kouri) is employed to obtain Volterra integral equations of the second kind for "modified electric field functions." In deriving the Volterra equations, one is led by analogy with quantum mechanical scattering to define a "Jost matrix" associated with electromagnetic scattering. A simple quadrature procedure is suggested for obtaining numerical solutions to the Volterra integral equations.

I. INTRODUCTION

Integral equations have long been of great importance in mathematical physics because they permit the succinct expression of both the local properties of physical quantities and their behavior at boundary surfaces. In the case of electromagnetic phenomena, most applications of integral equations have involved kernals which are of specialized character, e.g., specialized to potential or diffraction problems with idealized boundary surfaces.[1–5] There do, however, exist formulations of general integral equations for electromagnetic scattering which are analogous to the well-known Lippmann–Schwinger integral equations used in quantum mechanical scattering theory.[3,4] These integral equations are Fredholm equations of the second kind and there exists a very extensive literature dealing with the analytic properties of such equations.[1,6] Indeed, because of the great importance in quantum mechanical scattering theory of iterative solutions to such equations, much effort has been expended in studying the behavior of essentially perturbative solutions of such integral equations. Such perturbative or iterative solutions are generally known as Born or Neumann iterative solutions.[1,6,7] One of the most powerful techniques for solving such integral equations is the Fredholm determinant solution procedure.[1,4,6] Indeed, solutions of this type possess much superior convergence properties compared to the Born–Neumann procedure (i.e., convergence is independent of the interaction strength).

Some years ago it was observed by Drukarev[8] (and recently rediscovered by Sams and Kouri[9]) that the Lippmann–Schwinger integral equation could be transformed into a Volterra integral equation of the second kind for a modified wavefunction.[10] The resulting Volterra integral equation could then also be interatively solved by the Born–Neumann procedure. However, the convergence properties of such a solution were now essentially the same as those of the Fredholm determinant solution.[4] Indeed, it has been shown by Brysk that the solution of the Lippmann–Schwinger equations via the Volterra equations is exactly equivalent to a construction of the Fredholm determinant solution.[11]

In addition to independently discovering Drukarev's transformation procedure for obtaining Volterra integral equations from Fredholm integral equations (having a specialized kernal form[11]), Sams and Kouri pointed out that such Volterra equations could be used as the basis for generating an extremely rapid, noniterative numerical solution to the original Lippmann–Schwinger equation.[9,12] Their procedure essentially generates the Jost matrix numerically, which matrix can then be used to construct the scattering wavefunction and scattering matrix according to well-known formalism.[4] Furthermore, the modified wavefunction satisfying the Volterra integral equations are, in fact, transformed into the physical wavefunctions by multiplication with the inverse of the Jost matrix.[4]

The present paper contains a treatment of the integral equations describing electromagnetic scattering using the Drukarev–Sams–Kouri transformation procedure. In the next section, we present the integral equations for electromagnetic scattering following the treatment given by Newton.[4] In Sec. III we derive the Volterra integral equations and discuss analogies to be made with quantum mechanical scattering. Finally, in Sec. IV the numerical procedure of Sams and Kouri[9] is briefly described.

II. INTEGRAL EQUATIONS FOR ELECTROMAGNETIC SCATTERING

We first present a brief summary of the equations for electromagnetic scattering expressed in integral form. Our discussion follows that of Newton[4] and is included to establish notation. The physical process to be described is that of scattering of an incident electromagnetic wave by some material medium of arbitrary size and shape.

Let the index of refraction n' of the dispersive medium be given by

$$n'^2 = \epsilon + 4\pi i\sigma/\omega, \tag{1}$$

where ϵ is the dielectric constant, σ is the conductivity, and ω is the circular frequency of the radiation. We denote the magnetic permeability of the medium by μ and note that, in general, the refractive index n' and permeability μ are tensor quantities and need not be uniform. Thus, the scattering medium need not be homogeneous or isotropic. (However, for simplicity, we shall treat only isotropic media. The analysis can be extended to include the more gneral case.)

For the present discussion, it is most convenient to treat the electric fields using a "partial wave" description. Thus we may express Maxwell's equations for the process of scattering of an incident electromagnetic wave as[1,4]

$$\mathcal{E}^{\lambda\lambda'}_{JM,J'M'}(r) = u_J(kr)\delta_{JJ'}\delta_{MM'}\delta_{\lambda\lambda'}(\delta_{\lambda o} - 1)$$
$$+ k^2 \sum_{\substack{J''M'' \\ \lambda'''\lambda''}} \int_0^\infty dr'\ \Gamma^J_{\lambda\lambda'''}(r_<, r_>)\, \mathcal{U}^{\lambda'''\lambda''}_{JM,J''M''}(r')\, \mathcal{E}^{\lambda''\lambda'}_{J''M'',J'M'}(r'). \tag{2}$$

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Thus $\mathcal{E}^{\lambda\lambda}_{JM,J'M'}$ is the radial coefficient in the expansion of the electric field $\vec{\mathcal{E}}(k,\nu,r)$ using vector spherical harmonics $\vec{Y}^{(\lambda)}_{JM}(\hat{r})$ and $\vec{Y}^{(\lambda')}_{J'M'}(\hat{k})$ describing the dependence on position $\vec{r}$ and propagation vector $\vec{k}$, and the polarization vectors $\vec{\chi}'_\nu$. In the above equation,

$$\Gamma^J_{ee}(k;r_<,r_>) = u'_J(kr_<)w^{(+)\prime}_J(kr_>), \tag{3}$$

$$\Gamma^J_{mm}(k;r_<,r_>) = -u_J(kr_<)w^{(+)}_J(kr_>), \tag{4}$$

$$\Gamma^J_{e0}(k;r_<,r_>) = \Gamma^J_{0e}(k;r_<,r_>) = \frac{[J(J+1)]^{1/2}}{k^2r'}\frac{\partial}{\partial r}[u_J(kr_<)w^{(+)}_J(kr_>)], \tag{5}$$

$$\Gamma^J_{00}(k;r_<,r_>) = -\frac{(J+1)}{k^2rr'}u_J(kr_<)w^{(+)}_J(kr_>), \tag{6}$$

and all other $\Gamma^J_{\lambda\lambda'}$ elements are zero; the $u_J(kr)$ is a Ricatti–Bessel function of order J, $w^{(+)}_J(kr)$ is a Ricatti–Hankel function of the first kind of order J, and by u'_J (or $w^{(+)\prime}_J$) we mean the derivative of u_J (or $w^{(+)}_J$) with respect to r; the function $\mathfrak{N}^{\lambda'''\lambda''}_{JM,J'''M''}(r)$ is defined by

$$\mathfrak{N}^{\lambda'''\lambda''}_{JM,J'''M''}(r) = i^{J+J''}\int d\hat{r}\,\vec{Y}^{(\lambda''')}_{JM}(\hat{r})\cdot\vec{1}(n^2-1)\cdot\vec{Y}^{(\lambda'')}_{J'''M''}(\hat{r}). \tag{7}$$

For the special case of a spherically symmetric scatterer, Eq. (7) reduces to

$$\mathfrak{N}^{\lambda'''\lambda''}_{JM,J'''M''}(r) = (-1)^J\delta_{JJ''}\delta_{MM''}\delta_{\lambda'''\lambda''}(n^2-1) \tag{8}$$

and our integral equation for $\mathcal{E}^{\lambda\lambda'}_{JM}(r)$ yields a set of three coupled integral equations given by

$$\mathcal{E}^{\lambda\lambda'}_{JM}(r) = u_J(r)\delta_{\lambda\lambda'}(\delta_{\lambda o}-1) + (-1)^J k^2\sum_{\lambda''}\int_0^\infty dr'\,\Gamma^J_{\lambda\lambda''}(r_<,r_>)[n^2(r')-1]\mathcal{E}^{\lambda''\lambda'}_{JM}(r') \tag{9}$$

for $\lambda,\lambda',\lambda''$ equal to e,m, and 0. (The above equation will constitute the starting point for our noniterative solution method since the more complicated nonspherically symmetric scatterer can be treated using the same analysis.)

We comment that these equations are very similar to those encountered in quantum mechanical scattering theory, where now the role of the potential is taken by the quantity $n^2(r)-1$. Thus, in the absence of any dispersive medium, $n=1$ so that the "potential" in Eq. (9) tends to zero as one moves from the scattering region into free space. If no medium is present, then n^2-1 vanishes everywhere and $\mathcal{E}^{\lambda\lambda'}_{JM}$ equals the incident wave, i.e., no scattering occurs. If one has a spherical region radius R where $n(r)$ is constant but different from one, the integral in Eq. (9) above extends from $r'=0$ up to $r'=R$ and for $r>R$, there are purely outgoing scattered waves with amplitude depending on, e.g., for $\lambda=e$, $\int_0^R u_J(kr')[n^2(r')-1]\mathcal{E}^{\lambda''\lambda'}_{JM}(r')dr'$. Thus, one expects the amplitude of the scattered waves to vary with the "size" of the scattering medium in this fashion. If $[n^2(r)-1]$ is bounded by Q, the product QR will be a measure of the strength of the scattering medium. This is similar to a sort of square barrier or well in quantum mechanics.

III. THE VOLTERRA EQUATIONS FOR ELECTROMAGNETIC SCATTERING

We now wish to discuss the application of the Drukarev–Sams–Kouri procedure for obtaining Volterra integral equations. The plan of presentation in this section is as follows. We first illustrate the procedure for solving the Lippmann–Schwinger equations for quantum mechanical scattering by transforming them to Volterra integral equations. Next, the discussion of the problem of electromagnetic scattering will be developed using completely analogous techniques. Furthermore, the discussion of various quantities appearing in the electromagnetic scattering case will be strongly dependent on analogies with the quantum mechanical problem. This is particularly true of the definition of an "electromagnetic Jost matrix" relating modified electric field functions with the physical electromagnetic field functions.

The transformation procedure depends on the appearance of $r_<$ and $r_>$ variables in the kernel[8,9,11] of the integral equations and can be illustrated using the single uncoupled Lippmann–Schwinger radial integral equation. We may eliminate the $r_<$ and $r_>$ variables explicitly by writing the equation for the wavefunction at r as

$$\psi^+_J(r) = u_J(kr) + \frac{(-1)^{J+1}}{k}\omega^{(+)}_J(kr)\int_0^r dr'\,u_J(kr')V(r')\psi^+_J(r') + \frac{(-1)^{J+1}}{k}u_J(kr)\int_r^\infty dr'\,\omega^{(+)}_J(kr')V(r')\psi^+_J(kr'). \tag{10}$$

Upon adding and subtracting $[(-1)^{J+1}/k]u_J(kr)\int_0^r dr'\,\omega^{(+)}_J(kr')V(r')\psi^+_J(r')$, we obtain

$$\psi^+_J(r) = u_J(kr)[1+C] + \frac{(-1)^{J+1}}{k}\omega^{(+)}_J(kr)\int_0^r dr' \times u_J(kr')V(r')\psi^+_J(r') + \frac{(-1)^J}{k}u_J(kr)\int_0^r dr'\,\omega^{(+)}_J(kr')V(r')\psi^+_J(r') \tag{11}$$

with

$$[1+C] = 1 + \frac{(-1)^{J+1}}{k}\int_0^\infty dr'\,\omega^{(+)}_J(kr')V(r')\psi^+_J(r'). \tag{12}$$

We now try a solution to Eq. (11) of the form

$$\psi^+_J(r) = \varphi_J(r)[1+C] \tag{13}$$

and substitution into Eq. (11) yields

$$\varphi_J(r) = u_J(kr) + \frac{(-1)^{J+1}}{k}\int_0^r dr' \times [\omega^{(+)}_J(kr)u_J(kr') - \omega^{(+)}_J(kr')u_J(kr)]V(r')\varphi_J(r') \tag{14}$$

as the equation which $\varphi_J(r)$ must satisfy. In addition, we may substitute Eq. (13) into Eq. (12) and formally rearrange it to obtain

$$1+C = \left(1 + \frac{(-1)^J}{k}\int_0^\infty dr\,\omega^{(+)}_J(kr)V(r)\varphi_J(r)\right)^{-1}, \tag{15}$$

provided $\{1+[(-1)^J/k]\int_0^\infty dr\,\omega^{(+)}_J V\varphi_J\}$ is nonzero. Thus, the equation satisfied by the "modified wavefunction" $\varphi_J(r)$ is a Volterra integral equation of the second kind.[10] It is seen that the variable upper limit r in this integral equation is automatically associated with the point r which is the argument of the scattering wavefunction. Furthermore, if the Volterra equation for $\varphi_J(r)$ can be solved, the quantity $\{1+[(-1)^J/k]\int_0^\infty dr\,\omega^{(+)}_J V\varphi_J\}$ can be computed and by Eq. (13) a complete solution to the original scattering problem obtained. In fact it has been shown by Brysk that the quantity $\{1+[(-1)^J/k]\int_0^\infty dr\,\omega^{(+)}_J V\varphi_J\}$ is the Fredholm determinant[11] for the original integral equation (10). Thus,

it has zeros only in the complex k plane, and solutions using Eqs. (14) and (15) for real energies may always be found. Of course, the zeros of $\{1 + [(-1)^J/k]\int_0^\infty dr\ \omega_J^{(+)} V\varphi_J\}$ in the complex k plane locate any resonances or bound states of the total system. Finally, we point out that the quantity $\{1 + [(-1)^J/k]\int_0^\infty dr\ \omega_J^{(+)} V\varphi_J\}$ is essentially the Jost function for the quantum mechanical scattering problem. In the present context it arises naturally as a transforming factor relating the functions φ_J (satisfying essentially *initial value* type boundary conditions) to the scattering wavefunctions ψ_J^+. We shall make use of this later in defining an electromagnetic analogue of the Jost function (or matrix).

In order to most conveniently discuss the application of this same procedure to electromagnetic scattering, we now rewrite Eq. (9) in matrix form as

$$\overleftrightarrow{\mathcal{E}}_{JM}(r) = \overleftrightarrow{u}_J(r) + (-1)^J k^2 \int_0^\infty dr' \times \overleftrightarrow{\Gamma}^J(r_<, r_>)\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r') \quad (16)$$

where

$$\{\overleftrightarrow{\mathcal{E}}_{JM}\}_{\lambda\lambda'} = \mathcal{E}_{JM}^{\lambda\lambda'}, \quad (17)$$

$$\{\overleftrightarrow{\Gamma}^J\}_{\lambda\lambda'} = \Gamma^J_{\lambda\lambda'}, \quad (18)$$

$$\{\overleftrightarrow{u}_J\}_{\lambda\lambda'} = u_J(kr)\delta_{\lambda\lambda'}[\delta_{\lambda o} - 1], \quad (19)$$

and

$$\{\overleftrightarrow{m}\}_{\lambda\lambda'} = \delta_{\lambda\lambda'}[n^2(r) - 1]. \quad (20)$$

It is then convenient to write $\overleftrightarrow{\Gamma}^J$ as a sum of matrix products, each factor of which depends only on $r_<$ or $r_>$. Thus,

$$\overleftrightarrow{\Gamma}^J(r_<, r_>) = \overleftrightarrow{\mathcal{F}}_1^J(r_<)\cdot\overleftrightarrow{\mathcal{F}}_2^J(r_>) + \frac{1}{r'}\frac{d}{dr}\left(\overleftrightarrow{\mathcal{F}}_3^J(r_<)\cdot\overleftrightarrow{\mathcal{F}}_4^J(r_>)\right) \quad (21)$$

with the diagonal $\overleftrightarrow{\mathcal{F}}_1^J$, $\overleftrightarrow{\mathcal{F}}_2^J$, and $\overleftrightarrow{\mathcal{F}}_3^J$ matrices given by

$$\mathcal{F}_{1oo}^J(r) = i\sqrt{J+1}\, u_J(kr)/kr, \quad (22)$$

$$\mathcal{F}_{1ee}^J(r) = \frac{d}{dr} u_J(kr), \quad (23)$$

$$\mathcal{F}_{1mm}^J(r) = iu_J(kr), \quad (24)$$

$$\mathcal{F}_{2oo}^J(r) = i\sqrt{J+1}\, \omega_J^{(+)}(kr)/kr, \quad (25)$$

$$\mathcal{F}_{2ee}^J(r) = \frac{d}{dr}\omega_J^{(+)}(kr), \quad (26)$$

$$\mathcal{F}_{2mm}^J(r) = i\omega_J^{(+)}(kr), \quad (27)$$

$$\mathcal{F}_{3oo}^J(r) = i[J(J+1)]^{1/4} u_J(kr)/k, \quad (28)$$

$$\mathcal{F}_{3ee}^J(r) = i[J(J+1)]^{1/4} u_J(kr)/k, \quad (29)$$

$$\mathcal{F}_{3mm}^J(r) = 0, \quad (30)$$

while $\overleftrightarrow{\mathcal{F}}_4^J$ has only two nonzero elements given by

$$\mathcal{F}_{4oe}^J(r) = \mathcal{F}_{4eo}^J(r) = i[J(J+1)]^{1/4}\omega_J^{(+)}(kr)/k. \quad (31)$$

Then Eq. (16) may be written as

$$\overleftrightarrow{\mathcal{E}}_{JM}(r) = \overleftrightarrow{u}_J(r) + (-1)^J k^2\Bigg[\overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\int_0^r dr'\,\overleftrightarrow{\mathcal{F}}_1^J(r')\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r') + \overleftrightarrow{\mathcal{F}}_1^J(r)\cdot\int_r^\infty dr'\,\overleftrightarrow{\mathcal{F}}_2^J(r')\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r') + \left\{\frac{d}{dr}\overleftrightarrow{\mathcal{F}}_4^J(r)\right\}\cdot\int_0^r dr'\,\frac{\overleftrightarrow{\mathcal{F}}_3^J(r')}{r'}\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM} + \left\{\frac{d}{dr}\overleftrightarrow{\mathcal{F}}_3^J(r)\right\}\cdot\int_r^\infty dr'\,\frac{\overleftrightarrow{\mathcal{F}}_4^J(r')}{r'}\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r')\Bigg], \quad (32)$$

where we have explicitly eliminated the $r_<, r_>$ variables. Now just as in the discussion of Eq. (10), we add and subtract the integrals[8,9]

$$(-1)^J k^2\overleftrightarrow{\mathcal{F}}_1^J(r)\cdot\int_0^r \overleftrightarrow{\mathcal{F}}_2^J(r')\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r')dr' \quad (33)$$

and

$$(-1)^J k^2\left\{\frac{d}{dr}\overleftrightarrow{\mathcal{F}}_3^J(r)\right\}\cdot\int_0^r \frac{\overleftrightarrow{\mathcal{F}}_4^J(r')}{r'}\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r')dr' \quad (34)$$

to obtain

$$\overleftrightarrow{\mathcal{E}}_{JM}(r) = \overleftrightarrow{u}_J(r) + (-1)^J k^2 \times\Bigg[\int_0^r dr'\{\overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\overleftrightarrow{\mathcal{F}}_1^J(r') - \overleftrightarrow{\mathcal{F}}_1^J(r)\cdot\overleftrightarrow{\mathcal{F}}_2^J(r')\}\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r') + \int_0^r dr'\left\{\frac{d}{dr}\overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{\mathcal{F}}_3^J(r') - \frac{d}{dr}\overleftrightarrow{\mathcal{F}}_3^J(r)\cdot\overleftrightarrow{\mathcal{F}}_4^J(r')\right\}\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r')\Bigg] + \overleftrightarrow{\mathcal{F}}_1^J(r)\cdot\overleftrightarrow{C}^J + \frac{d}{dr}\overleftrightarrow{\mathcal{F}}_3^J(r)\cdot\overleftrightarrow{D}^J. \quad (35)$$

Here the constant matrices $\overleftrightarrow{C}^J$ and $\overleftrightarrow{D}^J$ are defined by analogy with Eq. (12) as

$$\overleftrightarrow{C}^J = (-1)^J k^2\int_0^\infty dr\,\overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r) \quad (36)$$

and

$$\overleftrightarrow{D}^J = (-1)^J k^2\int_0^\infty dr\,\overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(r). \quad (37)$$

In order to solve Eq. (35), we now write the electric field $\overleftrightarrow{\mathcal{E}}_{JM}(r)$ as

$$\overleftrightarrow{\mathcal{E}}_{JM}(r) = \overleftrightarrow{\mathcal{E}}_{JM}(0|r) + \overleftrightarrow{\mathcal{E}}_{JM}(1|r)\cdot\overleftrightarrow{C}^J + \overleftrightarrow{\mathcal{E}}_{JM}(2|r)\cdot\overleftrightarrow{D}^J. \quad (38)$$

This expression is substituted into Eq. (35), and if the functions $\overleftrightarrow{\mathcal{E}}_{JM}(p|r)$, $p = 0, 1, 2$ are taken to satisfy

$$\overleftrightarrow{\mathcal{E}}_{JM}(p|r) = \overleftrightarrow{I}_J(p|r) + (-1)^J k^2 \times\Bigg[\int_0^r dr'\{\overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\overleftrightarrow{\mathcal{F}}_1^J(r') - \overleftrightarrow{\mathcal{F}}_1^J(r)\cdot\overleftrightarrow{\mathcal{F}}_2^J(r')\}\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(p|r') + \int_0^r dr'\left\{\frac{d}{dr}\overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{\mathcal{F}}_3^J(r') - \frac{d}{dr}\overleftrightarrow{\mathcal{F}}_3^J(r)\cdot\overleftrightarrow{\mathcal{F}}_4^J(r')\right\}\cdot\overleftrightarrow{m}(r')\cdot\overleftrightarrow{\mathcal{E}}_{JM}(p|r')\Bigg], \quad p = 0, 1, 2 \quad (39)$$

with

$$\overleftrightarrow{I}_J(0|r) = \overleftrightarrow{u}_J(r), \quad (40)$$

$$\overleftrightarrow{I}_J(1|r) = \overleftrightarrow{\mathcal{F}}_1^J(r), \quad (41)$$

and

$$\overleftrightarrow{I}_J(2|r) = \frac{d}{dr}\overleftrightarrow{\mathcal{F}}_3^J(r), \quad (42)$$

then Eq. (38) represents the solution of Maxwell's equations expressed in integral form. The equations satisfied by the functions $\overleftrightarrow{\mathcal{E}}_{JM}(p|r)$, $p = 0, 1, 2$ are clearly Volterra equations of the second kind and in analogy with Eq. (14), it is again observed that the variable upper limit r appearing is the same as the radial posi-

tion variable in the physical electromagnetic function $\overleftrightarrow{\mathcal{E}}_{JM}(r)$. Assuming that Eq. (39) may be solved (by iterative or noniterative procedures), we now substitute Eq. (38) into Eqs. (36), (37) to obtain

$$\overleftrightarrow{C}^J = (-1)^J k^2 \int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\overleftrightarrow{m}(r)\cdot[\overleftrightarrow{\mathcal{E}}_{JM}(0|r) + \overleftrightarrow{\mathcal{E}}_{JM}(1|r)\cdot\overleftrightarrow{C}^J + \overleftrightarrow{\mathcal{E}}_{JM}(2|r)\cdot\overleftrightarrow{D}^J] \quad (43)$$

and

$$\overleftrightarrow{D}^J = (-1)^J k^2 \int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{m}(r)\cdot[\overleftrightarrow{\mathcal{E}}_{JM}(0|r) + \overleftrightarrow{\mathcal{E}}_{JM}(1|r)\cdot\overleftrightarrow{C}^J + \overleftrightarrow{\mathcal{E}}_{JM}(2|r)\cdot\overleftrightarrow{D}^J]. \quad (44)$$

Since the equations for the $\overleftrightarrow{\mathcal{E}}_{JM}(p|r)$ do not depend on the $\overleftrightarrow{C}^J$ and $\overleftrightarrow{D}^J$ matrices, they may be computed independently by solving Eqs. (38). Then $\overleftrightarrow{C}^J$ and $\overleftrightarrow{D}^J$ may be computed from the above two equations treating them as simultaneous equations for the two matrices. Indeed, these equations may be written in compact form using supermatrices defined by

$$\vec{\mathfrak{B}} = \begin{pmatrix} \overleftrightarrow{C}^J \\ \overleftrightarrow{D}^J \end{pmatrix}, \quad (45)$$

$$\vec{\mathfrak{K}} = \begin{pmatrix} [\int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(1|r)][\int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(2|r)] \\ [\int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(2|r)][\int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(1|r)] \end{pmatrix}, \quad (46)$$

and

$$\vec{\mathcal{G}} = \begin{pmatrix} [\int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_2^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(0|r)] \\ [\int_0^\infty dr\ \overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{m}(r)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(0|r)] \end{pmatrix}. \quad (47)$$

Then Eqs. (43)-(44) become

$$\vec{\mathfrak{B}} = \vec{\mathcal{G}} + \overleftrightarrow{\mathfrak{K}}\cdot\vec{\mathfrak{B}} \quad (48)$$

so that

$$\vec{\mathfrak{B}} = (\overleftrightarrow{I} - \overleftrightarrow{\mathfrak{K}})^{-1}\cdot\vec{\mathcal{G}} \quad (49)$$

whereupon the solution of the original field equations is given by

$$\overleftrightarrow{\mathcal{E}}_{JM}(r) = \overleftrightarrow{\mathcal{E}}_{JM}(0|r) + \vec{\mathcal{E}}^T\cdot\vec{\mathfrak{B}} \quad (50)$$

Here we define

$$\vec{\mathcal{E}}^T = \overbrace{\overleftrightarrow{\mathcal{E}}_{JM}(1|r)\,\overleftrightarrow{\mathcal{E}}_{JM}(2|r)}. \quad (51)$$

This then leads to

$$\overleftrightarrow{\mathcal{E}}_{JM}(r) = \overleftrightarrow{\mathcal{E}}_{JM}(0|r) + \vec{\mathcal{E}}^T\cdot(\overleftrightarrow{I} - \overleftrightarrow{\mathfrak{K}})^{-1}\cdot\vec{\mathcal{G}}. \quad (52)$$

It is interesting to compare these expressions with the corresponding quantum mechanical scattering equations. It is evident that the elements of $(\overleftrightarrow{I} - \overleftrightarrow{\mathfrak{K}})$ are analogues of the quantity $\{1 + [(-1)^J/k]\int_0^\infty \omega_J^{(+)} V\varphi_J\, dr\}$ so that $(\overleftrightarrow{I} - \overleftrightarrow{\mathfrak{K}})$ now plays the role of the Jost matrix for electromagnetic scattering. In particular, under circumstances where $\det(\overleftrightarrow{I} - \overleftrightarrow{\mathfrak{K}})$ vanishes, one expects resonant scattering just as in the quantum mechanical case.

Finally, in Eq. (38) the physical electric field is expressed in terms of the $\overleftrightarrow{\mathcal{E}}_{JM}(p|r)$, $p = 0, 1, 2$ which we call "modified field functions." It is of interest to explore briefly the differences between these modified fields and the physical field. By far the most significant difference may be appreciated by contrasting the Volterra equations satisfied by the $\overleftrightarrow{\mathcal{E}}_{JM}(p|r)$ and the Fredholm equation for $\overleftrightarrow{\mathcal{E}}_{JM}(r)$. One sees immediately that the true field at a point r is influenced by the value of the field everywhere else. That is, the integral equation for $\overleftrightarrow{\mathcal{E}}_{JM}(r)$, Eq. (18), involves an integration over the entire region where the refractive index differs from the free space value of 1. Essentially, this implies that a wave propagating in the medium of refractive index $n(r)$ undergoes scattering and interferes with portions of the wave scattered by all other regions within the medium. On the other hand, the modified field functions $\overleftrightarrow{\mathcal{E}}_{JM}(p|r)$ at $r = R$ are determined solely by their preceeding values and are *completely uninfluenced* by the modified field at points $r > R$. There is no interference between portions of the modified wave scattered at different points in the medium. These interference effects are introduced when one combines the modified fields, together with the "electromagnetic Jost matrix" to construct the physical wave. Then the amplitude of the reference modified wave $\overleftrightarrow{\mathcal{E}}_{JM}(0|r)$ is changed by the contributions $\overleftrightarrow{\mathcal{E}}_{JM}(1|r)\cdot\overleftrightarrow{C}^J$ and $\overleftrightarrow{\mathcal{E}}_{JM}(2|r)\cdot\overleftrightarrow{D}^J$ which either interfere constructively or destructively.

IV. NUMERICAL PROCEDURE

We now briefly discuss a numerical procedure for solving Eqs. (39) for the $\overleftrightarrow{\mathcal{E}}_{JM}(p|r)$, $p = 0, 1, 2$. The approach is based on the approximation of the integral terms by a Newton-Coates quadrature. Eq. (39) then becomes

$$\overleftrightarrow{\mathcal{E}}_{JM}(p|r_n) = \overleftrightarrow{I}_J(p|r_n) + (-1)^J k^2 \sum_{t=1}^{n} w_t \times \left[\begin{array}{l} \overleftrightarrow{\mathcal{F}}_2^J(r_n)\cdot\overleftrightarrow{\mathcal{F}}_1^J(r_t) - \overleftrightarrow{\mathcal{F}}_1^J(r_n)\cdot\overleftrightarrow{\mathcal{F}}_2^J(r_t) \\ + \overleftrightarrow{\mathcal{F}}_4^{J'}(r_n)\cdot\overleftrightarrow{\mathcal{F}}_3^J(r_t) - \overleftrightarrow{\mathcal{F}}_3^{J'}(r_n)\cdot\overleftrightarrow{\mathcal{F}}_4^J(r_t) \end{array}\right] \cdot\overleftrightarrow{m}(r_t)\cdot\overleftrightarrow{\mathcal{E}}_{JM}(p|r_t) \quad (53)$$

It is of interest to examine the quantity in brackets above for $t = n$. It is readily seen to equal $\overleftrightarrow{V}_n$ where

$$\overleftrightarrow{V}_n = \left\{\frac{d}{dr}[\overleftrightarrow{\mathcal{F}}_4^J(r)\cdot\overleftrightarrow{\mathcal{F}}_3^J(r)]\right\}_{r=r_n} \quad (54)$$

since the first term vanishes. [Here we see an important difference between the electromagnetic scattering problem and the quantum mechanical problem. Unless there are velocity dependent potentials occurring in the quantum mechanical problem, only the term $\underleftrightarrow{\mathcal{F}}_2^J(r_n)\cdot\underleftrightarrow{\mathcal{F}}_1^J(r_t) - \underleftrightarrow{\mathcal{F}}_1^J(r_n)\cdot\underleftrightarrow{\mathcal{F}}_2^J(r_t)$ occurs and this is readily seen to vanish at $r_t = r_n$. The result is that for quantum mechanical problems, the analog of Eq. (53) may be solved without necessitating any matrix inversions.] Thus, in order to solve Eq. (53) for the "modified field functions" $\underleftrightarrow{\mathcal{E}}_{JM}(p\,|\,r)$ at the point r_n it is necessary to compute the inverse of the matrix $1 - \underleftrightarrow{V}_n\cdot\underleftrightarrow{m}(r_n)\times(-1)^J k^2 w_n$. However, it is stressed that, for the present problem, this is simply a 3×3 matrix and, in general, the dimensionality of the matrix to be inverted is the same as the dimensionality of the matrix $\underleftrightarrow{\mathcal{E}}_{JM,J'M'}(r)$. This may be contrasted with what one encounters in a direct quadrature solution of Eq. (16), where one obtains

$$\underleftrightarrow{\mathcal{E}}_{JM}(r_n) = \underleftrightarrow{u}_J(r_n) + (-1)^J k^2 \sum_{t=1}^{N} \tilde{w}_t\,\underleftrightarrow{\Gamma}^J(r_n, r_t)\cdot\underleftrightarrow{m}(r_t)\cdot\underleftrightarrow{\mathcal{E}}_{JM}(r_t). \tag{55}$$

Even if one uses a quadrature scheme which takes account of the cusp occurring in $\underleftrightarrow{\Gamma}^J$ one must invert a matrix of dimension $3N\times 3N$, where N is the *total* number of quadrature points employed. Clearly, the solution of the Volterra equations is considerably simpler than the corresponding Fredholm equations.[12] In order to effect the numerical evaluation of the $\underleftrightarrow{\mathcal{E}}_{JM}(p\,|\,r_n)$ then, one simply requires the initial condition on the modified field functions at $r = 0$ which is given by

$$\underleftrightarrow{\mathcal{E}}_{JM}(p\,|\,0) = 0. \tag{56}$$

It follows that Eq. (55) can then be used to step the function out into the region where $\underleftrightarrow{m}(r)$ is zero. Using these pointwise values of $\underleftrightarrow{\mathcal{E}}_{JM}(p\,|\,r_n)$, $n = 0, 1, 2, \ldots$, the integrals required to obtain $\underleftrightarrow{I} - \underleftrightarrow{\mathcal{K}}$ and $\mathcal{J}$ can be constructed. Finally, $(\underleftrightarrow{I} - \underleftrightarrow{\mathcal{K}})^{-1}$ is constructed and the physical fields obtained using Eq. (52).

Finally, it is noted that one might also desire to attempt the solution of Eqs. (39) by iteration. In contrast to an iterative solution of Eq. (16), the convergence of which is governed by the same conditions as the Born–Neumann procedure in quantum mechanics,[4] the conditions for convergence of iteration of Eqs. (39) are those of an integral equation with a triangular kernal [i.e., $K(r, r') = 0$ for $r' > r$]. Thus, one expects the convergence of such iterative solutions to be independent of the "strength" of $\underleftrightarrow{m}(r)$.

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Minimal extensions as generalized semidirect products*

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An extension of a two-element symmetry group Z_2 (defined, e.g., by C, P, or T) by another symmetry group K is called a minimal extension (ME). From the general theory of group extensions it follows that a ME is determined by an element ϕ of K and an automorphism F in K which are related in a certain way. It is shown that every ME can be expressed as a generalized semidirect product (GSP): $(K \circledS H)/K'_0$, where the homomorphism τ is defined by F, and K'_0, H are cyclic groups of order m and $2m$, respectively, m being the order of ϕ. The simplest GSP form of any ME is obtained depending on ϕ being outside or inside the center of K (in particular, ϕ may be equal to the unit element), and F being an inner or an outer automorphism. A complete classification of inequivalent ME's is presented, and its possible significance for magnetic space and point groups is indicated. The usefulness of the GSP form for finding the irreducible representations of a ME is pointed out.

1. INTRODUCTION

As it is well known,[1] a group G can be extended by a group K into a group E if and only if a mapping $\Psi: G \to \mathrm{Aut}(K)$, as well as a mapping $\omega: G \times G \to K$, can be found so that the following relations are satisfied $\forall \alpha \in K, \forall a, b, c \in G$:

$$\Psi[a](\Psi[b](\alpha)) = \omega(a,b)\Psi[ab](\alpha)\omega(a,b)^{-1}, \tag{1a}$$

$$\omega(a,b)\omega(ab,c) = \Psi[a](\omega(b,c))\omega(a,bc). \tag{1b}$$

The maps Ψ and ω are assumed to be normalized, i.e.,

$$\Psi[e] = I \tag{2a}$$

$$\omega(e,e) = \omega(a,e) = \omega(e,a) = \epsilon, \forall a \in G \tag{2b}$$

(e, I, and ϵ being the unit elements in G, $\mathrm{Aut}(K)$ and K, respectively). Then

$$E = \{(\alpha, a) \mid \alpha \in K, a \in G\}, \tag{3a}$$

with the composition law

$$(\alpha, a)(\beta, b) = (\alpha\Psi[a](\beta)\omega(a,b), ab). \tag{3b}$$

The isomorphism $i: \alpha \to (\alpha, e), \forall \alpha \in K$ defines an invariant subgroup $i(K)$ in E such that $E/i(K) \cong G$, i.e., we have the exact sequence.

$$1 \to K \xrightarrow{i} E \to G \to 1.$$

When G is of order two, i.e., $G = Z_2 = \{e, a\}$ (e.g., the generating element "a" can be C, P, or T), E is called a *minimal extension* (ME).[2] Owing to Eqs. (2) the maps Ψ and ω are now determined by $F = \Psi[a]$ and $\phi = \omega(a,a)$. The necessary and sufficient conditions (1) boil down to

$$F^2(\alpha) = \phi\alpha\phi^{-1} \equiv I_\phi(\alpha), \quad \forall \alpha \in K, \tag{4a}$$

$$F(\phi) = \phi. \tag{4b}$$

Equation (4a) by itself means that F cannot give any extension at all unless it belongs to a coset $\in \mathrm{Aut}(K)/I(K)$ [$I(K)$ being the invariant subgroup of all inner automorphisms in K] whose square is $I(K)$, i.e., to an involutive coset.

Two ME's determined by F, ϕ and F', ϕ' are equivalent if and only if there exists $\alpha \in K$, such that:[2]

$$F' = I_\alpha F, \tag{5a}$$

$$\phi' = \alpha F(\alpha)\phi. \tag{5b}$$

It is an immediate consequence of Eqs. (5) that if F gives a solution, then F' gives an equivalent one if and only if it belongs to the same coset in $\mathrm{Aut}(K)$.

From now on we shall consider suitable representatives F, ϕ from the classes of equivalent extensions so that F is simplest possible. All the classes in which an F can be found such that $F^2 = I$ (an involution) we group together to obtain a category consisting of, what we call, *involutive* ME's. Section 2 is devoted to the discussion of these extensions. Section 3 treats the remaining *noninvolutive* ME's, which are characterized by the nonexistence of an involutive F in the class of equivalent extensions. An example is presented as an illustration for the noninvolutive ME's.

2. INVOLUTIVE MINIMAL EXTENSIONS

Let F, ϕ be an arbitrary solution of Eqs. (4) such that F is in the same coset of $\mathrm{Aut}(K)$ [with respect to $I(K)$] with at least one involution F_0. It is an immediate consequence of Eqs. (4) that there exists an equivalent solution F_0, ϕ_0 satisfying

$$F_0^2 = I, \quad \phi_0 \in C^{F_0}, \tag{6}$$

where by C^{F_0} we denote the subgroup of the center C of K consisting of all elements in C which are invariant under F_0.

A. The complete classification of nonequivalent ME's

Two solutions F, ϕ and F', ϕ' are equivalent if and only if the corresponding F_0, ϕ_0 and F'_0, ϕ'_0 are equivalent. Therefore, it is sufficient to classify only the latter.

Lemma 1: All the nonequivalent involutive ME's of a group K are enumerated firstly by the cosets of $\mathrm{Aut}(K)$ [with respect to $I(K)$] which contain an involution, and secondly, after having chosen an involution F_0 in each such coset, by the elements of the factor group $C^{F_0}/$

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$CF_0(C)^d$, where $CF_0(C)^d = \{\gamma F_0(\gamma) | \gamma \in C\}$ is an invariant subgroup of C^{F_0}. In the second step one may use alternatively a set of representatives, one from each coset of C^{F_0} with respect to $CF_0(C)^d$.

Proof: The first claim follows from the definition of involutive ME's and (5a). Further, as was already pointed out, one can replace any given involutive solution F, ϕ by F_0, ϕ_0, where F_0 is the chosen involution in the same coset as F, and ϕ_0 is some element of C^{F_0}. It is seen from Eqs. (5) that F_0, ϕ_0 and F_0, ϕ_0' are equivalent if and only if there exists $\alpha \in C$, such that $\phi_0' = \alpha F_0(\alpha)\phi_0$, i.e., if and only if ϕ_0 and ϕ_0' are in the same coset $\in C^{F_0}/CF_0(C)^d$. All that remains to be shown is that $CF_0(C)^d$ is an invariant subgroup in C^{F_0}, which follows easily. QED

The proof of Lemma 1 can also be obtained using cohomology theory, where it is shown that the nonequivalent extensions of G by K are enumerated by the elements of the second cohomology group $H^2(G, C)$, which, for cyclic G, is given by[3] $\mathrm{Ker}(T)/\mathrm{Im}(N)$. For $G = Z_2(a)$ the mappings T and N are $T(\gamma) = \gamma F_0(\gamma^{-1})$ and $N(\gamma) = \gamma F_0(\gamma)$, $\forall \gamma \in C$. Therefore, $\mathrm{Ker}(T) = C^{F_0}$ and $\mathrm{Im}(N) = CF_0(C)^d$ as claimed in the lemma.

B. The central GSP form

The central generalized semidirect product (GSP) form[4,5] of any extension E of G by K exists provided that the mapping Ψ can be a homomorphism denoted by $\sigma: G \to \mathrm{Aut}(K)$. Each central GSP is based on an extension H of G by a central subgroup C_0 of K, i.e.,

$$1 \to C_0 \xrightarrow{l} H \xrightarrow{n} G \to 1.$$

Here C_0 is invariant under every $\sigma[a], a \in G$, and H is obtained using $\sigma: G \to \mathrm{Aut}(C_0)$. It consists in a simple construction:

$$E = (K \textcircled{T} H)/C_0', \tag{7}$$

where the semidirect product $K \textcircled{T} H$ is determined by the homomorphism $\tau = \sigma \circ n$, and $C_0' = \{(\gamma, l(\gamma^{-1})) | \gamma \in C_0\}$.

In general, the main problem in this approach lies in finding a σ and an H. In the case of involutive ME's both of these problems disappear because every F_0 and ϕ_0 satisfying (6) provide us with σ and H, respectively. Namely, having chosen F_0 to be an involution, the mapping Ψ obviously becomes a homomorphism σ, i.e.,

$$\sigma[a] = F_0. \tag{8}$$

The cycle of ϕ_0 gives the central subgroup C_0, i.e.,

$$C_0 = Z_m(\phi_0), \tag{9}$$

where m is the order of the element ϕ_0. Any cyclic group of the order $2m$ can be taken for H, i.e.,

$$H = Z_{2m}(x), \tag{10}$$

with x as the generating element. The isomorphism $l: C_0 \to H$ we define by $l(\phi_0^p) = x^{2p}$, $p = 1, \ldots, m$. The kernel of the homomorphism $n: H \to Z_2(a)$ is $l(C_0)$, so that $n(x^q) = a^q$, $q = 1, \ldots, 2m$ (remembering that $a^2 = e$). The homomorphism $\tau: H \to \mathrm{Aut}(K)$ equals $\sigma \circ n$, i.e., keeping in mind that $F_0^2 = I$,

$$\tau[x^q] = F_0^q, \quad q = 1, \ldots, 2m. \tag{11}$$

Thus we have established the following:

Lemma 2: For an arbitrary involutive $F_0 \in \mathrm{Aut}(K)$ and any $\phi_0 \in C^{F_0}$, whose order is m, the central GSP form of the corresponding ME is the factor group

$$E = [K \textcircled{T} Z_{2m}(x)]/C_0', \tag{12}$$

where the composition law in $K \textcircled{T} Z_{2m}(x)$ is

$$(\alpha, x^q)(\beta, x^r) = (\alpha F_0^q(\beta), x^{q+r}), \qquad \alpha, \beta \in K,\ q, r = 1, \ldots 2m, \tag{13}$$

and

$$C_0' = \{(\phi_0^p, x^{2(m-p)}) | p = 1, \ldots, m\}. \tag{14}$$

Different choices of x give equivalent realizations of E.

It is useful to notice [cf. Ref. 4, Sec. 5(C)] that after having constructed E by (12), it is a product of two subgroups. The first is invariant in E and isomorphic to K, the second is isomorphic to $Z_{2m}(x)$, and they intersect in a third subgroup isomorphic to $C_0 = Z_m(\phi_0)$.[6]

C. Canonical forms

Lemma 1 gives a systematic way of choosing F_0, ϕ_0 as representatives from well-defined cosets to obtain one involutive ME from each class of mutually equivalent ones. There is an obvious freedom in this selection, which can be used to make the central GSP form simplest possible, i.e., canonical.

First we distinguish between F_0 being an inner automorphism and its being an outer one. In the former case one takes $F_0 = I$. According to Eq. (11) this causes τ to become the trivial homomorphism (i.e., one has the case of the central extensions), and E from (12) to take up the form[4,7]

$$E = [K \otimes Z_{2m}(x)]/C_0', \tag{15}$$

which we call the generalized direct product (GDP). When F_0 is an outer (involutive) automorphism, τ is necessarily nontrivial, and therefore the GSP form cannot simplify to the GDP one.

As to ϕ_0, irrespectively of F_0 being an inner or outer automorphism, the lower its order m is the smaller $Z_{2m}(x)$ becomes. Hence in each coset of C^{F_0} one should single out a ϕ_0 of minimal order. In $CF_0(C)^d$ itself $\phi_0 = \epsilon$ is the unique choice, which makes C_0' trivial. This reduces the GDP form to the direct product (DP), and the GSP to the semidirect product (SP).

To summarize and to compare this rough classification according to the simplicity of form with the classification from A_1 to B_2 of Lee and Wick,[2] we give the table

ϕ_0 \ F_0	$F_0 = I$	F_0 involutive outer automorphisms
$\phi_0 = \epsilon$	DP (A_1)	SP (B_1)
$\phi_0 \neq \epsilon$, $\phi_0 \in C^{F_0}$	GDP (A_2, A_3)	central GSP (B_2)

3. NONINVOLUTIVE MINIMAL EXTENSIONS

Let K be a given non-Abelian group, and F an outer automorphism in K belonging to an involutive coset [element of $\mathrm{Aut}(K)/I(K)$ whose square is $I(K)$] which does not contain an involution. As a consequence, F defines via Eq. (4a) a coset in K (element of K/C distinct from C) because $1 \to C \to K \to I(K) \to 1$. On the other hand, Eq. (4b) gives the subgroup of elements in K invariant under F. If this coset and this subgroup have a nonempty intersection, then there exists a solution F, ϕ of Eqs. (4a) and (4b), which we assume fixed. In contrast, in the case of involutive ME's the coset is always C itself, and the intersection C^F contains at least ϵ.

From another point of view, a pair F, ϕ satisfying (4) gives a noninvolutive ME if and only if there is no equivalent F', ϕ' such that $\phi' \in C$.

A. The complete classification of nonequivalent ME's

For the classification we turn to F_τ, the automorphism F reduced to C, which (4a) shows to be necessarily an involution, and consider the ME's of C determined by F_τ.

Lemma 3: All the nonequivalent noninvolutive ME's of a group K for a given F are in a one-to-one correspondence with the factor group $C^{F_\tau}/CF_\tau(C)^d$.

Proof: It is easily verified that F, ϕ' is also a solution of Eqs. (4a) and (4b) if $\phi' = \phi_0\phi$, $\phi_0 \in C^{F_\tau}$, where F, ϕ is the fixed solution. This form of ϕ' is also a necessary condition because Eq. (4a) implies $\phi'\phi^{-1} \in C$, and (4b) entails that $\phi'\phi^{-1}$ is invariant under F, so that $\phi'\phi^{-1} \in C^{F_\tau}$. Therefore, all solutions F, ϕ' (with the fixed F) are in one-to-one correspondence with all solutions F_τ, ϕ_0 for ME's of C. If two solutions F_τ, ϕ_0' and F_τ, ϕ_0'' are equivalent, then Eq. (5b) entails the equivalence of $F, \phi_0'\phi$ and $F, \phi_0''\phi$. Contrariwise, if F, ϕ' and F, ϕ'' are equivalent, then there exists $\alpha \in K$, such that $I_\alpha = I$ and $\phi'' = \alpha F(\alpha)\phi'$. Replacing here $\phi' = \phi_0'\phi$ and $\phi'' = \phi_0''\phi$, it follows that F_τ, ϕ_0' and F_τ, ϕ_0'' are also equivalent. Since F_τ, ϕ_0 always give involutive ME's of C, Lemma 1 is valid for them. Therefore, translation by the fixed ϕ establishes Lemma 3.

Remark 1: In the proof of Lemma 3 one has a simple illustration of the important statement of the cohomology theory that the nonequivalent extensions of K and those of C stand in a one-to-one correspondence.

B. The noncentral GSP form

In the case of noninvolutive ME's the map Ψ is not a homomorphism (because $\Psi[a] = F$ could not be an involution), so that the theory of central GSP [see Sec. 2B] is not applicable. Nevertheless, the approach of i-unifications to GSP[5] makes it possible to put also these ME's into a GSP form.

To sum up this approach, let K and H be two groups, and let τ be a homomorphism: $H \to \mathrm{Aut}(K)$. Furthermore, let there exist a subgroup K_0 of K and an invariant subgroup H_0 of H which are isomorphic via $l: K_0 \to H_0$ so that the following necessary and sufficient conditions are satisfied:

$$\tau[x](\gamma) = l^{-1}(xl(\gamma)x^{-1}), \quad \forall\gamma \in K_0, \ \forall x \in H, \tag{16a}$$

$$\tau[l(\gamma)](\alpha) = \gamma\alpha\gamma^{-1}, \quad \forall\alpha \in K, \ \forall\gamma \in K_0. \tag{16b}$$

Then the GSP

$$E = (K \textcircled{T} H)/K_0', \tag{17}$$

with

$$K_0' = \{(\gamma, l(\gamma^{-1})) \mid \gamma \in K_0\} \tag{18}$$

is a unification of K and H, as well as an extension of $G \equiv H/H_0$ by K.

If K_0 is a noncentral subgroup of K, and only then, Ψ is not a homomorphism[5] and (17) is called noncentral GSP.

Lemma 4: The noninvolutive ME determined by F, ϕ (ϕ necessarily noncentral) has the noncentral GSP form (17), where $H = Z_{2m}(x)$, m being the order of ϕ; $\tau[x^q] = F^q, q = 1, \ldots, 2m$; $K_0 = Z_m(\phi)$; $l(\phi^p) = x^{2p}$, $p = 1, \ldots, m$.

Proof: It is sufficient to verify the validity of condition (16a) only for the generating element of H using (4b), and the validity of (16b) only for $\gamma = \phi$ with the help of (4a). QED

Remark 2: When dealing with involutive ME's one might choose a noninvolutive F and arrive at a noncentral GSP. This appears to be useful when the corresponding ϕ could be ϵ, i.e., when the GSP simplifies to SP (cf. case A_2 in Ref. 2).

It is noteworthy that every ME (involutive or not) has a GSP form which is determined by F, ϕ.

Remark 3: The usefulness of the GSP form of a ME lies in the fact that one can easily find the irreducible representations (IR's) of a GSP.[4] Namely, finding the IR's of a semidirect product with the second factor being a cyclic group is well known.[8] The IR's of the factor group $(K \textcircled{T} H)/K_0'$ are a selection of the IR's of $K \textcircled{T} H$, consisting of those whose kernels contain K_0'.

We expect that the GSP form of ME's, their complete classification and canonical forms will prove valuable in the theory of linear–antilinear representations, a continuation of Wigner's corepresentation theory,[8] which we intend to undertake.

C. An example

Lee and Wick[2] presented a number of examples of ME's discussing discrete symmetries of elementary particles. Noninvolutive ME's (B_3 in their notation) did not occur among them. Also in a different field—in the magnetic groups of solid state physics—ME's appear to be important.[9] For example, among the 1651 magnetic space groups there are 1191 in which time reversal occurs only in combination with other operations, and not by itself. Groups of this type can be obtained systematically by finding all index-2 subgroups of all (classical) space groups. Namely, if $\underline{M}'$ is one of the latter and $\underline{G}$ its subgroup of index 2, i.e.,

$$\underline{M}' = \underline{G} + R\underline{G}, (R \in \underline{M}', R \notin \underline{G}),$$

then

$$\underline{M} = \underline{G} + \Theta R\underline{G}$$

(Θ being the time reversal) is a magnetic space group. Obviously, $\underline{M}'$ and $\underline{M}$ are ME's of $\underline{G}$, and we expect that

the complete classification of ME's presented in this paper will prove useful.

Here we give only an example of an $\underline{M}'$ which is a noninvolutive ME of a $\underline{G}$. Let $\underline{M}'$ be the space group $P4$ (in the International notation), i.e., the set of transformations

$$(\alpha|\mathbf{t}), \alpha \in \{E, C_{4z}, C_{4z}^2, C_{4z}^3\},$$
$$\mathbf{t} \in \{\sum_{i=1}^{3} n_i \mathbf{a}_i \,|\, n_i = 0, \pm 1, \pm 2, \ldots;$$
$$|\mathbf{a}_1| = |\mathbf{a}_2| \neq |\mathbf{a}_3|; \mathbf{a}_1 \perp \mathbf{a}_2 \perp \mathbf{a}_3 \perp \mathbf{a}_1\},$$

with the composition law

$$(\alpha|\mathbf{t})(\alpha'|\mathbf{t}') = (\alpha\alpha'|\alpha\mathbf{t}' + \mathbf{t}).$$

Let $\underline{G}$ be its subgroup obtained by restricting α to $\{E, C_{4z}^2\}$, which clearly is of index 2. Then any coset representative R is of the form $(C_{4z}|\mathbf{O})(\alpha|\mathbf{t})$, $(\alpha|\mathbf{t}) \in \underline{G}$. Now, $\phi = R^2$, and $F(\alpha|\mathbf{t}) = R(\alpha|\mathbf{t})R^{-1}$, $\forall(\alpha|\mathbf{t}) \in \underline{G}$, and different choices of R give equivalent ME forms of $\underline{M}'$. It is easy to show that no R can give $\phi \in C$, the center C being the subgroup of translations along the z axis. Thus $\underline{M}'$ is a noninvolutive ME with respect to $\underline{G}$.

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Symmetry transformations of the classical Kepler problem

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The finite, canonical symmetry transformations of the negative energy motions of the classical Kepler problem are constructed by solving the fundamental differential equations of the dynamical invariance group. The geometric interpretation of the transformations is discussed.

1. MOTIVATION

The nonrelativistic Kepler problem has long been a subject of theoretical interest because it is an important example of a dynamical system possessing so-called hidden symmetry. The invariance transformations of its Hamiltonian form a representation of the orthogonal group in four dimensions whereas the obvious geometric symmetry of its potential function is only that of the orthogonal group in three dimensions. The additional symmetry results from the particular functional form of the force law governing the motion. Thus the symmetry group of the Kepler problem is referred to as a dynamical symmetry group, and the additional symmetry is called an internal symmetry. The harmonic oscillator is another important problem in mechanics which has received extensive study because of its hidden symmetry.

A transformation of the dynamical variables in phase space is a symmetry, or invariance transformation of a dynamical system if the transformed Hamiltonian $H'(q,p)$ is related to the original Hamiltonian $H(q,p)$ by the relation

$$H'(q,p) = H(q,p), \tag{1.1}$$

where q and p are generic symbols for a complete set of coordinates in phase space. Symmetry transformations of the Hamiltonian are canonical and map any given solution of the equations of motion into another solution having the same total energy. The continuous symmetry transformations of a dynamical system are generated by those constants of its motion which are not explicitly time dependent. If these constants of the motion form a Lie algebra, the transformations furnish a representation of the appropriate group.

The three-dimensional harmonic oscillator is a well-known example of such a system. The invariance transformations of its Hamiltonian form a representation of the group $SU(3)$. The finite transformations of the group can be written down rather easily because the primitive dynamical variables are very well adapted to the symmetry of the problem. Also one is able to obtain some insight into the transformations from a geometric standpoint.

The example of the Kepler problem is different, however. The primitive dynamical variables are badly adapted to the symmetry of the problem. As a result the finite, symmetry transformations of the Kepler Hamiltonian are very complicated and have received little attention in the literature. In particular, a really sufficient geometric interpretation of the problem has, to our knowledge, never been given.

Because of the preeminence of the nonrelativistic Kepler problem in classical mechanics, it therefore seemed desirable to construct the finite symmetry transformations of its negative energy motions and to discuss their geometric significance.

2. HISTORICAL REMARKS

A major advance in the classical treatment of the Kepler problem was made many years ago by Laplace[1] when he discovered the existence of three new constants of the motion in addition to the components of the angular momentum. These additional conserved quantities are the components of a vector which determines the direction of the perihelion of the motion and whose magnitude is the eccentricity of the orbit. The Laplace vector was later rediscovered by Jacobi[2] and has since been rediscovered several times under different names. In 1926 Pauli[3] used the Laplace vector to solve for the energy spectrum of the hydrogen atom by purely algebraic means. Hulthén and Klein[4] then showed that, suitably chosen, the six constants of the motion of the Kepler problem form a Lie algebra isomorphic to that of O(4), the orthogonal group in four dimensions. Shortly thereafter, Fock[5] showed explicitly the O(4) degeneracy of the wave functions of the quantum mechanical problem. In 1936 Bargmann[6] established the connection between Pauli's algebraic treatment and the group theoretical approach used by Fock by showing that the constants of motion of the Kepler problem generate Fock's group.

In the last thirty years the Kepler problem has been one of the most exhaustively studied in analytical dynamics. Many significant papers[7-15] have been devoted to the hydrogen atom and its symmetry group. In recent years the use of invariance groups and the study of symmetries have played an important role in the classification of elementary particles. Since particle symmetries are usually broken, noninvariance groups have come into prominent usage. The nonrelativistic Kepler problem is an excellent prototype of a system possessing a dynamical symmetry group and even of one displaying a broken symmetry (if its various energy levels are considered as arising from a symmetry breaking mechanism). Thus renewed interest in the Kepler problem has centered primarily around noninvariance groups of its Hamiltonian.[16-21]

The problem of finding the finite, canonical symmetry transformations of the negative energy states of the Kepler problem has been addressed in several interesting papers.[22-25] The high degree of nonlinearity of the equations has limited the success of the investigations and has not allowed a tractable geometric interpretation of the results.

3. FORMULATION OF THE PROBLEM

The Hamiltonian of the nonrelativistic Kepler problem will be written as

$$H = p^2/2m - k/r, \quad k > 0. \tag{3.1}$$

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The constants of the negative energy motions are given by the expressions

$$\vec{L} = \vec{q} \times \vec{p},$$
$$\vec{A} = \frac{1}{(-2mH)^{1/2}} \left[\frac{\vec{p} \times \vec{L}}{km} - \frac{\vec{q}}{r} \right] \tag{3.2}$$

which are, respectively, the angular momentum vector and the Laplace vector divided by $(-2mH)^{1/2}$. The notation used throughout is standard and should require only a minimum of explanation.

The components of $\vec{L}$ and $\vec{A}$ are closed under the Poisson bracket operation and form a Lie algebra which is isomorphic to that of O(4). This can be put into evidence by defining the linear combinations

$$\vec{M} = \tfrac{1}{2}(\vec{L} + \vec{A}), \quad \vec{N} = \tfrac{1}{2}(\vec{L} - \vec{A}). \tag{3.3}$$

These new quantities obey the following bracket relations.

$$\{M_i, M_j\} = \epsilon_{ijk} M_k,$$
$$\{N_i, N_j\} = \epsilon_{ijk} N_k, \quad \{M_i, N_j\} = 0 \tag{3.4}$$

In (3.4) the latin indices run from 1 to 3, repeated indices are summed, and ϵ_{ijk} is the Levi–Civita tensor density. The structure of the algebra is thus seen to be that of O(3) × O(3), i.e., O(4).

If the generator of the group of transformations is denoted by G, the differential equation describing the action of the group upon any coordinate of the system, say F, may be written in terms of the Poisson bracket of F with G as

$$\frac{dF(s)}{ds} = \{F(s), G\}. \tag{3.5}$$

Here s is a parameter defined along the group trajectory in such a manner that $s = 0$ corresponds to the identity transformation. For the Kepler problem the generator will be written in the form

$$G = \tfrac{1}{2}[\vec{Y}\cdot(\vec{L} + \vec{A}) + \vec{Z}\cdot(\vec{L} - \vec{A}], \tag{3.6}$$

where $\vec{Y}$ and $\vec{Z}$ are vectors, independent of s, which parameterize the group. It should be noted that, while the components of $\vec{Y}$ and $\vec{Z}$ are essential parameters, s is not and is introduced simply for convenience. Thus G generates a six parameter group of transformations.

The difficulty of the problem is almost immediately obvious. If one chooses, most naturally, the primitive dynamical variables $\vec{q}$ and $\vec{p}$ as coordinates, the structure of the Laplace vector is such that the resulting differential equations are highly nonlinear. In reality, of course, the trouble arises because these coordinates are badly adapted to the symmetry of the problem. One approach that suggests itself, therefore, is to try to find a coordinate set which is more suitable in the hope that the differential equations will become manageable. At the same time, though, one should not make so much of a concession to manageability that it becomes impossible to picture what the transformations look like. For instance, using constants of the motion as coordinates yields considerably simpler equations, but any geometric insight into the transformations of the $\vec{q}$ and $\vec{p}$ in such a coordinate system is out of the question.

In searching for a new coordinate set one naturally thinks of the approach used by Fock. By projecting the momentum space stereographically onto the surface of a unit hypersphere, he was able to exibit the higher rotational invariance of the problem in terms of the coordinates on the sphere. Even though Fock was dealing with the quantum mechanical problem, it seems that the stereographic sphere should also be useful in the classical description. The reason is that the hodographs of the negative energy motions of the Kepler problem are circles. Under stereographic projection circles in the momentum space are mapped into circles on the sphere. Thus the problem of mapping orbits into orbits in momentum space is equivalent to mapping circles into circles on the sphere.

With these thoughts in mind we tentatively introduce in place of the p_j, the four coordinates

$$\vec{P} = \frac{2p_0\vec{p}}{p_0^2 + p^2}, \quad P_4 = \frac{p^2 - p_0^2}{p_0^2 + p^2}, \tag{3.7}$$

where $p_0 = (-2mH)^{1/2}$. In order that the treatment not be restricted to a single energy hypersurface though, we regard H as the Hamiltonian function rather than some given absolute constant. The four new coordinates satisfy one side condition:

$$P^2 + P_4^2 = 1. \tag{3.8}$$

Only three are independent, therefore.

Intuitively, it is desirable at the same time to introduce a coordinate set in configuration space that complements the one in momentum space. The orbits in configuration space are ellipses in general. An ellipse, however, can be viewed as the parallel projection of a circle on a hypersphere. Accordingly then we introduce the four coordinates on a unit hypersphere in configuration space:

$$\vec{Q} = \frac{\vec{q}}{r} - \frac{\vec{q}\cdot\vec{p}}{km}\vec{p}, \quad Q_4 = \frac{p_0\vec{q}\cdot\vec{p}}{km}. \tag{3.9}$$

Again only three of the coordinates are independent as they satisfy the side condition

$$Q^2 + Q_4^2 = 1. \tag{3.10}$$

It is important to note that the eight new coordinates are subject to an additional constraint. They are orthogonal:

$$\vec{Q}\cdot\vec{P} + Q_4 P_4 = 0. \tag{3.11}$$

Thus, in all, we have eight quantities subject to three side conditions. Consequently, they do not form a complete set in the six dimensional phase space. An additional coordinate is required, and we choose for it the Hamiltonian H.

The inverse transformations can now be written down. They are

$$\vec{q} = -\frac{k}{2H}[(1 - P_4)\vec{Q} + Q_4\vec{P}],$$
$$\vec{p} = (-2mH)^{1/2}\frac{\vec{P}}{1 - P_4}. \tag{3.12}$$

Again the reason for introducing coordinates other than $\vec{q}$ and $\vec{p}$ is to simplify the differential equations of the

group. If the calculation is performed, the new equations are in fact simpler than the original ones. It is possible at this point, however, to use an additional device which reduces the complexity of the equations even further. One knows that, in general, quaternions provide a natural and even elegant way in which to represent the transformations of O(4). It turns out that if the new coordinates in configuration and momentum space are considered as being the components of quaternions, and if the differential equations of the group are written in quaternion form, the structure of the equations is dramatically simplified.

As quaternions are not frequently used in physics today, it may be well to list a few of their algebraic properties.

4. QUATERNION ALGEBRA

If a Cartesian coordinate system is introduced into a four-dimensional Euclidean space, and the four unit vectors along the axes are denoted by $\mathbf{e}_\mu$, the resulting vector space over the field of real numbers may be converted into an algebra by prescribing the following multiplication table for the $\mathbf{e}_\mu$.

$$\begin{aligned} &(\mathbf{e}_4)^2 = \mathbf{e}_4, \quad \mathbf{e}_4\mathbf{e}_i = \mathbf{e}_i\mathbf{e}_4 = \mathbf{e}_i, \\ &(\mathbf{e}_i)^2 = -\mathbf{e}_4, \quad \mathbf{e}_i\mathbf{e}_j = \epsilon_{ijk}\mathbf{e}_k. \end{aligned} \tag{4.1}$$

The vectors in this space form an algebra of rank four over the field of real numbers, and they are called quaternions. Quaternion multiplication is both distributive and associative, but not commutative. A given nonzero quaternion possesses both a left and a right inverse, and it is possible to divide by a nonzero quaternion. Thus quaternions form a skew field.

If $\mathbf{a}$ and $\mathbf{b}$ are quaternions one writes

$$\begin{aligned} \mathbf{a} &= a^\mu\mathbf{e}_\mu = a^4\mathbf{e}_4 + \vec{a}\cdot\vec{\mathbf{e}}, \\ \mathbf{b} &= b^\mu\mathbf{e}_\mu = b^4\mathbf{e}_4 + \vec{b}\cdot\vec{\mathbf{e}}, \end{aligned} \tag{4.2}$$

where the components a^μ and b^μ are real numbers. The product of $\mathbf{a}$ with $\mathbf{b}$ is given by

$$\mathbf{ab} = (a^4b^4 - \vec{a}\cdot\vec{b})\mathbf{e}_4 + [a^4\vec{b} + b^4\vec{a} + \vec{a}\times\vec{b}]\cdot\vec{\mathbf{e}}. \tag{4.3}$$

The quaternion conjugate to $\mathbf{a}$, $\mathbf{a}^*$ is defined as

$$\mathbf{a}^* = a^4\mathbf{e}_4 - \vec{a}\cdot\vec{\mathbf{e}}. \tag{4.4}$$

The product of a nonzero quaternion with its conjugate is a positive, nonzero number which is called the norm of the quaternion. A vectorial quaternion is, by definition, a quaternion which has a zero scalar part, that is, a zero value for its fourth component. Finally, the scalar product of $\mathbf{a}$ and $\mathbf{b}$ is prescribed as

$$\mathbf{a}\cdot\mathbf{b} = \tfrac{1}{2}[\mathbf{ab}^* + \mathbf{ba}^*]. \tag{4.5}$$

These are by no means all the properties of quaternions, but they are the only ones that will be needed in this paper.

5. THE DIFFERENTIAL EQUATIONS AND THEIR SOLUTIONS

The calculation proceeds now along the following lines. The coordinate set consists of the quaternions.

$\mathbf{H}$, $\mathbf{Q}$, and $\mathbf{P}$, where

$$\mathbf{H} = H\mathbf{e}_4,$$

$$\begin{aligned} \mathbf{Q} &= Q_4\mathbf{e}_4 + Q_1\mathbf{e}_1 + Q_2\mathbf{e}_2 + Q_3\mathbf{e}_3, \\ \mathbf{P} &= P_4\mathbf{e}_4 + P_1\mathbf{e}_1 + P_2\mathbf{e}_2 + P_3\mathbf{e}_3. \end{aligned} \tag{5.1}$$

It proves useful to define the dimensionless, vectorial quaternions

$$\begin{aligned} \mathbf{U} &= p_0(\vec{L} + \vec{A})\cdot\vec{\mathbf{e}}, \\ \mathbf{V} &= p_0(\vec{L} - \vec{A})\cdot\vec{\mathbf{e}}. \end{aligned} \tag{5.2}$$

Then if the components of the vectors $\vec{Y}$ and $\vec{Z}$ are taken to be the components of the vectorial quaternions $\mathbf{Y}$ and $\mathbf{Z}$, the generator of the group of transformations may be written as

$$G = \frac{1}{2p_0}[\mathbf{Y}\cdot\mathbf{U} + \mathbf{Z}\cdot\mathbf{V}]. \tag{5.3}$$

The algebra involved in expressing the differential equations of the group in terms of quaternions is straightforward, but tedious. The result is

$$\begin{aligned} &\frac{d\mathbf{H}(s)}{ds} = 0, \\ &\frac{d\mathbf{Q}(s)}{ds} = \tfrac{1}{2}[\mathbf{ZQ}(s) - \mathbf{Q}(s)\mathbf{Y}] + \mathbf{K}(s)\mathbf{P}(s), \\ &\frac{d\mathbf{P}(s)}{ds} = \tfrac{1}{2}[\mathbf{ZP}(s) - \mathbf{P}(s)\mathbf{Y}] - \mathbf{K}(s)\mathbf{Q}(s), \end{aligned} \tag{5.4}$$

where $\mathbf{K}(s)$ is a scalar quaternion given by

$$\mathbf{K}(s) = \frac{dQ_4(s)}{ds}\mathbf{e}_4. \tag{5.5}$$

Two relations that are particularly important are

$$\begin{aligned} \mathbf{Q} &= \mathbf{PU} = -\mathbf{VP}, \\ \mathbf{P} &= -\mathbf{QU} = \mathbf{VQ}. \end{aligned} \tag{5.6}$$

Equations (5.6) allow the Eqs. (5.4) to be rewritten in the more symmetrical manner

$$\begin{aligned} &\frac{d\mathbf{H}(s)}{ds} = 0, \\ &\frac{d\mathbf{Q}(s)}{ds} = \tfrac{1}{2}[\mathbf{Z} + \mathbf{K}(s)\mathbf{V}(s)]\mathbf{Q}(s) - \tfrac{1}{2}\mathbf{Q}(s)[\mathbf{Y} + \mathbf{K}(s)\mathbf{U}(s)], \\ &\frac{d\mathbf{P}(s)}{ds} = \tfrac{1}{2}[\mathbf{Z} + \mathbf{K}(s)\mathbf{V}(s)]\mathbf{P}(s) - \tfrac{1}{2}\mathbf{P}(s)[\mathbf{Y} + \mathbf{K}(s)\mathbf{U}(s)]. \end{aligned} \tag{5.7}$$

The solution to the above set of equations can be deduced by inspection and is

$$\begin{aligned} &\mathbf{H}(s) = \mathbf{H}(0), \\ &\mathbf{Q}(s) = e^{(s/2)\mathbf{Z}}[e^{[R(s)/2]\mathbf{V}(0)}\mathbf{Q}(0)e^{-[R(s)/2]\mathbf{U}(0)}]e^{-(s/2)\mathbf{Y}}, \\ &\mathbf{P}(s) = e^{(s/2)\mathbf{Z}}[e^{[R(s)/2]\mathbf{V}(0)}\mathbf{P}(0)e^{-[R(s)/2]\mathbf{U}(0)}]e^{-(s/2)\mathbf{Y}}. \end{aligned} \tag{5.8}$$

In (5.8) the function $R(s)$ is defined as

$$R(s) = Q_4(s) - Q_4(0) \tag{5.9}$$

and the exponential quaternion $e^{s/2\mathbf{Z}}$ is given by

$$e^{s/2\mathbf{Z}} = \left[\cos\frac{s}{2}|\vec{Z}|\right]\mathbf{e}_4 + \left[\sin\frac{s}{2}|\vec{Z}|\right]\frac{\vec{Z}\cdot\vec{\mathbf{e}}}{|\vec{Z}|} \tag{5.10}$$

with similar expressions for the other exponential terms.

Written in this form the solution is obviously implicit because of the appearance of one of the unknowns, $Q_4(s)$ on the right-hand side of the equations. The solution is complete nevertheless because $Q_4(s)$ can be solved for by inverting the scalar component of the equation for $\mathbf{Q}(s)$. The result can then be substituted in the appropriate places to yield the explicit solution. For our purposes though this inversion is not really a useful thing to do because, using elementary functions, it is not possible to express Q_4 as a function of s in closed form.

At this point the parameter s can be set equal to unity. All the transformations of the group can be obtained by allowing the parameters $\mathbf{Y}$ and $\mathbf{Z}$ to vary appropriately in magnitude and direction. Equations (5.8) then are equivalent to

$$\begin{aligned}
&\mathbf{H}(Y,Z) = \mathbf{H}(0),\\
&\mathbf{Q}(Y,Z) = e^{\mathbf{Z}/2}\left[e^{[R(Y,Z)/2]\mathbf{V}(0)}\mathbf{Q}(0)e^{-[R(Y,Z)/2]\mathbf{U}(0)}\right]e^{-\mathbf{Y}/2},\\
&\mathbf{P}(Y,Z) = e^{\mathbf{Z}/2}\left[e^{[R(Y,Z)/2]\mathbf{V}(0)}\mathbf{P}(0)e^{-[R(Y,Z)/2]\mathbf{U}(0)}\right]e^{-\mathbf{Y}/2}
\end{aligned} \tag{5.11}$$

where now

$$R(Y,Z) = Q_4(Y,Z) - Q_4(0). \tag{5.12}$$

If one selects an arbitrary point in phase space, one can, by using Eqs. (3.12) and (5.11), transform to any other point in the phase space which lies on the same energy hypersurface as the initial point. The formal solution to the problem is thus complete.

Using (5.6) and (5.11) one finds that the constants of the motion of the original orbit transform according to

$$\begin{aligned}
&\mathbf{U}(Y,Z) = e^{\mathbf{Y}/2}\mathbf{U}(0)e^{-\mathbf{Y}/2},\\
&\mathbf{V}(Y,Z) = e^{\mathbf{Z}/2}\mathbf{V}(0)e^{-\mathbf{Z}/2}
\end{aligned} \tag{5.13}$$

whence it follows that if $\mathbf{Y} \propto \mathbf{U}(0)$ and $\mathbf{Z} \propto \mathbf{V}(0)$ these quantities remain unchanged. In this case the orbit simply undergoes an automorphism.

One further observation is called for. The fact that the coordinates used do not consist of canonically conjugate pairs makes it desirable to demonstrate that the underlying transformations of the $\vec{q}$ and $\vec{p}$ are in fact canonical. One can prove by simple substitution that Eqs. (5.11) leave invariant the differential form

$$\omega = (-2mH)^{1/2}\,[\mathbf{P}\cdot d\mathbf{Q} - dQ_4]. \tag{5.14}$$

In terms of the original dynamical variables, ω is expressable as

$$\omega = \vec{p}\cdot d\vec{q} - 2d(\vec{q}\cdot\vec{p}). \tag{5.15}$$

The invariance of this form proves that the transformations are canonical as they should be.

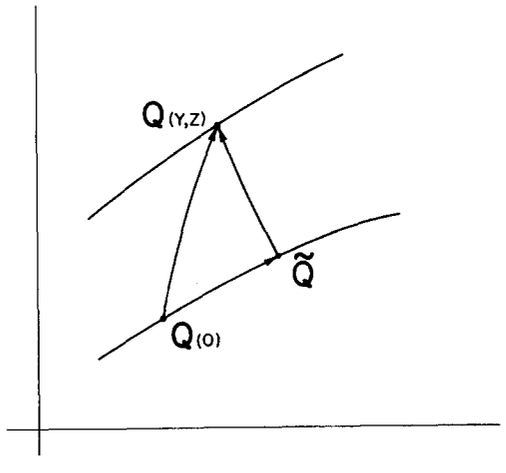

FIG. 1. Finite motion of $\mathbf{Q}(0)$ to $\mathbf{Q}(Y,Z)$ pictured as an automorphism followed by a rigid rotation.

6. GEOMETRIC INTERPRETATION OF THE TRANSFORMATIONS

It may be tempting to conjecture that the symmetry transformations, when expressed in terms of the coordinates used here, should manifest themselves as rigid rotations on the respective spheres. The fact though that the differential equations (5.4) contain terms which are nonlinear in $\mathbf{Q}$ and $\mathbf{P}$ shows that the finite group motions are of a more complicated nature. A simple and direct geometric interpretation of the transformations is possible, however, in spite of the nonlinear character of the problem. Since the equations for $\mathbf{Q}$ and $\mathbf{P}$ are structurally identical, we will confine our remarks to $\mathbf{Q}$ space.

It is possible to write the transformation for $\mathbf{Q}$ formally in terms of two equations. First we define the quantity $\tilde{\mathbf{Q}}$ by the relation

$$\tilde{\mathbf{Q}} = e^{[R(Y,Z)/2]\mathbf{V}(0)}\mathbf{Q}(0)e^{-[R(Y,Z)/2]\mathbf{U}(0)}. \tag{6.1}$$

From the considerations of the last section, it follows that $\tilde{\mathbf{Q}}$ and $\mathbf{Q}(0)$ lie in the same orbit. Using (6.1) now, the transformation for $\mathbf{Q}(Y,Z)$ can be written as

$$\mathbf{Q}(Y,Z) = e^{\mathbf{Z}/2}\tilde{\mathbf{Q}}e^{-\mathbf{Y}/2}. \tag{6.2}$$

The nature of these last two equations is clear. Equation (6.1) represents a rotation which repositions the initial point in the original orbit. Equation (6.2) then describes a rotation of the intermediate point $\tilde{\mathbf{Q}}$ into the final point $\mathbf{Q}(Y,Z)$. The geometric representation of the transformation of $\mathbf{Q}$ is shown schematically in Fig. 1. The transformation of $\mathbf{P}$ can be sketched in the same manner.

One concludes that the finite symmetry transformations of the Kepler problem, when expressed in term of $\mathbf{Q}$ and $\mathbf{P}$, can be viewed as an automorphism of the original orbit followed by a rigid rotation of the original orbit into the new orbit. It should be noted that the automorphism of a particular point differs from that of other points in general. Thus the symmetry transformations do not represent rigid mappings of the spheres into themselves. It is clear from this interpretation that orbits are mapped into orbits since, under the composite motion just described, circles are mapped into circles on the respective spheres.

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A new basis for the representations of the rotation group. Lamé and Heun polynomials

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The representation theory of the rotation group $O(3)$ is developed in a new basis, consisting of eigenfunctions of the operator $E = -4(L_1^2 + rL_2^2)$, where $0 < r < 1$ and L_i are generators. This basis $|J\lambda\rangle$ is shown to be a unique nonequivalent alternative to the canonical basis (eigenfunctions of L_3). The functions $|J\lambda\rangle$ are constructed as linear combinations of canonical basis functions and are shown to fall into four symmetry classes, distinguished by their behavior under reflections of the inidividual space axes. Algebraic equations for the eigenvalues λ of E are derived. When realized in terms of functions on an $O(3)$ sphere, the basis $|J\lambda\rangle$ consists of products of two Lamé polynomials, obtained by separating variables in the corresponding Laplace equation in elliptic coordinates. When realized in a space of functions of one complex variable, $|J\lambda\rangle$ are Heun polynomials. Applications of the new basis in elementary particle, nuclear, and molecular physics are pointed out, due in particular to the symmetric form of $|J\lambda\rangle$ as functions on a sphere and to the fact that they are the wavefunctions of an asymmetrical top.

1. INTRODUCTION

The three-dimensional rotation group $O(3)$, or its universal covering group $SU(2)$, is quite definitely the one single Lie group, which has the most extensive applications in essentially all branches of physics. Not surprisingly the representation theory of $O(3)$ has received much attention and has been summarized in many excellent books.[1] It would thus seem that the topic of representations of the group $O(3)$ has received full coverage and that little new can be added.

The aim of this paper is to stress that this is not so and in particular to construct the representation theory of $O(3)$ [and SU(2)] in a new basis, different from the "canonical" one, in which the basis functions are eigenfunctions of one of the generators of angular momentum, usually L_3. A systematic investigation of possible bases for constructing representations of Lie groups was initiated some time ago.[2,3] It was shown that a classification of second order polynomials in the generators of a Lie group leads to a classification of different possible bases and that this problem is related to the problem of separating variables in Laplace equations on homogeneous manifolds. A detailed treatment was given for the little groups of the Poincaré group, corresponding to timelike, spacelike, and lightlike vectors [the groups $O(3)$, $O(2,1)$, and E_2, respectively][2,3] and also of the Lorentz group $O(3,1)$ and the E_3 Euclidean group.[4]

Two different bases were shown to exist for $O(3)$. The first is the canonical one, which is a "subgroup type" basis, in that it corresponds to the group reduction $O(3) \supset O(2)$. The basis functions are eigenfunctions of the complete set of operators

$$\Delta = -(L_1^2 + L_2^2 + L_3^2) \text{ and } L_3, \tag{1}$$

where L_i is the generator of rotations about the ith axis and Δ is the Casimir operator of $O(3)$. The second basis is new, it is of the "nonsubgroup" type, in that the basis functions are eigenfunctions of an operator E that is not the generator of any subgroup and of some additional discrete operators. The complete set of commuting operators can be chosen to be

$$\Delta, E = -4(L_1^2 + rL_2^2), X \text{ and } PZ, \quad 0 < r < 1, \tag{2}$$

where X and Z correspond to reflections in the yz and xy planes and P is the parity operator.

Let us emphasize that a study of group representation theory in different bases is of interest both from the mathematical and physical points of view. The intimate connection between the representations of Lie groups and the special functions of mathematical physics has long been recognized (and treated in textbooks[5-10]). The special functions, actually appearing as basis functions, transformation matrices, kernels of integral transformations, Clebsch–Gordan coefficients, etc., depend not only on the group that is being considered, but also on the choice of basis. A systematic study of different possible bases will thus very considerably enlarge the class of special functions, that obtain a group theoretical interpretation and that can be studied using the powerful techniques of Lie theory.

In particular, consider the rotation group $O(3)$. The connection between this group and the Legendre and Jacobi polynomials is well known and has been made full use of. Less well known is the fact that other important functions, namely the Lamé polynomials,[11,12] and as we shall show below, a certain class of Heun functions[12] (distinct from the Lamé polynomials), is equally intimately related to the rotation group. These polynomials make their appearance as basis functions in the nonsubgroup type basis, determined by the operators (2).

An alternative way of viewing the appearance of nonsubgroup bases in general and the Lamé polynomials in particular, is the following. For the group $O(3)$ the Laplace equation on the sphere $\Delta\psi = J(J+1)\psi$ allows the separation of variables in two coordinate systems.[13] The usual spherical coordinates correspond to the diagonalization of the operators (1) and hence to spherical functions. Elliptic coordinates on the sphere (see below) correspond to the operators (2) and to the solutions of the Laplace equation which are also eigenfunctions of the operator $E = -4(L_1^2 + rL_2^2)$ and can be written as

$$\psi_{Jh}(\alpha,\beta) = \Lambda_{Jh}(\alpha)\Lambda_{Jh'}(\beta), \tag{3}$$

where α and β are the elliptic coordinates and $\Lambda_{Jh}(\alpha)$ are the Lamé polynomials.

Let us mention some of the possible applications of nonsubgroup type bases in physics. The first application that comes to mind is due to the fact that the $O(3)$ basis functions (3) can be identified with the wavefunctions of an asymmetric quantum mechanical top and that the eigenvalues of the operator E are intimately related

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to the energy levels of this physical system.[14-19] The importance of these eigenfunctions and eigenvalues in nuclear physics[20] and molecular physics[15] is obvious, since they make it possible to calculate energy levels, transition probabilities, etc. for nonaxial nuclei or molecules). Lamé and Heun functions of various types occur in numerous other physical problems like potential scattering,[21] the construction of solvable potentials in quantum mechanics,[22] the two-center Coulomb problem (i.e., the H_2^+ ion),[23] quadrupole interactions of various types,[16,24] etc. Further, the classification of second order operators, commuting with a Laplace operator, that lead to the consideration of nonsubgroup bases for group representations, has a direct application in the study of canonical transformations in quantum and classical mechanics.[25,26]

Finally, let us mention the applications of nonsubgroup bases in elementary particle physics, that actually lie at the root of our interest in such bases. A scattering amplitude for the reaction $1 + 2 \to 3 + 4$ is usually expanded in terms of the irreducible representations of $O(3)$ (partial wave analysis[27]) for fixed energy s or $O(2,1)$ (Regge pole theory[28]) for fixed momentum transfer t. Alternatively, Lorentz invariance can be used to obtain two-variable expansions of amplitudes in terms of the irreducible unitary representations of the Lorentz group $O(3,1)$ (a review containing references to older work is given in the lecture, Ref. 29; for more recent work see Refs. 30, 31). Nonsubgroup bases, on the other hand, make it possible to obtain explicitly crossing symmetric two-variable expansions.[30] Indeed, formula (3) shows that a separation of variables in elliptic coordinates on a sphere leads to basis functions that are products of two identical functions (that happen to be Lamé polynomials). The same is true for certain types of elliptic coordinates on $O(2,1)$ and $O(3,1)$ hyperboloids,[13] where one obtains Lamé functions (that are not polynomials).

Another interesting application of the nonsubgroup basis for the $O(3)$ group in elementary particle physics is in strong coupling theory. Indeed, the problem of finding the spectrum of nucleon resonances in the strong coupling limit of a fixed source pseudoscalar theory has been shown to be equivalent to the problem of diagonalizing the asymmetric top Hamiltonian.[32] A study of the representations of $O(3)$ in the nonsubgroup basis, should thus supply information on resonance masses and widths, decay rates, etc., in the strong coupling theory.

The rest of this paper is devoted to the representations of $O(3)$ in the nonsubgroup basis, corresponding to the diagonalization of the operators (2). In Sec. 2 we give a brief discussion of the algebra of $O(3)$, of second order operators in general and the operator E in particular. We show how E arises as a unique alternative to L_3 as an operator, defining basis functions. In Sec. 3 we consider the eigenfunctions and eigenvalues of the operator E and construct the nonsubgroup type basis functions $|J\lambda\rangle$ as sums of the usual angular momentum eigenfunctions $|JM\rangle$. We derive recursion relations and general formulas for the coefficients in the corresponding expansions and also obtain algebraic equations for the eigenvalues λ. We show that the basis functions naturally separate into four symmetry classes (with different properties under reflections). In Sec. 4 we briefly mention the matrix elements of the generators in the new basis, "shifting operators" that are analogous to raising and lowering operators in the canonical basis, finite transformation matrices and Clebsch–Gordan coefficients. Half-integer values of angular momentum are discussed in Sec. 5. In Sec. 6 we construct a two-dimensional realization of the representations of $O(3)$ in a space of functions defined over the unit sphere. We show how the nonsubgroup basis leads to Lamé functions. Section 7 is devoted to a one-dimensional realization in a space of functions of one complex variable. The basis functions in this case are Heun functions (polynomials) of a specific type. In the final Sec. 8 we discuss some of the implications of our results and outline our future program, concerning the nonsubgroup type representation bases for $O(3)$ and for other groups, in particular the other little groups of the Poincaré group.

2. THE ALGEBRA OF $O(3)$ AND SECOND ORDER OPERATORS

In order to establish notation, let us write out a few trivial formulas. The group $O(3)$ is generated by the operators L_i, $i = 1, 2, 3$, satisfying the commutation relations

$$[L_i, L_k] = \epsilon_{ikl} L_l . \tag{4}$$

We shall also make use of the operators

$$H_+ = iL_1 - L_2,\ H_- = iL_1 + L_2, H_3 = iL_3. \tag{5}$$

The most general second order operator in the enveloping algebra of $O(3)$ can be written as

$$Q = \sum_{i,k=1}^{3} A_{ik} L_i L_k \tag{6}$$

and without loss of generality we can restrict ourselves to symmetric operators, satisfying $A_{ik} = A_{ki}$ (i.e., A is a real symmetric matrix).

The operator Q can be simplified[3] by an inner automorphism, i.e., by a rotation, that transforms Q into some operator Q' and by taking linear combinations of Q' and Δ.

We are interested in bases for the representations of $O(3)$. Any first order operator in the algebra can be rotated into say L_3. Hence, basis functions defined as eigenfunctions of a first order operator will simply constitute a canonical basis. Let us now consider eigenfunctions of the second order "diagonal" operator Q', which can be so chosen that the corresponding matrix A' is diagonal.[33] Three distinct cases arise: (i) All eigenvalues of A are equal. Then $Q' \sim \Delta$ and does not determine a basis. (ii) Only two of the eigenvalues are equal. Then Q can be transformed into L_3^2, so its eigenfunctions will again constitute a canonical basis. (iii) All eigenvalues of A are distinct. Then Q can be transformed into E, defined in (2). Thus, in this case we do obtain a new operator and the rest of this paper will be devoted to an investigation of the basis, consisting of the eigenfunctions of this operator:

$$E = -4(L_1^2 + rL_2^2) = (1 - r)(H_+^2 + H_-^2) + 2(1 + r)[J(J + 1) - H_3^2]. \tag{7}$$

We have not been able to discover any particularly illuminating algebraic properties of the operator E. For instance, we have not succeeded in finding any closed subalgebras in the enveloping algebra of $O(3)$, involving operator E. The importance of E is thus not in its algebraic properties, but in the fact that it represents a unique alternative to L_3 in a possible complete set of commuting operators, defining a basis.

3. THE NONSUBGROUP BASIS FUNCTIONS AND SPECTRUM OF THE OPERATOR E

A. Expansion of the nonsubgroup basis in terms of the canonical one

The canonical basis $|JM\rangle$ for $O(3)$ is defined by the usual relation

$$H_{\pm}|JM\rangle = [(J \mp M)(J \pm M + 1)]^{1/2}|JM \pm 1\rangle,$$
$$H_3|JM\rangle = M|JM\rangle. \tag{8}$$

The nonsubgroup basis $|J\lambda\rangle$ satisfies

$$E|J\lambda\rangle = \lambda|J\lambda\rangle, \tag{9}$$

and our first aim is to find the spectrum of E, i.e., the values of λ, for which the basis functions form a complete orthonormal set, and also to construct the functions $|J\lambda\rangle$.

Let us expand $|J\lambda\rangle$ in terms of $|JM\rangle$:

$$|J\lambda\rangle = \sum_{M=-J}^{J} (X_J)_{\lambda M}|JM\rangle. \tag{10}$$

The expansion coefficients are elements of a $(2J+1)$-dimensional matrix and we shall obtain recursion relations for them. Indeed, let us apply the operator E to both sides of (10). Using (7) and (8) we have

$$E|JM\rangle = A_M|JM+2\rangle + B_M|JM\rangle + A_{M-2}|JM-2\rangle \tag{11}$$

with

$$A_M = (1-\gamma)[(J-M)(J+M+1)\times(J-M-1)(J+M+2)]^{1/2}, \tag{12}$$

$$B_M = 2(1+\gamma)[J(J+1) - M^2]. \tag{13}$$

The coefficients in (11) obey the following symmetry relations:

$$A_{-M} = A_{M-2}, \quad B_{-M} = B_M. \tag{14}$$

Applying $(E-\lambda)$ to both sides of (10), we have

$$(E-\lambda)|J\lambda\rangle = \sum_M \{(X_J)_{\lambda,M-2}A_{M-2} + (X_J)_{\lambda,M}(B_M - \lambda) + (X_J)_{\lambda,M+2}A_M\}|JM\rangle = 0. \tag{15}$$

Equation (15) implies a three-term recursion relation for the matrix elements of X_J:

$$(X_J)_{\lambda,M-2}A_{M-2} + (X_J)_{\lambda,M}(B_M - \lambda) + (X_J)_{\lambda,M+2}A_M = 0. \tag{16}$$

B. Eigenvalues of E and discussion of the recursion relations for integer values of J

From now on unless we specifically state the opposite, we shall assume that J is integer. The recursion relations (15) can be rewritten in the form of two sets of homogeneous linear equations for the coefficients $(X_J)_{\lambda,M}$. Starting from $M = J$ we have

$$\begin{aligned} &X_{\lambda,J}(B_J - \lambda) + X_{\lambda,J-2}A_{J-2} = 0,\\ &X_{\lambda,J}A_{J-2} + X_{\lambda,J-2}(B_{J-2} - \lambda) + X_{\lambda,J-4}A_{J-4} = 0,\\ &\cdots\\ &X_{\lambda,-J+2}A_{J-2} + X_{\lambda,-J}(B_J - \lambda) = 0. \end{aligned} \tag{17}$$

Starting from $M = J-1$ we obtain a supplementary system of equations:

$$\begin{aligned} &X_{\lambda,J-1}(B_{J-1} - \lambda) + X_{\lambda,J-3}A_{J-3} = 0,\\ &X_{\lambda,J-1}A_{J-3} + X_{\lambda,J-3}(B_{J-3} - \lambda) + X_{\lambda,J-5}A_{J-5} = 0,\\ &\cdots\\ &X_{\lambda,-J+3}A_{J-3} + X_{\lambda,-J+1}(B_{J-1} - \lambda) = 0. \end{aligned} \tag{18}$$

We have made use of the symmetries (14) and simplified notations by putting $(X_J)_{\lambda,M} = X_{\lambda,M}$.

The condition for Eqs. (17) and (18) to have a nontrivial solution is that the determinants of these two sets of homogeneous linear equations be equal to zero. This condition immediately provides us with algebraic equations for the eigenvalues λ of the operator E. The situation can be further simplified by noting that the Eqs. (17) and (18) are consistent with the symmetry conditions

$$X_{\lambda,-M} = pX_{\lambda,M}, \quad p = \pm 1. \tag{19}$$

For any given value of J, we obtain four different secular equations for the eigenvalues λ, which thus fall into four classes. We shall denote these classes (p,q), where $p = \pm 1$ as in (19) and $q = (-1)^M$. Let us consider the equations in the individual classes:

(i) $(pq) = (++)$, i.e., $M =$ even, $\quad X_{\lambda,-M} = X_{\lambda,M}$,

$$\begin{vmatrix} (B_K - \lambda) & A_{K-2} & & \\ A_{K-2} & (B_{K-2} - \lambda) & A_{K-4} & \\ \cdots & & & \\ & A_2 & (B_2 - \lambda) & A_0 \\ & & 2A_0 & (B_0 - \lambda) \end{vmatrix} = 0 \tag{20}$$

where

$$K = \begin{cases} J \text{ for } J = \text{even} \\ J-1 \text{ for } J = \text{odd}. \end{cases} \tag{21}$$

(ii) $(pq) = (-+)$, i.e., $M =$ even, $\quad X_{\lambda,-M} = -X_{\lambda,M}$,

$$\begin{vmatrix} (B_K - \lambda) & A_{K-2} & & \\ A_{K-2} & (B_{K-2} - \lambda) & A_{K-4} & \\ \cdots & A_4 & (B_4 - \lambda) & A_2 \\ & & A_2 & (B_2 - \lambda) \end{vmatrix} = 0, \tag{22}$$

with K as in (21)

(iii) $(pq) = (p-)$, i.e., $M =$ odd, $\quad X_{\lambda,-M} = pX_{\lambda,M}$.

$$\begin{vmatrix} (B_R - \lambda) & A_{R-2} & & \\ A_{R-2} & (B_{R-2} - \lambda) & A_{R-5} & \\ \cdots & & & \\ & A_3 & (B_3 - \lambda) & A_1 \\ & & A_1 & (B_1 + pA_{-1} - \lambda) \end{vmatrix} = 0, \tag{23}$$

with $R = J$ for J odd and $R = J-1$ for J even.

The coefficients A_M and B_M in the above determinants are given by (12) and (13), all omitted entries are equal to zero. For numerical calculations it may be convenient to replace $(X_J)_{\lambda,M}$ in (10) by a new coefficient $(Y_J)_{\lambda,M}$, putting

$$(X_J)_{\lambda,M} = \left[\frac{(2J)!(J-M)!}{(J+M)!}\right]^{1/2} (Y_J)_{\lambda,M}.$$

We then obtain an equivalent set of secular equations for the eigenvalues λ. These equations will be less symmetric than (20)–(23), but all the coefficients in the determinants will be integers multiplied by $(1-r)$ or $(1+r)$ (in other words, we get rid of the square roots).

C. General properties of the eigenvalues and eigenfunctions

The eigenvalues λ are thus obtained by solving certain algebraic equations given above. For each integer value of J, we obtain $2J+1$ different values of λ. They are functions of the parameter r in (7) and, in general, they are not integers and are not equally spaced. The eigenvalues can be evaluated explicitly as functions of r for low values of J. Indeed for $J \leq 3$ we need only solve quadratic equations, the case $3 < J \leq 7$ involves cubic and quartic ones. For $J \geq 8$ the equations must be solved numerically for each value of r. The eigenvalues λ are directly related to the eigenvalues of the equation for Lamé polynomials, which have been extensively tabulated (for more details, see Sec. 6).

Several properties of the eigenvalues λ are of interest:

(i) Sums of eigenvalues. It follows directly from the secular equations (20), (22), and (23) that the sum of all eigenvalues within each class is equal to the sum of all diagonal coefficients in the corresponding determinant. We thus have

$$\begin{aligned}
&\sum_{\lambda\in(++)} \lambda = \tfrac{2}{3}(1+r)J(J+1)(J+2),\\
&\sum_{\lambda\in(-+)} \lambda = \tfrac{2}{3}(1+r)(J-1)J(J+1),\\
&\sum_{\lambda\in(+-)} \lambda = \tfrac{1}{3}(1+r)J(J+1)(2J+1) + (1-r)J(J+1),\\
&\sum_{\lambda\in(--)} \lambda = \tfrac{1}{3}(1+r)J(J+1)(2J+1) - (1-r)J(J+1).
\end{aligned} \tag{24}$$

(ii) Symmetry under replacement $r \to 1/r$. If we put $E(r) = -4(L_1^2 + rL_2^2)$, then $E(1/r) = -(1/r)4(rL_1^2 + L_2^2)$. Hence, if $\lambda(r)$ is an eigenvalue, then so is $r\lambda(1/r)$ and the two may or may not coincide. From (20) and (22) we see that for M even, the eigenvalue equation contains only even powers of A_M. We have $A_M(1/r) = -(1/r)A_M(r)$ and $B_M(1/r) = (1/r)B_M(r)$. For M odd the term pA_{-1} in (23) spoils the symmetry. It follows that the eigenvalues satisfy

$$\begin{aligned}
&r\lambda(1/r) = \lambda(r) \quad \text{for } M = \text{even},\\
&r\lambda_1(1/r) = \lambda_2(r) \neq \lambda_1(r) \quad \text{for } M = \text{odd},
\end{aligned} \tag{25}$$

where $\lambda_2(r)$ is also an eigenvalue of the operator $E(r)$ corresponding to the same J; if $\lambda_1(r)$ belongs to a state from the subspace (pq), then $\lambda_2(r)$ belongs to $(-pq)$.

(iii) Limiting values of $\lambda(r)$. For $r \to 0$ or $r \to 1$ the "elliptic" basis reduces to a canonical one. Obviously we have

$$\lambda(r) \underset{r\to 0}{\to} 4M^2, \qquad \lambda(r) \underset{r\to 1}{\to} 4[J(J+1) - M^2]. \tag{26}$$

It is only in these limiting cases that the eigenvalues $\lambda(r)$ become degenerate (a twofold degeneracy for $M \neq 0$).

Having calculated the eigenvalues λ, we can easily obtain the basis functions $|J\lambda)$, or rather the expansion coefficients $X_{\lambda,M}$ in (10), by solving Eqs. (17) and (18). Indeed, let us impose the symmetries (19), eliminate all equations containing $X_{\lambda,M}$ with $M < 0$ and obtain separate equations for each class (pq). If λ is an eigenvalue, then we obtain consistent sets of homogeneous equations, which means that in each class we can eliminate one equation. Let us eliminate the last equation in each class, i.e., the one containing $(B_0 - \lambda)X_{\lambda,0}$ in the $(++)$ class $(B_2 - \lambda)X_{\lambda,2}$ in the $(-+)$ one and $(B_1 + pA_{-1} - \lambda)X_{\lambda,1}$ in the $(p-)$ classes. All four systems of equations then have the same structure and can be used to express all $X_{\lambda,M}$ in terms of the "highest" one, i.e., $X_{\lambda,K}$ or $X_{\lambda,R}$. The general formula can be written in a somewhat symbolic form, which should however be useful for computer calculations. For M even, i.e., for the classes $(p+)$, we have

$$X_{\lambda K-k-2} = \left(\prod_{j=0,2,\cdots}^{k} D_{K-j}\right)\left[1 + \sum_{j_1=0,2\cdots}^{k-2} \frac{E_{K-j_1}}{D_{K-j_1}D_{K-j_1-2}} \times\left[1 + \sum_{j_2=0,2\cdots}^{j_1-4} \frac{E_{K-j_2}}{D_{K-j_2}D_{K-j_2-2}}[1+\cdots]\right]\cdots\right]X_{\lambda,K}, \tag{27}$$

where

$$\begin{aligned}
&k = 0,2,4\cdots K-2 \quad \text{for class } (++),\\
&k = 0,2,4\cdots K-4 \quad \text{for class } (-+).
\end{aligned} \tag{28}$$

For M odd, i.e., for the classes $(p-)$ we have

$$X_{\lambda,R-k-2} = \left(\prod_{j=1,3,\cdots}^{k} D_{R-j}\right)\left[1 + \sum_{j_1=1,3\cdots} \frac{E_{R-j_1}}{D_{R-j_1}D_{R-j_1-2}} + \sum_{j_2=1,3,\cdots}^{j_1} \frac{E_{R-j_2}}{D_{R-j_2}D_{R-j_2-2}}[1+\cdots]\right]\cdots\right]X_{\lambda,R}, \tag{29}$$

where

$$k = 0,2,4,\cdots,R-3. \tag{30}$$

In the above formulas we have

$$D_M = (\lambda - B_M)/(A_M - 2), \qquad E_M = -(A_{M-2})/(A_{M-4}). \tag{31}$$

The basis functions in the individual classes can finally be expressed as

$$\begin{aligned}
|J\lambda\,++\rangle &= \{X^+_{\lambda 0}|J\,0\rangle + \sum_{M=2,4,\cdots}^{K} X^+_{\lambda M}\{|JM\rangle + |J-M\rangle\},\\
|J\lambda\,-+\rangle &= \sum_{M=2,4,\cdots}^{K} X^-_{\lambda M}\{|JM\rangle - |J-M\rangle\},\\
|J\lambda p\,-\rangle &= \sum_{M=1,3,\cdots}^{R} X^p_{\lambda M}\{|JM\rangle + p|J-M\rangle\}.
\end{aligned} \tag{32}$$

Formulas (32) can be combined into one expression, putting

$$|J\lambda pq\rangle = \sum_{k=0} (X^p_J)_{\lambda,2k+1/2-q/2} \times\left\{\left|J, 2k+\frac{1}{2}-\frac{q}{2}\right\rangle + p\left|J, -2k-\frac{1}{2}+\frac{q}{2}\right\rangle\right\}, \tag{33}$$

with

$$(X^p_J)_{\lambda,2k+1/2-q/2} = \kappa_{kq} X^p_{\lambda,2k+1/2-q/2},$$
$$\kappa_{0+} = \tfrac{1}{2}, \qquad \kappa_{kq} = 1 \quad (k \neq 0,\ q \neq +). \tag{34}$$

We choose the constants $X_{\lambda,K}$ and $X_{\lambda,R}$ in (27) and (29) in such a way as to normalize the functions

$$\langle J'\lambda'p'q' \mid J\lambda pq\rangle = \delta_{JJ'}\delta_{\lambda\lambda'}\delta_{pp'}\delta_{qq'}. \tag{35}$$

Notice also that the functions $|J\lambda pq\rangle$ are real if the coefficients satisfy

$$(X_J^p)^*_{\lambda,M} = pq(X_J^p)_{\lambda,M}. \tag{36}$$

Since both the left and right hand sides of (36) satisfy Eqs. (17) and (18), the reality condition (36) can always be imposed.

The notation $|J\lambda pq\rangle$ is actually somewhat redundant, in that the functions $|J\lambda\rangle$ are, at least for integer values of J, not degenerate (see Sec. 6 for half-integer spins). The value of λ itself characterizes the symmetry class of the eigenfunction. In view of the importance of the symmetry properties of the basis functions we prefer to indicate the class explicitly.

D. Inversion of expansion

Formula (33) provides an expansion of the nonsubgroup basis functions in terms of the canonical ones. The expansion can easily be inverted. Ignoring, for a moment, the individual classes of functions, we can write

$$|J\lambda\rangle = \sum_M X^J_{\lambda,M}|JM\rangle,$$

where X is a $(2J+1)$-dimensional matrix. Since both $|JM\rangle$ and $|J\lambda\rangle$ form orthonormal sets, the matrix X must be unitary $X^{-1} = X^*$.

Hence we have

$$|JM\rangle = \sum_\lambda X^{J*}_{\lambda,M}|J\lambda\rangle, \tag{37}$$

where the sum is over all values of λ.

Within each class (pq) we can invert (33) to obtain

$$|J, 2K + \tfrac{1}{2} - \tfrac{q}{2}\rangle + p\,|J, -2K - \tfrac{1}{2} + \tfrac{q}{2}\rangle = \sum_\lambda (X_j^p)^*_{\lambda,2k+1/2-q/2}|J\lambda pq\rangle, \tag{38}$$

where the star denotes complex conjugation and the sum is over all λ's in the class (pq).

E. Comments on the symmetry classes

The investigation of the expansion (10) of the eigenfunctions $|J\lambda\rangle$ and of the recursion relations (17) and (18) for the expansion coefficients has lead to the introduction of four classes of functions $|J\lambda pq\rangle$ with $p = \pm$ and $q = \pm$. Each class can be characterized by its behavior under reflections, i.e., the set of operators Δ and E, determining the eigenfunctions, should be supplemented by certain discrete reflection operators.

Let us assume that the canonical basis functions (for integer J) $|JM\rangle$ have the usual properties under reflections, i.e., the properties of the spherical harmonics $Y_{JM}(\theta,\phi)$. These are:

(i) Parity $P: x \to -x, y \to -y, z \to -z$
$P\,|JM\rangle = (-1)^J\,|JM\rangle$.

(ii) Reflection in xy plane $Z: x \to x, y \to y, z \to -z$
$Z\,|JM\rangle = (-1)^{J-M}\,|JM\rangle$.

(iii) Reflection in yz plane $X: x \to -x, y \to y, z \to z$
$X\,|JM\rangle = |J-M\rangle$.

(iv) Reflection in zx plane $Y: x \to x, y \to -y, z \to z$
$Y\,|JM\rangle = (-1)^M\,|J-M\rangle$.

Applying these discrete operators to both sides of expansion (33), we find

$$\begin{aligned} P\,|J\lambda pq\rangle &= (-1)^J\,|J\lambda pq\rangle,\\ Z\,|J\lambda pq\rangle &= (-1)^J q\,|J\lambda pq\rangle,\\ X\,|J\lambda pq\rangle &= p\,|J\lambda pq\rangle,\\ Y\,|J\lambda pq\rangle &= pq\,|J\lambda pq\rangle. \end{aligned} \tag{39}$$

The complete set of operators, defining the $O(3)$ basis functions in the nonsubgroup basis can finally be written as

$$\begin{aligned} \Delta\,|J\lambda pq\rangle &= J(J+1)\,|J\lambda pq\rangle,\\ E\,|J\lambda pq\rangle &= \lambda\,|J\lambda pq\rangle,\\ X\,|J\lambda pq\rangle &= p\,|J\lambda pq\rangle,\\ XY\,|J\lambda pq\rangle &= q\,|J\lambda pq\rangle. \end{aligned} \tag{40}$$

As we mentioned in the Introduction, the functions $|J\lambda pq\rangle$ can be identified with the wave functions of the quantum-mechanical asymmetric top. These are usually divided into four symmetry classes,[14] transforming according to the irreducible representations A, B_1, B_2, and B_3 of the discrete group D_2, consisting of the identity e and the rotations through π about the x, y, and z axes (i.e., of e and the reflections YZ, XZ, and XY). The two classifications are clearly equivalent, since we have $YZ = (-1)^J p, XZ = (-1)^J pq$, and $XY = q$. The classification (40) may be somewhat more straightforward and can be directly generalized to other groups. Indeed, a very similar classification of nonsubgroup type basis functions was obtained previously[30] for the group $O(2,1)$.

Finally, let us give the number of states in each class:

J = even: $\frac{J}{2}+1$ states in class $(++)$,
$\frac{J}{2}$ states in all other classes.

J = odd: $\frac{J-1}{2}$ states in class $(-+)$,
$\frac{J+1}{2}$ states in all other classes.

F. Examples

In order to elucidate the above considerations let us consider two simple but nontrivial examples.

$J = 1$:

$$\begin{aligned} &\lambda_1 = 4(1+r), && |1\lambda_1{+}{+}\rangle = |10\rangle,\\ &\lambda_2 = 4 && |1\lambda_2{+}{-}\rangle = 2^{-1/2}[\,|11\rangle + |1-1\rangle],\\ &\lambda_3 = 4r && |1\lambda_3{-}{-}\rangle = 2^{-1/2}[\,|11\rangle - |1-1\rangle]. \end{aligned} \tag{41}$$

$J = 2$:

$$\begin{aligned} \lambda_{1,2} &= 8[1 + r \pm (r^2 - r + 1)^{1/2}],\\ |2\lambda_{1,2}{+}{+}\rangle &= (3^{1/2}/2)(1-r)(r^2-r+1)^{-1/4}\\ &\quad\times[2(r^2-r+1)^{1/2} \mp (1+r)]^{-1/2}\\ &\quad\times\{|20\rangle + \frac{-(1+r) \pm 2(r^2-r+1)^{1/2}}{\sqrt{6}(1-r)}\\ &\quad\times(|22\rangle + |2-2\rangle)]\}, \end{aligned}$$

$$\lambda_3 = 4(4+r), \quad |2\lambda_3 +-\rangle = 2^{-1/2}[\,|21\rangle + |2-1\rangle],$$
$$\lambda_4 = 4(1+r), \quad |2\lambda_4 -+\rangle = 2^{-1/2}[\,|22\rangle - |2-2\rangle],$$
$$\lambda_5 = 4(1+4r), \quad |2\lambda_5 --\rangle = 2^{-1/2}[\,|21\rangle - |2-1\rangle]. \tag{42}$$

It can easily be checked that these eigenfunctions are orthogonal and normalized and that the eigenvalues satisfy the general properties (24)–(26).

4. MATRIX ELEMENTS OF GENERATORS, D FUNCTIONS, AND CLEBSCH-GORDAN COEFFICIENTS

In order to establish how the generators $H_\pm$ and H_3 act on the basis that we have constructed, one uses the expansion (33), the inverse expansion (38), and formulas (8) which give the matrix elements of the generators in the canonical basis. The matrix elements in the nonsubgroup type basis are then expressed as functions of the coefficients X_J^P which themselves are known only when the eigenvalues λ have been found. As a consequence, raising and lowering operators can be defined, but they are not as useful as in the case of the canonical basis, since they involve the coefficients X_J^P. Thus the eigenvalue problem of Sec. 2 must be solved completely, before formulas generating arbitrary basis vectors from a given one can be written. These formulas are lengthy and not particularly illuminating, so we do not present them here. Figure 1 summarizes how H_3 and $H_+ \pm H_-$ shift vectors between the classes (pq).

The standard parametrization of the rotation group in terms of Euler angles is convenient for calculating matrix elements of finite transformations in the canonical basis, because the operator L_3 is diagonal. Since none of the generators is diagonal in the nonsubgroup basis, it is difficult to find a straightforward similarly convenient parametrization of the group. Therefore we make use of the Euler angles ϕ, θ, and ψ, putting

$$D^J_{\lambda pq,\lambda' p'q'}(\phi,\theta,\psi) = \langle J\lambda pq\,|\,e^{-iL_3\phi}e^{-iL_2\theta}e^{-iL_3\psi}\,|J\lambda' p'q'\rangle. \tag{43}$$

Using expansion (33) one easily finds the matrix elements $D^J_{\lambda pq,\lambda' p'q'}(\phi,\theta,\psi)$ and the expansion coefficients X_J^P.

Similarly as the D functions, the Clebsch–Gordan coefficients in the nonsubgroup basis can also be expressed in terms of the corresponding quantities in the canonical basis. Let us define the Clebsch–Gordan coefficients by the relation

$$|J_1\lambda_1 p_1 q_1\rangle|J_2\lambda_2 p_2 q_2\rangle = \sum_{J\lambda pq} (J_1\lambda_1 p_1 q_1\; J_2\lambda_2 p_2 q_2\,|J\lambda pq)\,|J\lambda pq\rangle. \tag{44}$$

Expanding both sides in terms of the canonical basis, we find

$$\begin{aligned}(J_1\lambda_1 p_1 q_1\; J_2\lambda_2 p_2 q_2\,|J\lambda pq) &= \delta[p, p_1 p_2 (-1)^{J_1+J_2-J}]\delta(q, q_1 q_2)\\ &\times \sum_{M_1\geq 0; M_2\geq 0} \{(X_{J_1}^{p_1})_{\lambda_1, M_1}(X_{J_2}^{p_2})_{\lambda_2, M_2}\\ &\times (X_J^p)^*_{\lambda, M_1+M_2}(J_1 M_1 J_2 M_2\,|JM_1+M_2)\\ &+ p_2 (X_{J_1}^{p_1})_{\lambda_1, M_1}(X_{J_2}^{p_2})_{\lambda_2, M_2}(X_J^p)^*_{\lambda, M_1-M_2}\\ &\times (J_1 M_1 J_2 - M_2\,|JM_1 - M_2)\\ &\times [\,p\,\theta(-M_1+M_2) + \theta(M_1 - M_2 - 1)]\}.\end{aligned} \tag{45}$$

Here $\delta(a,b)$ denotes the Kronecker delta δ_{ab}, $(J_1 M_1 J_2 M_2\,|JM)$ are the usual Clebsch–Gordan coefficients, $\theta(N) = 1$ for $N \geq 0$ and $\theta(N) = 0$ for $N < 0$. It is a trivial matter to verify the symmetry

$$(J_1\lambda_1 p_1 q_1\; J_2\lambda_2 p_2 q_2\,|J\lambda pq) = (-1)^{J_1+J_2-J}(J_2\lambda_2 p_2 q_2\; J_1\lambda_1 p_1 q_1\,|J\lambda pq), \tag{46}$$

as well as the fact that the Clebsch–Gordan coefficients are alternatively real and pure imaginary, if we adopt the convention (36) for all basis functions:

$$(J_1\lambda_1 p_1 q_1\; J_2\lambda_2 p_2 q_2\,|J\lambda pq)^* = (-1)^{J_1+J_2-J}(J_1\lambda_1 p_1 q_1\; J_2\lambda_2 p_2 q_2\,|J\lambda pq\rangle. \tag{47}$$

The orthogonality conditions for the Clebsch–Gordan coefficients follow in the usual manner from the orthogonality of the basis. Finally, let us make a comment on the ranges of summation. In actual fact, only the J summation ($|J_1 - J_2| \leq J \leq J_1 + J_2$) is present in (44) since the Kronecker deltas in (45) prescribe the values of p and q. For each given J (and fixed indices on the left hand side) λ can have only one value. This value can be obtained by applying the operator E to both sides of (44) and then multiplying by $\langle J\lambda pq\,|$.

5. HALF-INTEGER VALUES OF ANGULAR MOMENTUM

The nonsubgroup basis can also be used for half-integer spin representations, but some modifications are necessary. The most important change is that the spectrum of λ becomes two-fold degenerate. Indeed, the coefficients $(X_J)_{\lambda M}$ of (10) still satisfy the recursion relation (16), however, the systems of linear equations (17) and (18) for half-odd-integer J have the form

$$\begin{aligned} X_{\lambda,J}(B_J - \lambda) + X_{\lambda,J-2}A_{J-2} &= 0,\\ X_{\lambda,J}A_{J-2} + X_{\lambda,J-2}(B_{J-2} - \lambda) + X_{\lambda,J-4}A_{J-4} &= 0,\\ &\cdots\\ X_{\lambda,-J+3}A_{-J+1} + X_{\lambda,-J+1}(B_{J+1} - \lambda) &= 0,\end{aligned} \tag{48}$$

and

$$\begin{aligned} X_{\lambda,J-1}(B_{J-1} - \lambda) + X_{\lambda,J-3}A_{J-3} &= 0,\\ X_{\lambda,J-1}A_{J-3} + X_{\lambda,J-3}(B_{J-3} - \lambda) + X_{\lambda,J-5}A_{J-5} &= 0,\\ &\cdots\\ X_{\lambda,-J+2}A_{-J} + X_{\lambda,-J}(B_{-J} - \lambda) &= 0.\end{aligned} \tag{49}$$

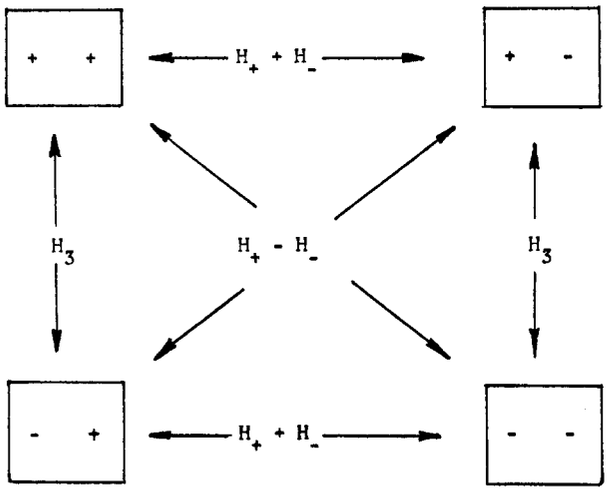

FIG. 1. Action of the generators of $O(3)$ on the individual symmetry classes of nonsubgroup basis functions.

Remembering that $A_{-M} = A_{M-2}$ and $B_{-M} = B_M$, (14), we see that the systems (48) and (49) coincide and hence each eigenvalue λ will occur twice.

The degeneracy can be lifted by introducing the discrete symmetries of Sec. 3E. We can put

$$P|JM\rangle = \eta(-1)^{[J]}|JM\rangle, \quad Z|JM\rangle = \eta(-1)^{[J]-[M]}|JM\rangle,$$
$$X|JM\rangle = \eta|J-M\rangle, \quad Y|JM\rangle = \eta(-1)^{[M]}|J-M\rangle, \tag{50}$$

where η is an intrinsic parity and $[K] = K - \frac{1}{2}$ for K half-odd-integer.

The two eigenfunctions corresponding to each given λ can be chosen to be eigenfunctions of the X reflection, and can be labelled by the symbol p.

The functions

$$|J\lambda p\rangle = \sum_{M\geq 0}(X_J)_{\lambda M}\{|JM\rangle + p|J-M\rangle\} \tag{51}$$

are again eigenfunctions of the complete set of commuting operators Δ, E, and X, as in (40), not however of XY, so there is no point in introducing the label q (e.g., as $q = (-1)^{[M]}$) for half-odd-integer J. The matrix elements of generators, shifting operators, D functions, Clebsch–Gordan coefficients, etc. will be given by similar formulas as in the integer case; we shall, however, not go into the details.

From the point of view of actual computations there is another important difference. In the integer case, functions with $p = \pm 1$ corresponded to different values of λ, whereas in the half-integer case $|J\lambda p\rangle$ and $|J\lambda - p\rangle$ correspond to the same λ. The secular equation for λ in the integer case reduced to four separate algebraic equations, whereas for half-odd-integer J it reduces only to two. We noted in Sec. 3C that the eigenvalues λ could be obtained by solving equations of order less or equal to 4 for $J \leq 7$. For half-odd-integer spins the situation is less favorable. Indeed, $J = \frac{3}{2}$ leads to a quadratic equation and $J = \frac{5}{2}$ and $\frac{7}{2}$ to cubic and quartic ones, respectively,

We can of course again sum all the eigenvalues λ for a given value of J. Since there are only two classes ($p = \pm 1$) and since the values of λ coincide in both classes, let us just give the sum over all eigenvalues:

$$\sum_{\lambda\in\text{all}}\lambda = (1+r)\tfrac{4}{3}J(J+1)(2J+1), \tag{52}$$

which coincides with the corresponding formula for integer spin. Also note that for half-integer J we always have

$$r\lambda(1/r) = \lambda(r)$$

and that (26) remains valid.

As an example, consider $J = \frac{3}{2}$. We have

$$\lambda_1 = \lambda_2 \equiv \lambda = 5(1+r) + 4(r^2 - r + 1)^{1/2},$$
$$|J\lambda p\rangle = N_1\Big\{[|\tfrac{3}{2}\tfrac{3}{2}\rangle + p|\tfrac{3}{2}-\tfrac{3}{2}\rangle] + p\,\frac{1+r+2(r^2-r+1)^{1/2}}{\sqrt{3}(1-r)}[|\tfrac{3}{2}\tfrac{1}{2}\rangle + p|\tfrac{3}{2}-\tfrac{1}{2}\rangle]\Big\}.$$

$$\lambda_3 = \lambda_4 \equiv \lambda' \equiv 5(1+r) - 4(r^2 - r + 1)^{1/2},$$
$$|J\lambda' p\rangle = N_2\Big\{[|\tfrac{3}{2}\tfrac{3}{2}\rangle + p|\tfrac{3}{2}-\tfrac{3}{2}\rangle] + p\,\frac{1+r-2(r^2-r+1)^{1/2}}{\sqrt{3}(1-r)}[|\tfrac{3}{2}\tfrac{1}{2}\rangle + p|\tfrac{3}{2}-\tfrac{1}{2}\rangle]\Big\},$$

where

$$N_{1,2} = \frac{\sqrt{3}(1-r)}{2\sqrt{2}[2(r^2-r+1) \pm (r^2-r+1)^{1/2}]^{1/2}}.$$

6. REALIZATION OF THE REPRESENTATIONS ON A THREE-DIMENSIONAL SPHERE

All our previous considerations concerning the $|J\lambda pq\rangle$ basis were model independent, i.e., did not depend on the space in which the representations are realized. In this section and the following one we shall consider two specific models and discuss the realization of $|J\lambda pq\rangle$ in terms of special functions.

Let us consider a Hilbert space of functions $F(x)$ defined over a unit sphere and satisfying

$$\int |F(x)|^2 \frac{dx_1 dx_2}{x_3} < \infty, \tag{53}$$

where the integration is over the entire sphere and $(dx_1 dx_2)/x_3$ is the invariant measure.

As was mentioned in the Introduction, two coordinate systems exist on the sphere, for which the Laplace equation $\Delta\psi(x) = J(J+1)\psi(x)$ (with J integer) allows the separation of variables.[13] The first are spherical coordinates and the separation of variables leads to the canonical basis for O(3), realized as spherical harmonics,[1] i.e., $|JM\rangle = Y_{JM}(\theta,\phi)$.

Let us now consider the second type of separable coordinates, namely elliptic ones.

A. Elliptic coordinates and the generators of $O(3)$

Elliptic coordinates on a sphere have been considered in several different but equivalent forms.

An algebraic form is

$$x_1^2 = \frac{(a-\rho_1)(a-\rho_2)}{(a-c)(a-b)}, \quad x_2^2 = \frac{(\rho_1-b)(b-\rho_2)}{(b-c)(a-b)},$$
$$x_3^2 = \frac{(\rho_1-c)(\rho_2-c)}{(a-c)(b-c)}, \quad c < \rho_2 < b < \rho_1 < a \tag{54}$$

(a, b, and c are real parameters).

Putting

$$(a-\rho_1) = (a-b)\cos^2\psi, \quad b-\rho_2 = (b-c)\sin^2\eta,$$

we obtain a trigonometric form

$$x_1 = \cos\psi(1-k'^2\cos^2\eta)^{1/2}, \quad x_2 = \sin\psi\sin\eta,$$
$$x_3 = \cos\eta(1-k^2\cos^2\psi)^{1/2},$$
$$0 \leq \eta \leq \pi, \quad 0 \leq \psi < 2\pi, \tag{55}$$
$$k^2 = (a-b)/(a-c), \quad k'^2 = (b-c)/(a-c).$$

Putting

$$(a-\rho_1) = (a-b)\,\mathrm{sn}^2(\alpha,k), \quad b-\rho_2 = (b-c)\,\mathrm{cn}^2(\beta,k'),$$

we obtain a Jacobi elliptic form

$$x_1 = \mathrm{sn}(\alpha,k)\mathrm{dn}(\beta,k'), \quad x_2 = \mathrm{cn}(\alpha,k)\mathrm{cn}(\beta,k'),$$
$$x_3 = \mathrm{dn}(\alpha,k)\mathrm{sn}(\beta,k'), \quad -K \leq \alpha \leq K,$$
$$-2K' \leq \beta \leq 2K', \tag{56}$$
$$k^2 + k'^2 = 1, \quad 0 \leq k \leq 1, \quad 0 \leq k' \leq 1.$$

Here, e.g., $\mathrm{sn}(\alpha,k)$, $\mathrm{cn}(\alpha,k)$, and $\mathrm{dn}(\alpha,k)$ are Jacobi elliptic functions[34] of argument α and modulus k. Their real quarter-period K is determined uniquely as a function of k[k and k' are the same as in (55)].

Other forms of elliptic coordinates exist, but we shall further use only (56). It is easy to see that the coordinates α and β in the regions indicated in (56) cover the whole sphere once. Note that under the reflection [$\alpha \to -\alpha$ the function $\mathrm{sn}(\alpha,k)$ is antisymmetric, whereas $\mathrm{cn}(\alpha,k)$ and $\mathrm{dn}(\alpha,k)$ are symmetric]. Thus the reflections of α and β are related to the reflections of Sec. 3E, namely

$$\begin{aligned} &\alpha \to -\alpha, \beta \to \beta \text{ is } X,\\ &\alpha \to \alpha, \beta \to -\beta \text{ is } Z,\\ &\alpha \to -\alpha, \beta \to \beta + 2K' \text{ is } P' \end{aligned} \tag{57}$$

The generators of $O(3)$ can be written as differential operators and are

$$\begin{aligned} L_1 &= \frac{1}{k^2\,\mathrm{cn}^2\alpha + k'^2\,\mathrm{cn}^2\beta} \times\left\{-k'^2\,\mathrm{sn}\alpha\,\mathrm{cn}\beta\,\mathrm{sn}\beta\frac{\partial}{\partial\alpha} - \mathrm{cn}\alpha\,\mathrm{dn}\alpha\,\mathrm{dn}\beta\frac{\partial}{\partial\beta}\right\},\\ L_2 &= \frac{1}{k^2\,\mathrm{cn}^2\alpha + k'^2\,\mathrm{cn}^2\beta} \times\left\{-\mathrm{cn}\alpha\,\mathrm{sn}\beta\,\mathrm{dn}\beta\frac{\partial}{\partial\alpha} + \mathrm{sn}\alpha\,\mathrm{dn}\alpha\,\mathrm{cn}\beta\frac{\partial}{\partial\beta}\right\},\\ L_3 &= \frac{1}{k^2\,\mathrm{cn}^2\alpha + k'^2\,\mathrm{cn}^2\beta} \times\left\{\mathrm{dn}\alpha\,\mathrm{cn}\beta\,\mathrm{dn}\beta\frac{\partial}{\partial\alpha} + k^2\,\mathrm{sn}\alpha\,\mathrm{cn}\alpha\,\mathrm{sn}\beta\frac{\partial}{\partial\beta}\right\} \end{aligned} \tag{58}$$

(we have dropped the moduli in the elliptic functions).

B. The complete set of commuting operators and Lamé polynomials

The operators Δ and E of (2) can readily be written as differential operators:

$$\begin{aligned} \Delta &= -\frac{1}{k^2\,\mathrm{cn}^2(\alpha,k) + k'^2\,\mathrm{cn}^2(\beta,k')}\left[\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial\beta^2}\right],\\ E &= -\frac{4}{k^2\,\mathrm{cn}^2(\alpha,k) + k'^2\,\mathrm{cn}^2(\beta,k')} \times\left[k'^2\,\mathrm{sn}^2(\beta,k')\frac{\partial^2}{\partial\alpha^2} + \mathrm{dn}^2(\alpha,k)\frac{\partial^2}{\partial\beta^2}\right], \end{aligned} \tag{59}$$

with

$$k'^2 = r,\ k^2 = 1 - r.$$

The equations

$$\begin{aligned} &\Delta\psi_{J\lambda}(\alpha,\beta) = J(J+1)\psi_{J\lambda}(\alpha,\beta),\\ &E\psi_{J\lambda}(\alpha,\beta) = \lambda\psi_{J\lambda}(\alpha,\beta) \end{aligned} \tag{60}$$

have a complete set of common solutions which we write as

$$\psi_{J\lambda}(\alpha,\beta) = A_{J\lambda}(\alpha)B_{J\lambda}(\beta), \text{ where}$$

$$\frac{d^2A_{J\lambda}(\alpha)}{d\alpha^2} + [-\frac{\lambda}{4} + J(J+1) - J(J+1)k^2\,\mathrm{sn}^2(\alpha,k)]A_{J\lambda}(\alpha) = 0,$$

$$\frac{d^2B_{J\lambda}(\beta)}{d\beta^2} + \left[\frac{\lambda}{4} - J(J+1)k'^2\,\mathrm{sn}^2(\beta,k')\right]B_{J\lambda}(\beta) = 0. \tag{61}$$

Both these equations are the Lamé equation in its Jacobian form.[11,12] The ordinary differential equations (61) must be supplemented by boundary conditions. In agreement with the general theory of Sec. 3 we use the boundary conditions to choose solutions that have the proper symmetry properties with respect to the reflections X and XY [see (40) and (57)]. Finally, we have

$$|J\lambda pq\rangle = \Lambda^p_{Jh}(\alpha)\,\Lambda^q_{Jh'}(\beta), \qquad h + h' = J(J+1), \tag{62}$$

where $\Lambda^p_{Jh}(\alpha)$ is a Lamé polynomial satisfying

$$\begin{aligned} &\frac{d^2\Lambda^p_{Jh}(\alpha)}{d\alpha^2} + [h - J(J+1)k^2\,\mathrm{sn}^2(\alpha,k)]\Lambda^p_{Jh}(\alpha) = 0,\\ &\Lambda^p_{Jh}(-\alpha) = p\Lambda^p_{Jh}(\alpha), \qquad k^2 = 1 - r,\\ &h = -\frac{\lambda}{4} + J(J+1). \end{aligned} \tag{63}$$

The function $\Lambda^q_{Jh'}(\beta)$ satisfies the same equations (with $\alpha \to \beta, k \to k', h \to h' = \lambda/4$ and $p \to q$).

The normalization is such that

$$\begin{aligned} \langle\widetilde{J\lambda pq}|J\lambda pq\rangle &= \int_{-K}^{K} d\alpha \int_{-2K}^{2K} d\beta(k^2\,\mathrm{cn}^2(\alpha,k) + k'^2\,\mathrm{cn}^2(\beta,k'))\Lambda^{\tilde p}_{J\tilde h}{}^*(\alpha)\Lambda^{\tilde q}_{J\tilde h}{}^*(\beta)\\ &\times\Lambda^p_{Jh}(\alpha)\Lambda^q_{Jh'}(\beta) = \delta_{J\tilde J}\delta_{h\tilde h}\delta_{p\tilde p}\delta_{q\tilde q}. \end{aligned} \tag{64}$$

Note that the symmetry (63) implies only that

$$\frac{d}{d\alpha}[\Lambda^+_{Jh}(\alpha)]\big|_{\alpha=0} = 0, \qquad \Lambda^-_{Jh}(0) = 0. \tag{65}$$

The values of $\Lambda^+_{Jh}(0)$ and $\Lambda^{-\prime}_{Jh}(0) \equiv d/d\alpha[\Lambda^-_{J\lambda}(\alpha)]|_{\alpha=0}$ must be so chosen that (64) is satisfied. This still leaves an arbitrary phase, which can be fixed, e.g., by taking $\Lambda^+_{J\lambda'}(0)$ and $\Lambda^{-\prime}_{J\lambda'}(0)$ to be real. The Lamé polynomials themselves will then be real and the expansion coefficients $(X^p_J)_{\lambda,M}$ of Sec. 3 will satisfy the reality condition (36).

Thus, the nonsubgroup type basis functions in this model turn out to be well-known functions—the Lamé polynomials. The corresponding eigenvalues λ as well as the functions themselves have been tabulated for a large range of values of J and r[35].

The functions $|J\lambda pq\rangle$ of (62) are called ellipsoidal harmonics. One of their useful applications is to provide symmetric expansions of functions, defined over a sphere. Indeed, for any function $F(x) = F(\alpha,\beta)$ satisfying (53), we can write

$$F(\alpha,\beta) = \sum_{J=0}^{\infty}\sum_{\lambda}\sum_{p,q} A^{pq}_{Jh}\,\Lambda^p_{Jh}(\alpha)\Lambda^q_{Jh'}(\beta), \tag{66}$$

where

$$A^{pq}_{Jh} = \int_{-K}^{K} d\alpha \int_{-2K}^{2K} d\beta[k^2\,\mathrm{cn}^2(\alpha,k) + k'^2\,\mathrm{cn}^2(\beta,k')] \times F(\alpha,\beta)\Lambda^{p*}_{Jh}(\alpha)\Lambda^{q*}_{Jh'}(\beta). \tag{67}$$

Symmetry conditions like

$$F(\alpha,\beta) = \pm F(\beta,\alpha)$$

can be imposed by putting

$$A^{pq}_{Jh} = \pm A^{qp}_{Jh'}. \tag{68}$$

Precisely this type of expansion has been used[30] to provide crossing symmetric expansions of physical scattering amplitudes in terms of products of Lamé functions (not polynomials), that occur as basis functions for irreducible representations of $O(2,1)$ in a nonsubgroup basis.

7. ONE-DIMENSIONAL REALIZATION OF THE REPRESENTATIONS

Let us consider a space of polynomials $f(z)$ of order less or equal to $2J$ of one complex variable.[5,7] An invariant scalar product is so defined that

$$(X^{J-M}, X^{J-N}) = (J-M)!(J+M)!\delta_{MN}.$$

Representations of $O(3)$ can be constructed in this space and the canonical basis is realized by the functions

$$|JM\rangle = \frac{z^{J-M}}{[(J-M)!(J+M)!]^{1/2}}, \quad -J \le M \le J. \tag{69}$$

The generators of $O(3)$ in this realization are

$$H_+ = \frac{d}{dz}, \quad H_- = 2Jz - z^2\frac{d}{dz}, \quad H_3 = J - z\frac{d}{dz} \tag{70}$$

Let us now construct the nonsubgroup basis. The operator E can be written as

$$\begin{aligned} E = {} & [(1-\sqrt{r})z^2 - (1+\sqrt{r})][(1+\sqrt{r})z^2 - (1-\sqrt{r})]\frac{d^2}{dz^2} \\ & + (2J-1)2z[1+r-z^2(1-r)]\frac{d}{dz} \\ & + 2J[1+r+(1-r)(2J-1)z^2]. \end{aligned} \tag{71}$$

The basis functions are determined by the condition

$$E\psi_{J\lambda}(z) = \lambda\psi_{J\lambda}(z). \tag{72}$$

However, let us make the substitution

$$y = [(1-\sqrt{r})/(1+\sqrt{r})]z^2, \tag{73}$$

and put

$$\psi_{J\lambda}(z) = \phi_{J\lambda}(y). \tag{74}$$

Substituting (71) into (72) we obtain an equation for the basis functions

$$\begin{aligned} \frac{d^2}{dy^2}\phi_{J\lambda}(y) + & \left(\frac{\gamma}{y} + \frac{\delta}{y-1} + \frac{\epsilon}{y-a^2}\right)\frac{d}{dy}\phi_{J\lambda}(y) \\ & + \frac{\alpha\beta y - q}{y(y-1)(y-a^2)}\phi_{J\lambda}(y) = 0, \end{aligned} \tag{75}$$

where

$$\begin{aligned} & \gamma = \tfrac{1}{2}, \quad \alpha = \delta = \epsilon = -J + \tfrac{1}{2}, \quad \beta = -J, \\ & q = -\tfrac{1}{16}[4J(1+a^2) - (1+a)^2\lambda], \\ & a = [(1-\sqrt{r})/(1+\sqrt{r})]. \end{aligned} \tag{76}$$

Equation (75) is the general form of the Heun equation[12] and when the parameters satisfy (76) its solutions are, by construction, polynomials in z. Note that the Lamé equation is obtained from the Heun one if $\gamma = \delta = \epsilon = \frac{1}{2}$.

Another useful transformation of Eq. (72) is obtained by putting

$$w = \left(\frac{1-\sqrt{r}}{1+\sqrt{r}}\right)^{1/2} z = \sqrt{a}z, \quad \psi_{J\lambda}(z) = \chi_{J\lambda}(w); \tag{77}$$

we then obtain

$$\begin{aligned} (1-w^2)(a^4-w^2)\frac{d^2\chi_{J\lambda}}{dw^2} + (2J-1)w(1+a^4-2w^2)\frac{d\chi_{J\lambda}}{dw} \\ - \frac{2(2J-1)}{J+1}[h - J(J+1)w^2]\chi_{J\lambda} = 0, \end{aligned} \tag{78}$$

with

$$h = \frac{(J+1)[(1+a^2)^2\lambda - 4J(1+a^4)]}{8(2J-1)}.$$

The symmetries of Eqs. (72), (75), and (78) are not immediately apparent; however, from the results of Sec. 3 we know that the solutions fall into four classes (pq). Indeed, consider Eq. (72). The solutions can be written as (for integer J):

$$\begin{aligned} |J\lambda pq\rangle = \psi^{pq}_{J\lambda}(z) = \sum_{M\ge 0}(X^p_J)_{\lambda,M}\frac{1}{[(J-M)!(J+M)!]^{1/2}} \\ \times (z^{J-M} + pz^{J+M}), \end{aligned} \tag{79}$$

where the coefficients $(X^p_J)_{\lambda,M}$ satisfy, e.g., (16) and $q = (-1)^M$.

Let us restrict ourselves to integer values of J. We have

$$\psi^{pq}_{J\lambda}(-z) = (-1)^J q\,\psi^{pq}_{J\lambda}(z). \tag{80}$$

Thus, the transformation $z \to -z$ corresponds exactly to the Z reflection of (39) in a three-dimensional Euclidean space. For a given (integer) value of J, the label q tells us whether $\psi^{pq}_{J\lambda}(z)$ is symmetric or antisymmetric under reflection of the complex variable z.

The label p in this model is related to the transformation

$$\psi^{pq}_{J\lambda}(z) \to z^{2J}\psi^{pq}_{J\lambda}\left(\frac{1}{z}\right). \tag{81}$$

Indeed, from (79) we have

$$z^{2J}\psi^{pq}_{J\lambda}(1/z) = p\,\psi^{pq}_{J\lambda}(z), \tag{82}$$

so that the transformation (81) corresponds to the X reflection of (39).

It is interesting to compare the two-dimensional model of the previous section with this one-dimensional one. The functions $\psi^{pq}_{J\lambda}(z)$, satisfying Eq. (72) and related to Heun polynomials by relations (73) and (74), are generating functions for the coefficients $(X^p_J)_{\lambda,M}$, figuring in the expansion of ellipsoidal harmonics in terms of spherical harmonics:

$$\Lambda^p_{Jh}(\alpha)\Lambda^q_{Jh'}(\beta) = \sum_{M\ge 0}(X^p_J)_{\lambda,M}[Y_{JM}(\theta,\phi) + pY_{J-M}(\theta,\phi)], \tag{83}$$

where

$$\begin{aligned} & x_1 = \mathrm{sn}(\alpha,k)\mathrm{dn}(\beta,k') = \sin\theta\cos\phi, \\ & x_2 = \mathrm{cn}(\alpha,k)\,\mathrm{cn}(\beta,k') = \sin\theta\sin\phi, \\ & x_3 = \mathrm{dn}(\alpha,k)\,\mathrm{sn}(\beta,k') = \cos\theta, \\ & h = -(\lambda/4) + J(J+1), \\ & h' = \lambda/4. \end{aligned}$$

The equations of this section define a new class of polynomials, related to Heun functions. It should be stressed that they can be constructed explicitly using formula (79) and that the values of λ, as well as the coefficients $(X^p_J)_{\lambda M}$, will simply coincide with the corresponding

quantities for the ellipsoidal harmonics of the previous section. Hence direct use can be made of existing tables of Lamé polynomials.[35]

8. CONCLUSIONS

The present approach, i.e., a systematic consideration of different possible bases for the representations of various groups, may be of interest for several reasons. One is that a great variety of special functions becomes amenable to a group theoretical treatment, so that they can be subjected to a unified systematic investigation. For the $O(3)$ group this has lead to Lamé and Heun polynomials (besides the obvious Legendre and Jacobi polynomials). For noncompact groups the variety of functions that occur is much larger, since many more subgroup and nonsubgroup type bases exist. Thus, already for the Euclidean group E_2 we obtain, besides the obvious Bessel functions and exponentials, also Mathieu functions and functions of the parabolic cylinder. The groups $O(2,1)$, $O(4)$, $O(3,1)$, and E_3 will also lead to many functions of interest (spheroidal functions, Mathieu functions, Weber functions, ellipsoidal functions, etc.).

The results of this paper and more generally of the present approach are also of interest in view of possible applications in physics and mathematical physics—these have been discussed in the Introduction. We consider the "symmetric" expansion (66)–(68) to be of particular importance in various applications. In some applications in elementary particle physics (crossing symmetry) one needs functions $F(s,t,u)$ that have definite symmetries under the permutations of three variables. We plan to investigate this problem in connection with the representation theory of the four-dimensional rotation group $O(4)$ and the Lorentz group $O(3,1)$.

Let us add a few words about the future outlook. Several problems remain concerning the representations of $O(3)$. Thus, it would be desirable to provide a new parametrization of the group element of $O(3)$, that would be as "natural" for the nonsubgroup basis, as the Euler angles are for the canonical one. This would make it possible to find a useful representation of the D functions, and, in particular, would lead to new special functions as matrix elements. In preparation is an article in which we study the $|J\lambda pq\rangle$ basis functions in greater detail for low values of J and also consider further the special functions figuring in the models.

A systematic study of the various subgroup and nonsubgroup basis for the E_2, $O(2,1)$, E_3, $O(4)$, and $O(3,1)$ groups is also in progress.

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Nonnegativity of the Yukawa Hamiltonian

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The Yukawa Hamiltonian $H = -\Delta - r^{-1}e^{-\mu r}$ is shown to be nonnegative for $\mu \geq [1+6\log 2-(9/2)\log 3]^{1/3} \approx (1.67)^{-1}$.

1. INTRODUCTION

In a recent article Piepenbrink[1] proves that the Yukawa Hamiltonian

$$H = -\Delta - r^{-1}e^{-\mu r} \tag{1}$$

is nonnegative if

$$\mu \geq (1.64)^{-1} \tag{2}$$

The purpose of the present note is to demonstrate that the sharper condition

$$\mu \geq [1 + 6\log 2 - \frac{9}{2}\log 3]^{1/3} \approx (1.67)^{-1} \tag{3}$$

can be obtained in a simple way.

2. CALCULATION

For the critical value μ_0 of μ the smallest eigenvalue of the Hamiltonian vanishes. The zero eigenvalue spherical symmetric eigenfunction $r^{-1}u(r)$ is determined as a *bounded* solution of the radial equation

$$\mu d^2u/dx^2 = -ux^{-1}e^{-x} \tag{4}$$

with $u(0) = 0$. Here $x = \mu r$. (These eigenfunctions are not square integrable since zero energy belongs to the continuous spectrum.) Bounded solutions of (4) exist only for a discrete set $\mu_0, \mu_1, \cdots$ of *positive* μ's, and we seek the largest among these.

Integrating (4) twice, taking the boundary conditions $u(0) = 0$ and $|u(\infty)| < \infty$ into account, we obtain

$$\mu u(x) = \int_x^\infty y^{-1}xe^{-y}u(y)dy + \int_0^x e^{-y}u(y)dy, \tag{5}$$

or in a symmetrized version,

$$\int_0^\infty K(x,y)\psi(y)dy = \mu\psi(y), \tag{6}$$

where $u(x) = x^{1/2}e^{x/2}\psi(x)$. The kernel

$$K(x,y) = (xy)^{-1/2}e^{-(x+y)/2}\min(x,y) \tag{7}$$

is Hilbert–Schmidt.

The traces of the iterated kernels $K^{(n)}(x,y)$,

$$T_n = \int_0^\infty K^{(n)}(x,x)dx, \tag{8}$$

can be evaluated for low n; in fact,

$$\begin{aligned} T_1 &= 1, \\ T_2 &= -1 + \log 4, \\ T_3 &= 1 + 6\log 2 - \frac{9}{2}\log 3. \end{aligned} \tag{9}$$

The integrations involved are elementary though somewhat tedious.

By Mercer's theorem, $\Sigma_i \mu_i^n = T_n$, and the positivity of the μ's, we have

$$\mu_0 \leq T_n^{1/n}, \tag{10}$$

which for $n = 3$ implies Eq. (3) above.

Both Piepenbrink's technique and the present one can be iterated to yield improved bounds.

3. COMMENT

The upper bound (3) approximates the exact value for μ_0 within 1%. This follows from the existence of a Rayleigh–Ritz lower bound[1] $(1.68)^{-1}$ for μ_0. Relative to μ_0 the improvement of (3) over (2) is therefore not insignificant.

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[1] J. Piepenbrink, J. Math. Phys. **13**, 1825 (1972).

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On analytic nonlocal potentials. I. A forward dispersion relation

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We propose a class of analytic short-ranged nonlocal potentials, and we obtain dispersion relations for the forward scattering amplitude. We use the Fredholm method for the Lippman–Schwinger equation for the scattering solution, and contour rotation in the analytic continuation of the forward scattering amplitude.

1. INTRODUCTION

Nonlocal potentials have been studied both in the separable form and simple generalizations,[1-12] and in more general forms.[13-19] They appear and have been used in problems of nuclear and atomic physics.[20-31] For example, meson theory suggests that any internucleon potential is nonlocal,[2 8] and the Hartree Fock equation contains a strongly nonlocal term.[23,27]

Analyticity in the k plane and dispersion relations in the energy variable for scattering amplitudes have been studied for separable nonlocal potentials and simple generalizations.[4,6,9] The nonlocal potentials which we shall consider are in general nonseparable. They are 'analytic' and short-ranged.

We shall consider any nonlocal potential $V(\mathbf{x},\mathbf{x}')$ satisfying the following conditions (A):

(A1) $V(\mathbf{x},\mathbf{x}')$ is real, $V(\mathbf{x},\mathbf{x}') = V(\mathbf{x}',\mathbf{x})$.

(A2) $V(\mathbf{x},\mathbf{x}')$ is rotationally invariant:

$$V(\mathbf{x},\mathbf{x}') = V(x,x',\cos\nu),$$

$$x = |\mathbf{x}| > 0, \quad x' = |\mathbf{x}'| > 0, 1 \geq \cos\nu \geq -1,$$

where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$.

(A3) $V(x,x',\cos\nu) = (e^{-\gamma x}/x^{\alpha})\tilde{V}(x,x',\cos\nu)e^{-\gamma x'}/x'^{\alpha}$,

$$\gamma > 0, \quad \tfrac{3}{2} > \alpha \geq 0,$$

where $\tilde{V}(x,x',\cos\nu)$ is holomorphic in x and x', in $\mathrm{Re}\, x > 0, \mathrm{Re}\, x' > 0$, for $1 \geq \cos\nu \geq -1$, and continuous in all these variables in $\mathrm{Re}\, x > 0, \mathrm{Re}\, x' > 0, 1 \geq \cos\nu \geq -1$, and

$$|\tilde{V}(x,x',\cos\nu)| \leq \text{const}.$$

for $\mathrm{Re}\, x > 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$.

Such a potential leads to a self-adjoint Hamiltonian operator in the space $L^2(R^3)$, with domain $W^{2,2}(R^3)$.[18]

We shall show that, for such a potential, the forward scattering amplitude is holomorphic in k in $\mathrm{Im}\, k > -\gamma$, cut from $i\gamma$ to $i\infty$, perhaps with the exception of poles in the interval $k = i\kappa, \gamma > \kappa > 0$, or in $0 > \mathrm{Im}\, k > -\gamma$, each of those on the upper imaginary axis, which are finite in number, corresponds to a negative energy bound state or bound states.[32] We obtain a substracted dispersion relation for the forward scattering amplitude.

We obtain an unsubtracted dispersion relation for the forward scattering amplitude for such a potential satisfying the following additional conditions (B):

(B1) $\tilde{V}(x,x',\cos\nu)$ is continuous in all its variables in $\mathrm{Re}\, x \geq 0, \mathrm{Re}\, x' \geq 0, 1 \geq \cos\nu \geq -1$, and in this region of x, x', and $\cos\nu$ we have

$$|\tilde{V}(x,x',\cos\nu)| \leq \frac{\text{const}}{[(1+|x|)(1+|x'|)]^{3+\beta-\alpha}}, \quad \text{some } \beta > 0.$$

(B2) $\tilde{V}(x,x',\cos\nu)$ is differentiable in $\cos\nu$ in $1 \geq \cos\nu \geq -1$, for $\mathrm{Re}\, x \geq 0, \mathrm{Re}\, x' \geq 0$. $(\partial/\partial\cos\nu)\tilde{V}(x,x',\cos\nu)$ is continuous in all its variables in $\mathrm{Re}\, x \geq 0$, $\mathrm{Re}\, x' \geq 0$, $1 \geq \cos\nu \geq -1$, and for such values of x, x', and $\cos\nu$, we have

$$\left|\frac{\partial}{\partial\cos\nu}\tilde{V}(x,x',\cos\nu)\right| \leq \frac{\text{const}}{[(1+|x|)(1+|x'|)]^{3+\beta-\alpha}}.$$

We give examples of classes of potentials satisfying conditions (A) but not necessarily conditions (B), for which we also have an unsubtracted dispersion relation for the forward scattering amplitude.

The analysis may be extended to give dispersion relations for the physical nonforward scattering amplitude.

In the following, $V(x,x',\cos\nu)$ is defined for $\mathrm{Re}\, x > 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$, in terms of $\tilde{V}(x,x',\cos\nu)$ by the relation in (A3).

2. THE SCATTERING SOLUTION, THE BOUND STATES, AND THE SCATTERING AMPLITUDE

A. The kernel

We define an integral operator $K(k)$ on the space of bounded measurable functions, for $k \geq 0$, by the following kernel:

$$K(k;\mathbf{x},\mathbf{x}') = \frac{-1}{4\pi}\int d\mathbf{x}''\, \frac{e^{ik|\mathbf{x}-\mathbf{x}''|}}{|\mathbf{x}-\mathbf{x}''|}V(\mathbf{x}'',\mathbf{x}'), \quad |\mathbf{x}'| > 0. \tag{2.1}$$

We have

$$K(k;\mathbf{x},\mathbf{x}') = A(k;\mathbf{x},\mathbf{x}')\frac{e^{-\gamma x'}}{x'^{\alpha}}, \tag{2.2}$$

$$|A(k;\mathbf{x},\mathbf{x}')| \leq \text{const}\int d\mathbf{x}''\frac{1}{|\mathbf{x}-\mathbf{x}''|}\frac{e^{-\gamma x''}}{x''^{\alpha}} \leq N, \quad x'' = |\mathbf{x}''| \tag{2.3}$$

where N is a constant.

The function $K(k;\mathbf{x},\mathbf{x}')$ depends on $x = |\mathbf{x}'|, x' = |\mathbf{x}'|$, and $\cos\nu$ only, where ν is the angle between $\mathbf{x}'$ and $\mathbf{x}''$:

$$K(k;\mathbf{x},x') = K(k;x,x',\cos\nu),$$

$$x \geq 0, \quad x' > 0, \quad 1 \geq \cos\nu \geq -1. \tag{2.4}$$

We now define $K(k;x,x',\cos\nu)$, for $\mathrm{Im}\, k > -\gamma$, $x \geq 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$ by

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$$K(k;x,x',\cos\nu)$$
$$= \frac{-1}{4\pi}\iiint x''^2 dx'' \sin\mu\, d\mu\, d\chi \times \frac{\exp[ik(x^2+x''^2-2xx''\cos\mu)^{1/2}]}{(x^2+x''^2-2xx''\cos\mu)^{1/2}} V(x'',x',\cos\lambda), \quad (2.5)$$

where

$$\cos\lambda = \cos\mu\cos\nu + \sin\mu\sin\nu\cos\chi.$$

This reduces to (2.1) for $k \geq 0$, $x \geq 0$, $x' > 0$, $1 \geq \cos\nu \geq -1$.

We find that $K(k;x,x',\cos\nu)$, so defined, is holomorphic in k and x' in Im $k > -\gamma$, Re $x' > 0$, for $x \geq 0$, $1 \geq \cos\nu \geq -1$, and continuous in $x, x', \cos\nu$, in $x \geq 0$,[33] Re $x' > 0$, $1 \geq \cos\nu \geq -1$, for Im $k > -\gamma$.

We have

$$K(k;x,x',\cos\nu) = A(k;x,x',\cos\nu)\, e^{-\gamma x'}/x'^{\alpha}, \quad (2.6)$$

$$|A(k;x,x',\cos\nu)| \leq N(\epsilon) e^{(\gamma-\epsilon)x}, \quad \text{Im } k \geq -(\gamma-\epsilon),\ \gamma \geq \epsilon > 0, \quad (2.7)$$

where $N(\epsilon)$ depends on ϵ only.

B. The Lippman-Schwinger equation for k real

The Lippman-Schwinger equation for the scattering solution $\psi(\mathbf{k};\mathbf{x})$ for $\mathbf{k}$ real is

$$\psi(\mathbf{k};\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi}\int d\mathbf{x}''\, \frac{e^{ik|\mathbf{x}-\mathbf{x}''|}}{|\mathbf{x}-\mathbf{x}''|}\int d\mathbf{x}' V(\mathbf{x}'',\mathbf{x}')\psi(\mathbf{k};\mathbf{x}'), \quad k = |\mathbf{k}| \geq 0. \quad (2.8)$$

This equation may be explicitly and uniquely solved in the space of bounded measurable functions, when the Fredholm determinant of the integral operator $K(k)$ is not zero, and the solution is continuous in $\mathbf{x}$.

We consider the following integral equation:

$$\psi(\mathbf{k};\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \int d\mathbf{x}' K(k;\mathbf{x},\mathbf{x}')\psi(\mathbf{k};\mathbf{x}'). \quad (2.9)$$

We define $\Delta_n(k)$ by

$$\Delta_0(k) = 1,$$
$$\Delta_n(k) = \int\cdots\int d\mathbf{x}_1\cdots d\mathbf{x}_n \begin{vmatrix} K(k;\mathbf{x}_1,\mathbf{x}_1)\cdots K(k;\mathbf{x}_1,\mathbf{x}_n) \\ \cdot \\ \cdot \\ \cdot \\ K(k;\mathbf{x}_n,\mathbf{x}_1)\cdots K(k;\mathbf{x}_n,\mathbf{x}_n) \end{vmatrix}$$
$$= \int\cdots\int d\mathbf{x}_1\cdots d\mathbf{x}_n \frac{e^{-\gamma x_1}}{x_1^{\alpha}}\cdots\frac{e^{-\gamma x_n}}{x_n^{\alpha}} \times \begin{vmatrix} A(k;\mathbf{x}_1,\mathbf{x}_1)\cdots A(k;\mathbf{x}_1,\mathbf{x}_n) \\ \cdot \\ \cdot \\ \cdot \\ A(k;\mathbf{x}_n,\mathbf{x}_1)\cdots A(k;\mathbf{x}_n,\mathbf{x}_n) \end{vmatrix}, \quad x_i = |\mathbf{x}_i|,\ n \geq 1. \quad (2.10)$$

We have

$$|\Delta_n(k)| \leq N^n M^n n^{n/2}, \quad n \geq 1, \quad (2.11)$$

using (2.3) and Hadamard's theorem,[34] where

$$M = \int d\mathbf{x}\, \frac{e^{-\gamma x}}{x^{\alpha}}, \quad x = |\mathbf{x}|.$$

Hence

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta_n(k).$$

is convergent and we write

$$\Delta(k) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta_n(k). \quad (2.12)$$

$\Delta(k)$ is the Fredholm determinant of the operator $K(k)$.

We define $\Delta_n(k;\mathbf{x},\mathbf{x}')$ by

$$\Delta_0(k;\mathbf{x},\mathbf{x}') = K(k;\mathbf{x},\mathbf{x}')$$
$$\Delta_n(k;\mathbf{x},\mathbf{x}') = \int\cdots\int d\mathbf{x}_1\cdots d\mathbf{x}_n \begin{vmatrix} K(k;\mathbf{x},\mathbf{x}')\cdots K(k;\mathbf{x},\mathbf{x}_n) \\ \cdot \\ \cdot \\ \cdot \\ K(k;\mathbf{x}_n,\mathbf{x}')\cdots K(k;\mathbf{x}_n,\mathbf{x}_n) \end{vmatrix}$$
$$= \int\cdots\int d\mathbf{x}_1\cdots d\mathbf{x}_n \frac{e^{-\gamma x'}}{x'^{\alpha}}\frac{e^{-\gamma x_1}}{x_1^{\alpha}}\cdots\frac{e^{-\gamma x_n}}{x_n^{\alpha}} \times \begin{vmatrix} A(k;\mathbf{x},\mathbf{x}')\cdots A(k;\mathbf{x},\mathbf{x}_n) \\ \cdot \\ \cdot \\ \cdot \\ A(k;\mathbf{x}_n,\mathbf{x}')\cdots A(k;\mathbf{x}_n,\mathbf{x}_n) \end{vmatrix},$$
$$x' = |\mathbf{x}'|,\ x_i = |\mathbf{x}_i|,\ n \geq 1; \quad (2.13)$$

We have

$$|\Delta_n(k;\mathbf{x},\mathbf{x}')| \leq N^{n+1}M^n(n+1)^{(n+1)/2}\, e^{-\gamma x'}/x'^{\alpha}, \quad (2.14)$$

using (2.3) and Hadamard's theorem again.

Hence

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta_n(k;\mathbf{x},\mathbf{x}')$$

is uniformly convergent in $\mathbf{x}$, and is a continuous function of $\mathbf{x}$. It is also a continuous function of $\mathbf{x}$ and $\mathbf{x}'$, in all $\mathbf{x}$, and $|\mathbf{x}'| > 0$. We write

$$\Delta(k;\mathbf{x},\mathbf{x}') = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta_n(k;\mathbf{x},\mathbf{x}'), \quad |\mathbf{x}| \geq 0, \quad |\mathbf{x}'| > 0 \quad (2.15)$$

We have

$$|\Delta(k;\mathbf{x},\mathbf{x}')| \leq \text{const}\ e^{-\gamma x'}/x'^{\alpha}, \quad x' = |\mathbf{x}'|. \quad (2.16)$$

Using (2.2), (2.3), and (2.16), and following Ref. 35, we find that, for $\Delta(k) \neq 0$, the function

$$\psi(\mathbf{k};\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \int d\mathbf{x}'\, \frac{\Delta(k;\mathbf{x},\mathbf{x}')}{\Delta(k)}\, e^{i\mathbf{k}\cdot\mathbf{x}'} \quad (2.17)$$

is a bounded continuous solution of (2.9) and, further, that any bounded measurable solution of (2.9) is necessarily given by (2.17).

We now return to (2.8). For $\Delta(k) \neq 0$, the solution (2.17) of (2.9) satisfies the relation

$$\psi(\mathbf{k};\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi}\int d\mathbf{x}'\psi(\mathbf{k};\mathbf{x}')\int d\mathbf{x}''\, \frac{e^{ik|\mathbf{x}-\mathbf{x}''|}}{|\mathbf{x}-\mathbf{x}''|}V(\mathbf{x}'',\mathbf{x}'). \quad (2.18)$$

Making use of the boundedness of $\psi(\mathbf{k};\mathbf{x})$, we may change the order of integrations and obtain (2.8). Conversely, suppose $\Delta(k) \neq 0$ and that $\psi(\mathbf{k};\mathbf{x})$ is a bounded measurable solution of (2.8). Then again we may change the order of integrations and obtain (2.9). Hence $\psi(\mathbf{k};\mathbf{x})$ is given by (2.17).

C. The functions $\Delta(k)$ and $\Delta(k; x, x', \cos\nu)$

1. The function $\Delta(k)$

From (2.6) and (2.7), we see that we may define $\Delta_n(k)$, for $\mathrm{Im}\, k > -\gamma$, by (2.10).

We consider $\mathrm{Im}\, k \geq -(\gamma - \epsilon)$, $\gamma \geq \epsilon > 0$. We have

$$|A(k;x,x',\cos\nu)| \leq N(\epsilon)e^{(\gamma-\epsilon)x}. \tag{2.19}$$

The integral in (2.10) is uniformly convergent in $\mathrm{Im}\, k > -(\gamma - \epsilon)$, and is therefore holomorphic in k in this region. We also have, for k in this region, the inequality

$$|\Delta_n(k)| \leq N(\epsilon)^n M(\epsilon)^n n^{n/2}, \qquad M(\epsilon) = \int d\mathbf{x}\frac{e^{-\epsilon x}}{x^\alpha}, \quad x = |\mathbf{x}|. \tag{2.20}$$

Hence

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta_n(k)$$

is uniformly convergent in $\mathrm{Im}\, k \geq -(\gamma - \epsilon)$, and the sum

$$\Delta(k) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta_n(k) \tag{2.21}$$

is holomorphic in $\mathrm{Im}\, k > -(\gamma - \epsilon)$, for all $\gamma \geq \epsilon > 0$, and therefore holomorphic in $\mathrm{Im}\, k > -\gamma$.

From (2.5), we have

$$K(-k^*;\mathbf{x},\mathbf{x}') = K(k;\mathbf{x},\mathbf{x}')^*. \tag{2.22}$$

Consequently, from (2.10), now extended to $\mathrm{Im}\, k > -\gamma$, we obtain

$$\Delta_n(-k^*) = \Delta_n(k)^*. \tag{2.23}$$

Hence, from (2.21), we have

$$\Delta(-k^*) = \Delta(k)^*, \quad \mathrm{Im}\, k > -\gamma. \tag{2.24}$$

We have, from (2.20) and (2.21), the following inequality:

$$|\Delta(k)| \leq \text{const}, \quad \mathrm{Im}\, k \geq -(\gamma - \epsilon), \quad \gamma \geq \epsilon > 0. \tag{2.25}$$

By a method of Khuri,[36] and using (2.7), we may demonstrate,[37] for any $\delta > 0$

$$|A(k;x,x',\cos\nu)| < \delta \tag{2.26}$$

for $\mathrm{Im}\, k \geq 0$, $x \geq 0$, $x' > 0$, $1 \geq \cos\nu \geq -1$, for k sufficiently large. Hence we obtain, from (2.21), using Hadamard's theorem,

$$\Delta(k) \underset{|k|\to\infty}{\to} 1, \quad \mathrm{Im}\, k \geq 0. \tag{2.27}$$

2. The function $\Delta(k; x, x', \cos\nu)$

The function $\Delta(k;\mathbf{x},\mathbf{x}')$, defined in (2.13) and (2.15), for $k \geq 0$, $|\mathbf{x}| \geq 0$, $|\mathbf{x}'| > 0$, is a function of $k, x = |\mathbf{x}|$, $x' = |\mathbf{x}'|$, and $\cos\nu$ only, where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$. We have, from (2.4) and (2.13),

$$\Delta_n(k;\mathbf{x},\mathbf{x}') = \int\cdots\int\prod_{i=1}^{n} x_i^2 dx_i \sin\mu_i d\mu_i d\chi_i$$

$$\times \begin{vmatrix} K(k;x,x',\cos\nu) & K(k;x,x_1,\cos\mu_1)\cdots & K(k;x,x_n,\cos\mu_n) \\ K(k;x_1,x',\cos\lambda_1) & K(k;x_1,x_1,1)\cdots & K(k;x_1,x_n,\cos\nu_{1n}) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ K(k;x_n,x',\cos\lambda_n) & K(k;x_n,x_1,\cos\nu_{n1})\cdots & K(k;x_n,x_n,1) \end{vmatrix} = \Delta_n(k;x,x',\cos\nu), \quad n \geq 1, \tag{2.28}$$

$$\cos\lambda_i = \cos\mu_i\cos\nu + \sin\mu_i\sin\nu\cos\chi_i, \qquad \cos\nu_{ij} = \cos\mu_i\cos\mu_j + \sin\mu_i\sin\mu_j\cos(\chi_i - \chi_j). \tag{2.29}$$

We now define $\Delta(k;x,x',\cos\nu)$, for $\mathrm{Im}\, k > -\gamma$, $x \geq 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$, by

$$\Delta(k;x,x',\cos\nu) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Delta_n(k;x,x',\cos\nu), \tag{2.30}$$

with

$$\Delta_0(k;x,x',\cos\nu) = K(k;x,x',\cos\nu), \tag{2.31}$$

and $\Delta_n(k;x,x',\cos\nu)$ given by (2.28), for $n \geq 1$. The series is indeed convergent since by (2.6) and (2.7), we have, for $\mathrm{Im}\, k \geq -(\gamma - \epsilon)$, $\gamma \geq \epsilon > 0$, $x \geq 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$,

$$|\Delta_n(k;x,x',\cos\nu)| \leq N(\epsilon)^{n+1}M(\epsilon)^n(n+1)^{(n+1)/2}e^{(\gamma-\epsilon)x}\,|e^{-\gamma x'}/x'^{\alpha}|. \tag{2.32}$$

The series is, moreover, uniformly convergent in $\mathrm{Im}\, k \geq -(\gamma - \epsilon)$, $\gamma \geq \epsilon > 0$, $a \geq x \geq 0$, $\mathrm{Re}\, x' \geq b$, $1 \geq \cos\nu \geq -1$, for any a and b satisfying $\infty > a > 0$, $\infty > b > 0$.

From the holomorphy of $K(k;x,x',\cos\nu)$ in k and x' in $\mathrm{Im}\, k > -\gamma$, $\mathrm{Re}\, x' > 0$, we find that $\Delta_n(k;x',x',\cos\nu)$ and $\Delta(k;x,x',\cos\nu)$ are holomorphic in k and x', in $\mathrm{Im}\, k > -\gamma$, $\mathrm{Re}\, x' > 0$, for $x \geq 0$, $1 \geq \cos\nu \geq -1$, using the uniform convergence of the series. We also find that $\Delta(k,x,x',\cos\nu)$ is continuous in x, x', and $\cos\nu$, in $x \geq 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$, for $\mathrm{Im}\, k > -\gamma$.

From conditions (A) of the potential and Schwartz reflection principle,[38] we find

$$V(x,x'^*,\cos\nu) = V(x,x',\cos\nu)^* \tag{2.33}$$

for $x > 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$. Hence from (2.22) and (2.28), we have

$$\Delta_n(-k^*;x,x'^*,\cos\nu) = \Delta_n(k;x,x',\cos\nu)^* \tag{2.34}$$

for $\mathrm{Im}\, k > -\gamma$, $x \geq 0$, $\mathrm{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$. Hence, from (2.30) we have

$$\Delta(-k^*;x,x'^*,\cos\nu) = \Delta(k;x,x',\cos\nu)^* \tag{2.35}$$

in the same region of the variables.

Further, we have, from (2.30) and (2.32)

$$|\Delta(k;x,x',\cos\nu)| \leq \text{const} \times e^{(\gamma-\epsilon)x}|e^{-\gamma x'}/x'^{\alpha}| \tag{2.36}$$

for $\text{Im } k \geq -(\gamma-\epsilon)$, $\gamma \geq \epsilon > 0$, $x \geq 0$, $\text{Re } x' > 0$, $1 \geq \cos\nu \geq -1$.

D. Zeroes of $\Delta(k)$ and bound states

We shall see that the zeroes of $\Delta(k)$ in $\text{Im } k \geq 0$ are related to the bound states of the system.

We suppose $\Delta(k) = 0$, $\text{Im } k \geq 0$. Following Ref. 35, and using (2.6) and (2.7), we can show that the equation

$$\chi(k;\mathbf{x}) = \int d\mathbf{x}'\, K(k;\mathbf{x},\mathbf{x}')\chi(k;\mathbf{x}') \tag{2.37}$$

has a finite number of bounded measurable solutions.

We can write (2.37) as

$$\chi(k;\mathbf{x}) = \frac{-1}{4\pi}\int d\mathbf{x}'\chi(k;\mathbf{x}')\int d\mathbf{x}''\,\frac{e^{ik|\mathbf{x}-\mathbf{x}''|}}{|x-x''|}\,V(\mathbf{x}'',\mathbf{x}') \tag{2.38}$$

For any such bounded measurable solution $\chi(k;\mathbf{x})$ of (2.37), we may change the order of integrations in (2.38), and obtain

$$\chi(k;\mathbf{x}) = \frac{-1}{4\pi}\int d\mathbf{x}''\,\frac{e^{ik|\mathbf{x}-\mathbf{x}''|}}{|\mathbf{x}-\mathbf{x}''|}\int d\mathbf{x}'\,V(\mathbf{x}'',\mathbf{x}')\chi(k;\mathbf{x}'). \tag{2.39}$$

We know, for $\text{Im } k \geq 0$, $k \neq 0$, from Ref. 18 that $\chi(k;\mathbf{x})$ belongs to $W^{2,2}$, and that

$$\nabla^2\chi(k;\mathbf{x}) + k^2\chi(k;\mathbf{x}) = \int d\mathbf{x}'V(\mathbf{x},\mathbf{x}')\ \chi(k;\mathbf{x}'). \tag{2.40}$$

Hence $\chi(k;\mathbf{x})$ is an eigenfunction of the Hamiltonian operator, and is a bound state solution. As the Hamiltonian operator for our system is self-adjoint, the eigenvalues $\hbar^2k^2/2m$ must be real. Hence the zeroes of $\Delta(k)$, in $\text{Im } k \geq 0$, $k \neq 0$, lead to bound states of the system, and can only lie on the real axis or the upper imaginary axis. We note that for nonlocal potentials, positive energy bound states can occur.

We now suppose that $\chi(k;\mathbf{x})$ is a bound state solution, i.e., $\chi(k;\mathbf{x})$ is an eigenfunction of the Hamiltonian operator. Then $\chi(k;\mathbf{x})$ belongs to $W^{2,2}$ and satisfies (2.40), and, from the self-adjointness of the Hamiltonian, k is real or pure imaginery. We may restrict ourselves to $k \geq 0$, or $k = i\kappa$, $\kappa > 0$.

As shown in Ref. 18, $\chi(k;\mathbf{x})$ necessarily satisfies (2.39). Hence we have

$$|\chi(k;\mathbf{x})| \leq \text{const} \times \int d\mathbf{x}''\,\frac{1}{|\mathbf{x}-\mathbf{x}''|}\,\frac{e^{-\gamma x''}}{x''^{\alpha}}\int d\mathbf{x}'\,\frac{e^{-\gamma x'}}{x'^{\alpha}}$$

$$\times|\chi(k;\mathbf{x}') \leq \text{const}, \quad x' = |\mathbf{x}'|, x'' = |\mathbf{x}''|, \tag{2.41}$$

where the integral $\int d\mathbf{x}'(e^{-\gamma x'}/x'^{\alpha})|\chi(k;\mathbf{x}')|$ exists as both $e^{-\gamma x'}/x'^{\alpha}$ and $\chi(k;\mathbf{x}')$ belong to L^2. Hence, by a change of the order of integrations, we find that $\chi(k;\mathbf{x})$ is a bounded measurable solution of (2.37). Further, from (2.39) and the boundedness of $\chi(k;\mathbf{x})$, we find that $\chi(k;\mathbf{x})$ is continuous in $\mathbf{x}$.[33]

We can show, again following Ref. 35 and using (2.6) and (2.7), that (2.37) has a bounded continuous solution only if $\Delta(k) = 0$. Hence a bound state solution leads to $\Delta(k) = 0$.

We note that, as $\Delta(k)$ is holomorphic in $\text{Im } k > -\gamma$ and not identically zero, its zeroes in $\text{Im } k > -\gamma$ are isolated ones with no finite accumulation point in $\text{Im } k > -\gamma$. And as $\Delta(k) \to 1$ as $|k| \to \infty$, in $\text{Im } k \geq 0$ [(2.27)], the number of zeroes of $\Delta(k)$ in $\text{Im } k \geq 0$ is finite. Hence the number of bound state is finite.

It will be of interest to show that the bound state eigenfunctions $\chi(k;\mathbf{x})$ are twice continuously differentiable at $|\mathbf{x}| > 0$.

E. The scattering amplitude for physical scattering angle

The scattering amplitude for scattering through angle θ, $\pi \geq \theta \geq 0$, for $k > 0$, is defined as

$$F(k;\cos\theta) = \frac{-1}{4\pi}\int d\mathbf{x}e^{-i\mathbf{k}'\cdot\mathbf{x}}\int d\mathbf{x}'V(\mathbf{x},\mathbf{x}')\psi(\mathbf{k},\mathbf{x}'), \tag{2.42}$$

where $\mathbf{k} = k\hat{k}$, $\mathbf{k}' = k\hat{k}'$, $\hat{k}$ and $\hat{k}'$ are real unit vectors with $\hat{k}\cdot\hat{k}' = \cos\theta$, and $\psi(\mathbf{k},\mathbf{x}')$ is given by (2.17). We have

$$F(k;\cos\theta) = \frac{-1}{4\pi}\iint d\mathbf{x}d\mathbf{x}'e^{-ik\hat{k}'\cdot\mathbf{x}}V(x,x',\cos\nu)e^{ik\hat{k}\cdot\mathbf{x}'}$$

$$-\frac{1}{4\pi}\iiint d\mathbf{x}d\mathbf{x}'d\mathbf{x}''e^{-ik\hat{k}'\cdot\mathbf{x}}V(x,x',\cos\nu)\,\frac{\Delta(k;x',x'',\cos\lambda)}{\Delta(k)}$$

$$\times e^{ik\hat{k}\cdot\mathbf{x}''} \tag{2.43}$$

where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$ and λ is the angle between $\mathbf{x}'$ and $\mathbf{x}''$.

Equation (2.43) enables us to define the scattering amplitude $F(k;\cos\theta)$ for k and $\cos\theta$ in $|\text{Im } k| < \gamma$, $\Delta(k) \neq 0$, and $1 \geq \cos\nu \geq -1$. We can show that it is holomorphic in k in $|\text{Im } k| < \gamma$, $\Delta(k) \neq 0$, for $1 \geq \cos\theta \geq -1$. Indeed, we have

$$F(k;\cos\theta) = F^{(1)}(k;\cos\theta) + F^{(2)}(k;\cos\theta)/\Delta(k), \tag{2.44}$$

where $F^{(1)}(k;\cos\theta)$ and $F^{(2)}(k;\cos\theta)$ are holomorphic in k in $|\text{Im } k| < \gamma$, for $1 \geq \cos\theta \geq -1$. Further, $F^{(1)}(k;\cos\theta)$ and $F^{(2)}(k;\cos\theta)$ are continuous in $\cos\theta$ in $1 \geq \cos\theta \geq -1$ for $|\text{Im } k| < \gamma$.

If we use the following expansion, for $k > 0$ and $\Delta(k) \neq 0$,

$$F(k;\cos\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[S_l(k)-1]P_l(\cos\theta), \tag{2.45}$$

where[15,17] $S_l(k) = 1 + 2iT_l(k) = e^{2i\delta_l(k)}$, $\delta_l(k)$ being the real lth phase shift,[15,17] and the result[17]

$$|T_l(k)| \leq (G/\sqrt{k})l^{-1}e^{-(\beta-\epsilon)l}(1-\beta^2)^{-1/2}, \quad \text{any } \epsilon > 0, \tag{2.46}$$

for $l > L$, where $\cosh\beta = 1 + 2\gamma^2/k^2$, $\beta > 0$, and G and L are constants, we find that $F(k;\cos\theta)$ is bounded as $k \to k_0$, along the positive real axis, where $k_0 > 0$ and $\Delta(k_0) = 0$, and

$$F(k;\cos\theta) \underset{k\to 0}{=} O(1/\sqrt{k}).$$

Hence from the holomorphy of $F^{(1)}(k;\cos\theta)$, $F^{(2)}(k;\cos\theta)$, and $\Delta(k)$ in k in $|\text{Im } k| < \gamma$, we conclude that $F(k;\cos\theta)$ is defined and is holomorphic in a neighborhood of the positive real axis of k, and using the relation $F(-k;\cos\theta) = F(k;\cos\theta)^*$, $k \geq 0$, which we may derive from (2.24), (2.35), and (2.43), we find that $F(k;\cos\theta)$ is defined and is holomorphic in a neighborhood of the whole real axis of k, for $1 \geq \cos\theta \geq -1$.

The same conclusion is reached if we do not use (2.45). Since the Hamiltonian operator H is self-adjoint, the

evolution operator $e^{-iHt/\hbar}$ is unitary; hence probability is conserved. Consequently, from the asymptotic behaviour of a suitable wavepacket,[2,3] from Taylor expansions of $F^{(2)}(k;\cos\theta)$ and $\Delta(k)$ about k_0, where $k_0 \geq 0$, $\Delta(k_0) = 0$, and from the continuity of $F^{(2)}(k;\cos\theta)$ in $\cos\theta$, we arrive at the holomorphy of $F(k;\cos\theta)$ in a neighborhood of the positive real axis of k.

3. ANALYTIC CONTINUATION OF THE FORWARD SCATTERING AMPLITUDE AND A FORWARD DISPERSION RELATION

A. Analytic continuation of the forward scattering amplitude

From (2.43), we obtain, for $|\mathrm{Im}\ k| < \gamma$, $\Delta(k) \neq 0$, the following expression for the forward scattering amplitude:

$$F(k) = F^{(1)}(k) + F^{(2)}(k)/\Delta(k), \tag{3.1}$$

where $F(k) = F(k;\cos\theta = 1)$, and

$$F^{(1)}(k) = \iiint \sin\theta\, d\theta d\varphi\, \sin\theta' d\theta' d\varphi' \times \int_0^\infty dx\, x^2 e^{-ikx\cos\theta} \frac{e^{-\gamma x}}{x^\alpha} \times \int_0^\infty dx'\, x'^2 \tilde{V}(x,x',\cos\nu) \frac{e^{-\gamma x'}}{x'^\alpha} e^{ikx'\cos\theta'}, \tag{3.2}$$

$$F^{(2)}(k) = \iiiint \sin\theta d\theta d\varphi\, \sin\theta' d\theta' d\varphi'\, \sin\theta'' d\theta'' d\varphi'' \times \int_0^\infty dx\, x^2 e^{-ikx\cos\theta} \frac{e^{-\gamma x}}{x^\alpha} \times \int_0^\infty dx'\, x'^2 \tilde{V}(x,x',\cos\nu) \frac{e^{-\gamma x'}}{x'^\alpha} \times \int_0^\infty dx''\, x''^2\, \Delta(k;x',x'',\cos\lambda)\, e^{ikx''\cos\theta''} \tag{3.3}$$

with

$$\cos\nu = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi'),$$
$$\cos\lambda = \cos\theta'\cos\theta'' + \sin\theta'\sin\theta''\cos(\varphi' - \varphi'').$$

We now analytically continue $F(k)$ to a function holomorphic in $\mathrm{Im}\ k > -\gamma$, for $\Delta(k) \neq 0$, and $k \neq i\kappa$ where $\kappa \geq \gamma$.

We consider, for $k = i\kappa$, $\gamma > \kappa > -\gamma$, the function

$$h(k;x,\cos\nu,\cos\theta') = \int_0^\infty dx'\, x'^2 \tilde{V}(x,x',\cos\nu) \frac{e^{-\gamma x'}}{x'^\alpha} e^{ikx'\cos\theta'}. \tag{3.4}$$

We write

$$h(i\kappa;x,\cos\nu,\cos\theta') = \int_0^\infty dx' p(i\kappa;x,x',\cos\nu,\cos\theta'), \tag{3.5}$$

$$p(i\kappa;x,x',\cos\nu,\cos\theta') = x'^2 \tilde{V}(x,x',\cos\nu) \frac{e^{-\gamma x'}}{x'^\alpha} e^{-\kappa x'\cos\theta'}. \tag{3.6}$$

We have

$$h(i\kappa;x,\cos\nu,\cos\theta') = \lim_{\epsilon\to 0+} \lim_{R\to\infty} \int_\epsilon^R dx' p(i\kappa;x,x',\cos\nu,\cos\theta'). \tag{3.7}$$

From condition (A3) on the potential, we see that $p(i\kappa;x,x',\cos\nu,\cos\theta')$ is holomorphic in x' in $\mathrm{Re}\ x' > 0$, and we may write

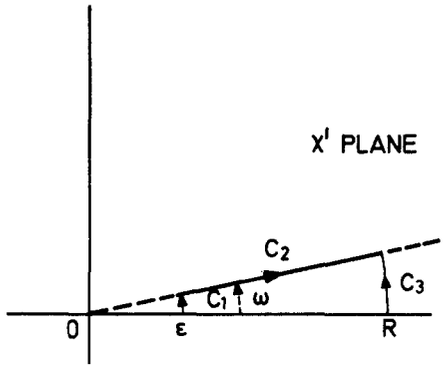

FIG. 1.

$$h(i\kappa;x,\cos\nu,\cos\theta') = \lim_{\epsilon\to 0+} \lim_{R\to\infty} \left\{ \int_{C_1} + \int_{C_2} - \int_{C_3} \right\} dx' \times p(i\kappa;x,x',\cos\nu,\cos\theta') \quad \text{(Fig. 1)}, \tag{3.8}$$

where C_1 and C_3 are circular arcs of angle ω, $\pi/2 > \omega > -\pi/2$.

Again from condition (A3) on the potential, we find

$$\lim_{\epsilon\to 0+} \int_{C_1} dx' p(i\kappa;x,x',\cos\nu,\cos\theta') = 0, \tag{3.9}$$

$$\lim_{R\to 0} \int_{C_3} dx' p(i\kappa;x,x',\cos\nu,\cos\theta') = 0. \tag{3.10}$$

Hence, we have

$$h(i\kappa;x,\cos\nu,\cos\theta') = \lim_{\epsilon\to 0+} \lim_{R\to\infty} \int_{C_2} dx' p(i\kappa;x,x',\cos\nu,\cos\theta') = \int_0^\infty d|x'|\, e^{i\omega} p(i\kappa;x,|x'|e^{i\omega},\cos\nu,\cos\theta'). \tag{3.11}$$

For $\gamma > \kappa > -\gamma$, $h(i\kappa;x,\cos\nu,\cos\theta')$ is holomorphic in x in $\mathrm{Re}\ x > 0$ and, for fixed κ, is a bounded function of x, $\cos\nu$, and $\cos\theta'$. Hence we may apply the same change of contour of integration to the integral,

$$\int_0^\infty dx\, x^2 e^{\kappa x\cos\theta} \frac{e^{-\gamma x}}{x^\alpha} h(i\kappa;x,\cos\nu,\cos\theta'),$$

and obtain

$$\int_0^\infty dx\, x^2 e^{\kappa x\cos\theta} \frac{e^{-\gamma x}}{x^\alpha} h(i\kappa;x,\cos\nu,\cos\theta') = \int_0^\infty d|x|\, |x|^2 e^{3i\omega} e^{\kappa|x|e^{i\omega}\cos\theta} \times \frac{e^{-\gamma|x|e^{i\omega}}}{|x|^\alpha e^{i\alpha\omega}} h(i\kappa;|x|e^{i\omega},\cos\nu,\cos\theta'). \tag{3.12}$$

Hence we arrive at, for $\gamma > \kappa > -\gamma$,

$$F^{(1)}(i\kappa) = F^{(1)\omega}(i\kappa), \tag{3.13}$$

where

$$F^{(1)\omega}(k) = \iiint \sin\theta\, d\theta d\varphi\, \sin\theta' d\theta' d\varphi' \times \int_0^\infty d|x|\, |x|^2 e^{3i\omega} e^{-ik|x|e^{i\omega}\cos\theta} \frac{e^{-\gamma|x|e^{i\omega}}}{|x|^\alpha e^{i\alpha\omega}} \times \int_0^\infty d|x'|\, |x'|^2 e^{3i\omega} \tilde{V}(|x|e^{i\omega}, |x'|e^{i\omega},\cos\nu) \frac{e^{-\gamma|x'|e^{i\omega}}}{|x'|^\alpha e^{i\alpha\omega}} e^{ik|x'|e^{i\omega}\cos\theta'} \tag{3.14}$$

is defined in the strip $|\mathrm{Im}\ ke^{i\omega}| < \gamma\cos\omega$, which is the strip $|\mathrm{Im}\ k| < \gamma\cos\omega$ rotated through ω in the clockwise direction about the origin (Fig. 2), from condition (A3)

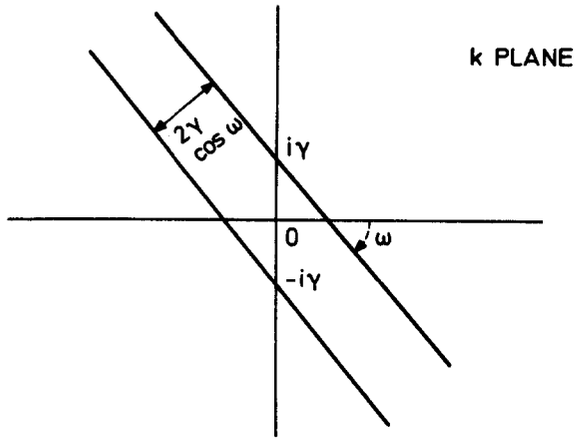

FIG. 2.

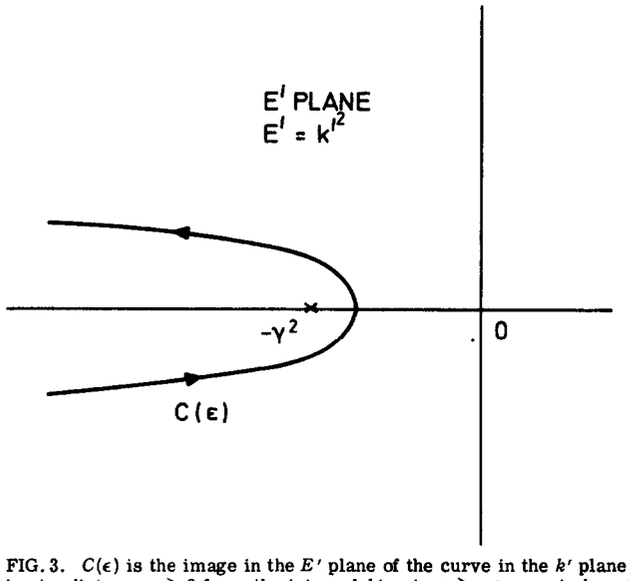

FIG. 3. $C(\epsilon)$ is the image in the E' plane of the curve in the k' plane which is at a distance $\epsilon > 0$ from the interval $k' = i\kappa, \infty > \kappa \geq \gamma$. ϵ is less than γ and is sufficiently small so that all E_i are on the right of $C(\epsilon)$. It coincides with part of a parabola for Re $E' \leq -(\gamma^2 - \epsilon^2)$.

on the potential. Further, $F^{(1)\omega}(k)$ is holomorphic in the strip $|\text{Im } ke^{i\omega}| < \gamma \cos\omega$.

Hence we have continued $F^{(1)}(k)$, originally defined and holomorphic in $|\text{Im } k| < \gamma$, to a function holomorphic in $|\text{Im } ke^{i\omega}| < \gamma \cos\omega$ as well, for any ω in the interval $\pi/2 > \omega > -\pi/2$. Since the union of all strips $|\text{Im } ke^{i\omega}| < \gamma \cos\omega$ is the whole k plane cut from $i\gamma$ to $i\infty$ and from $-i\gamma$ to $-i\infty$, we have continued $F^{(1)}(k)$ to a function holomorphic in this cut plane. We denote this function by $F^{(1)}(k)$ also:

$$F^{(1)}(k) = F^{(1)\omega}(k), \quad |\text{Im } ke^{i\omega}| < \gamma \cos\omega. \tag{3.15}$$

Using condition (A3) on the potential, the holomorphy of $\Delta(k;x',x'', \cos\lambda)$ in k and x'', in Im $k > -\gamma$, Re $x'' > 0$, for $x' \geq 0, 1 \geq \cos\lambda \geq -1$, and (2.36), we find that $F^{(2)}(k)$ can be similarly continued to a function holomorphic in Im $k > -\gamma$, cut from $i\gamma$ to $i\infty$. We denote this function by $F^{(2)}(k)$ also. We have the following representation for $F^{(2)}(k)$ in Im $k > -\gamma$, $|\text{Im } ke^{i\omega}| < \gamma \cos\omega$:

$$F^{(2)}(k) = \iiiint \sin\theta d\theta d\varphi \sin\theta' d\theta' d\varphi' \sin\theta'' d\theta'' d\varphi''$$
$$\times \int_0^\infty d|x| \; |x|^2 e^{3i\omega} e^{-ik|x|e^{i\omega}\cos\theta} \frac{e^{-\gamma|x|e^{i\omega}}}{|x|^\alpha e^{i\alpha\omega}}$$
$$\times \int_0^\infty dx' \, x'^2 \tilde{V}(|x|e^{i\omega}, x', \cos\nu) \frac{e^{-\gamma x'}}{x'^\alpha}$$
$$\times \int_0^\infty d|x''| \; |x''|^2 e^{3i\omega} \Delta(k;x', |x''|e^{i\omega}, \cos\lambda) e^{ik|x''|e^{i\omega}\cos\theta''}. \tag{3.16}$$

Hence $F(k)$ can be continued to a function holomorphic in Im $k > -\gamma$, perhaps with the exception of poles at the nonreal zeroes of $\Delta(k)$, and cut from $i\gamma$ to $i\infty$. We denote this function by $F(k)$ also. We have, for k in this region,

$$F(k) = F^{(1)}(k) + F^{(2)}(k)/\Delta(k). \tag{3.17}$$

B. Symmetry, asymptotic behavior, and dispersion relations for the forward scattering amplitude

From the reality of the potential $V(x,x', \cos\nu)$, for $x > 0$, $x' > 0$, and from the Schwartz reflection principle,[38,39] we obtain

$$V(x^*,x'^*, \cos\nu) = V(x,x', \cos\nu)^* \tag{3.18}$$

for Re $x > 0$, Re $x' > 0$, $1 \geq \cos\nu \geq -1$. Hence, from (3.14), we have

$$F^{(1)\omega}(-k^*) = F^{(1)\omega}(k)^*. \tag{3.19}$$

Hence, from (3.15), we obtain

$$F^{(1)}(-k^*) = F^{(1)}(k)^* \tag{3.20}$$

in the whole k plane cut from $i\gamma$ to $i\infty$ and from $-i\gamma$ to $-i\infty$. Similarly, using (2.35), (3.16) and (3.18), we obtain

$$F^{(2)}(-k^*) = F^{(2)}(k)^* \tag{3.21}$$

in Im $k > -\gamma$ cut from $i\gamma$ to $i\infty$. Hence, using (2.24), we have the following symmetry property:

$$F(-k^*) = F(k)^*. \tag{3.22}$$

We now study the asymptotic behavior of $F(k)$. From (2.27), (2.36), (3.15), and (3.16) and using a theorem on Laplace transform,[40] we immediately obtain, for $k = |k|e^{-i\omega}$, $0 \geq \omega > -\pi/2$ and $k = -|k|e^{-i\omega}$, $\pi/2 > \omega \geq 0$, and for $|k|$ sufficiently large,

$$|F(k)| \leq \text{const} / \cos^{(6-2\alpha)}\omega \tag{3.23}$$

for all such ω. Since $|\text{Re } k| = |k||\cos\omega|$, we have, for Im $k \geq 0$ and for $|k|$ sufficiently large,

$$|F(k)| \leq \text{const} \; (|k|/|\text{Re } k|)^{6-2\alpha}, \tag{3.24}$$

where $\frac{3}{2} > \alpha \geq 0$.

From the holomorphy property, the above asymptotic behavior, and the symmetry property of $F(k)$ in Im $k \geq 0$, we obtain the following substracted dispersion relation for $f(E) = F(k)$:

$$f(E) = \sum_{i=0}^{p} d_i (E - E_S)^i + (E - E_S)^{p+1} \sum_{i=1}^{I} \sum_{j=1}^{J_i} \frac{dij}{(E - E_i)^j}$$
$$+ \frac{(E - E_S)^{p+1}}{\pi} \int_0^\infty dE' \frac{\text{Im } [f(E')]}{(E' - E_S)^{p+1}} \frac{1}{E' - E}$$
$$- \frac{(E - E_S)^{p+1}}{2\pi i} \int_{C(\epsilon)} dE' \frac{f(E')}{(E' - E_S)^{p+1}} \frac{1}{E' - E},$$
$$E = k^2 \quad \text{(Fig. 3)}. \tag{3.25}$$

Here $E \neq E_i, E$ is not on the cut from 0 to ∞ and is on the right of the contour $C(\epsilon)$, the E_i are negative bound state energies which are greater than $-\gamma^2, E_S$ is a constant $\neq E_i$, for all E_i, and not on the cut from 0 to ∞, and on the right of $C(\epsilon)$, d_i and d_{ij} are constants, and $p = 3 - \alpha$, if the latter is an integer, and is the integer smaller than and nearest to $3 - \alpha$ otherwise. The limit $\epsilon \to 0$ may be taken.

The physical amplitude at $E > 0$ is

$$f(E) = \lim_{\epsilon \to 0+} f(E + i\epsilon). \tag{3.26}$$

The number of subtractions is reduced to one, in the above dispersion relation, if instead of the contour $C(\epsilon)$ we use the contour $C'(\epsilon)$ (Fig. 4).

If we assume conditions (B) as well, then we get, using (2.27), (3.15) and (3.16) and using integration by parts in the $\cos\theta$ variable, the result

$$|F(k)| \leq \text{const}/|k|, \quad \text{Im } k \geq 0 \tag{3.27}$$

for $|k|$ sufficiently large.

We note that, in obtaining (3.27), we have also used the following relationship:

$$|\Delta(k; x, x', \cos\nu)| \leq \text{const } |e^{-\gamma x'}/x'^{\alpha}|(1 + |x'|)^{-(3+\beta-\alpha)} \tag{3.28}$$

for Im $k \geq 0$, $x \geq 0$, Re $x' > 0$, $1 \geq \cos\nu \geq -1$, which may be derived from (2.5), (2.30), and using conditions (B).

Hence for potentials satisfying both conditions (A) and (B), we may write an unsubstrated dispersion relation for $f(E)$:

$$f(E) = \sum_{i=1}^{I} \sum_{j=1}^{J_i} \frac{d_{ij}}{(E - Ei)^j} + \frac{1}{\pi} \int_0^{\infty} dE' \frac{\text{Im}\,[f(E')]}{E' - E} - \frac{1}{2\pi i} \int_{C''(\epsilon)} \frac{f(E')}{E' - E} \quad \text{(Fig. 5)} \tag{3.29}$$

with E on the right of $C''(\epsilon)$, not on the cut from 0 to ∞, and $E \neq E_i$, for all E_i. The limit $\epsilon \to 0$ may be taken.

We note that for a potential satisfying conditions (A), with $\alpha = 0, \frac{1}{2}, 1$, and with $\tilde{V}(x, x', \cos\nu)$ of the following form,

$$\tilde{V}(x, x', \cos\nu) = \sum_{l=0}^{L} P_l(\cos\nu) \sum_{p,q=1}^{N_l} C_{lpq} e^{-\gamma_{lp} x} e^{-\gamma_{lq} x'},$$

$$\gamma_{lp} \geq 0, \ \min \gamma_{lp} = 0, \ C_{lpq} \text{ real}, \ C_{lpq} = C_{lqp}, \tag{3.30}$$

we can carry out the integrations in the radial variables first in (3.2) and (3.3), thereby obtaining the analytic continuation of $F(k)$, defined and holomorphic in $|\text{Im } k| < \gamma$, perhaps with the exception of poles at the nonreal zeroes of $\Delta(k)$, to a function holomorphic in Im $k > -\gamma$, perhaps with the exception of poles at the nonreal zeroes of $\Delta(k)$, and poles or branch points at $k = i(\gamma + \gamma_{lp})$. Indeed, for $\alpha = 0, 1$, $\tilde{V}(x, x', \cos\nu) =$ const, $F(k)$ has a pole at $k = i\gamma$, and for $\alpha = \frac{1}{2}$, $\tilde{V}(x, x', \cos\nu) =$ const, $F(k)$ has a branch point at $k = i\gamma$ and approaches infinity as k approaches $i\gamma$.

Further, for $\tilde{V}(x, x', \cos\nu)$ of the form (3.30), we obtain, using (2.27) and the relations

$$|(\gamma + \gamma_{lp}) \pm ik\cos\theta|^{-1}$$

$$= [(\gamma + \gamma_{lp})^2 \mp 2(\text{Im } k)(\gamma + \gamma_{lp})\cos\theta + |k|^2]^{-1/2}$$

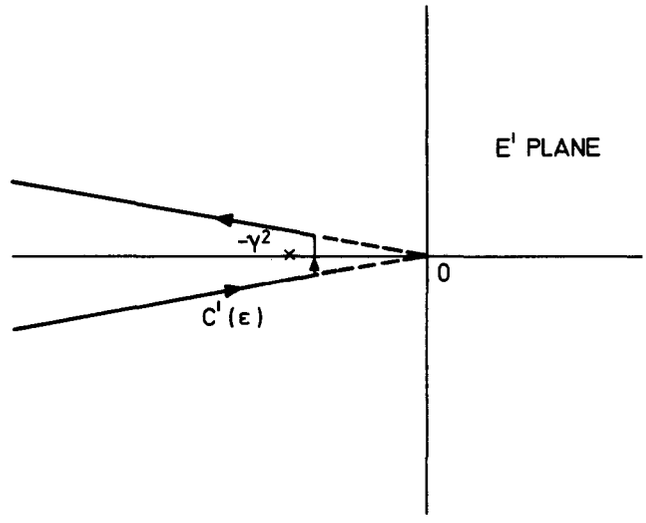

FIG. 4. $C'(\epsilon)$ is the curve consisting of parts of the two half-lines each at an angle $\epsilon > 0$ with the negative real axis and on the left of the imaginary axis, and part of a straight line parallel to the imaginary axis and at a distance $\gamma^2\epsilon/2$ to the right of $E' = -\gamma^2$. ϵ is less than $\pi/2$ and is sufficiently small so that all E_i are on the right of $C'(\epsilon)$.

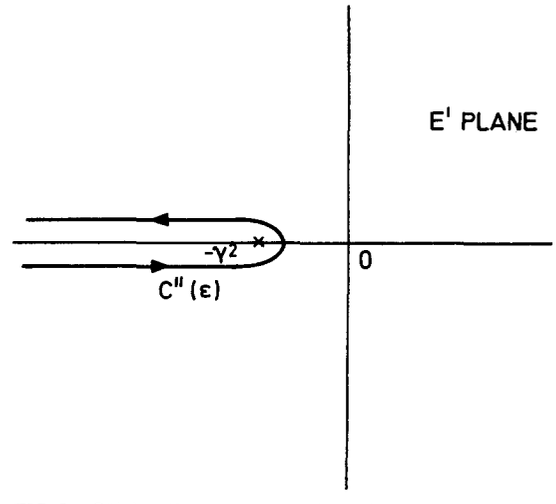

FIG. 5. $C''(\epsilon)$ is the curve consisting of all points at a distance $\epsilon > 0$ from the interval $-\gamma^2 \geq E' > -\infty$. ϵ is less than γ^2 and is sufficiently small so that all E_i are on the right of $C''(\epsilon)$.

$$= |k|^{-1}\{1 + [(\gamma + \gamma_{lp})^2 \mp 2(\text{Im } k)(\gamma + \gamma_{lp}) \times \cos\theta]/|k|^2\}^{-1/2} \tag{3.31}$$

the following asymptotic behavior for $|k|$ sufficiently large:

$$|F(k)| \leq \text{const}/|k|^{6-2\alpha}, \quad \alpha = 0, \tfrac{1}{2}, 1, \ \text{Im } k \geq 0 \tag{3.32}$$

and we obtain an unsubtracted dispersion relation for $f(E)$ of the form (3.29).

We now consider potentials satisfying conditions (A) with $\alpha = 0, \frac{1}{2}, 1$, and $\tilde{V}(x, x', \cos\nu)$ satisfying condition (C)[41]:

$$\text{(C)} \quad \tilde{V}(x, x', \cos\nu) = \int_0^{\infty} \int_0^{\infty} d\beta d\beta' \, e^{-\beta x} e^{-\beta' x'} \sigma(\beta, \beta', \cos\nu),$$

$$\text{Re } x > 0, \quad \text{Re } x' > 0, \quad 1 \geq \cos\nu \geq -1, \tag{3.33}$$

where $\sigma(\beta, \beta', \cos\nu)$ satisfies the following:

(i) $\sigma(\beta, \beta', \cos\nu)$ is real, $\sigma(\beta, \beta', \cos\nu) = \sigma(\beta', \beta, \cos\nu)$.
(ii) $\sigma(\beta, \beta', \cos\nu)$ is continuous in all its variables in $\infty > \beta \geq 0$, $\infty > \beta' \geq 0$, $1 \geq \cos\nu \geq -1$, and in this region

$$|\sigma(\beta,\beta',\cos\nu)| \leq \sum(\beta,\beta') \leq \text{const},$$

where $\Sigma(\beta,\beta')$ is continuous in its variables in $\infty > \beta \geq 0$, $\infty > \beta' \geq 0$, and satisfies $\Sigma(\beta,\beta') = \Sigma(\beta',\beta)$, and

$$\int_0^\infty \int_0^\infty d\beta d\beta' \sum(\beta,\beta') < \infty,$$

$$\int_0^\infty d\beta \sum(\beta,\beta') \leq \text{const}.$$

We obtain, for[42] $\text{Im}\, k \geq -(\gamma-\epsilon)$, $\gamma \geq \epsilon > 0$, $x \geq 0$, $\text{Re}\, x' > 0$, $1 \geq \cos\nu \geq -1$,

$$K(k;x,x',\cos\nu) = \frac{e^{-\gamma x'}}{x'^{\alpha}} \int_0^\infty d\beta'\, e^{-\beta' x'} \rho_0(k;x,\beta',\cos\nu), \tag{3.34}$$

$$\Delta(k;x,x',\cos\nu) = \frac{e^{-\gamma x'}}{x'^{\alpha}} \int_0^\infty d\beta'\, e^{-\beta' x'} \rho(k;x,\beta',\cos\nu), \tag{3.35}$$

where $\rho_0(k;x,\beta',\cos\nu)$ and $\rho(k;x,\beta',\cos\nu)$ are continuous in $x, \beta', \cos\nu$, in $x \geq 0$, $\infty > \beta' \geq 0$, $1 \geq \cos\nu \geq -1$, and satisfy[42]

$$|\rho_0(k;x,\beta',\cos\nu)| \leq \text{const} \times e^{(\gamma-\epsilon)x} \int_0^\infty d\beta''\, \Sigma(\beta'',\beta'), \tag{3.36}$$

$$|\rho(k;x,\beta',\cos\nu)| \leq \text{const} \times e^{(\gamma-\epsilon)x} \int_0^\infty d\beta''\, \Sigma(\beta'',\beta'). \tag{3.37}$$

We now carry out the integrations in the radial variables first in (3.2) and (3.3), making use of (3.35) and (3.37). We obtain

$$|F^{(1)}(k)| \leq \text{const} \times I_\alpha^{(+)}(k) I_\alpha^{(-)}(k), \tag{3.38}$$

$$|F^{(2)}(k)| \leq \text{const} \times I_\alpha^{(+)}(k) I_\alpha^{(-)}(k), \tag{3.39}$$

$$\alpha = 0, \tfrac{1}{2}, 1, \qquad \text{Im}\, k \geq -(\gamma-\epsilon), \qquad \gamma \geq \epsilon > 0,$$

with

$$I_\alpha^{(\pm)}(k) = \int_{-1}^{+1} d\cos\theta \int_0^\infty d\beta \frac{1}{|(\gamma+\beta) \pm ik\cos\theta|^{3-\alpha}}$$

$$= \int_{-1}^{+1} d\cos\theta \int_0^\infty d\beta \times \frac{1}{[|k|^2 \mp 2k_2(\gamma+\beta)\cos\theta + (\gamma+\beta)^2]^{(3-\alpha)/2}} \tag{3.40}$$

where $k_1 = \text{Re}\, k \neq 0$, $k_2 = \text{Im}\, k \neq 0$. We have[43]

$$|I_0^{(\pm)}(k)| = \int_{-1}^{+1} d\cos\theta \frac{1}{(|k|^2 - k_2^2\cos^2\theta)} \times \left(1 + \frac{k_2\cos\theta - \gamma}{(|k|^2 \mp 2k_2\gamma\cos\theta + \gamma^2)^{1/2}}\right)$$

$$\leq \text{const} \times \int_{-1}^{+1} d\cos\theta \frac{1}{|k|^2 - k_2^2\cos^2\theta}, \qquad |k| \gg \gamma, \tag{3.41}$$

$$\therefore |I_0^{(\pm)}(k)| \leq \frac{\text{const}}{|k||k_2|} \ln\frac{|k|+|k_2|}{|k|-|k_2|}, \qquad |k| \gg \gamma.$$

Using

$$\ln(1+\xi) < \xi, \qquad 0 < \xi < 1,$$

$$|\ln(1-\xi)| \leq 1/(1-\xi)^\eta, \qquad 0 \leq \xi < 1, \text{ any } \eta > 0,$$

and

$$|k| - |k_2| = (|k|^2 - |k_2|^2)/(|k| + |k_2|) > |k_1|^2/2|k|,$$

we obtain, for $|k| \gg \gamma$,

$$|I_0^{(\pm)}(k)| \leq \frac{\text{const}}{|k|^2} + \frac{\text{const}}{|k|^{1-2\eta}} \frac{1}{|k_2|} \frac{1}{|k_1|^{2\eta}},$$

$$\therefore |I_0^{(\pm)}(k)| \leq \frac{\text{const}}{|k|^{1-2\eta}}, \quad \begin{cases} |k_1| \geq a_1 > 0, \\ |k_2| \geq a_2 > 0, \end{cases} \tag{3.42}$$

$$|I_0^{(\pm)}(k)| \leq \frac{\text{const}}{|k|^{1-2\eta}} \frac{1}{|k_1|^{2\eta}}, \quad \begin{cases} a_1 > |k_1| > 0, \\ |k| \gg a_1, \end{cases} \tag{3.43}$$

and a_1 and a_2 are constants. Further, from (3.41), we have

$$|I_0^{(\pm)}(k)| \leq \frac{\text{const}}{|k|^2}, \quad \begin{cases} a_2 > |k_2| > 0, \\ |k| \gg a_2. \end{cases} \tag{3.44}$$

We now consider $I_1^{(\pm)}(k)$. We have[43]

$$|I_1^{(\pm)}(k)| = \int_{-1}^{+1} d\cos\theta \frac{1}{(|k|^2 - k_2^2\cos^2\theta)^{1/2}} \times \left[\frac{\pi}{2} \pm \tan^{-1}\left(\frac{k_2\cos\theta \mp \gamma}{(|k|^2 - k_2^2\cos^2\theta)^{1/2}}\right)\right]$$

$$\leq \int_{-1}^{+1} d\cos\theta \frac{\pi}{(|k|^2 - k_2^2\cos^2\theta)^{1/2}} = \frac{2\pi}{|k_2|} \sin^{-1}\left|\frac{k_2}{k}\right|,$$

$$\therefore |I_1^{(\pm)}(k)| \leq \frac{\text{const}}{|k_2|}, \qquad |k_2| \geq a, \tag{3.45}$$

$$|I_1^{(\pm)}(k)| \leq \frac{\text{const}}{|k|}, \quad \begin{cases} a_2 > |k_2| > 0, \\ |k| \gg a_2. \end{cases} \tag{3.46}$$

Lastly, we consider $I_{1/2}^{(\pm)}(k)$. We have

$$|I_{1/2}^{(\pm)}(k)| = \int_{-1}^{+1} d\cos\theta \int_0^\infty d\beta \frac{1}{X_{(\pm)}^{5/4}}$$

$$= \int_{-1}^{+1} d\cos\theta \int_0^\infty d\beta \frac{1}{X_{(\pm)}^{3/4} X_{(\pm)}^{1/2}}$$

$$\leq \int_{-1}^{+1} d\cos\theta \left(\int_0^\infty d\beta \frac{1}{X_{(\pm)}^{3/2}}\right)^{1/2} \left(\int_0^\infty d\beta \frac{1}{X_{(\pm)}}\right)^{1/2},$$

where

$$X_{(\pm)}(k) = |k|^2 \mp 2k_2(\gamma+\beta)\cos\theta + (\gamma+\beta)^2,$$

$$\therefore |I_{1/2}^{(\pm)}(k)| \leq \text{const} \times \int_{-1}^{+1} d\cos\theta \frac{1}{(|k|^2 - k_2^2\cos^2\theta)^{3/4}}, \qquad |k| \gg \gamma,$$

$$\therefore |I_{1/2}^{(\pm)}(k)| \leq \text{const} \times \left(\int_{-1}^{+1} d\cos\theta\right)^{1/2} \times \left(\int_{-1}^{+1} d\cos\theta \frac{1}{(|k|^2 - k_2^2\cos^2\theta)^{3/2}}\right)^{1/2}.$$

∴ We have[43]

$$|I^{(\pm)}_{1/2}(k)| \leq \frac{\text{const}}{|k|\,|k_1|^{1/2}}, \qquad |k| \gg \gamma. \tag{3.47}$$

For $k_2 = 0$, we have (3.38), (3.39), and (3.40), with

$$|I^{(\pm)}_{\alpha}(k)| \leq \text{const}/|k_1|^{3-\alpha}, \qquad |k_1| \gg \gamma. \tag{3.48}$$

The results (3.42)—(3.48) on $I^{(\pm)}_{\alpha}(k)$, together with (2.27), (3.38), (3.39) and the holomorphy and symmetry properties previously obtained for $F(k)$, enable us to write an unsubtracted dispersion relation for $f(E)$ of the form (3.29) for the class of potentials satisfying conditions (A) and (C), for $\alpha = 0, \frac{1}{2}, 1$.

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APPENDIX A

We now prove (2.26).

We have

$$A(k; x, x', \cos\nu) = \int d\mathbf{x}''\, e^{ik|\mathbf{x}-\mathbf{x}''|}\, Q(\mathbf{x}, \mathbf{x}', \mathbf{x}''),$$
$$x = |\mathbf{x}|, \quad x' = |\mathbf{x}'|, \quad \mathbf{x}\cdot\mathbf{x}' = xx'\cos\nu$$

with

$$Q(\mathbf{x}, \mathbf{x}', \mathbf{x}'') = \frac{1}{|\mathbf{x}-\mathbf{x}''|}\,\frac{e^{-\gamma x''}}{x''^{\alpha}}\,\tilde{V}(\mathbf{x}'', \mathbf{x}'), \qquad x'' = |\mathbf{x}''|.$$

We have

$$\int d\mathbf{x}''\,|Q(\mathbf{x}, \mathbf{x}', \mathbf{x}'')| < \infty.$$

Hence, since $C^1_0(R^3)$ is dense in $L^1(R_3)$, there exists, for every $\delta > 0$, a function $Q_\delta(\mathbf{x}, \mathbf{x}', \mathbf{x}'')$ such that, as a function of $\mathbf{x}''$, $Q_\delta(\mathbf{x}, \mathbf{x}', \mathbf{x}'')$ vanishes outside a sphere with center at the origin $\mathbf{x}'' = 0$, has continuous first derivatives, and satisfies

$$\int d\mathbf{x}''\,|Q(\mathbf{x}, \mathbf{x}', \mathbf{x}'') - Q_\delta(\mathbf{x}, \mathbf{x}', \mathbf{x}'')| < \delta/2.$$

Hence

$$|A(k; x, x', \cos\nu)| \leq \delta/2 + \left|\int d\mathbf{x}''\, e^{ik|\mathbf{x}-\mathbf{x}''|}\, Q_\delta(\mathbf{x}, \mathbf{x}', \mathbf{x}'')\right|.$$

We have

$$\left|\int d\mathbf{x}''\, e^{ik|\mathbf{x}-\mathbf{x}''|}\, Q_\delta(\mathbf{x}, \mathbf{x}', \mathbf{x}'')\right|$$
$$= \left|\int_{-\Delta}^{\Delta} dx_1''\iint dx_2'' dx_3''\, e^{ik|\mathbf{x}-\mathbf{x}''|}\, Q_\delta(\mathbf{x}, \mathbf{x}', \mathbf{x}'')\right.$$
$$\left. + \left\{\int_{-\infty}^{-\Delta} + \int_{\Delta}^{\infty}\right\} dx_1''\iint dx_2'' dx_3''\, e^{ik|\mathbf{x}-\mathbf{x}''|}\, Q_\delta(\mathbf{x}, \mathbf{x}', \mathbf{x}'')\right|$$
$$\leq \Delta\cdot L_1(\mathbf{x}, \mathbf{x}', \delta) + (1/|k|)\, L_2(\mathbf{x}, \mathbf{x}', \delta), \qquad k \neq 0,$$

where $\Delta > 0$, $L_1(\mathbf{x}, \mathbf{x}', \delta) > 0$, $L_2(\mathbf{x}, \mathbf{x}', \delta) > 0$, using integration by parts. Hence, for any $\delta > 0$, we have

$$|A(k; x, x', \cos\nu)| \leq \delta/2 + \Delta\cdot L_1(\mathbf{x}, \mathbf{x}', \delta) + (1/|k|)\, L_2(\mathbf{x}, \mathbf{x}', \delta).$$

From (2.7), we find that

$$|L_1(\mathbf{x}, \mathbf{x}', \delta)| \leq \text{const},$$
$$|L_2(\mathbf{x}, \mathbf{x}', \delta)| \leq \text{const},$$

for all $\mathbf{x}, \mathbf{x}'$, and δ. Hence we may choose Δ so small and $|k|$ so large that

$$|A(k; x, x', \cos\nu)| \leq \delta.$$

APPENDIX B

Here we obtain a result which enables us to give a set of sufficient conditions for $\tilde{V}(x, x', \cos\nu)$ to satisfy condition (C).

We introduce a class of functions $f(z_1; z_2)$ of two complex variables z_1 and z_2, $\mathrm{Re}\, z_1 \geq 0$, $\mathrm{Re}\, z_2 \geq 0$, defined in the following way:

$f(z_1; z_2)$ satisfies the following set of sufficient conditions:

(i) $f(z_1; z_2) = f(z_2; z_1)$.

(ii) $f(z_1; z_2)$ is holomorphic in z_1 in $\mathrm{Re}\, z_1 > 0$, for each z_2 in $\mathrm{Re}\, z_2 \geq 0$.

(iii) $f(z_1; z_2)$ is continuous in z_1 and z_2, in $\mathrm{Re}\, z_1 \geq 0$, $\mathrm{Re}\, z_2 \geq 0$.

(iv) $f(z_1; z_2)$ satisfies the bound:

$$|f(z_1; z_2)| \leq \text{const}/|(1 + z_1)(1 + z_2)|^{1+\lambda}$$

for some $\lambda > 0$, in $\mathrm{Re}\, z_1 \geq 0$, $\mathrm{Re}\, z_2 \geq 0$.

We then have the following result:

(I)

$$f(z_1; z_2) = \int_0^\infty\int_0^\infty d\beta_1 d\beta_2 e^{-\beta_1 z_1} e^{-\beta_2 z_2}\sigma(\beta_1; \beta_2) \tag{B1}$$

for $\mathrm{Re}\, z_1 > 0$, $\mathrm{Re}\, z_2 > 0$, where $\sigma(\beta_1; \beta_2)$ is continuous, bounded, and symmetric in β_1 and β_2, in $\infty > \beta_1 \geq 0$, $\infty > \beta_2 \geq 0$.

Such a representation is unique when the restriction that $\sigma(\beta_1; \beta_2)$ is continuous in β_1 and β_2, in $\infty > \beta_1 \geq 0$, $\infty > \beta_2 \geq 0$, is imposed. The unique spectral function is determined by

$$\sigma(\beta_1; \beta_2) = \left(\frac{1}{2\pi i}\right)^2 \int_{-i\infty}^{+i\infty}\int_{-i\infty}^{+i\infty} dz_1 dz_2\, e^{\beta_1 z_1} e^{\beta_2 z_2} f(z_1; z_2) \tag{B2}$$

Further, $\sigma(\beta_1; \beta_2)$ is real in $\infty > \beta_1 \geq 0$, $\infty > \beta_2 \geq 0$, if $f(z_1; z_2)$ is real in $\infty > z_1 \geq 0$, $\infty > z_2 \geq 0$. For then, by the Schwartz reflection principle,[44] we have

$$f(z_1^*; z_2^*) = f(z_1; z_2)^*.$$

Hence the reality of $\sigma(\beta_1; \beta_2)$ follows from (B2).

Let us now impose a further condition on $f(z_1; z_2)$:

(v) $\dfrac{d}{dv_1} f(iv_1; iv_2)$, $\dfrac{d}{dv_1^2} f(iv_1; iv_2)$, $\dfrac{d}{dv_2}\dfrac{d^2}{dv_1^2} f(iv_1; iv_2)$,

and

$$\frac{d^2}{dv_2^2}\frac{d^2}{dv_1^2} f(iv_1; iv_2)$$

all exist, are continuous in v_1 and v_2, and are bounded by

$\text{const}/|(1+iv_1)(1+iv_2)|^{1+\lambda}$, in $\infty > v_1 > -\infty$, $\infty > v_2 > -\infty$.

For functions $f(z_1; z_2)$ satisfying conditions (i)–(v), we have the stronger result:

(II)

$$f(z_1; z_2) = \int_0^\infty \int_0^\infty d\beta_1 d\beta_2 \; e^{-\beta_1 z_1} e^{-\beta_2 z_2} \sigma(\beta_1; \beta_2) \quad \text{(B3)}$$

in $\text{Re}\, z_1 \geq 0$, $\text{Re}\, z_2 \geq 0$, where $\sigma(\beta_1; \beta_2)$ is continuous in β_1 and β_2, bounded, symmetric, and absolutely integrable in $\infty > \beta_1 \geq 0$, $\infty > \beta_2 \geq 0$, and satisfies

$$|(1+\beta_1)^2 \sigma(\beta_1; \beta_2)(1+\beta_2)^2| \leq \text{const}, \quad \infty > \beta_1 \geq 0, \; \infty > \beta_2 \geq 0. \quad \text{(B4)}$$

The representation is unique when the restriction that $\sigma(\beta_1; \beta_2)$ is continuous in β_1 and β_2, in $\infty > \beta_1 \geq 0$, $\infty > \beta_2 \geq 0$, is imposed. The unique spectral function is given by (B2).

We note that the following lemma leads to the above results:

Lemma: If $f(z)$ is holomorphic in $\text{Re}\, z > 0$ and continuous in $\text{Re}\, z \geq 0$, and satisfies the bound

$$|f(z)| \leq \text{const}/|1+z|^{1+\lambda}, \quad \text{Re}\, z \geq 0,$$

then

$$f(z) = \int_0^\infty d\beta \; e^{-\beta z} \rho(\beta), \quad \text{Re}\, z > 0,$$

where $\rho(\beta)$ is continuous and bounded in $\infty > \beta \geq 0$. The representation is unique when the restriction that $\rho(\beta)$ is continuous in $\infty > \beta \geq 0$ is imposed. The unique spectral function is given by

$$\rho(\beta) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} dz \; e^{\beta z} f(z).$$

To prove the lemma, we define

$$\rho(\beta) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} dz \; e^{\beta z} f(z).$$

$\rho(\beta)$ is continuous and bounded in $\infty > \beta \geq 0$.

We consider

$$\mathbf{f}(z) = \int_0^\infty d\beta \; e^{-\beta z} \rho(\beta) = \int_0^\infty d\beta \; e^{-\beta z} \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} d\omega \, e^{\beta\omega} f(\omega).$$

We have the absolute convergence of the double integral

$$\int_0^\infty \int_{-\infty}^\infty d\beta dv \; |e^{-\beta z} e^{i\beta v} f(iv)| \leq \text{const} \times \int_0^\infty \int_{-\infty}^\infty d\beta dv \; e^{-\beta z} \frac{1}{|1+iv|^{1+\lambda}} < \infty, \quad \text{Re}\, z > 0.$$

Hence we can change the order of integrations, for $\text{Re}\, z > 0$, and obtain

$$\mathbf{f}(z) = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} d\omega \, \frac{f(\omega)}{\omega - z}.$$

We have

$$\lim_{a\to 0} \int_{a-i\infty}^{a+i\infty} d\omega \, \frac{f(\omega)}{\omega - z} - \int_{-i\infty}^{+i\infty} d\omega \, \frac{f(\omega)}{\omega - z} = \lim_{a\to 0} \int_{-i\infty}^{+i\infty} d\omega \, \frac{f(\omega + a) - f(\omega)}{\omega - z + a}, \quad \text{Re}\, z > 0, \; a > 0.$$

The last limit may be proved to be zero. Hence we have

$$f(z) = \lim_{a\to 0} \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} d\omega \, \frac{f(\omega)}{\omega - z} = \mathbf{f}(z), \quad \text{Re}\, z > 0,$$

$$\therefore f(z) = \int_0^\infty d\beta \; e^{-\beta z} \rho(\beta), \quad \text{Re}\, z > 0.$$

The uniqueness follows from the identity theorem in Laplace transform theory.

APPENDIX C

We prove (3.35) and (3.37).

From (3.28), extended to $\text{Im}k > -\gamma$, $x \geq 0$, $\text{Re}x' > 0$, $1 \geq \cos\nu \geq -1$, we have

$$\begin{aligned}\Delta_n(k; x, x', \cos\nu) &= \Delta_n(k) K(k; x, x', \cos\nu) \\ &\quad - n\Delta_{n-1}(k) \iiint x''^2 dx'' \, \sin\mu \, d\mu d\chi \, K(k; x, x'', \cos\mu) \\ &\quad \times K(k; x'', x', \cos\lambda) \\ &\quad + \sum_{\substack{i,j=1 \\ i\neq j}}^{n} \iiint\iiint x_i^2 dx_i \, \sin\mu_i d\mu_i d\chi_i x_j^2 dx_j \, \sin\mu_j \, d\mu_j d\chi_j \\ &\quad \times K(k; x, x_i, \cos\mu_i) K(k; x_j, x', \cos\lambda_j) \\ &\quad \times f_{ij}(k; x_i, \mu_i, \chi_i, x_j, \mu_j, \chi_j), \quad n \geq 1,\end{aligned}$$

where

$$\cos\lambda = \cos\mu \cos\nu + \sin\mu \sin\nu \cos\chi,$$

$$\cos\lambda_j = \cos\mu_j \cos\nu + \sin\mu_j \sin\nu \cos\chi_j,$$

with $f_{ij}(k; x_i, \mu_i, \chi_i, x_j, \mu_j, \chi_j)$ given by the following expression, where $\mathbf{x}_i$ and $\mathbf{x}_j$ are the vectors with x_i, μ_i, χ_i, and x_j, μ_j, χ_j, as their polar coordinates respectively:

$$\begin{aligned}f_{ij}(k; \mathbf{x}_i, \mathbf{x}_j) &= (-1)^{i+j-1} \int\cdots\int d\mathbf{x}_1 \cdots d\mathbf{x}_{i-1} d\mathbf{x}_{i+1} \\ &\quad \cdots d\mathbf{x}_{j-1} d\mathbf{x}_{j+1} \cdots d\mathbf{x}_n \\ &\quad \times g_{ij}(k; \mathbf{x}_1, \ldots, \mathbf{x}_n), \quad i < j, \; n \geq 2, \\ f_{ij}(k; \mathbf{x}_i, \mathbf{x}_j) &= (-1)^{i+j-1} \int\cdots\int d\mathbf{x}_1 \cdots d\mathbf{x}_{j-1} d\mathbf{x}_{j+1} \\ &\quad \cdots d\mathbf{x}_{i-1} d\mathbf{x}_{i+1} \cdots d\mathbf{x}_n \\ &\quad \times g_{ij}(k; \mathbf{x}_1, \ldots, \mathbf{x}_n), \quad i > j, \; n \geq 2,\end{aligned}$$

and

$$g_{ij}(k; \mathbf{x}_1, \ldots, \mathbf{x}_n) = \begin{vmatrix} K(k; \mathbf{x}_1, \mathbf{x}_1) \cdots K(k; \mathbf{x}_1, \mathbf{x}_{i-1}) & K(k; \mathbf{x}_1, \mathbf{x}_{i+1}) \cdots K(k; \mathbf{x}_1, \mathbf{x}_n) \\ \vdots & \\ K(k; \mathbf{x}_{j-1}, \mathbf{x}_1) & \\ K(k; \mathbf{x}_{j+1} \mathbf{x}_1) & \\ \vdots & \\ K(k; \mathbf{x}_n, \mathbf{x}_1) \cdots K(k; \mathbf{x}_n, \mathbf{x}_{i-1}) & K(k; \mathbf{x}_n, \mathbf{x}_{i+1}) \cdots K(k; \mathbf{x}_n, \mathbf{x}_n) \end{vmatrix}, n \geq 2.$$

We have, using (2.6) and (2.7),

$$|f_{ij}(k;\mathbf{x}_i,\mathbf{x}_j)| \leq e^{(\gamma-\epsilon)x_i}(e^{-\gamma x_j}/x_j^{\alpha})N(\epsilon)^{n-1}M(\epsilon)^{n-2}(n-1)^{(n-1)/2}.$$

Hence, using (3.34) and (3.36), we obtain

$$\Delta_n(k;x,x',\cos\nu) = e^{-\gamma x}/x'^{\alpha}\int_0^{\infty} d\beta' \times e^{-\beta' x'}\rho_n(k;x,\beta',\cos\nu)$$

with

$$|\rho_n(k;x,\beta',\cos\nu)| \leq e^{(\gamma-\epsilon)x}\int_0^{\infty} d\beta''\,\Sigma(\beta'',\beta') \times \{\text{const} \times \Delta_n(k) + \text{const} \times n \times \Delta_{n-1}(k) + \text{const} \times N(\epsilon)^{n-1}M(\epsilon)^{n-2}n(n-1)^{(n-1)/2}\}, \quad n \geq 1.$$

Hence, using (2.20), we obtain

$$\Delta(k;x,x',\cos\nu) = \frac{e^{-\gamma x'}}{x'^{\alpha}}\int_0^{\infty} d\beta'\, e^{-\beta' x'}\rho(k;x,\beta',\cos\nu),$$

$$\rho(k;x,\beta',\cos\nu) = \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\rho_n(k;x,\beta',\cos\nu),$$

$$|\rho(k;x,\beta',\cos\nu)| \leq \text{const} \times e^{(\gamma-\epsilon)x}\int_0^{\infty} d\beta''\,\Sigma(\beta'',\beta'),$$

for $\mathrm{Im}k \geq -(\gamma-\epsilon)$, $\gamma \geq \epsilon > 0$, $\infty > x \geq 0$, $\infty > \beta' \geq 0$, $1 \geq \cos\nu \geq -1$.

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Erratum: Neutron transport equations with spin-orbit coupling [J. Math. Phys. 14, 97 (1973)]

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Eq. (2.26): F should be a subscript.

Eq. (3.15): The square brackets of the integral should contain

$$C_0\Pi + C_1\hat{u}'n - C_2(\hat{u}'\wedge\Pi) + C_3(\hat{u}'\wedge\hat{u}'\wedge\Pi).$$

Erratum: A stochastic Gaussian beam [J. Math. Phys. 14, 84 (1973)]

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The third line of Eq. (3.13) should be:

$$-\frac{1}{2}\int_0^\infty R(s)\sin(2s)ds\,\frac{\partial P^{(0)}}{\partial\chi} - 2\gamma\,\frac{\coth\theta}{\sinh\theta}\,\frac{\partial^2 P^{(0)}}{\partial\chi\partial\phi}.$$

Errata: Gauge transformations of second type and their implementations. I. Fermions [J. Math. Phys. 13, 2002 (1972)]

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The first equation of the second column, p. 2002 should read

$$\pi'(B(\psi^j_k)) = \bigotimes_j \bigotimes_1^{k-1} \pi'_j(\epsilon_j\,\Theta_j)\otimes\pi'_k(B(\psi^j_k))\bigotimes_j\bigotimes_{k+1}^{\infty} I_j.$$

The second equation of the second column p. 2002 should read

$$\pi(B(\psi^j_k)) = \bigotimes_l \bigotimes_1^{k-1} \pi_l(\Theta_l)\otimes\pi_k(B(\psi^j_k))\otimes\bigotimes_l\bigotimes_{k+1}^{\infty} I_l.$$

Inequality (ii) in 2. *Necessity* should read

$$\text{(ii)}\quad \sum_{k,\,|\lambda_k|\le 1} x_k(1-x_k)\lambda^2_k < +\infty.$$

The inclusion of line 24 of the first column, p. 2005 should read

$$\mathfrak{A}_e(E_n^+, s)\oplus\Theta_{1,n}\mathfrak{A}_0(E_n^+, s)\supset\bigcup_{k+1}^{\infty}(\mathfrak{A}_e(E_{n+1,k}, s)\oplus\Theta_{1,n}\mathfrak{A}_0(E_{n+1,k}, s).$$

The inequality and equality of lines 27–30 of the first column, p. 2005 should read

$$\begin{aligned}\|(\omega_\Omega-\omega_\Omega\circ\tau_\theta)|\mathfrak{A}(E_n,s)^c\| &= \|(\omega_\Omega-\omega_\Omega\circ\tau_\theta)|\mathfrak{A}_e(E_n^+,s)\oplus\Theta_{1,n}\mathfrak{A}_0(E_n^+,s)\| \\ &\geqslant \lim_{k,\infty}\|(\omega_\Omega-\omega_\Omega\circ\tau_\theta)|\mathfrak{A}_e(E_{n+1,k},s)\oplus\Theta_{1,n}\mathfrak{A}_0(E_{n+1,k},s)\|.\end{aligned}$$

Reference 10 should read E. Balslev and A. Verbeure, Commun. Math. Phys. 7, 55 (1968).

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