Relations among elements of the density matrix. I. Definiteness inequalities

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The statistical operator of quantum theory may be determined empirically by computations based upon the measured mean values of a set of observables we have called a quorum. The requirement that a statistical operator be positive semidefinite is then used to generate a family of inequalities connecting these quorum means. Like the simpler uncertainty relations, these inequalities are universal, valid for all quantum states. In the special case of pure states, the method yields a family of equalities.

1. THE QUORUM CONCEPT

According to quantum mechanics, every reproducible state preparation scheme Π is characterized by a statistical operator ρ in the sense that

$$\mathrm{Tr}(\rho A) = \langle A \rangle, \tag{1}$$

where A is the Hermitian operator for an observable of interest and $\langle A \rangle$ denotes the arithmetic mean of data for that observable gathered from an ensemble of systems each prepared in the manner Π. Recently we have explored[1,2,3] the problem of empirical state determination, formulated as follows: given Π and the means to measure any A, how much data is needed in order to determine the unknown ρ? This problem has been attacked in the past by several authors, including Feenberg,[4] Kemble,[5] and Gale, Guth, and Trammell.[6]

For an N-dimensional Hilbert space, any matrix representation of relation (1) contains $N^2 - 1$ independent real unknowns in the statistical matrix ρ (also commonly called the density matrix). This is a consequence of the Hermiticity of ρ and of its unit trace. The unknowns occur linearly; hence, if $N^2 - 1$ observables $\{A\}$ are chosen so that the associated $N^2 - 1$ linear algebraic equations like (1) possess a unique solution set, then the elements of the ρ matrix may be determined in terms of the $N^2 - 1$ mean values $\{\langle A \rangle\}$ by standard methods for solving linear systems of equations.

We have elsewhere called a set of observables $\{A\}$ whose mean values $\{\langle A \rangle\}$ constitute sufficient information to deduce the statistical operator ρ a *quorum* of observables.

In the present paper it is sufficient to acknowledge simply that such quorums exist, that the statistical operator ρ may be expressed as a function of quorum means $\{\langle A \rangle\}$. It will be demonstrated below that such representations of ρ, when considered in the light of an old theorem in matrix algebra, permit us to generate families of quantal inequalities reminiscent of, but more elaborate than, the uncertainty relations. In the sequel (Paper II) we shall investigate a new class of conserved quantities which are revealed by the study of quorums.

The present authors have developed systematic procedures for the construction of quorums for physical systems with N-dimensional Hilbert spaces and, under certain circumstances, for systems with infinite-dimensional Hilbert spaces.

Directly verifiable illustrations of density matrices as functions of quorum means will be given below; the reader interested in the philosophical and mathematical origins of the quorum theory is referred to the literature cited earlier.

2. DEFINITENESS OF THE STATISTICAL MATRIX

Three independent defining properties are customarily attributed to the statistical operator:

(i) hermiticity,

(ii) unit trace,

(iii) positive semidefiniteness.

Characteristics (i) and (ii) have already been incorporated into the quorum theory; every matrix representation of ρ which satisfies (1) and whose elements are functions of quorum means will automatically be Hermitian, and of trace unity.

Property (iii) may be derived[7] from the consistency condition that a dichotomic observable, represented by a projector $|\phi\rangle\langle\phi|$ onto a Hilbert vector ϕ, must have a nonnegative mean value since the eigenvalues of the projector are 0 and 1. Thus,

$$\mathrm{Tr}(\rho|\phi\rangle\langle\phi|) = \langle\phi|\rho|\phi\rangle \geq 0. \tag{2}$$

But ϕ is arbitrary; hence by definition ρ is positive semidefinite, or nonnegative definite.

It follows that the quorum means of which statistical-matrix elements are functions must be interrelated in such a manner that the statistical matrix will be nonnegative definite. Such a connection among the quorum observables is established by application of the old algebraic theorem[8] which states that all principal minor determinants of a nonnegative definite matrix must be nonnegative.

To be explicit, consider an $N \times N$ statistical matrix ρ with (k, l) element ρ_{kl}. An n-dimensional principal minor matrix is obtained by striking out $N - n$ rows and their *corresponding* columns; thus, the common element of each struck row-column pair will be in the principal diagonal of ρ. The standard proof that the determinants of these minor matrices are all nonnegative is based on the Hermiticity of the quadratic form (2) and on the invariance of determinants under similarity transformations.

Since each ρ_{kl} is a function of quorum means $\{\langle A \rangle\}$, the nonnegativity of principal minor determinants is ultimately expressible as a family of inequalities involving the quorum means. Like the celebrated uncertainty relations, these *definiteness inequalities* are valid for all preparations of state.

The family of definiteness inequalities becomes a family of equalities for $n > 1$ whenever the preparation is pure. For a pure state, ρ is a projector $|\psi\rangle\langle\psi|$; in terms of matrix elements,

$$\rho_{kl} = \psi_k \psi_l^*. \quad (3)$$

A typical minor determinant of a pure statistical matrix will therefore have the form

$$e^{b_1 b_2 \cdots b_n} (\psi_{a_1}\psi_{b_1}^*)(\psi_{a_2}\psi_{b_2}^*)\cdots(\psi_{a_n}\psi_{b_n}^*) = (\psi_{a_1}\psi_{a_2}\cdots\psi_{a_n})\, e^{b_1 b_2 \cdots b_n}\, \psi_{b_1}^*\psi_{b_2}^*\cdots\psi_{b_n}^*. \quad (4)$$

Since the e-system is totally skew-symmetric and $\psi_{b_1}^*\psi_{b_2}^*\cdots\psi_{b_n}^*$ is completely symmetric, the minor determinant vanishes, provided $n > 1$. Hence for a pure statistical matrix all principal minor determinants with $n > 1$ vanish; we can therefore generate a family of definiteness *equalities* relating the various quorum means in any *pure* state.

3. ILLUSTRATIONS

Several expressions are given below for matrix elements of the statistical operator expressed as functions of quorum means. As noted above, the procedures[9] used to discover quorum observables will not be reproduced here, nor will the straightforward but sometimes lengthy algebra by which the matrix elements are obtained from systems of linear equations. There is, however, no need for the reader to accept the matrix elements on faith; their validity may be checked directly by using (1).

A. Spin-½ system

Quorum: $\sigma_x, \sigma_y, \sigma_z$ (standard Pauli matrices).

Statistical matrix:

$$(\rho) = \tfrac{1}{2}\begin{pmatrix} 1 + \langle\sigma_z\rangle & \langle\sigma_x\rangle - i\langle\sigma_y\rangle \\ \langle\sigma_x\rangle + i\langle\sigma_y\rangle & 1 - \langle\sigma_z\rangle \end{pmatrix}. \quad (5)$$

Definiteness inequalities:

(1) One-dimensional minors:

$$1 + \langle\sigma_z\rangle \ge 0, \qquad 1 - \langle\sigma_z\rangle \ge 0. \quad (6)$$

The relations (6), involving only one component of the polarization vector $\langle\boldsymbol{\sigma}\rangle$, are uninteresting since they convey no information not already obvious from the spectrum $\{-1, +1\}$ of σ_z.

(2) Two-dimensional minor (detρ):

$$\tfrac{1}{4}(1 - \langle\sigma_z\rangle^2 - \langle\sigma_x\rangle^2 - \langle\sigma_y\rangle^2) \ge 0$$
or
$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 \le 1. \quad (7)$$

Pure state definiteness equality:

$$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \langle\sigma_z\rangle^2 = 1. \quad (8)$$

By subtracting (8) from the familiar equation

$$\langle\sigma_x^2\rangle + \langle\sigma_y^2\rangle + \langle\sigma_z^2\rangle = 3, \quad (9)$$

we obtain the following relation among uncertainties for any pure spin-$\frac{1}{2}$ state:

$$(\Delta\sigma_x)^2 + (\Delta\sigma_y)^2 + (\Delta\sigma_z)^2 = 2. \quad (10)$$

B. Spin-½ system (alternative quorum)

Quorum: P_x, P_y, P_z, where P_k denotes the projector onto the σ_k-eigenvector belonging to eigenvalue + 1, etc. $\langle P_k\rangle$ is the probability that a σ_k-measurement will yield + 1.

Statistical matrix:

$$(\rho) = \begin{pmatrix} \langle P_z\rangle & (\langle P_x\rangle - \frac{1}{2}) - i(\langle P_y\rangle - \frac{1}{2}) \\ (\langle P_x\rangle - \frac{1}{2}) + i(\langle P_y\rangle - \frac{1}{2}) & 1 - \langle P_z\rangle \end{pmatrix}. \quad (11)$$

Definiteness inequalities:

(1) One-dimensional minors:

$$0 \le \langle P_z\rangle \le 1. \quad (12)$$

(2) Two-dimensional minor (detρ):

$$(\langle P_x\rangle + \langle P_y\rangle + \langle P_z\rangle) - (\langle P_x\rangle^2 + \langle P_y\rangle^2 + \langle P_z\rangle^2) \ge \tfrac{1}{2}. \quad (13)$$

C. Harmonic oscillator with 2-level energy cutoff

Quorum theory is readily applicable to systems with infinite-dimensional Hilbert spaces whenever it is known that the state preparation Π has this property: there is an observable C (the cutoff observable[10]) whose probability distribution vanishes except for a finite number n of C-eigenvalues. Thus in a representation diagonal in C the (infinite) statistical matrix will have only n nonzero diagonal elements. From the inequality[11]

$$|\rho_{kl}| \le (\rho_{kk}\rho_{ll})^{1/2} \quad (14)$$

valid for any positive semidefinite ρ, it then follows that all elements of the statistical matrix vanish except for an $n \times n$ submatrix.

In the present example, the cutoff observable is energy H and $n = 2$; specifically, only the two lowest energy levels have nonzero probability.

Quorum: x (position), p (momentum),

$$H = (p^2/2m) + (m\omega^2/2)x^2.$$

Statistical matrix:

Let ρ_c denote the 2×2 nonzero submatrix of ρ. Then

$$\rho_c = \tfrac{1}{2}\begin{pmatrix} 3 - \langle K\rangle & \langle X\rangle - i\langle P\rangle \\ \langle X\rangle + i\langle P\rangle & -1 + \langle K\rangle \end{pmatrix}, \quad (15)$$

where

$$K \equiv (2/\hbar\omega)H, \qquad X \equiv (2m\omega/\hbar)^{1/2}x, \qquad P \equiv (2/m\hbar\omega)^{1/2}p. \quad (16)$$

Definiteness inequalities:

(1) One-dimensional minors:

$$1 \le \langle K\rangle \le 3$$
or
$$\hbar\omega/2 \le \langle H\rangle \le 3\hbar\omega/2. \quad (17)$$

Relation (17) is expected for a harmonic oscillator certain to yield upon energy measurement one of its two lowest eigenvalues.

(2) Two-dimensional minor:

$$\mathcal{E}(\langle x\rangle, \langle p\rangle) \le 2\langle H\rangle - (\hbar\omega)^{-1}\langle H\rangle^2 - (3/4)\hbar\omega \quad (18)$$

where

$$\mathcal{E}(\langle x\rangle, \langle p\rangle) \equiv (\langle p\rangle^2/2m) + (m\omega^2/2)\langle x\rangle^2.$$

The expression (18) is of interest in connection with the classical limit problem since $\mathcal{E}$ is the classical energy function with quantal means $\langle x\rangle$ and $\langle p\rangle$ as arguments; thus, (18) reflects a basic disparity between classical and quantal energy concepts. We intend to investigate the quorum theory approach to the classical limit problem in another publication.

The foregoing illustrations in a two-dimensional Hilbert space yielded several inequalities derivable also from the well known relation

$$\mathrm{Tr}\rho^2 \le 1. \tag{19}$$

However, in higher dimensional spaces a matrix of unit trace may satisfy this inequality and yet fail to be nonnegative definite. Thus our approach will in general produce additional inequalities which are not derivable from (19).

D. Spin-1 system

Quorum: J_x, J_y, J_z (angular momentum components), J_x^2, J_y^2, J_{xy}, J_{zx}, where $J_{ab} \equiv J_aJ_b + J_bJ_a$. A discussion concerning measurement of quorum members J_{ab} is given in Ref. 3.

Statistical matrix (representation diagonal in J_z; $\hbar = 1$):

$$(\rho) = \begin{pmatrix} 1 + \frac{1}{2}(\langle J_z\rangle - \langle J_x^2\rangle - \langle J_y^2\rangle) & (1/2\sqrt{2})[\langle J_x\rangle + \langle J_{zx}\rangle - i(\langle J_y\rangle + \langle J_{yz}\rangle)] & \frac{1}{2}(\langle J_x^2\rangle - \langle J_y^2\rangle - i\langle J_{xy}\rangle) \\ (1/2\sqrt{2})[\langle J_x\rangle + \langle J_{zx}\rangle + i(\langle J_y\rangle + \langle J_{yz}\rangle)] & -1 + \langle J_x^2\rangle + \langle J_y^2\rangle & (1/2\sqrt{2})[\langle J_x\rangle - \langle J_{zx}\rangle - i(\langle J_y\rangle - \langle J_{yz}\rangle)] \\ \frac{1}{2}(\langle J_x^2\rangle - \langle J_y^2\rangle + i\langle J_{xy}\rangle) & (1/2\sqrt{2})[\langle J_x\rangle - \langle J_{zx}\rangle + i(\langle J_y\rangle - \langle J_{yz}\rangle)] & 1 - \frac{1}{2}(\langle J_z\rangle + \langle J_y^2\rangle + \langle J_x^2\rangle) \end{pmatrix}. \tag{20}$$

Definiteness inequalities:

(1) One-dimensional minors: Consider for instance the (2, 2) element, which yields

$$\langle J_x^2\rangle + \langle J_y^2\rangle \ge 1. \tag{21}$$

This is expected, since for spin-1 we know that

$$\langle J_x^2\rangle + \langle J_y^2\rangle + \langle J_z^2\rangle = 2 \tag{22}$$

and

$$\langle J_z^2\rangle \le 1 \tag{23}$$

(2) Two-dimensional minors: At this level the method begins to reveal complicated new relationships among the quorum observables that are not anticipated intuitively. As an example, we compute the upper left minor determinant of (20).

$$[1 + \tfrac{1}{2}(\langle J_z\rangle - \langle J_x^2\rangle - \langle J_y^2\rangle)][-1 + \langle J_x^2\rangle + \langle J_y^2\rangle] - \tfrac{1}{8}[(\langle J_x\rangle + \langle J_{zx}\rangle)^2 + (\langle J_y\rangle + \langle J_{yz}\rangle)^2] \ge 0. \tag{24}$$

The first term in (24) may be simplified by applying (22) to obtain

$$\tfrac{1}{2}(\langle J_z\rangle + \langle J_z^2\rangle)(1 - \langle J_z^2\rangle) - \tfrac{1}{8}[(\langle J_x\rangle + \langle J_{zx}\rangle)^2 + (\langle J_y\rangle + \langle J_{yz}\rangle)^2] \ge 0. \tag{25}$$

The expression (25) typifies the complex interconnections among the means of quantal observables that may be discovered by generating definiteness inequalities. Moreover, the equality case of (25) is illustrative of the definiteness equalities which link quorum means for systems prepared in pure quantum states.

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A new expansion method in the Feynman path integral formalism: Application to a one-dimensional delta-function potential

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An expansion method in the path-integral formulation of quantum mechanics, as proposed in a previous paper, is extended to account for states with odd parity. The method is tested on the case of a one-dimensional attractive delta-function potential and the well-known solutions for both bound and scattering states are obtained analytically by an exact summation of the expansion series. The applicability of the method is discussed and it is shown how the energy spectrum could be determined by means of Stieltjes theory of moments.

I. INTRODUCTION

In a previous paper[1] two of us (M.J.G. and J.T.D.) proposed a new expansion procedure to solve the quantum-mechanical problems starting from Feynman's path-integral formalism. This method allows us to treat states corresponding to even wavefunctions and was successfully applied to get the well-known spectrum of the hydrogen atom. In the present paper we indicate how this expansion method can be extended in order to account for states with odd parity. In our procedure the general term of the series expansion may be expressed in analytic form and therefore the convergence problem could be examined in detail. For cases of practical interest the summation of this series cannot generally be carried out explicitly, except for some special situations. But knowing the formal expressions of all the terms of the expansions for the quantities W and W_1, defined by Eqs. (3) and (11), respectively, we can determine, at least in principle, the energy spectrum of the problem with the desired degree of accuracy (and in some cases this can be done by means of Stieltjes theory of moments). To illustrate the method we give the quantum-mechanical description of the one-dimensional attractive delta-function potential, starting from the path-integral formulation. We show that by an exact summation of the expansion series one gets the results known from solving the corresponding Schrödinger equation with appropriate boundary conditions. The applicability and the limitations of the method are discussed in the last section of the present paper.

II. A NEW EXPANSION METHOD IN THE FEYNMAN PATH INTEGRAL FORMALISM

We start from the density matrix $\rho(\mathbf{r}_\beta, \mathbf{r}_0)$ expressed as a Feynman path integral[2]

$$\rho(\mathbf{r}_\beta,\mathbf{r}_0)=\int \exp\left[-\int_0^\beta H(\mathbf{p},\mathbf{r},t)dt\right]D\mathbf{r}(t), \tag{1}$$

where the integration is done over all possible paths of the particle between the endpoints $\mathbf{r}_\beta$ and $\mathbf{r}_0$. $H(\mathbf{p}, \mathbf{r}, t)$ is the Hamiltonian of the system and it will be assumed to have the form

$$H(\mathbf{p},\mathbf{r},t)=\tfrac{1}{2}\mathbf{p}^2+V(\mathbf{r})=\tfrac{1}{2}\dot{\mathbf{r}}^2+V(\mathbf{r}) \tag{2}$$

(the units are chosen such that $\hbar=m=1$). The method proposed in I consists of evaluating the quantity

$$W(\mathbf{r}_0)=\int d^3\mathbf{r}_\beta\,\rho(\mathbf{r}_\beta,\mathbf{r}_0) \tag{3}$$

by taking in (1) the series expansion of the exponential function $\exp[-\int_0^\beta V(\mathbf{r})dt]$. Each term of this expansion leads to Feynman's "Gaussian integrals" and after a straightforward calculation one obtains the following result for the density matrix

$$\rho(\mathbf{r}_\beta,\mathbf{r}_0)=\frac{1}{(2\pi\beta)^{3/2}}\exp\left(-\frac{1}{2\beta}(\mathbf{r}_\beta-\mathbf{r}_0)^2\right)+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta dt_1\cdots\int_0^\beta dt_n\int\frac{d^3\mathbf{k}_1}{(2\pi)^3}f(\mathbf{k}_1)\cdots\times\int\frac{d^3\mathbf{k}_n}{(2\pi)^3}f(\mathbf{k}_n)P_n(\mathbf{r}_\beta,\mathbf{r}_0), \tag{4}$$

where $f(\mathbf{k})$ is the Fourier transform of the potential function

$$f(\mathbf{k})=\int V(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{r}, \tag{4a}$$

and $P_n(\mathbf{r}_\beta, \mathbf{r}_0)$ is defined by

$$P_n(\mathbf{r}_\beta,\mathbf{r}_0)=(2\pi\beta)^{-3/2}\exp[S_{n,cl}(\mathbf{r}_\beta,\mathbf{r}_0)], \tag{4b}$$

with

$$S_{n,cl}(\mathbf{r}_\beta,\mathbf{r}_0)=-\frac{1}{2\beta}(\mathbf{r}_\beta-\mathbf{r}_0)^2+\frac{i}{\beta}\sum_{j=1}^{n}t_j\mathbf{k}_j(\mathbf{r}_\beta-\mathbf{r}_0)+i\mathbf{r}_0\cdot\sum_{j=1}^{n}\mathbf{k}_j-\frac{1}{2}\sum_{i,j=1}^{n}T'_{ij}\mathbf{k}_i\cdot\mathbf{k}_j. \tag{4c}$$

Here T'_{ij} is a n-dimensional symmetric matrix, whose elements are

$$T'_{ij}=-(t_it_j/\beta)+\tfrac{1}{2}(t_i+t_j)-\tfrac{1}{2}|t_i-t_j|. \tag{4d}$$

Inserting expansion (4) in (3) and interchanging the order of integrations and summation, we get

$$W(\mathbf{r}_0)=1+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{1}{(2\pi)^{3n}}\int d^3\mathbf{k}_1 f(\mathbf{k}_1)\cdots\int d^3\mathbf{k}_n f(\mathbf{k}_n)\times\int_0^\beta dt_1\cdots\int_0^\beta dt_n\int d^3\mathbf{r}_\beta P_n(\mathbf{r}_\beta,\mathbf{r}_0). \tag{5}$$

It has been shown in I that the aim of the integration over $\mathbf{r}_\beta$ is to get rid of terms of the form t_it_j which appear in T'_{ij} and consequently in the exponential of $P_n(\mathbf{r}_\beta, \mathbf{r}_0)$. After eliminating such nonlinear terms the integration over time variables is easily performed by making use of the Laplace transform. Then the expansion for $W(\mathbf{r}_0)$ becomes

$$W(\mathbf{r}_0)=1+\sum_{n=1}^{\infty}\frac{(-1)^n}{(2\pi)^{3n}}L^{-1}\left(\int d^3\mathbf{k}_1 f(\mathbf{k}_1)e^{i\mathbf{k}_1\cdot\mathbf{r}_0}\cdots\right.$$
$$\left.\times\int d^3\mathbf{k}_n f(\mathbf{k}_n)e^{i\mathbf{k}_n\cdot\mathbf{r}_0}\frac{1}{s[s+\frac{1}{2}\mathbf{k}_1^2]\cdots[s+\frac{1}{2}(\mathbf{k}_1+\cdots+\mathbf{k}_n)^2]},\beta\right), \tag{6}$$

where

$$L^{-1}\{f(s),\beta\}=F(\beta)$$

denotes the inverse Laplace transform of the function $f(s)$. In Eq. (6) the transform L^{-1} can be evaluated in the general case,[3] but the corresponding expressions are lengthy and we shall not write them down.

It is easy to show that only the states with even parity contribute to $W(\mathbf{r}_0)$. Indeed, the density matrix $\rho(\mathbf{r}_\beta,\mathbf{r}_0)$ can be written as

$$\rho(\mathbf{r}_\beta,\mathbf{r}_0)=\sum_n \phi_n(\mathbf{r}_\beta)\phi_n^*(\mathbf{r}_0)e^{-\beta E_n}, \tag{7}$$

where the summation runs over both bound and scattering states of the system. From definition (3) it follows that

$$W(\mathbf{r}_0)=\int d^3\mathbf{r}_\beta\sum_n \phi_n^*(\mathbf{r}_0)\phi_n(\mathbf{r}_\beta)e^{-\beta E_n}; \tag{8a}$$

so that it is obvious that the states with odd parity $\phi_n^{\text{odd}}(-\mathbf{r}_\beta)=-\phi_n^{\text{odd}}(\mathbf{r}_\beta)$ do not contribute to $W(\mathbf{r}_0)$. By comparing Eqs. (8) and (6) we can determine the eigenvalues E_n and eigenfunctions $\phi_n(\mathbf{r}_0)$ corresponding to states with even parity.

Generally it is quite difficult to handle a formula of type (6). But if we are interested only in the energy spectrum of the system, we may considerably reduce the computational effort by choosing $\mathbf{r}_0=0$ (as it has been done in I for the energy spectrum of the hydrogen atom). Then Eq. (8) becomes

$$W_0=W(0)=\int d^3\mathbf{r}_\beta\sum_n \phi_n^*(0)e^{-\beta E_n}\phi_n(\mathbf{r}_\beta), \tag{8b}$$

so that the information concerning wavefunctions is entirely lost. Unfortunately the states described by wavefunctions which vanish in the origin of coordinates will be excluded from (8b). Therefore for this particular choice of the endpoint $\mathbf{r}_0$, we may also lose part of information concerning the energy spectrum corresponding to even states (the odd states are eliminated from the very beginning, as we pointed it out above).[4]

By choosing $\mathbf{r}_0=0$, formula (6) reduces to a simple form for potentials which are homogeneous functions of coordinates

$$V(\lambda\mathbf{r})=\lambda^h V(\mathbf{r}), \tag{9a}$$

which implies for the corresponding Fourier transforms

$$f(\lambda\mathbf{k})=\lambda^{3-h}f(\mathbf{k}), \tag{9b}$$

h being the homogeneity order. In this case, working up the inverse Laplace transform, one obtains the final formula (see I)

$$W_h=1+\sum_{n=1}^{\infty}\frac{(-1)^n}{(2)^{3n}}\frac{1}{(2)^{hn/2}}\frac{\beta^{n+h/2}}{\Gamma(n+\frac{1}{2}h+1)}$$
$$\times\int\frac{d^3\mathbf{k}_1 f(\mathbf{k}_1)}{1+\mathbf{k}_1^2}\cdots\int d^3\mathbf{k}_n\frac{f(\mathbf{k}_n)}{1+(\mathbf{k}_1+\cdots+\mathbf{k}_n)^2}, \tag{10}$$

where W_h represents the quantity W corresponding to a potential whose homogeneity order is h and Γ denotes, as usually, the "gamma function."

In order to give the quantum-mechanical description of the system by means of an expansion procedure as discussed above, we note that any solution can be written as a linear combination of odd and even functions and therefore it only remains to indicate how to take into account states with odd parity. We shall do it starting from the evaluation of the quantity

$$W_1(\mathbf{r}_0)=\int d^3\mathbf{r}_\beta\mathbf{r}_\beta\cdot\nabla_{\mathbf{r}_0}\rho(\mathbf{r}_\beta,\mathbf{r}_0). \tag{11a}$$

From expression (7) for the density matrix we can immediately see that only the states with odd parity contribute to $W_1(\mathbf{r}_0)$:

$$W_1(\mathbf{r}_0)=\int d^3\mathbf{r}_\beta\sum_n \mathbf{r}_\beta\cdot\nabla_{\mathbf{r}_0}\phi_n^*(\mathbf{r}_0)\phi_n(\mathbf{r}_\beta)e^{-\beta E_n}. \tag{11b}$$

By inserting expansion (4) into definition (11) and using Eqs. (4b)—(4d), we find

$$W_1(\mathbf{r}_0)=3+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{1}{(2\pi)^{3n}}\int d^3\mathbf{k}_1 f(\mathbf{k}_1)\cdots$$
$$\times\int d^3\mathbf{k}_n f(\mathbf{k}_n)\int_0^\beta dt_1\cdots\int_0^\beta dt_n$$
$$\times\exp\left(-\frac{1}{2}\sum_{i,j=1}^{n}T_{ij}\mathbf{k}_i\cdot\mathbf{k}_j\right)S_n(\mathbf{r}_0), \tag{12}$$

where

$$T_{ij}=\tfrac{1}{2}(t_i+t_j)-\tfrac{1}{2}|t_i-t_j| \tag{12'}$$

and

$$S_n(\mathbf{r}_0)=\frac{1}{(2\pi\beta)^{3/2}}\int d^3\mathbf{r}_\beta\mathbf{r}_\beta\cdot\nabla_{\mathbf{r}_0}$$
$$\times\exp\left[-\frac{1}{2\beta}\left(\mathbf{r}_\beta-\mathbf{r}_0-i\sum_{j=1}^{n}t_j\mathbf{k}_j\right)^2+i\mathbf{r}_0\cdot\sum_{j=1}^{n}\mathbf{k}_j\right]. \tag{12''}$$

In Cartesian coordinates $S_n(\mathbf{r}_0)$ can be written as a sum of three integrals of the type

$$S_n^x(\mathbf{r}_0)=\frac{1}{(2\pi\beta)^{3/2}}$$
$$\times\exp\left(i\mathbf{r}_0\cdot\sum_{j=1}^{n}\mathbf{k}_j\right)\int_{-\infty}^{\infty}dy\exp\left(-\frac{y^2}{2\beta}\right)\int_{-\infty}^{\infty}dz\exp\left(-\frac{z^2}{2\beta}\right)$$
$$\times\int_{-\infty}^{\infty}dx\left(x+x_0+i\sum_{j=1}^{n}t_jk_{j,x}\right)\left(\frac{1}{\beta}x+i\sum_{j=1}^{n}k_{j,x}\right)\exp\left(-\frac{x^2}{2\beta}\right). \tag{13}$$

The integrations in (13) are elementary and one gets

$$S_n^x(\mathbf{r}_0)=\exp\left(i\mathbf{r}_0\cdot\sum_{j=1}^{n}\mathbf{k}_j\right)\left(1+ix_0\sum_{j=1}^{n}k_{j,x}-\sum_{i,j=1}^{n}t_jk_{i,x}k_{j,x}\right), \tag{14}$$

so that

$$S_n(\mathbf{r}_0)=S_n^x(\mathbf{r}_0)+S_n^y(\mathbf{r}_0)+S_n^z(\mathbf{r}_0)$$
$$=\exp\left(i\mathbf{r}_0\cdot\sum_{j=1}^{n}\mathbf{k}_j\right)\left(3+i\mathbf{r}_0\cdot\sum_{j=1}^{n}\mathbf{k}_j-\sum_{i,j=1}^{n}t_j\mathbf{k}_i\cdot\mathbf{k}_j\right). \tag{15}$$

Therefore the quantity $W_1(\mathbf{r}_0)$ can be written as

$$W_1(\mathbf{r}_0)=3W(\mathbf{r}_0)+\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{1}{(2\pi)^{3n}}\int d^3\mathbf{k}_1 f(\mathbf{k}_1)e^{i\mathbf{k}_1\mathbf{r}_0}\cdots \times\int d^3\mathbf{k}_n f(\mathbf{k}_n)e^{i\mathbf{k}_n\cdot\mathbf{r}_0}\int_0^\beta dt_1\cdots\int_0^\beta dt_n \times\left(i\mathbf{r}_0\cdot\sum_{j=1}^n\mathbf{k}_j-\sum_{i,j=1}^n t_j\mathbf{k}_i\cdot\mathbf{k}_j\right)\exp\left(-\frac{1}{2}\sum_{i,j=1}^n T_{ij}\mathbf{k}_i\cdot\mathbf{k}_j\right) \tag{16}$$

The integrations over time variables may be performed as above, by making use of the Laplace transform. Denoting

$$V_n(\beta;t_j)=\int_0^\beta dt_1\int_0^{t_1}dt_2\cdots\int_0^{t_{n-1}}dt_n t_j\exp\left(-\sum_{i,j=1}^n T_{ij}\mathbf{k}_i\cdot\mathbf{k}_j\right), \tag{17}$$

we have

$$L[V_n(\beta;t_j),s]=\frac{\partial}{\partial\alpha_j}\left(\frac{1}{s[s+\mathbf{k}_1^2]\cdots[s-\alpha_j+(\mathbf{k}_1+\cdots\mathbf{k}_j)^2]\cdots}\times\frac{1}{[s-\alpha_j+(\mathbf{k}_1+\cdots+\mathbf{k}_n)^2]}\right)\Bigg|_{\alpha_j=0}$$
$$=\frac{1}{s[s+\mathbf{k}_1^2]\cdots[s+(\mathbf{k}_1+\cdots+\mathbf{k}_n)^2]}\times\sum_{p=j}^n\frac{1}{[s+(\mathbf{k}_1+\cdots+\mathbf{k}_p)^2]}. \tag{18}$$

For completeness we write down the Laplace transform (see I)

$$L[H_n(\beta),s]=1/s[s+\mathbf{k}_1^2]\cdots[s+(\mathbf{k}_1+\cdots+\mathbf{k}_n)^2] \tag{19}$$

for the function $H_n(\beta)$ defined by

$$H_n(\beta)=\int_0^\beta dt_1\int_0^{t_1}dt_2\cdots\int_0^{t_{n-1}}dt_n\exp\left(-\sum_{i,j=1}^n T_{ij}\mathbf{k}_i\cdot\mathbf{k}_j\right). \tag{20}$$

Now we can express $W_1(\mathbf{r}_0)$ by means of inverse Laplace transform. From the well-known relation

$$\sum_{j=1}^n\sum_{p=j}^n F(j,p)=\sum_{p=1}^n\sum_{j=1}^p F(j,p),$$

it follows that

$$\sum_{i,j=1}^n\mathbf{k}_i\mathbf{k}_j\sum_{p=j}^n\frac{1}{s+(\mathbf{k}_1+\cdots+\mathbf{k}_p)^2}=\sum_{i=1}^n\mathbf{k}_i\cdot\sum_{p=1}^n\frac{\mathbf{k}_1+\cdots+\mathbf{k}_p}{s+(\mathbf{k}_1+\cdots+\mathbf{k}_p)^2}, \tag{21}$$

so that

$$W_1(\mathbf{r}_0)=3W(\mathbf{r}_0)+\sum_{n=1}^\infty\frac{(-1)^n}{(2\pi)^{3n}}L^{-1}\Bigg[\int d^3\mathbf{k}_1 f(\mathbf{k}_1)e^{i\mathbf{k}_1\cdot\mathbf{r}_0}\cdots\times\int d^3\mathbf{k}_n f(\mathbf{k}_n)e^{i\mathbf{k}_n\cdot\mathbf{r}_0}$$
$$\times\left(i\mathbf{r}_0\cdot\sum_{j=1}^n\mathbf{k}_j\frac{1}{s[s+\frac{1}{2}\mathbf{k}_1^2]\cdots}\frac{1}{[s+\frac{1}{2}(\mathbf{k}_1+\cdots+\mathbf{k}_n)^2]}-\sum_{j,p=1}^n\mathbf{k}_j\cdot\frac{(\mathbf{k}_1+\cdots+\mathbf{k}_p)}{[s+\frac{1}{2}(\mathbf{k}_1+\cdots+\mathbf{k}_p)^2]}\times\frac{1}{s[s+\frac{1}{2}\mathbf{k}_1^2]\cdots[s+\frac{1}{2}(\mathbf{k}_1+\cdots+\mathbf{k}_n)^2]}\right),\beta\Bigg]. \tag{22}$$

The inverse Laplace transform may always be expressed in an analytic form,[3] but the remaining integrations over k cannot generally be exactly performed. The evaluation of formula (22) is considerably simplified if we choose $\mathbf{r}_0$ to be in the center of coordinate; but then we lose again all information concerning eigenfunctions. Moreover, from Eq. (11b) it follows that the odd states having a zero of order higher than one for $\mathbf{r}_0=0$ do not contribute to $W_1(0)=W_1$.

As we already mentioned it, the results are much simpler for potentials which are homogeneous functions of coordinates and in the present paper we shall write down an explicit solution for W_1 only in this case. Making use of the homogeneity condition (9b) and remembering that

$$L^{-1}\left[\frac{1}{s^{n+(hn/2)+1}},\beta\right]=\frac{\beta^{[(h/2)+1]n}}{\Gamma\{[(h/2)+1]n+1\}}, \tag{23}$$

we find

$$W_1^h=3W_h-2\sum_{n=0}^\infty\frac{(-1)^n}{(2\pi)^{3n}}\frac{1}{2^{hn/2}}\frac{\beta^{[(h/2)+1]n}}{\Gamma\{[(h/2)+1]n+1\}}\times\int d^3\mathbf{k}_1 f(\mathbf{k}_1)\cdots\int d^3\mathbf{k}_n f(\mathbf{k}_n)\frac{1}{[1+\mathbf{k}_1^2]\cdots[1+(\mathbf{k}_1+\cdots\mathbf{k}_n)^2]}\times\sum_{j=1}^n\mathbf{k}_j\cdot\sum_{p=1}^n\frac{(\mathbf{k}_1+\cdots+\mathbf{k}_p)}{1+(\mathbf{k}_1+\cdots+\mathbf{k}_p)^2}, \tag{24}$$

h being the homogeneity order of the potential.

III. APPLICATION TO A ONE-DIMENSIONAL ATTRACTIVE DELTA FUNCTION POTENTIAL

In order to illustrate the applicability of the expansion procedure we proposed in the previous section, let us consider a one-dimensional attractive potential, described by the function

$$V(x)=-\gamma\delta(x), \tag{25}$$

where γ is a positive constant.

We start by evaluating the quantities

$$W(x_0)=\int_{-\infty}^{+\infty}dx_\beta\rho(x_\beta,x_0) \tag{26}$$

and

$$W_1(x_0)=\int_{-\infty}^{+\infty}dx_\beta x_\beta\frac{d}{dx_0}\rho(x_\beta,x_0), \tag{27}$$

which characterize the even and odd states, respectively, for the case of one-dimensional systems. Expansions (6) and (22) for the three-dimensional quantities $W(\mathbf{r}_0)$ and $W_1(\mathbf{r}_0)$ are reduced in the one-dimensional case to

$$W(x_0)=1+\sum_{n=1}^\infty\frac{(-1)^n}{(2\pi)^n}L^{-1}\left\{\int_{-\infty}^{+\infty}dk_1 f(k_1)e^{ik_1x_0}\cdots\times\int_{-\infty}^{+\infty}dk_n f(k_n)e^{ik_nx_0}\frac{1}{s[s+\frac{1}{2}k_1^2]\cdots[s+\frac{1}{2}(k_1+\cdots+k_n)^2]},\beta\right\} \tag{28}$$

and

$$W_1(x_0)=W(x_0)+\sum_{n=1}^\infty\frac{(-1)^n}{(2\pi)^n}L^{-1}\left\{\int_{-\infty}^{+\infty}dk_1 f(k_1)e^{ik_1x_0}\cdots\int_{-\infty}^{+\infty}dk_n f(k_n)e^{ik_nx_0}\times\left(ix_0\sum_{j=1}^n\frac{1}{s[s+\frac{1}{2}k_1^2]\cdots[s+\frac{1}{2}(k_1+\cdots+k_n)^2]}-\sum_{j,p=1}^n k_j\frac{(k_1+\cdots+k_p)}{[s+\frac{1}{2}(k_1+\cdots+k_p)^2]}\frac{1}{s[s+\frac{1}{2}k_1^2]\cdots[s+\frac{1}{2}(k_1+\cdots+k_n)^2]}\right),\beta\right\}. \tag{29}$$

The Fourier transform of the potential (25) being

$$f(\mathbf{k}) = -\gamma, \tag{25'}$$

Eq. (28) becomes

$$W(x_0) = 1 + \sum_{n=1}^{\infty} \frac{\gamma^n}{(2\pi)^n} L^{-1}\left\{ \frac{2^{n/2}}{s^{n/2+1}} \int_{-\infty}^{+\infty} dk_1 \cdots \int_{-\infty}^{+\infty} dk_n \times \frac{1}{1+k_1^2} \cdots \frac{e^{ix_0\sqrt{2s}(k_1+\cdots+k_n)}}{1+(k_1+\cdots+k_n)^2}, \beta \right\}. \tag{30}$$

The integrations over the k are trivial and we get

$$W(x_0) = L^{-1}\left\{ \frac{1}{s} + \sum_{n=1}^{\infty} \frac{\gamma^n}{2^{n/2}} \frac{e^{-|x_0|\sqrt{2s}}}{s^{(n/2)+1}}, \beta \right\} = L^{-1}\left\{ \frac{1}{s} + \frac{\gamma}{\sqrt{2}} \frac{e^{-|x_0|\sqrt{2s}}}{s(\sqrt{s}-\gamma/\sqrt{2})}, \beta \right\}. \tag{31}$$

Making use of tables for inverse Laplace transform,[5] one finally has

$$W(x_0) = \mathrm{Erf}(|x_0|/\sqrt{2\beta}) + e^{-\gamma|x_0|} e^{\gamma^2\beta/2} \times \mathrm{Erfc}[(|x_0|/\sqrt{2\beta}) - \gamma\sqrt{\beta/2}\,], \tag{32}$$

where the complementary error function Erfc is related to the error function Erf by

$$\mathrm{Erfc}(x) = 1 - \mathrm{Erf}(x) = (2/\sqrt{\pi}) \int_x^{\infty} e^{-t^2} dt. \tag{33}$$

By inserting (25′) into (29) and taking into account (28), one finds after an integration by parts that

$$W_1(x_0) = 1. \tag{34}$$

From an expression of type (7) for the density matrix $\rho(x_\beta, x_0)$ and the definitions (26) and (27), it follows that

$$W(x_0) = \int_{-\infty}^{+\infty} dx_\beta \left(\sum_s \phi_s^*(x_0) e^{-\beta E_s} \phi_s(x_\beta) + \int_0^{\infty} dk\, e^{-\beta k^2/2} \phi^*(x_0;k)\phi(x_\beta;k) \right) \tag{35}$$

and

$$W_1(x_0) = \int_{-\infty}^{+\infty} dx_\beta x_\beta \left(\sum_s \frac{d}{dx_0} \phi_s^*(x_0) e^{-\beta E_s} \phi_s(x_\beta) + \int_0^{\infty} dk\, e^{-\beta k^2/2} \phi^*(x_0;k)\phi(x_\beta;k) \right), \tag{36}$$

where the summation over s accounts for the bound states of the system and the integration over k characterizes the continuous spectrum.

The explicit solution of our problem can be obtained by equating expressions (32) with (35), and (34) with (36), corresponding to $W(x_0)$ and $W_1(x_0)$, respectively. Since the resulting equations are valid for a continuous range of β,[6] the coefficients of $e^{-\beta E}$ on both sides of these equalities have to be equal; we get (see Appendix)

(a) one bound state (ground state of the system), with the energy

$$E_0 = -\tfrac{1}{2}\gamma^2 \tag{37a}$$

and the wavefunction

$$\phi_0(x) = \sqrt{\gamma} e^{-\gamma|x_0|}; \tag{37b}$$

(b) scattering states, characterized by

$$\phi_{\text{even}}(x;k) \sim e^{-ik|x|} + \frac{(k+i\gamma)^2}{k^2+\gamma^2} e^{ik|x|} \tag{38a}$$

for states with even parity, and

$$\phi_{\text{odd}}(x;k) \sim e^{ikx} - e^{-ikx} \tag{38b}$$

for states with odd parity.

We may generally remark that for a free particle one has $W(x_0) = 1$ and $W_1(x_0) = 1$ and therefore we might have seen from Eq. (34) without doing any calculation that the states with odd parity are not affected at all by a delta-function potential.

In scattering problems we do not need solutions having a well-defined parity, because from the physical point of view we have to study asymmetric situations. Indeed, usually we are interested in the picture with a particle which approaches from the region of negative (or, respectively, positive) x, and after the collision on the potential $V(x)$ either turns back or continues to move to the right (respectively, to the left). Therefore, for a particle coming from the left our asymptotic solution will have the form

$$\phi_{\text{left}}(x;k) = e^{ikx} + A(k)e^{-ikx} \quad \text{for } x<0, \qquad \phi_{\text{left}}(x;k) = B(k)e^{+ikx} \quad \text{for } x>0, \tag{39a}$$

and analogously for the particle approaching from the right

$$\phi_{\text{right}}(x;k) = e^{-ikx} + C(k)e^{ikx} \quad \text{for } x>0, \qquad \phi_{\text{right}}(x;k) = D(k)e^{-ikx} \quad \text{for } x<0. \tag{39b}$$

Then the wavefunctions of the scattering problem will be linear combinations of symmetric and antisymmetric solutions (38a) and (38b), which satisfy the corresponding boundary conditions (39a) or (39b). For instance, let us consider that

$$\alpha_1 \phi_{\text{even}}(x;k) + \alpha_2 \phi_{\text{odd}}(x;k) \tag{40}$$

satisfies condition (39a); then the coefficients α_1, α_2 will be solutions of the following set of linear equations

$$\alpha_1\{e^{ikx} + [(k+i\gamma)^2/(k^2+\gamma^2)]\,e^{-ikx}\} + \alpha_2(e^{ikx} - e^{-ikx}) = e^{ikx} + A(k)e^{-ikx} \quad \text{for } x<0,$$

$$\alpha_1\{e^{-ikx} + [(k+i\gamma)^2/(k^2+\gamma^2)]\,e^{+ikx}\} + \alpha_2(e^{+ikx} - e^{-ikx}) = B(k)e^{ikx} \quad \text{for } x>0. \tag{41}$$

By solving (41) we can determine the coefficients $A(k)$ and $B(k)$, which characterize the amplitude of reflected and transmitted waves, respectively; one obtains

$$A(k) = \frac{1}{2}\left(\frac{(k+i\gamma)^2}{k^2+\gamma^2} - 1 \right) = -\frac{\gamma^2 - ik}{k^2+\gamma^2}, \tag{42}$$

$$B(k) = \frac{1}{2}\left(\frac{(k+i\gamma)^2}{k^2+\gamma^2} + 1 \right) = \frac{k^2 + ik\gamma}{k^2+\gamma^2}. \tag{43}$$

As we expected, solutions (37a), (37b), (42), and (43) for both bound and scattering states are identical with those found by solving directly the corresponding Schrödinger equation.

IV. CONCLUSION

The procedure proposed in I in connection with the hydrogen atom energy spectrum calculation in the Feynman's path integral formalism and extended in the present paper provides a method for solving quantum mechanical problems for potentials having Fourier transform (the method may easily be adapted to cases when the Fourier transform does not exist, as it has been done for Coulomb[1] or harmonic oscillator potentials[3]).

Starting from Feynman's formulation of quantum mechanics, we may reduce the problem of solving the Schrödinger equation to that of evaluating expressions which involve only "classical calculations". Moreover, the general term of the corresponding expansions may be expressed analytically and therefore the convergence of the series could be examined in detail.[1,3] The summations cannot generally be carried out explicitly, except for particular types of potentials; but the knowledge of the general term of the expansions allows, at least in principle, to get numerical results with the desired degree of accuracy. In a forthcoming paper a numerical investigation of the rapidity of the convergence of this expansion will be performed on some exactly soluble models.

Unfortunately for potentials of a general form it is rather difficult to evaluate expressions (6) and (22) for the quantities $W(\mathbf{r}_0)$ and $W_1(\mathbf{r}_0)$. The calculations become much simpler if we put $\mathbf{r}_0 = 0$ in both these formulas, but the price to be paid for reducing the amount of computations is rather high: We lose all information on wavefunctions and possibly part of information concerning the energy spectrum. Indeed, as we have seen from (8b), all the states with even parity contribute to $W = W(0)$ except for those having zero's in the origin of coordinates. Similarly, from (11b) it follows that only the odd states contribute to $W = W_1(0)$, apart from those having zero's of higher order than one for $\mathbf{r}_0 = 0$. In fact the situation is not so bad as it seems to be at the first sight. For one-dimensional systems the quantities W and W_1 will generally describe the whole energy spectrum. In the three-dimensional case the problem is more complex. For instance, for central potentials which are less divergent than $1/r^2$ at $\mathbf{r}_0 = 0$ (condition which is satisfied by all the potentials of practical interest), the regular solutions will behave like r^l in the neighborhood of the origin, so that only the s and p states contribute to W and W_1, respectively. But for many practical purposes the knowledge of only s and p states seems to be rather satisfactory.

For completeness we remark that the ground state E_0 of the system may be easily obtained from (6) or (10) by applying the obvious formula

$$E_0 = -\lim_{\beta\to\infty}\left(\frac{\partial W}{\partial \beta}\right)\Big/ W. \tag{44}$$

After evaluating the quantities W and W_1 we still have to identify the eigenvalues for the discrete spectrum. That may be done by making use of the general theory of the problem of moments.[7] Indeed, according to (8a) and (12a), W and W_1 can be written as

$$W(\beta) = \int d^3\mathbf{r}_\beta \rho(\mathbf{r}_\beta, \mathbf{r}_0)\big|_{\mathbf{r}_0=0} = \int d^3\mathbf{r}_\beta \sum_n \phi_n(\mathbf{r}_\beta)\phi_n^*(0)e^{-\beta E_n} = \int_{-\infty}^{+\infty} e^{-\beta E} d\psi(E) \tag{45a}$$

and

$$W_1(\beta) = \int d^3\mathbf{r}_\beta \mathbf{r}_\beta \cdot \nabla_{\mathbf{r}_0}\rho(\mathbf{r}_\beta, \mathbf{r}_0)\big|_{\mathbf{r}_0=0} = \int d^3\mathbf{r}_\beta \sum_n \phi_n(\mathbf{r}_\beta)\mathbf{r}_\beta\cdot\nabla_{\mathbf{r}_0}\phi_n^*(\mathbf{r}_0)\big|_{\mathbf{r}_0=0} e^{-\beta E_n} = \int_{-\infty}^{+\infty} e^{-\beta E} d\psi_1(E), \tag{45b}$$

where $\int_{-\infty}^{+\infty}\cdots d\psi(E)$ and $\int_{-\infty}^{+\infty}\cdots d\psi_1(E)$ are Stieltjes integrals, the densities-of-states $d\psi(E)$ and $d\psi_1(E)$ being defined from Eqs. (45a) and (45b), respectively.

By introducing new quantities $S(z)$ and $S_1(z)$,

$$S(z) \equiv \int_0^\infty e^{-\beta z} W(\beta)d\beta = \int_{-\infty}^{+\infty} \frac{d\psi(E)}{z+E} \tag{46a}$$

and

$$S_1(z) \equiv \int_0^\infty e^{-\beta z} W_1(\beta)d\beta = \int_{-\infty}^{+\infty} \frac{d\psi_1(E)}{z+E}, \tag{46b}$$

we see that the moments μ_k and $\mu_k^{(1)}$, corresponding to these quantities $S(z)$ and $S_1(z)$ and defined by

$$\mu_k \equiv \int_{-\infty}^{+\infty} E^k d\psi(E) \tag{47a}$$

and

$$\mu_k^{(1)} \equiv \int_{-\infty}^{+\infty} E^k d\psi_1(E), \tag{47b}$$

can be expressed as derivatives of $W(\beta)$ and $W_1(\beta)$:

$$\mu_k = (-1)^k \frac{d^k}{d\beta^k} W(\beta)\Big|_{\beta=0} \tag{48a}$$

and

$$\mu_k^{(1)} = (-1)^k \frac{d^k}{d\beta^k} W_1(\beta)\Big|_{\beta=0}. \tag{48b}$$

If the quantities $W(\beta)$ and $W_1(\beta)$ and therefore the corresponding moments μ_k and $\mu_k^{(1)}$ are known, we may use the mathematical results from the theories of continued fractions and the moment problem in order to determine the eigenvalues of the problem. For applications we may use, for instance, an algorithm proposed by Gordon[8] in connection with the study of the canonical partition function. But such an algorithm can be used only if the moments of the problem are finite. That is true for instance in the case of the harmonic oscillator. The density matrix is then given by[9]

$$\rho(x_\beta, x_0) = (\omega/2\pi \sinh\beta\omega)^{1/2} \times \exp\{-(\omega/2\sinh\omega)[(x_\beta^2 + x_0^2)\cosh\beta\omega - 2x_\beta x_0]\}, \tag{49}$$

so that

$$W_0 = W(0) = (\cosh\beta\omega)^{-1/2} \tag{50a}$$

and

$$W_1 = W_1(0) = (\cosh\beta\omega)^{-3/2}, \tag{50b}$$

and therefore all the moments will be finite. It is possible to show in the general case[3] that the divergencies may appear only from the contribution to W_0 and W_1 of the continuous part of the spectrum. The case of infinite moments is more difficult from the practical point of view, because we cannot apply any more the theorems known from the theory of moments. However, the case of the Coulomb potential (where the moments are infinite) has been solved in I by making use of some of Grosjean theorems.[10]

Note added in proof: Starting from the method exposed in the present paper the δ-function density matrix itself has been evaluated by C. C. Grosjean, M. Goovaerts, and F. Broeckx in a paper entitled "Evaluation of the density matrix of one-dimensional systems in the path-integral formalism" (to be published).

APPENDIX

In order to determine the eigenvalues and eigenfunctions corresponding to states with even parity, we can equate (32) with (35). But it is more convenient, first, to work up expression (32), putting it in a form similar to (35). Indeed, taking into account definition (33), Eq. (32) becomes

$$W(x_0)=2e^{-\gamma|x_0|}e^{\gamma^2\beta/2}+K(x_0), \tag{A1}$$

where

$$K(x_0)=\frac{1}{\sqrt{2\pi\beta}}\int_0^{|x_0|}e^{-u^2/2\beta}du-\frac{1}{\sqrt{2\pi\beta}}e^{-\gamma|x_0|}\int_{-\infty}^{|x_0|}e^{-(u^2/2\beta)+u\gamma}du \tag{A2}$$

and making use of the equality

$$e^{-u^2/2\beta}=\sqrt{\frac{\beta}{2\pi}}\int_{-\infty}^{+\infty}e^{-\beta k^2/2}e^{iuk}dk, \tag{A3}$$

one gets

$$\begin{aligned}K(x_0)&=\frac{1}{\pi i}\int_{-\infty}^{+\infty}\frac{\gamma^2-ik\gamma}{k(k^2+\gamma^2)}e^{-\beta k^2/2}e^{ik|x_0|}dk\\&=\frac{1}{\pi i}\int_0^{\infty}dk\frac{\gamma^2-ik\gamma}{k(k^2+\gamma^2)}e^{-\beta k^2/2}\left(e^{ik|x_0|}+\frac{(k-i\gamma)^2}{k^2+\gamma^2}e^{-ik|x_0|}\right),\end{aligned} \tag{A4}$$

so that equating (A1) with (35) we find that

$$e^{-\beta E_s}\phi_s^*(x_0)\sim e^{\beta\gamma^2/2}e^{-\gamma|x_0|}, \tag{A5a}$$

or after normalization of the wavefunction

$$\phi_s(x_0)=\sqrt{\gamma}\,e^{-\gamma|x_0|},\quad E_s=-\tfrac{1}{2}\gamma^2, \tag{A5b}$$

and

$$\phi^*(x_0;k)\sim e^{ik|x_0|}+[(k-\gamma i)^2/(k^2+\gamma^2)]\,e^{-ik|x_0|}. \tag{A6}$$

Similarly from Eq. (34) and equality (A3) we get

$$\begin{aligned}W_1(x_0)&=\frac{1}{\sqrt{2\pi\beta}}\int_{-\infty}^{+\infty}e^{-u^2/2\beta}du=-\frac{1}{\sqrt{2\pi\beta}}\int_{-\infty}^{+\infty}u\frac{d}{du}(e^{-u^2/2\beta})du\\&=-\frac{1}{4\pi}\int_{-\infty}^{+\infty}udu\int_{-\infty}^{+\infty}dk\,e^{-\beta k^2/2}(e^{iku}+e^{-iku}),\end{aligned} \tag{A7}$$

so that finally we obtain

$$\begin{aligned}W_1(x_0)&=\frac{1}{4\pi}\int_{-\infty}^{+\infty}x_\beta dx_\beta\\&\times\int_0^{\infty}dk\,e^{-\beta k^2/2}(e^{ikx_\beta}-e^{-ikx_\beta})\frac{d}{dx_0}(e^{-ikx_0}-e^{ikx_0})\end{aligned} \tag{A8}$$

and, by comparing it with Eq. (34),

$$\psi(x_0;k)\sim(e^{+ikx_0}-e^{-ikx_0}). \tag{A9}$$

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Lattice Green's function for the simple cubic lattice in terms of a Mellin–Barnes type integral. II

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The series representation of the lattice Green's function for the simple cubic lattice $I(a)=\pi^{-3}\int_0^\pi\int_0^\pi\int_0^\pi D^{-1}\,dxdydz$, where $D=a-i\epsilon-\cos x-\cos y-\cos z$, around the singularity $a=1$ is obtained in fractional powers of a^2-1 (convergent for $|a^2-1|<1$), by the method of analytic continuation using a Mellin–Barnes type integral and also by use of the analytic continuation of ${}_3F_2\,(\,,\,,\,;\,,\,;1)$ as a function of the parameter. It gives leading and full expansions near the singularity $a=1$.

1. INTRODUCTION

In the previous paper[1] lattice Green's function of the simple cubic lattice at the origin

$$I(a)=\frac{1}{\pi^3}\int\int\int_0^\pi \frac{dx\,dy\,dz}{a-i\epsilon-\cos x-\cos y-\cos z}\,, \tag{1.1}$$

which has singularities at $a=1$ and $a=3$, was evaluated in series representation for $a\geq 3$ in powers of $1/a^2$, for $0\leq a\leq 1$ in powers of a^2, and for $1\leq a\leq 3$ in powers of $(a^2-5)/4$ by the method of analytic continuation using a Mellin–Barnes type integral. The exact values of $I(0)$, $I(1)$, $I(\sqrt{5})$ were also given in terms of a product of complete elliptic integrals. The method was successfully applied for the bcc lattice,[2] the rectangular and the square lattices[3] and the tetragonal lattice.[4] In this paper the expansion of the lattice Green's function of the simple cubic lattice around the singularity $a=1$, which was not given in the previous paper, is presented.

First $I(a)$ is expressed as a Mellin–Barnes type integral with the argument a^2-1. The integrand is a sum of two series expressed in terms of the generalized hypergeometric function ${}_3F_2(\,,\,,\,;\,,\,;1)$ which includes the integration variable as a parameter. In order to obtain the expansion in powers of a^2-1, it is necessary to know the behavior of the integrand in the left-half plane of the integration variable. The difficulty is that the series in the integrand are divergent in the left-half parameter plane while they are convergent in the right-half parameter-plane. We have succeeded in finding the behavior of the integrand in the left-half parameter-plane by constructing the analytic continuation of ${}_3F_2$ in the parameter plane. Then the series representation of $I(a)$ around $a^2=1$, which is convergent for $|a^2-1|<1$, is obtained by residue calculations in fractional powers of a^2-1.

2. SERIES REPRESENTATION AROUND $a^2=1$

For large absolute values of a ($a>3$), the following integral expression using a hypergeometric function has been derived in the previous paper[1]:

$$I(a)=\frac{1}{\pi a}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} ds\,\frac{\Gamma(-s)[\Gamma(s+\frac{1}{2})]^2}{\Gamma(s+1)}\left(\frac{-4}{a^2}\right)^s \times {}_2F_1\left(s+\tfrac{1}{2},s+1;1;\frac{1}{a^2}\right), \tag{2.1}$$

$$|\arg(-4/a^2)|<\pi, \tag{2.1'}$$

where δ is a small positive number and the path of integration is taken as a straight line parallel to the imaginary axis. The restriction (2.1′) ensures the convergence of the integration, and -4 is taken to be $4e^{-i\pi}$ since we consider a in the lower half plane.[5]

Applying a formula

$${}_2F_1(\alpha,\beta;\gamma;z)=(1-z)^{-\alpha}\,{}_2F_1(\alpha,\gamma-\beta;\gamma;z/(z-1))$$

to the hypergeometric function in the rhs of the Eq. (2.1) with $\alpha=s+\frac{1}{2}$, we obtain

$$I(a)=\frac{1}{\pi}\frac{1}{2\pi i}\int_{-\delta-i\infty}^{-\delta+i\infty} ds\,\frac{\Gamma(-s)[\Gamma(s+\frac{1}{2})]^2(4e^{-i\pi})^s}{\Gamma(s+1)}\left(\frac{1}{a^2-1}\right)^{s+1/2} \times {}_2F_1\left(s+\tfrac{1}{2},-s;1;\frac{1}{(1-a^2)}\right). \tag{2.2}$$

Here we take the branch where $(a^2)^{1/2}=a$.

Using the representation of the hypergeometric function by a Mellin–Barnes type integral, we have

$$I(a)=\frac{1}{\pi}\left(\frac{1}{2\pi i}\right)^2\int_{-\delta-i\infty}^{-\delta+i\infty} ds \times\int_{-\delta'-i\infty}^{-\delta'+i\infty} dt\,\frac{\Gamma(s+\frac{1}{2})\Gamma(-t)\Gamma(s+t+\frac{1}{2})\Gamma(-s+t)(4e^{-i\pi})^s}{\Gamma(s+1)\Gamma(t+1)} \times\left(\frac{1}{a^2-1}\right)^{s+t+1/2}, \tag{2.3}$$

where δ' is a small positive number chosen so as to make $\mathrm{Re}(-s+t)>0$, i.e., $\delta'<\delta$.

Introducing a new variable $u=s+t$ and changing the order of integration, we have

$$I(a)=\frac{1}{\pi}\left(\frac{1}{2\pi i}\right)^2\int_{-\delta''-i\infty}^{-\delta''+i\infty} du\,\Gamma(u+\tfrac{1}{2})(a^2-1)^{-u-1/2} \times\int_{-\delta-i\infty}^{-\delta+i\infty} ds\,\frac{\Gamma(s+\frac{1}{2})\Gamma(s-u)\Gamma(u-2s)(4e^{-i\pi})^s}{\Gamma(s+1)\Gamma(1+u-s)}, \tag{2.4}$$

where $\delta''=\delta+\delta'$. Note that $\mathrm{Re}(s-u)=-\delta'<0$ and $\mathrm{Re}(u-2s)=\delta'-\delta<0$.

Now the s-integration is carried out by collecting the residues of the poles at $s=\frac{1}{2}u+q$ and $\frac{1}{2}u+\frac{1}{2}+q$, $q=0,1,2,\ldots$, in the right-half s-plane. Then we have

$$\frac{1}{2\pi i}\int ds\cdots=\frac{1}{2}\sum_{q=0}^{\infty}\frac{\Gamma(\frac{1}{2}u+q+\frac{1}{2})\Gamma(q-\frac{1}{2}u)}{(2q)!\,\Gamma(\frac{1}{2}u+q+1)\Gamma(1+\frac{1}{2}u-q)}(4e^{-i\pi})^{u/2+q} -\frac{1}{2}\sum_{q=0}^{\infty}\frac{\Gamma(\frac{1}{2}u+q+1)\Gamma(q-\frac{1}{2}u+\frac{1}{2})}{(2q+1)!\,\Gamma(\frac{1}{2}u+q+\frac{3}{2})\Gamma(\frac{1}{2}+\frac{1}{2}u-q)}(4e^{-i\pi})^{u/2+q+1/2}. \tag{2.5}$$

It is shown that the summations with respect to q are divergent for $\mathrm{Re}\,u \le -1$, while the integration path in the u plane is to be closed to the left-half plane where $\mathrm{Re}\,u < 0$ to obtain the series valid for $|a^2| < 1$. Therefore it is necessary to transform the summations of Eq. (2.5) and to get other expressions which are valid for $\mathrm{Re}\,u \le 1$.

The rhs of the Eq. (2.5) is expressed in terms of a generalized hypergeometric function ${}_3F_2$ with argument equal to unity, and leads to

$$\frac{1}{2\pi i}\int ds \cdots = -\frac{1}{2\sqrt{\pi}}(4e^{-i\pi})^{u/2}\sin\tfrac{1}{2}u\pi \frac{\Gamma(\frac{1}{2}+\frac{1}{2}u)[\Gamma(-\frac{1}{2}u)]^2}{\Gamma(\frac{1}{2})\Gamma(1+\frac{1}{2}u)} \times {}_3F_2\left[\begin{matrix}\frac{1}{2}+\frac{1}{2}u, -\frac{1}{2}u, -\frac{1}{2}u; 1\\ \frac{1}{2}, 1+\frac{1}{2}u\end{matrix}\right] + \frac{i}{2\sqrt{\pi}}(4e^{-i\pi})^{u/2}\cos\tfrac{1}{2}u\pi \frac{\Gamma(1+\frac{1}{2}u)[\Gamma(\frac{1}{2}-\frac{1}{2}u)]^2}{\Gamma(\frac{3}{2})\Gamma(\frac{3}{2}+\frac{1}{2}u)} \times {}_3F_2\left[\begin{matrix}1+\frac{1}{2}u, \frac{1}{2}-\frac{1}{2}u, \frac{1}{2}-\frac{1}{2}u; 1\\ \frac{3}{2}, \frac{3}{2}+\frac{1}{2}u\end{matrix}\right]. \tag{2.6}$$

The expansion of a generalized hypergeometric function in terms of hypergeometric functions of lower order[6] [Eq. (5.1) in Ref. 3] and the value of ${}_2F_1$ with the argument equal to unity lead to a formula

$$\frac{\Gamma(\alpha_3)}{\Gamma(\beta_1)\Gamma(\beta_2)}\,{}_3F_2\left[\begin{matrix}\alpha_1, \alpha_2, \alpha_3; 1\\ \beta_1, \beta_2\end{matrix}\right] = \frac{\Gamma(\beta_1+\beta_2-\alpha_1-\alpha_2-\alpha_3)}{\Gamma(\beta_1+\beta_2-\alpha_1-\alpha_3)\Gamma(\beta_1+\beta_2-\alpha_2-\alpha_3)} \times {}_3F_2\left[\begin{matrix}\beta_1-\alpha_3, \beta_2-\alpha_3, \beta_1+\beta_2-\alpha_1-\alpha_2-\alpha_3; 1\\ \beta_1+\beta_2-\alpha_1-\alpha_3, \beta_1+\beta_2-\alpha_2-\alpha_3\end{matrix}\right]. \tag{2.7}$$

Applying the formula[7] (2.7) to the two ${}_3F_2$'s in (6) with $\alpha_3 = -\frac{1}{2}u$ and $\alpha_3 = \frac{1}{2}-\frac{1}{2}u$, respectively, we have

$$\frac{\Gamma(-\frac{1}{2}u)}{\Gamma(\frac{1}{2})\Gamma(1+\frac{1}{2}u)}\,{}_3F_2\left[\begin{matrix}\frac{1}{2}+\frac{1}{2}u, -\frac{1}{2}u, -\frac{1}{2}u; 1\\ \frac{1}{2}, 1+\frac{1}{2}u\end{matrix}\right] = \frac{\Gamma(1+u)}{\Gamma(1+\frac{1}{2}u)\Gamma(\frac{3}{2}+\frac{1}{2}u)}\,{}_3F_2\left[\begin{matrix}\frac{1}{2}+\frac{1}{2}u, 1+u, 1+u; 1\\ 1+\frac{1}{2}u, \frac{3}{2}+\frac{1}{2}u\end{matrix}\right], \tag{2.8}$$

and

$$\frac{\Gamma(\frac{1}{2}-\frac{1}{2}u)}{\Gamma(\frac{3}{2})\Gamma(\frac{3}{2}+\frac{1}{2}u)}\,{}_3F_2\left[\begin{matrix}1+\frac{1}{2}u, \frac{1}{2}-\frac{1}{2}u, \frac{1}{2}-\frac{1}{2}u; 1\\ \frac{3}{2}, \frac{3}{2}+\frac{1}{2}u\end{matrix}\right] = \frac{\Gamma(1+u)}{\Gamma(\frac{3}{2}+\frac{1}{2}u)\Gamma(2+\frac{1}{2}u)}\,{}_3F_2\left[\begin{matrix}1+\frac{1}{2}u, 1+u, 1+u; 1\\ \frac{3}{2}+\frac{1}{2}u, 2+\frac{1}{2}u\end{matrix}\right]. \tag{2.9}$$

The two hypergeometric series in the lhs of Eq. (8) and (9) are convergent for $\mathrm{Re}\,u > -1$ while those in the rhs of Eqs. (8) and (9) are convergent for $\mathrm{Re}\,u < 0$ and $\mathrm{Re}\,u < 1$, respectively. The rhs gives the analytic continuation of the lhs as a function of u.

Using the above transformations (8) and (9) and the series representation of ${}_3F_2$ (in the rhs) and changing the order of summation and integration, we obtain

$$I(a) = -\tfrac{1}{2}(\pi)^{-3/2}(a^2-1)^{-1/2}\sum_{p=0}^{\infty}\frac{1}{p!} \times \frac{1}{2\pi i}\int du \frac{\Gamma(\frac{1}{2}+u)\Gamma(-\frac{1}{2})\Gamma(\frac{1}{2}+\frac{1}{2}u+p)[\Gamma(1+u+p)]^2\sin\frac{1}{2}u\pi}{\Gamma(1+u)\Gamma(1+p+\frac{1}{2}u)\Gamma(\frac{3}{2}+p+\frac{3}{2}u)} \times\left(\frac{2e^{-i\pi/2}}{a^2-1}\right)^u + \frac{i}{2}(\pi)^{-3/2}(a^2-1)^{-1/2}\sum_{p=0}^{\infty}\frac{1}{p!}\frac{1}{2\pi i} \times\int du \frac{\Gamma(\frac{1}{2}+u)\Gamma(\frac{1}{2}-\frac{1}{2}u)\Gamma(1+p+\frac{1}{2}u)[\Gamma(1+p+u)]^2\cos\frac{1}{2}u\pi}{\Gamma(1+u)\Gamma(\frac{3}{2}+p+\frac{1}{2}u)\Gamma(2+p+\frac{3}{2}u)} \times\left(\frac{2e^{-i\pi/2}}{a^2-1}\right)^u. \tag{2.10}$$

Closing the integration path to the left-half u-plane, the evaluation of the integrals is carried out by summing residues of poles in the left-half u-plane. The poles of the integrand are located at $u = -\frac{1}{2}-q$, $q = 0, 1, 2, \ldots$, and at $u = -1-p-q$, where $p+q+1$ is odd integer for the first integrand of Eq. (10) and is even integer for the second integrand with $q \ge 0$. The calculation is straightforward but tedious, and we finally obtain

$$I(a) = I_{\mathrm{reg}}(a) + I_{\mathrm{irreg}}(a), \tag{2.11a}$$

$$I_{\mathrm{reg}}(a) = \frac{1}{4\sqrt{2}\,\pi}\sum_{q=0}^{\infty}\frac{i^q}{q!}\left\{(1+i)\frac{\Gamma(\frac{1}{4}+\frac{1}{2}q)\Gamma(\frac{1}{4}+\frac{3}{2}q)}{[\Gamma(\frac{3}{4}+\frac{1}{2}q)]^2} \times {}_3F_2\left[\begin{matrix}\frac{1}{4}-\frac{1}{2}q, \frac{1}{2}-q, \frac{1}{2}-q; 1\\ \frac{3}{4}-\frac{1}{2}q, \frac{3}{4}-\frac{3}{2}q\end{matrix}\right] - (1-i)\frac{\Gamma(-\frac{1}{4}+\frac{1}{2}q)\Gamma(-\frac{1}{4}+\frac{3}{2}q)}{[\Gamma(\frac{1}{4}+\frac{1}{2}q)]^2} \times {}_3F_2\left[\begin{matrix}\frac{3}{4}-\frac{1}{2}q, \frac{1}{2}-q, \frac{1}{2}-q; 1\\ \frac{5}{4}-\frac{1}{2}q, \frac{5}{4}-\frac{3}{2}q\end{matrix}\right]\right\}\left(\frac{a^2-1}{4}\right)^q, \tag{2.11b}$$

$$I_{\mathrm{irreg}}(a) = -i\frac{3}{2\pi}\sum_{r=0}^{\infty}\frac{[(\frac{1}{2})_r]^3}{r!(\frac{3}{4})_r(\frac{5}{4})_r}\,{}_3F_2\left[\begin{matrix}1+2r, \frac{1}{2}, -r; 1\\ 1+r, 1+r\end{matrix}\right](a^2-1)^{2r+1/2} + i\frac{1}{4\pi}\sum_{r=0}^{\infty}\frac{(1)_r[(\frac{3}{2})_r]^3}{[(2)_r]^2(\frac{5}{4})_r(\frac{7}{4})_r}\,{}_3F_2\left[\begin{matrix}2+2r, \frac{1}{2}, -r; 1\\ 2+r, 2+r\end{matrix}\right](a^2-1)^{2r+3/2}, \tag{2.11c}$$

where $I_{\mathrm{reg}}(a)$ and $I_{\mathrm{irreg}}(a)$ represent regular and irregular parts of $I(a)$ at $a=1$, and the leading singularity is $(a^2-1)^{1/2}$. For $a^2 < 1$, the irregular part does not contribute to the imaginary part but to the real part of $I(a)$. ${}_3F_2$'s in the irregular part are finite series and give rational numbers.

The generalized hypergeometric function ${}_3F_2(\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2; 1)$ converges when $\sigma \equiv \sum\beta_i - \sum\alpha_i > 0$, and the convergence becomes faster as σ increases, i.e., the degree of the convergence is of the order of $\sum_{n=1}^{\infty}(1/n^{\sigma+1})$. From the point of view of the convergence of ${}_3F_2(1)$, it is more convenient to transform $I_{\mathrm{reg}}(a)$ into another form, though Eq. (2.11) is a desirable expression as far as it goes. Using a transformation[8] of ${}_3F_2$, we have

$$I_{\mathrm{reg}}(a) = \frac{1}{\sqrt{2}}\frac{1}{\pi^{3/2}}\sum_{q=0}^{\infty}\frac{\Gamma(q-\frac{1}{2})}{q!}\,{}_3F_2\left[\begin{matrix}\frac{1}{2}-q, \frac{1}{2}-q, \frac{1}{2}; 1\\ \frac{3}{4}-\frac{1}{2}q, \frac{5}{4}-\frac{1}{2}q\end{matrix}\right]\left(\frac{a^2-1}{8}\right)^q + \frac{1}{(2\pi)^{3/2}}\sum_{q=0}^{\infty}[(-1)^q+i]\frac{\Gamma(\frac{1}{2}+q)[\Gamma(\frac{1}{4}+\frac{1}{2}q)]^2}{q![\Gamma(\frac{3}{4}+\frac{1}{2}q)]^2} \times {}_3F_2\left[\begin{matrix}\frac{1}{4}-\frac{1}{2}q, \frac{1}{4}-\frac{1}{2}q, \frac{1}{4}+\frac{1}{2}q; 1\\ \frac{1}{2}, \frac{3}{4}+\frac{1}{2}q\end{matrix}\right]\left(\frac{a^2-1}{2}\right)^q + \frac{1}{\sqrt{2}\,\pi^{3/2}}\sum_{q=0}^{\infty}\frac{[(-1)^q-i]\Gamma(\frac{1}{2}+q)[\Gamma(\frac{3}{4}+\frac{1}{2}q)]^2}{q!\,\Gamma(\frac{5}{4}+\frac{1}{2}q)\Gamma(\frac{1}{4}+\frac{1}{2}q)} \times {}_3F_2\left[\begin{matrix}\frac{3}{4}-\frac{1}{2}q, \frac{3}{4}-\frac{1}{2}q, \frac{3}{4}+\frac{1}{2}q; 1\\ \frac{3}{2}, \frac{5}{4}+\frac{1}{2}q\end{matrix}\right]\left(\frac{a^2-1}{2}\right)^q. \tag{2.11d}$$

The convergence indices σ in ${}_3F_2$'s in (2.11d) are all $\frac{1}{2}+q$, while those in (2.11b) are $\frac{1}{4}+\frac{1}{2}q$ and $\frac{3}{4}+\frac{1}{2}q$, showing better convergence than the original ${}_3F_2$ in (2.11b).

Now we investigate the radius of the convergence of Eq. (2.11). Consider the double series $\sum\sum A_{qp}x^q y^p$ generalized from the first term of (2.11d), where

$$A_{qp}=\frac{[\Gamma(\frac{1}{2}-q+p)]^2\Gamma(\frac{1}{2}+p)\Gamma(\frac{3}{4}-\frac{1}{2}q)\Gamma(\frac{5}{4}-\frac{1}{2}q)}{q!\,p!\,8^q[\Gamma(\frac{1}{2}-q)]\Gamma(\frac{3}{4}-\frac{1}{2}q+p)\Gamma(\frac{5}{4}-\frac{1}{2}q+p)}\,.$$

Put $p=\lambda q$; then from

$$\frac{1}{r}\equiv\lim_{q\to\infty}\left|\frac{A_{q+1,p}}{A_{q,p}}\right|=\left|\frac{1-2\lambda}{8(1-\lambda)^2}\right|$$

and

$$\frac{1}{s}\equiv\lim_{q\to\infty}\left|\frac{A_{q,p+1}}{A_{q,p}}\right|=\left|\frac{4(1-\lambda)^2}{(1-2\lambda)^2}\right|$$

we have

$$1/r=|(\pm\sqrt{s}-s)/2| \tag{2.12}$$

by eliminating λ. The double series $\sum A_{qp}x^q y^p$ converges absolutely in the region $|x|<r$ and $|y|<s$, where r and s are determined by Eq. (2.12). For $s=1$, we have $r=1$. That is, the first term in Eq. (2.11d) converges for $|a^2-1|<1$, i.e., $0<a<\sqrt{2}$ for real a. The radii of convergence of other terms in Eqs. (2.11d) and (2.11c) are also shown to be $|a^2-1|<1$.

The expression (2.11) includes only a^2, while the original form (1.1) depends on a such that $I(a-i\epsilon)=-I(-a+i\epsilon)$. This suggests that the expression (2.1) has a branch point at $a^2=0$. That is the reason why Eq. (2.11) is convergent for $|a^2-1|<1$.

For $a^2=1$, only the terms of $q=0$ in Eq. (2.11d) [or Eq. (2.11b)] do not vanish, and ${}_3F_2(1)$ for $q=0$ can be expressed in gamma functions[9] and the exact value of $I(1)$ announced in the previous paper [Eq. (33) in Ref. 1] is derived. The leading term is given by

$$I(a)=\tfrac{1}{2}\pi(1+\sqrt{2}i)[\Gamma(\tfrac{5}{8})\Gamma(\tfrac{7}{8})]^{-2}-(3i/2\pi)(a^2-1)^{1/2}+O(a^2-1). \tag{2.13}$$

The third term gives a real part for $a^2<1$.

Equations (2.11a), (2.11c), and (2.11d) are the series representation of $I(a)$ around $a=1$, convergent for $|a^2-1|<1$.

Note added in proof: The coefficient of the second term in (2.13), $-3/2\pi$, can also be calculated by the method of Morita and Horiguchi [J. Phys. A 5, 67 (1972)].

3. CONCLUSION

The lattice Green's function of the simple cubic lattice is expanded at the singularity $a=1$ by the method of analytic continuation in terms of a Mellin–Barnes type integral. In the process of calculation it is shown that the analytic continuation of a generalized hypergeometric function ${}_3F_2(\ ,\ ,\ ;\ ,\ ;1)$ in a complex-parameter plane allows us to obtain the series representation of $I(a)$ in fractional powers of a^2-1. The result is given in Eq. (2.11) and the series is convergent for $|a^2-1|<1$. It gives insights into the nature of the singularity and simple and rapid subroutines for numerical calculations near the singularity.

The numerical calculation of Eq. (2.11) reproduces the values in the table by Morita and Horiguchi.[10] The values of the first few terms of ${}_3F_2$ used are listed in the Appendix.

TABLE A1.

q	$F_a(q)$	$F_b(q)$	$F_c(q)$
0	$2^{-3/2}\pi^2[\Gamma(\frac{7}{8})\Gamma(\frac{5}{8})]^{-2}$	$\pi[\Gamma(\frac{3}{4})]^2[\Gamma(\frac{5}{8})]^{-4}$	$\pi[\Gamma(\frac{5}{8})]^2[\Gamma(\frac{7}{8})]^{-4}$
	0.142 812 5286 E+01	0.111 401 8565 E+01	0.183 079 6988 E+01
1	0.176 439 0652 E+01	0.109 540 4946 E+01	0.104 637 2345 E+01
2	−0.208 641 1048 E+02	0.182 137 5871 E+01	0.103 696 1127 E+01
3	0.182 583 5244 E+03	0.347 711 7660 E+01	0.131 077 8150 E+01
4	−0.151 852 3862 E+04	0.683 259 6365 E+01	0.189 170 7243 E+01
5	0.124 130 0083 E+05	0.135 354 5539 E+02	0.294 861 7544 E+01
6	−0.100 673 3423 E+06	0.269 047 1748 E+02	0.482 468 1185 E+01
7	0.813 044 4869 E+06	0.535 764 1342 E+02	0.815 923 8967 E+01
8	−0.654 957 8345 E+07	0.106 807 6513 E+03	0.141 306 0823 E+02
9	0.526 746 0718 E+08	0.213 083 6520 E+03	0.249 148 5647 E+02
10	−0.423 158 9025 E+09	0.425 323 6238 E+03	0.445 481 5485 E+02
11	0.339 671 5097 E+10	0.849 276 2411 E+03	0.805 505 8548 E+02
12	−0.272 495 2366 E+11	0.169 628 1019 E+04	0.146 992 2940 E+03
13	0.218 506 5481 E+12	0.338 873 7729 E+04	0.270 299 3008 E+03

APPENDIX: VALUES OF ${}_3F_2$

The values of ${}_3F_2(\ ,\ ,\ ;\ ,\ ;1)$ in Eqs. (2.11c) and (2.11d) are calculated by a subroutine based on the definition of ${}_3F_2$. Those in $I_{\text{irreg}}(a)$ are finite series and give rational numbers. Those in Eq. (2.11d) are infinite series with $\sigma=\frac{1}{2}+q$ and the convergence becomes faster as q increases. Here we list the values of ${}_3F_2$'s in Eq. (2.11d) for the first several terms of q. The values of them for large q can be calculated rapidly:

$$F_a(q)\equiv{}_3F_2\left[\begin{matrix}\frac{1}{2}-q,\frac{1}{2}-q,\frac{1}{2};1\\ \frac{3}{4}-\frac{1}{2}q,\frac{5}{4}-\frac{1}{2}q\end{matrix}\right],$$

$$F_b(q)\equiv{}_3F_2\left[\begin{matrix}\frac{1}{4}-\frac{1}{2}q,\frac{1}{4}-\frac{1}{2}q,\frac{1}{4}+\frac{1}{2}q;1\\ \frac{1}{2},\frac{3}{4}+\frac{1}{2}q\end{matrix}\right],$$

$$F_c(q)\equiv{}_3F_2\left[\begin{matrix}\frac{3}{4}-\frac{1}{2}q,\frac{3}{4}-\frac{1}{2}q,\frac{3}{4}+\frac{1}{2}q;1\\ \frac{3}{2},\frac{5}{4}+\frac{1}{2}q\end{matrix}\right].$$

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On the Green's functions for the Bethe-Salpeter equation. II*

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Considering the Bethe-Salpeter equation as a relativistic equation, we have studied the free particle Green's functions for unequal mass scalar bosons, interacting via a translationally invariant potential. The scattering Green's function found by Huang and DeFacio (HD) is presented for all possible Ω-plane contours for the unequal masses case. Only two k-plane contours are found to be physically interesting. The causal, advanced, and retarded Green's functions are listed in an appendix for unequal masses for the physical contour. The timelike Green's functions again require severe restrictions on the interaction potential as found by HD, and possible Bethe-Salpeter bound states are briefly discussed.

1. INTRODUCTION

The Bethe–Salpeter equation (BSE) was first postulated as a configuration space differential equation by Nambu,[1] although it was later named after Bethe and Salpeter,[2,3] who obtained the BSE from a Feynman graphical analysis. Many other early workers independently proposed the BSE on different grounds and a detailed history is available, including all BSE references through late 1969, in the long and careful review article by Nakanishi.[4]

Most workers[4,5] on the BSE have taken, as a fundamental requirement on the Bethe–Salpeter (BS) amplitude, that it should reproduce the Feynman–Dyson perturbation series, or at least the (renormalized) ladder graph series. A soluble model, called the Wick–Cutkosky[6,7] model, is obtained by combining a Euclidean propagator for the zero mass exchanged particles in the ladder graph series. But the BSE is not analytically soluble when the exchanged mass is nonzero, and this fact has led Schwartz,[8] Schwartz and Zemach,[9] and Kershaw *et al*,[10,11] to an analytical analysis which leads naturally to computer (numerical) studies of the BSE in configuration space. Further references to many other authors who have performed similar analysis in momentum space and with various approximation methods are available in Ref. 4 and Refs. 7–10. Other workers[12–16] have used the BSE as a basis for a dynamical theory with the perturbation expansion as a fundamental requirement. Although several workers[17–19] studied causal propagation in the BSE and agreed with Schwartz and Zemach in Ref. 9, Huang and DeFacio[20] (hereafter HD) found that a careful examination of the k-plane singularities lead to very different results. HD showed that the causal boundary conditions originally used could not lead to scattering boundary conditions, and in its place they presented an equal mass scattering Green's function.

The view point taken in HD was that the configuration space BSE

$$(p_1^2 + m_1^2)(p_2^2 + m_2^2)\Psi(1,2) = V(1,2;1',2')\Psi(1',2') \quad (1)$$

is of considerable interest in its own right and therefore should be studied without imposing such restrictions as causal propagation and ladder graphs in perturbation theory. HD then studied equal mass free particle Green's functions for causal, advanced, retarded, and scattering Green's functions using contour integration methods. HD found that the scattering Green's function was well behaved for spacelike separations of the two particles but that the interaction had to vanish exponentially for timelike separations of the two particles if the Bethe–Salpeter amplitude is to be meaningful.

The present work extends HD's equal mass study to unequal masses with an emphasis on the scattering Green's functions. The scattering Green's function is studied for all possible k-plane contours, a few remarks concerning Bethe–Salpeter bound states are presented, and the causal, advanced, and retarded Green's functions are listed for the "physical" k-plane contour.

In Sec. 2 our notation and conventions are presented and pole structure for unequal masses are given. In Sec. 3 the scattering Green's function is given for the following (complete) set of k-plane contours:

(1) the outgoing wave contour: $(k+q)(k-q) \to (k+q+i\epsilon)(k-q-i\epsilon)$;

(2) the incoming wave contour: $(k+q)(k-q) \to (k+q-i\epsilon)(k-q+i\epsilon)$;

(3) the first mixed contour: $(k+q)(k-q) \to (k+q+i\epsilon)(k-q+i\epsilon)$;

(4) the second mixed contour: $(k+q)(k-q) \to (k+q-i\epsilon)(k-q-i\epsilon)$.

In Sec. 4 the results and conclusions are presented. Appendix A contains the real integrals with all singularities removed, and Appendix B lists the unequal mass Green's functions satisfying causal, advanced, and retarded boundary conditions for the outgoing wave k-plane contour.

2. NOTATION AND POLE STRUCTURE

All notations are the same as in HD and again only translationally invariant interactions, i.e. $V(x_1, x_2, x_1', x_2') = V(x_1 - x_2, x_1' - x_2')$ are considered. Define the quantities

$$\begin{aligned} X &= x_1 + x_2, \\ P &= p_1 + p_2, \\ p &= \mu_2 p_1 - \mu_1 p_2 = (\mathbf{p}, p_0), \\ x &= \mu_1 x_1 - \mu_2 x_2 = (\boldsymbol{x}, t), \\ p\cdot x &= \mathbf{p}\cdot\boldsymbol{x} - p_0 t, \end{aligned} \quad (2)$$

where $\mu_1 + \mu_2 = 1$ is the only condition placed upon the μ's and where X is the cm coordinate and P is the 4-momentum canonically conjugate to X. x is a relative coordinate and $\hat{p}$ is the momentum canonically conjugate to x. By letting ω_1 and ω_2 denote the energy of particles 1 and 2 in the center of momentum frame, it is useful to define

$$\nu = \mu_2\omega_1 - \mu_1\omega_2$$

when

$$\omega_{1k}^2 = k^2 + m_1^2 \quad \text{and} \quad \omega_{2k}^2 = k^2 + m_2^2$$

with $k = |\boldsymbol{k}|$.

Let us also define

$$R = |\mathbf{x} - \mathbf{x}'|, \qquad T = t - t'. \tag{3}$$

An interval $x - x'$ is called *timelike* if $T > R$ and spacelike if $R > T$. For translationally invariant interactions, the BSE in Eq. (1) can be reduced to the fourth order (in the ∂_μ) partial differential equation

$$[\mathbf{p}^2 - (p_0 - \nu + \omega_1)^2 + m_1^2][\mathbf{p}^2 - (p_0 - \nu - \omega_2)^2 + m_2^2]\psi(x) = V(x', x)\psi(x'). \tag{4}$$

The full solution $\psi(x)$ to the BSE can be related to the free particle Green's functions ${}^{\pm}G_i^{\alpha}$, where $\pm$ denotes sgn (T), (α) signifies timelike intervals (τ) or spacelike intervals (σ), and i denotes one of the physical boundary conditions (scattering, causal, advanced, or retarded) and $\phi(x)$ the homogeneous solution to the BSE, according to the integral equation

$$\psi(x) = \phi(x) + \int {}^{\pm}G_i^{\alpha}(x - x')V(x')\psi(x')d^4x'. \tag{5}$$

By following HD and using Fourier methods, the unequal mass configuration space Green's function can be written as (neglecting the super and subscripts for the time being)

$$G(x - x') = \frac{e^{-i\nu T}}{4\pi^3 R}\int_0^{\infty} k \sin(kR) I(\omega_1, \omega_2) dk, \tag{6}$$

where

$$I(\omega_1, \omega_2) = \int_{-\infty}^{+\infty} \frac{e^{-i\Omega T}}{[\omega_{1k}^2 - (\Omega + \omega_1)^2][\omega_{2k}^2 - (\Omega - \omega_2)^2]} d\Omega. \tag{7}$$

By extending the integrand of Eq. (7) to the complex (Ω) plane, the four poles of the integrand for unequal masses are given by

$$\Omega_1 = -(\omega_{1k} + \omega_1), \qquad \Omega_2 = \omega_{1k} - \omega_1,$$
$$\Omega_3 = -(\omega_{2k} - \omega_2), \qquad \text{and } \Omega_4 = \omega_{2k} + \omega_2. \tag{8}$$

The $\pm$ to the upper left of Green's functions from now on indicates sgn (T) required to close over the contour at (∞) for the complex extention of Eq. (7). The four residues at the poles in Eqs. (8) written as ${}^{\pm}G_i$ $(i = 1, 2, 3, 4)$ become for the unequal mass case

$${}^{\pm}G_1 = \mp \frac{ie^{i(\omega_1 - \nu)T}}{4\pi^2 R}\int_0^{\infty} \frac{k \sin(kR) e^{i\omega_{1k}T} dk}{\omega_{1k}[\omega_{2k}^2 - (\omega_{1k} + \omega_1 + \omega_2)^2]},$$

$${}^{\pm}G_2 = \mp \frac{ie^{i(\omega_1 - \nu)T}}{4\pi^2 R}\int_0^{\infty} \frac{k \sin(kR) e^{-i\omega_{1k}T} dk}{\omega_{1k}[(\omega_{1k} - \omega_1 - \omega_2)^2 - \omega_{2k}^2]},$$

$${}^{\pm}G_3 = \mp \frac{ie^{-i(\omega_2 + \nu)T}}{4\pi^2 R}\int_0^{\infty} \frac{k \sin(kR) e^{+i\omega_{2k}T} dk}{\omega_{2k}[\omega_{1k}^2 - (\omega_1 + \omega_2 - \omega_{2k})^2]},$$

$${}^{\pm}G_4 = \mp \frac{ie^{-i(\omega_2 + \nu)T}}{4\pi^2 R}\int_0^{\infty} \frac{k \sin(kR) e^{-i\omega_{2k}T} dk}{\omega_{2k}[(\omega_{2k} + \omega_2 + \omega_1)^2 - \omega_{1k}^2]}. \tag{9}$$

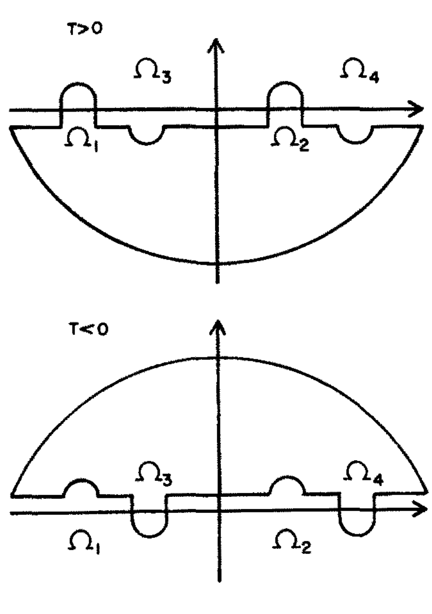

FIG. 1. Contour for the scattering Green's function in the complex Ω plane.

3. THE SCATTERING GREEN'S FUNCTIONS

The causal, advanced, and retarded Green's functions are defined and listed in Appendix B. The scattering Green's functions are defined in terms of the quantities in Eqs. (9) by the relations

$${}^{+}G_s = {}^{+}G_1 + {}^{+}G_2 \quad \text{and} \quad {}^{-}G_3 + {}^{-}G_4, \tag{10}$$

which is equivalent to the contour[13] shown in Fig. 1. As in HD, it is necessary to study integrals of the form

$$L(\pm, \pm) = \int \frac{k e^{\pm i(kR \pm \omega_{1k}T)} dk}{(k + q \pm i\epsilon)(k - q \mp i\epsilon)} \tag{11}$$

in order to evaluate integrals of the form

$$K_1(q \pm i\epsilon, R, T) = \int_0^{\infty} \frac{k \sin(kR) e^{\mp i\omega_{1k}T} dk}{(k + q \pm i\epsilon)(k - q \mp i\epsilon)}. \tag{12}$$

In order to close over the contours as $k \to \infty$, we must require that the quantity in the exponential of Eq. (11)

$$\alpha(\pm) = k_1 R \pm a_2 T \tag{13}$$

satisfy $\pm\,\alpha(\pm) < 0$, where

$$k = k_R + ik_I$$

and

$$\omega_{1k} = a_1 + ia_2 \tag{14}$$

Using the relationship between a_2 and k_I,

$$a_2 = (1/\sqrt{2})\{[k_R^2 - k_I^2 + m_1^2)^2 + 4k_R k_I]^{1/2} - (k_R^2 - k_I^2 + m_1^2)^{1/2}\}^{1/2}, \tag{15}$$

one constructs Table I which lists all possible contours for each sgn (T) and for all possible space–time intervals. In Fig. 2 the (UHP) and (LHP) contours[14] are shown for the $q \to q + i\epsilon$ prescription for the two poles of $L(\pm, \pm)$ and the contours show how to avoid the branch cut from $-im_1$ to $+im_1$ along the Im (k) axis. The information in Table I and Fig. 2 are adequate for the spacelike scattering Green's functions.

However, for the timelike scattering Table I and Fig. 2 are inadequate because it is necessary to evaluate integrals of the form

$$F_1(q + i\epsilon, R, T) = \int_{m_1}^{\infty} \frac{\omega_{1k} e^{\mp i\omega_{1k}T} \sin(kR) d\omega_{1k}}{(\omega_{1k} + \omega_1 \pm i\epsilon)(\omega_{1k} - \omega_1 \mp i\epsilon)}. \tag{16}$$

As in HD, we study integrals of the form

$$J(\pm,\pm) = \int \frac{\omega_{1k} e^{\pm i(kR \pm \omega_{1k} T)} d\omega_{1k}}{(\omega_{1k} + \omega_1 \pm i\epsilon)(\omega_{1k} - \omega_1 \mp i\epsilon)}, \quad (17)$$

which has simple poles at $\omega_{1k} = -\omega_1 \mp i\epsilon$ and $\omega_{1k} = \omega_1 \pm i\epsilon$ and two branch points at $(-m_1, +m_1)$ which are connected by a branch cut between these points. The relationship between k_I [note that $k = (\omega_{1k}^2 - m_1^2)^{1/2}$] and the real and imaginary parts of ω_{1k} from Eq. (14) is given by

$$k_I = (1/\sqrt{2})\{[a_1^2 - a_2^2 - m_1^2)^2 + 4a_1^2 a_2^2]^{1/2} - (a_1^2 - a_2^2 - m_1^2)^{1/2}\}^{1/2}. \quad (18)$$

By using Eq. (18) it is straightforward to construct Table II which requires quarter-plane contours as shown in Fig. 3.

Now one can evaluate the scattering Green's function for all possible cases. It is expressed in terms of the real integrals in Appendix A which have all of the poles and singularities removed. For the contour shown in Fig. 2, the scattering Green's functions include

$$^{+}G_s^{\sigma}(q + i\epsilon, R, T) = \frac{ie^{-i\nu T}}{8\pi(\omega_1 + \omega_2)} \frac{e^{iqR}}{R}, \quad (19)$$

$$^{+}G_s^{\tau}(q + i\epsilon, R, T) = \frac{ie^{i(\omega_1 - \nu)T}}{4\pi^2(\omega_1 + \omega_2)R}\{\tfrac{1}{4}\pi e^{iqR} - \tfrac{1}{2}M_1(R, -T) + \tfrac{1}{2}i[W_1(R, -T) + N_1(R, -T)] + \tfrac{1}{2}\omega_1[W_1'(R, -T) + iM_1'(R, T) + N_1'(R, -T)]\}, \quad (20)$$

$$^{-}G_s^{\sigma}(q + i\epsilon, R, T) = \frac{ie^{-i\nu T}}{8\pi(\omega_1 + \omega_2)} \frac{e^{iqR}}{R}, \quad (21)$$

and

$$^{-}G_s^{\tau}(q + i\epsilon, R, T) = \frac{ie^{-i(\omega_2 + \nu)T}}{4\pi^2(\omega_1 + \omega_2)R}\{\tfrac{1}{4}\pi e^{iqR} + \tfrac{1}{2}M_2(R, T) - \tfrac{1}{2}\omega_2[W_2'(R, T) + N_2'(R, T)] + \tfrac{1}{2}i[W_2(R, T) + N_2(R, T) + \omega_2 M_2'(R, T)]\}. \quad (22)$$

Another set of scattering Green's functions are obtained from the incoming wave contour. These Green's functions include

$$^{+}G_s^{\sigma}(q - i\epsilon, R, T) = [ie^{-i\nu T}/8\pi(\omega_1 + \omega_2)]e^{-iqR}/R, \quad (23)$$

$$^{+}G_s^{\tau}(q - i\epsilon, R, T) = [ie^{i(\omega_1 - \nu)T}/8\pi^2(\omega_1 + \omega_2)R] \times \{i[W_1(R, -T) + N_1(R, -T)] - \pi e^{-i\omega_1 T}\cos(qR) + \tfrac{1}{2}\pi e^{-iqR}e^{i\omega_1 T} - M_1(R, T)\} + [\omega_1 e^{i(\omega_1 - \nu)T}/8\pi^2(\omega_1 + \omega_2)R] \times \{i[W_1'(R, -T) + N_1'(R, -T) - \omega_1 M_1'(R, T) + \pi/\omega_1(e^{-i\omega_1 T} - 1)\cos(qR) + \pi/2\omega_1(e^{i\omega_1 T} - 1)e^{-iqR}]\}, \quad (24)$$

$$^{-}G_s^{\sigma}(q - i\epsilon, R, T) = [ie^{-i\nu T}/8\pi(\omega_1 + \omega_2)]e^{-iqR}/R, \quad (25)$$

and

$$^{-}G_s^{\tau}(q - i\epsilon, R, T) = [ie^{-i(\omega_2 + \nu)T}/8\pi^2(\omega_1 + \omega_2)R] \times \{i[W_2(R, T) + N_2(R, T)] + M_2(R, T) + \pi e^{-iqR}e^{-i\omega_2 T} - 2\pi e^{i\omega_2 T}\cos(qR) - i\omega_2[W_2'(R, T) + N_2'(R, T)] - \omega_2 M_2'(R, T) - \pi\omega_2 e^{-iqR}(e^{-i\omega_2 T} - 1) + 2\pi\omega_2(e^{i\omega_2 T} - 1)\cos(qR)\}. \quad (26)$$

TABLE I. Contours in the complex k plane with UHP referring to upper half-plane, LHP referring to lower half-plane, and σ, τ referring to spacelike and timelike spacetime intervals, respectively.

$\alpha(+)$	T	Space-time interval	Contour
+	+	σ	UHP
+	+	τ	UHP
−	+	σ	LHP
+	+	τ	LHP
+	−	σ	UHP
−	−	τ	UHP
−	−	σ	LHP
−	−	τ	LHP
$\alpha(-)$	T	Space-time interval	Contour
+	+	σ	UHP
−	+	τ	UHP
−	+	σ	LHP
−	+	τ	LHP
+	−	σ	UHP
+	−	τ	UHP
−	−	σ	LHP
+	−	τ	LHP

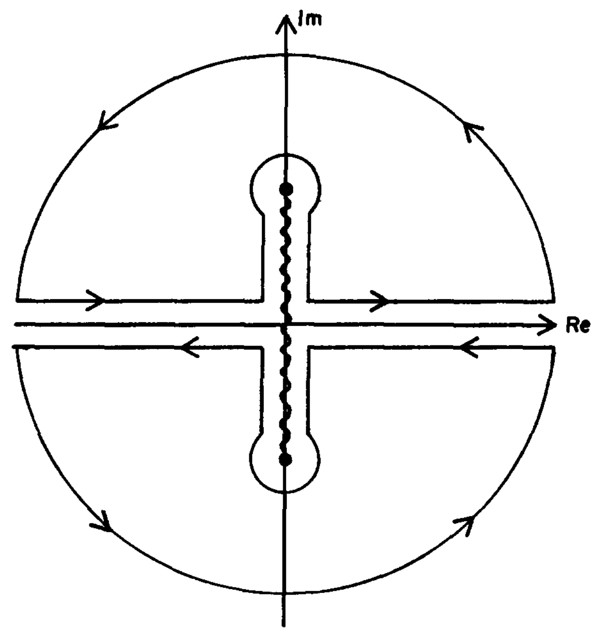

FIG. 2. Contours for the integrals $L(+,+)$ and $L(-,+)$ in the complex k plane. The solid line is for the integral $L(+,+)$ and the dotted line is for the integral $L(-,+)$. Both contours are for the outgoing wave treatment of the $k = \pm q$ poles (x) and different pole displacements must be used for these poles for the q-$i\epsilon$ and mixed contour cases.

Next we treat the first and second mixed contours. From Sec. 1, $(k + q)(k - q) \to (k + q + i\epsilon)(k - q + i\epsilon)$ defines the *first mixed contour*. Placing $q \pm i\epsilon$ in the argument of $^{\pm}G_s$ to indicate this treatment of the k-plane poles, the scattering Green's functions for the first mixed contour become

$$^{+}G_s^{\sigma}(q \pm i\epsilon, R, T) = [ie^{i(\omega_1 - \nu)T}/4\pi(\omega_1 + \omega_2)R] \times (2e^{-i\omega_1 T} - 1)\cos(qR), \quad (27)$$

$$^{+}G_s^{\tau}(q \pm i\epsilon, R, T) = [ie^{i(\omega_1 - \nu)T}/8\pi^2(\omega_1 + \omega_2)R] \times \{i[W_1(R, -T) + N_1(R, -T) + \pi e^{-i\omega_1 T}\cos(qR)] - \tfrac{1}{2}M_1(R, T) + \tfrac{1}{2}\omega[W_1'(R, -T) + N_1'(R, -T) - (2\pi i/\omega_1)(e^{-i\omega_1 T} - 1)\cos(qR) - \tfrac{1}{2}M_1'(R, T)]\}, \quad (28)$$

TABLE II. Contours in the complex ω_{ik} plane using the same notation as Table I.

$\alpha(+)$	T	Space–time interval	Contour
+	+	σ	UHP
+	+	τ	UHP
+	+	σ	LHP
—	+	τ	LHP
+	—	σ	UHP
—	—	τ	UHP
—	—	σ	LHP
—	—	τ	LHP
$\alpha(-)$	T	Space–time interval	Contour
+	+	σ	UHP
—	+	τ	UHP
+	+	σ	LHP
+	+	τ	LHP
+	—	σ	UHP
—	—	τ	UHP
—	—	σ	LHP
—	—	τ	LHP

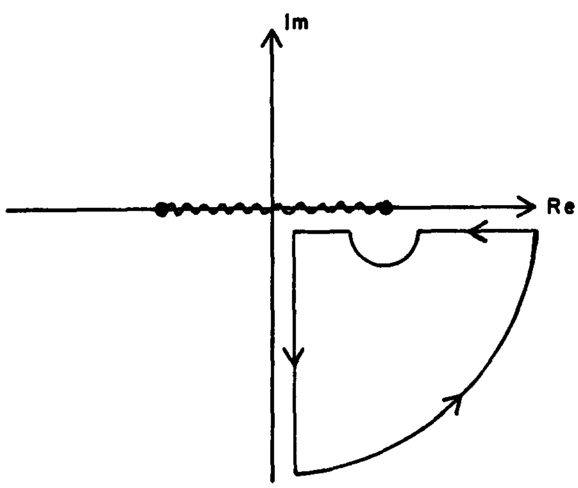

FIG. 3. Contour for the integrals $J(+,+)$ and $J(-,-)$ in the complex ω_{ik} plane.

$$^{-}G_s^{\sigma}(q \pm i\epsilon, R, T) = [ie^{-(\omega_2+\nu)T}/4\pi(\omega_1+\omega_2)R]\cos(qR), \tag{29}$$

and

$$\begin{aligned} ^{-}G_s^{\tau}(q \pm i\epsilon, R, T) &= [ie^{-i(\omega_2+\nu)T}/8\pi^2(\omega_1+\omega_2)R] \\ &\times \{i[W_2(R,-T) + N_2(R,-T) \\ &- iM_2(R,T)] - \omega_2[W_2'(R,T) + N_2'(R,T) - iM_2'(R,T) \\ &+ (\pi i/\omega_2)(e^{i\omega_2 T} - 1)\cos(qR)]\}. \end{aligned} \tag{30}$$

Finally, we consider the second mixed contour $(k+q)(k-q) \to (k+q-i\epsilon)(k-q-i\epsilon)$ placing $q \mp i\epsilon$ into the argument of $^{\pm}G_s$ to distinguish this scattering Green's functions from the previous ones, the scattering Green's functions for the second mixed contour become

$$^{+}G_s^{\sigma}(q \mp i\epsilon, R, T) = [ie^{-i\nu T}/4\pi(\omega_1+\omega_2)]\cos(qR)/R, \tag{31}$$

$$\begin{aligned} ^{+}G_s^{\tau}(q \mp i\epsilon, R, T) &= [ie^{i(\omega_1-\nu)T}/8\pi^2(\omega_1+\omega_2)R] \\ &\times \{i[W_1(R,-T) + iM_1(R,T) \\ &+ N_1(R,-T) + \pi e^{i\omega_1 T}\cos(qR)] \\ &- \omega_1 M_1'(R,T) + \pi(e^{i\omega_1 T} - 1)\cos(qR) \\ &+ i\omega_1[W_1'(R,-T) + N_1'(R,-T)]\} \end{aligned} \tag{32}$$

$$^{-}G_s^{\sigma}(q \mp i\epsilon, R, T) = [ie^{-i(\omega_2+\nu)T}/8\pi(\omega_1+\omega_2)]\cos(qR)/R, \tag{33}$$

and

$$\begin{aligned} ^{-}G_s^{\tau}(q \mp i\epsilon, R, T) &= [ie^{-i(\omega_2+\nu)T}/8\pi^2(\omega_1+\omega_2)R]\{M_2(R,T) \\ &+ i[W_2(R,T) + N_2(R,T)] - i\omega_2[W_2'(R,T) + N_2'(R,T)] \\ &- \omega_2 M_2(R,T)\}. \end{aligned} \tag{34}$$

The even numbered equations from Eq. (20) to Eq. (34) give the scattering Green's functions for timelike intervals and the odd numbered equations from Eq. (21) to Eq. (33) give the scattering Green's functions for spacelike intervals. One sees from the properties of the real integrals in Appendix A that all of the timelike scattering Green's functions become undefined as

$$\lim_{R\to\infty} {}^{\pm}G_s^{\tau}(q, R, T) \to \infty, \tag{35}$$

as was first observed by HD for the equal mass case. For the outgoing wave contour in k space, the spacelike scattering Green's function satisfied outgoing spherical wave boundary conditions *with no approximation for R large*. For the extension of the spacelike scattering Green's function, we obtain an incoming spherical wave with no approximations, but the two mixed contours lead to incoming and outgoing waves and therefore cannot satisfy scattering boundary conditions.

4. RESULTS AND CONCLUSIONS

There are no well-behaved timelike Green's functions, including the Green's functions in Appendix B, because of the real integrals $N_{\pm}(R, \pm T)$, and $N_i'(R, \pm T)$, $i = 1,2$, become infinite as $R \to \infty$. All of the spacelike Green's functions are finite as $R \to \infty$ but only the scattering Green's function from the outgoing wave contour $q \to q + i\epsilon$ in the k plane has the correct asymptotic behavior for scattering states. This $q \to q + i\epsilon$ condition is also used to derive the nonrelativistic scattering amplitude from the Lippmann–Schwinger equation. As already mentioned, the spacelike scattering Green's function has the exact scattering boundary condition form without making any approximation for large R. The scattering amplitude follows from the full solution to the BSE as in Eq. (5) if we demand that the interaction $V(x')$ vanish whenever $x - x'$ is timelike, for then we have

$$\psi(x) = \phi(x) + \frac{ie^{-i\nu T}}{8\pi(\omega_1+\omega_2)} \int \frac{e^{iqR}}{R} V(x')\psi(x')d^4x'. \tag{36}$$

With the usual approximation $|x| > |x'|$, we have

$$\psi(x) = \phi(x) + \frac{e^{iq|x|-i\nu T}}{8\pi(\omega_1+\omega_2)x} \int e^{i\nu\tau' - i\mathbf{q}\cdot\mathbf{x}'} V(x')\psi(x')d^4x', \tag{37}$$

which allows us to identify the scattering amplitude

$$f(\mathbf{q}' \leftarrow \mathbf{q}) = \frac{i}{8\pi(\omega_1+\omega_2)} \int e^{i(\nu\tau' - \mathbf{q}\cdot\mathbf{x}')} V(x')\psi(x')d^4x'. \tag{38}$$

For negative energies the homogeneous solution $\phi(x)$ no longer occurs and the relative three momentum q becomes $i|q|$ where $|q|$ is the real modulus of the pure imaginary q. Then the spatial behavior of the spacelike scattering Green's function becomes

$$^{\pm}G_s^{\sigma}(q + i\epsilon, R, T) \underset{R\to\infty}{\longrightarrow} e^{-|q|R}/R \tag{39}$$

which is the correct Green's function for a bound state.

The causal Green's function for spacelike intervals contains linear combinations of incoming and outgoing spatial waves and therefore cannot represent a scattering solution, as first reported by HD. And the causal Green's function cannot represent a bound state for negative energies because it is not *stationary*.

The $q \to q - i\epsilon$ solutions correspond to incoming spherical waves as in nonrelativistic scattering theory and are useful in final state interaction theories. The two mixtures are *genuine* solutions to the Bethe–Salpeter equation but are unrelated to physical scattering problems.

With the exception of a few minor changes, the Green's functions for the unequal mass bosons is similar to the equal mass boson case. Unlike some other problems[21] no new complications in analytic structure arise as a consequence of the unequal masses.

APPENDIX A

The real integrals with all poles and singularities removed are listed below:

$$M_1(R,T) = -\int_0^{m_1} \frac{k e^{-kR} \sin[\sqrt{m_1^2 - k^2}\,T]\,dk}{k^2 + q^2},$$

$$M_2(R,T) = -\int_0^{m_2} \frac{k e^{-kR} \sin[\sqrt{m_2^2 - k^2}\,T]\,dk}{k^2 + q^2},$$

$$N_1(R,T) = \int_0^{m_1} \frac{k \exp[i\sqrt{m_1^2 - k^2}\,T] \sinh(kR)\,dk}{k^2 + q^2},$$

$$N_2(R,T) = \int_0^{m_2} \frac{k \exp[i\sqrt{m_2^2 - k^2}\,T] \sinh(kR)\,dk}{k^2 + q^2},$$

$$W_1(R,T) = \int_0^{\infty} \frac{\omega_{1k} e^{\omega_{1k}T} \sinh[(\omega_{1k}^2 + m_1^2)^{1/2} R]\,d\omega_{1k}}{\omega_{1k}^2 + \omega_1^2},$$

$$W_2(R,T) = \int_0^{\infty} \frac{\omega_{2k} e^{\omega_{2k}T} \sinh[(\omega_{2k}^2 + m_2^2)^{1/2} R]\,d\omega_{2k}}{\omega_{2k}^2 + \omega_2}, \tag{A1}$$

For $X_i(R,T)$ a generic member of the list in Eq. (A1) the quantity $X_i'(R,T)$ is defined for $i = 1, 2$ as

$$X_i'(R,T) = \int_0^T X_i(R,T')\,dT'. \tag{A2}$$

Also, it is sometimes necessary to have $X_i(R,-T)$ or $X_i'(R,-T)$ but the substitution $T \to -T$ into Eqs. (A1) and (A2) give these real integrals.

APPENDIX B

In this appendix we define and list the causal, advanced and retarded Green's functions for the outgoing wave contour. We have also calculated the above Green's function[22] for the $q \to q - i\epsilon$ and the two mixed k-plane contours, but they do not seem interesting enough to list here. The causal Green's functions ${}^{\pm}G_c$ are defined by

$${}^{+}G_c = {}^{+}G_1 + {}^{+}G_2, \quad {}^{-}G_c = {}^{-}G_3 + {}^{-}G_4. \tag{B1}$$

Using the methods of HD, as in Sec. 3 for the scattering Green's function, we find that

$$\begin{aligned}{}^{+}G_c^{\sigma}(q + i\epsilon, R, T) &= [i/8\pi^2(\omega_1 + \omega_2)R] \\ &\times \{e^{i(\omega_1-\nu)T}[M_1(R,T) - i\omega_1 M_1'(R,T) \\ &+ i\pi(e^{-i\omega_1 T} - 1)e^{iqR}] - e^{-i(\omega_2+\nu)T} \\ &\times [M_2(R,T) + i\omega_2 M_2'(R,T) + \tfrac{1}{2}\pi e^{iqR}]\},\end{aligned} \tag{B2}$$

$$\begin{aligned}{}^{+}G_c^{\tau}(q + i\epsilon, R, T) &= [i/8\pi^2(\omega_1 + \omega_2)R] \\ &\times \{e^{-i(\nu-\omega_1)T}[iW_1(R,-T) + iN_1(R,-T) \\ &- \omega_1 W_1'(R,-T) - \omega_1 N_1'(R,-T)] \\ &- e^{-i(\nu+\omega_2)T}[iW_2(R,-T) + iN_2(R,-T) \\ &- \omega_2 W_2'(R,-T) - \omega_2 N_2'(R,-T)]\},\end{aligned} \tag{B3}$$

$$\begin{aligned}{}^{-}G_c^{\sigma}(q + i\epsilon, R, T) &= -[i/8\pi^2(\omega_1 + \omega_2)R] \\ &\times \{e^{i(\omega_1-\nu)T}[\tfrac{1}{2}\pi e^{iqR} - \tfrac{1}{2}M_1(R,T) \\ &+ i\omega_1 M_1'(R,T)] - e^{-i(\omega_2+\nu)T}[M_2(R,T) \\ &+ i\omega_2 M_2'(R,T) + \pi(e^{i\omega_2 T} - \tfrac{1}{2}e^{iqR}]\},\end{aligned} \tag{B4}$$

and

$$\begin{aligned}{}^{-}G_c^{\tau}(q + i\epsilon, R, T) &= -[i/8\pi^2(\omega_1 + \omega_2)R] \\ &\times \{e^{i(\omega_1-\nu)T}[W_1(R,T) + N_1(R,T) + i\omega_1 W_1'(R,T) \\ &+ i\omega_1 N_1'(R,T)] + e^{-i(\omega_2+\nu)T}[iW_2(R,T) + iN_2(R,T) \\ &- \omega_2 W_2'(R,T) - \omega_2 N_2'(R,T)]\}.\end{aligned} \tag{B5}$$

The advanced Green's functions G_A are defined in terms of the residues from Eq. (9) as

$${}^{+}G_A = 0 \quad \text{and} \quad {}^{-}G_A = {}^{-}G_1 + {}^{-}G_2 + {}^{-}G_3 + {}^{-}G_4. \tag{B6}$$

The outgoing wave k-plane contours together with Eq. (B6) give for the advanced Green's functions

$${}^{+}G_A^{\tau}(q + i\epsilon, R, T) = {}^{+}G_A^{\sigma}(q + i\epsilon, R, T) = 0, \tag{B7}$$

$${}^{-}G_A^{\sigma}(q + i\epsilon, R, T) = 0, \tag{B8}$$

and

$$\begin{aligned}{}^{-}G_A^{\tau}(q + i\epsilon, R, T) &= [i/8\pi^2(\omega_1 + \omega_2)R] \\ &\times \{e^{-i(\omega_2+\nu)T}[iW_2(R,T) + \tfrac{1}{2}\pi e^{iqR} \\ &+ iN_2(R,T) - \omega_2 W_2'(R,T) - \omega_2 N_2'(R,T) \\ &+ M_2(R,T) - i\omega_2 M_2'(R,T)] \\ &- e^{i(\omega_1-\nu)T}[iW_1(R,T) + iN_1(R,T) \\ &+ \omega_1 W_1'(R,T) + \omega_1 N_1'(R,T) \\ &+ \pi e^{-i\omega_1 T} e^{iqR} + M_1(R,T)]\}.\end{aligned} \tag{B9}$$

The retarded Green's functions G_R are defined in terms of the residues from Eq. (9) as

$${}^{-}G_R = 0,$$

and

$${}^{+}G_R = {}^{+}G_1 + {}^{+}G_2 + {}^{+}G_3 + {}^{+}G_4. \tag{B10}$$

By using the outgoing wave k-plane contour and Eq. (B10), the retarded Green's functions become

$${}^{-}G_R^{\tau}(q + i\epsilon, R, T) = {}^{-}G_R^{\sigma}(q + i\epsilon, R, T) = 0, \tag{B11}$$

$${}^{+}G_R^{\sigma}(q + i\epsilon, R, T) = 0, \tag{B12}$$

and

$$\begin{aligned}{}^{+}G_R^{\tau}(q + i\epsilon, R, T) &= [i/8\pi^2(\omega_1 + \omega_2)R] \\ &\times \{e^{-i(\nu-\omega_1)T}[iW_1(R,-T) \\ &+ iN_1(R,-T) + i\omega_1 M_1'(R,T) + \omega_1 W_1'(R,T) \\ &+ \omega_1 N_1'(R,-T) - \tfrac{1}{2}M_1(R,T) + \tfrac{1}{2}\pi e^{iqR}] \\ &+ e^{-(\nu+\omega_2)T}[\omega_2 W_2'(R,-T) + \omega_2 N_2'(R,-T) \\ &+ i\omega_2 M_2'(R,-T) + M_2(R,T) - \pi(e^{i\omega_2 T} - \tfrac{1}{2})e^{iqR} \\ &- iW_2(R,-T) - iN_2(R,-T)]\}.\end{aligned} \tag{B13}$$

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On matrix superpropagators. II

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The techniques developed in a previous paper (I) to compute the T product $<\phi^N{}_{\alpha\beta}(x), \phi^N{}_{\gamma\delta}(o)>$ for arbitrary N are extended to cover the case when $\phi(x)$ is a Hermitian matrix-valued field in ν dimensions. We obtain a closed expression which is used to determine superpropagators like $<[\exp\kappa\phi(x)]_{\alpha\beta}, [\exp\kappa\phi(o)]_{\gamma\delta}>$, which occur in strong interaction physics when ϕ is an SU(3) field, say.

1. INTRODUCTION

In a recent paper (I) bearing the same title,[1] a new method was developed for computing the vacuum expectation value $\langle \phi^N(x)_{\alpha\beta}, \phi^N(0)_{\gamma\delta}\rangle$ of matrix-valued symmetric fields ϕ in ν dimensions. The result for $\nu = 4$ was applied to finding the exponentially parameterized gravity superpropagator

$$\langle g_{\alpha\beta}(x), g_{\gamma\delta}(0)\rangle, \quad \text{where } g_{\alpha\beta}(x) = [\exp\kappa\phi(x)]_{\alpha\beta},$$

which occurs in localizable nonpolynomial models of quantized gravity.

In strong interaction physics the interest in nonpolynomial Lagrangians is mainly centred on nonlinear realizations of chiral $SU(\nu)$. The purpose of this paper is to show how the techniques of I are readily extended to Hermitian fields ϕ making it possible to deal with chiral $SU(3)$ matrix interactions of the type

$$m\overline{\psi}^\alpha F_\alpha^\beta(\phi)\psi_\beta, \quad F = \text{unitary function of } \gamma_5\phi,$$

which previous methods[2,3] were at great pains to tackle. We shall deduce the superpropagator $\langle F(\phi(x))_\alpha^\beta, F(\phi(0))_\gamma^\delta\rangle$ in closed form when ϕ propagates as

$$\langle \phi_\alpha^\beta(x), \phi_\gamma^\delta(0)\rangle = (\delta_\gamma^\beta\delta_\alpha^\delta - c\delta_\alpha^\beta\delta_\gamma^\delta)\Delta(x). \tag{1}$$

(Taking $c = 0$, ϕ has the interpretation of a nonet, while $c = \frac{1}{3}$ corresponds to an octet of pseudoscalar mesons.) The power of the method allows one to calculate the superpropagators for arbitrary parameterizations of the matrix group, such as the exponential or Cayley parameterizations:

$$F = e^{\gamma_5\kappa\phi} \text{ or } (1 + \tfrac{1}{2}\gamma_5\kappa\phi)(1 - \tfrac{1}{2}\gamma_5\kappa\phi)^{-1}.$$

Central to the whole approach of I was an integral representation due to Siegel giving the determinant $|Y|$ of a $\nu \times \nu$ symmetric matrix Y to an arbitrary power:

$$\left.\begin{aligned} &\int dX|X|^\mu e^{-\mathrm{Tr}(XY)} = \pi^{\nu(\nu-1)/4}\Gamma_\nu(\mu)|Y|^{-\mu-(\nu+1)/2},\\ &\Gamma_\nu(\mu) \equiv \Gamma(\mu+1)\Gamma(\mu+\tfrac{3}{2})\cdots\Gamma[\mu+\tfrac{1}{2}(\nu+1)]\\ &dX = \prod_{i\le j} dx_{ij}\end{aligned}\right\}, \tag{2}$$

the integration being taken over the space of all real, positive definite *symmetric* matrices. Formula (2) is therefore perfectly adequate for dealing with quantum gravity. However for Hermitian fields one needs a generalization of (2), and this reads

$$\left.\begin{aligned} &\int dZ|Z|^\mu e^{-\mathrm{Tr}(ZY)} = \pi^{\nu(\nu-1)/2}\Gamma_\nu^*(\mu)|Y|^{-\mu-\nu},\\ &\Gamma_\nu^*(\mu) \equiv \Gamma(\mu+1)\Gamma(\mu+2)\cdots\Gamma(\mu+\nu)\\ &dZ = \prod_{i=1} dz_{ii}\prod_{i<j} d^2z_{ij}\end{aligned}\right\}, \tag{3}$$

where the ν^2-fold integral is taken over the space of all positive definite Hermitian matrices $Z = (z_{ij})$. The proof of (3) is to be found in the Appendix. It turns out that the calculations evolving from (3) although similar to the ones evolving from (2) are in some respects simpler—for instance there is no distinction between even and odd dimensions—and this seems to be a reflexion of the phenomenon that real analysis is often harder than complex analysis.

The plan of the paper is as follows: In Sec. 2 we show how the matrix-valued superpropagator may be deduced from a knowledge of $\langle \mathrm{Tr}\phi^N, \mathrm{Tr}\phi^N\rangle$ and in Sec. 3 we indicate how this quantity may be explicitly computed by a use of representation (3). Finally in Sec. 4 we write down the superpropagators for chiral $SU(3)$ in exponential and Cayley coordinates. In places we shall be a little sketchy since most of the algebraic steps are to be found in I.

2. MATRIX SUPERPROPAGATORS

As in I we first show that the problem of arriving at the general superpropagator

$$\langle F(\phi(x))_\alpha^\beta, F(\phi(0))_\gamma^\delta\rangle, \quad F(z) = \sum_N F_N z^N/N! \tag{4}$$

is completely determined by a knowledge of the coefficients a_N in

$$\langle \mathrm{Tr}(\phi^N(x)), \mathrm{Tr}(\phi^N(0))\rangle \equiv N!\nu a_N\Delta^N(x). \tag{5}$$

For, making the ansatz,

$$\langle \phi^N{}_\alpha^\beta(x), \phi^N{}_\gamma^\delta(0)\rangle = N!(\delta_\alpha^\delta\delta_\gamma^\beta b_N - \delta_\alpha^\beta\delta_\gamma^\delta c_N)\Delta^N(x), \tag{6}$$

we obtain directly from Wick's theorem the pair of recurrence relations

$$\begin{aligned} a_N &= b_N - \nu c_N,\\ a_N &= (\nu - c)b_{N-1} - (1 - c\nu)c_{N-1}.\end{aligned} \tag{7}$$

Therefore writing the generating function of (5) as

$$\begin{aligned} a(\kappa^2\Delta) &= \nu^{-1}\langle \mathrm{Tr}\,[\exp\kappa\phi(x)], \mathrm{Tr}\,[\exp\kappa\phi(0)]\rangle\\ &= \sum_N a_N(\kappa^2\Delta)^N/N!,\end{aligned} \tag{8}$$

we find the generating function of the matrix-valued fields (6) to be

$$\langle [\exp\kappa\phi(x)]_\alpha^\beta, [\exp\kappa\phi(0)]_\lambda^\delta\rangle$$

$$= (\nu^2 - 1)^{-1}\begin{pmatrix}\{\nu\delta_\alpha^\delta\delta_\gamma^\beta - \delta_\alpha^\beta\delta_\gamma^\delta\}d/d(\kappa^2\Delta) + \\ \{(c\nu - 1)\delta_\alpha^\delta\delta_\gamma^\beta + (\nu - c)\delta_\alpha^\beta\delta_\gamma^\delta\}\end{pmatrix} a(\kappa^2\Delta). \tag{9}$$

Hence when we come to the general case (4) it is only necessary to represent the coefficients F_N as moments, $F_N = \int t^N d\mu(t)$ to make these superpropagators integral transforms, e.g.,

$$\langle \mathrm{Tr}F(\phi), \mathrm{Tr}F(\phi')\rangle = \iint d\mu(t)d\mu(t')\nu a(tt'\Delta).$$

3. EVALUATION OF $\langle \mathrm{Tr}\phi^N, \mathrm{Tr}\phi^N \rangle$

Take the vacuum expectation value of two integrals such as (3), making the substitution $Y = 1 + \kappa\phi$ and remembering that

$$\langle \exp[\mathrm{Tr}Z\phi(x)],\ \exp[\mathrm{Tr}Z'\phi(x)]\rangle = \exp[\mathrm{Tr}(ZZ') - c\ \mathrm{Tr}Z\ \mathrm{Tr}Z']\Delta(x)$$

from (1). Following the same steps as in I we arrive at

$$\langle \mathrm{Tr}(\phi^N(x)),\ \mathrm{Tr}(\phi^N(0))\rangle = N\Delta^N\left(\frac{\partial}{\partial\mu}\right)_{\mu=-\nu} I_\nu^{(c)}(\mu, N), \tag{10}$$

where

$$I_\nu^{(c)}(\mu,N) = \int \frac{dZ}{\pi^{\nu(\nu-1)/2}} \frac{|Z|^\mu}{\Gamma_\nu^*(\mu)} e^{-\mathrm{Tr}Z} T_\nu((Z - c\ \mathrm{Tr}Z)^N)$$
$$= \sum_{n=0}^{\infty} \binom{N}{n}(-c)^{N-n} \frac{\Gamma(N + \mu\nu + \nu^2)}{\Gamma(n + \mu\nu + \nu^2)} I_\nu^{(0)}(\mu, n). \tag{11}$$

To make tractable the integral $I_\nu^{(0)}(\mu, N)$, one notes that the integrand is a function only of the eigenvalues of the matrices involved which are necessarily real and positive. Changing to this set of variables, we have

$$dZ \to \gamma_\nu \prod_{k=1}^{\nu} d\lambda_k \prod_{i<j} (\lambda_j - \lambda_i)^2,$$

where γ_ν is a normalization constant [determined by $I_\nu^{(0)}(\mu, 0) = \nu$] coming from the angular integrations of parameters of $SU(\nu)$ which diagonalize Z. Hence the integral (11) reduces to

$$I_\nu^{(0)}(\mu,N) = \frac{\gamma_\nu}{\Gamma_\nu^*(\mu)} \prod_k \left(\int d\lambda_k e^{-\lambda_k} \lambda_k^\mu\right) \prod_{i<j} (\lambda_j - \lambda_i)^2 \sum_{l=1}^{\nu} \lambda_l^N \tag{12}$$

and involves the square of the Vandermonde determinant $\Pi(\lambda_j - \lambda_i)$ rather than its absolute value as we had in I; so we can apply a well-known identity[4] originally due to Lagrange for integrals involving products of determinants

$$\int_a^b d^\nu\lambda\ \det(\psi_i(\lambda_j))\ \det(\chi_i(\lambda_j)) = \nu!\ \det\int d\lambda \psi_i(\lambda)\chi_j(\lambda) \tag{13}$$

to (12) and obtain the basic form

$$I_\nu^{(0)}(\mu,N) = \frac{\nu!\gamma_\nu}{\Gamma_\nu^*(\mu)} \sum_{ij} a_{ij}^{(N)} \frac{\partial}{\partial a_{ij}} |A| \tag{14}$$

with

$$a_{ij}^{(N)} = \int_0^\infty d\lambda\ e^{-\lambda} \lambda^{N+\mu+i+j-2} = \Gamma(\mu + i + j + N - 1)$$

and

$$a_{ij}^{(0)} = a_{ij}. \tag{15}$$

This should be contrasted with the expression one encounters in the real symmetric case, where in place of of the determinant in (14) one meets a Pfaffian (= $\det^{1/2}$) possessing much more complicated matrix elements.

4. CHIRAL $SU(3)$ PROPAGATORS

Nonlinear realizations of $SU(\nu) \otimes SU(\nu)$ bring in unitary functions $F(\phi)$ of pseudoscalar meson fields transforming under the $(\nu, \nu) \oplus (\bar{\nu}, \nu)$ representation, and derivatives thereof. Correspondingly one is faced with superpropagators (4) when one performs a perturbation expansion in the Lagrangian rather than the coupling constant κ. For $\nu = 2$ there exist perfectly adequate and simple transform methods[2] for dealing with matrix interactions F; but for $\nu = 3$ these transform methods already become far too difficult to apply in practice even if they are still valid in principle. It is, therefore, when $\nu \geqslant 3$ that our new techniques can be used to advantage. We shall show below how they work for chiral $SU(3) \otimes SU(3)$ in the exponential and Cayley parameterizations of F.

To begin we need the basic coefficients a_N of (5) which are in this case given by

$$a_N = 3!\gamma_3 \sum_n \binom{N}{n}(-c)^{N-n} \frac{\partial}{\partial\mu}\Big|_{-3} \frac{1}{\Gamma^*(\mu)\Gamma(n + 3\mu + 9)} \times \sum_{ij} a_{ij}^{(n)} \frac{\partial |A|}{\partial a_{ij}}$$

with the A matrix elements (15). The differentiation is straightforwardly carried out to yield

$$a_N = \sum_{n=0}^{N} \binom{N}{n}(-c)^{N-n}[2\delta_{n0} - \delta_{n1} - \tfrac{1}{3}\delta_{n2} + \tfrac{1}{6}(n + 2)(n + 3)], \tag{16}$$

so the first few coefficients are

$$a_0 = 3, \quad a_1 = 1 - 3c, \quad a_2 = 3 - 2c + 3c^2,$$
$$a_3 = 5 - 9c + 3c^2 - 3c^3, \quad \text{etc.},$$

as can be checked by direct Wick expansion. More relevant is the generating function of (8):

$$a(\zeta) = [2 - \zeta - (\zeta^2/6)]e^{-c\zeta} + [1 + \zeta + (\zeta^2/6)]e^{(1-c)\zeta}, \tag{17}$$

where $\zeta = \kappa^2\Delta$.

For definiteness now suppose we have a nonet of pseudoscalar mesons, so that $c = 0$ in (1), and consider firstly the exponential parameterization

$$F(\phi) = e^{\gamma_5\kappa\phi} = \cos\kappa\phi + \gamma_5 \sin\kappa\phi. \tag{18}$$

By taking even and odd parts in κ^2 in (9) we get the desired superpropagator

$$16\ \langle [\exp\gamma_5\kappa\phi(x)]_\alpha^\beta, [\exp\gamma_5\kappa\phi(0)]_\gamma^\delta\rangle$$
$$= 1 \otimes 1\begin{pmatrix}(3\delta_\alpha^\delta\delta_\gamma^\beta - \delta_\alpha^\beta\delta_\gamma^\delta)a'(-\kappa^2\Delta) - \\ -(\delta_\alpha^\delta\delta_\gamma^\beta - 3\delta_\alpha^\beta\delta_\gamma^\delta)a(-\kappa^2\Delta)\end{pmatrix}$$
$$+ (\kappa^2 \leftrightarrow -\kappa^2),$$
$$+ \gamma_5 \otimes \gamma_5\begin{pmatrix}(3\delta_\alpha^\delta\delta_\gamma^\beta - \delta_\alpha^\beta\delta_\gamma^\delta)a'(-\kappa^2\Delta) - \\ -(\delta_\alpha^\delta\delta_\gamma^\beta - 3\delta_\alpha^\beta\delta_\gamma^\delta)a(-\kappa^2\Delta)\end{pmatrix}$$
$$- (\kappa^2 \leftrightarrow -\kappa^2) \tag{19}$$

with

$$a(\zeta) = 3 + [1 + \zeta + (\zeta^2/6)](e^\zeta - 1), \tag{20}$$

which demonstrates that the exponential superpropagator[5] is nothing more than polynomials multiplying hyperbolic functions of Δ, as was found[2] with chiral $SU(2)$; thus it is an entire function of Δ as expected. Indeed as $\Delta \to \infty$,

$$\langle(\exp\gamma_5\kappa\phi)_\alpha^\beta, (\exp\gamma_5\kappa\phi')_\gamma^\delta\rangle \sim (1 \otimes 1 - \gamma_5 \otimes \gamma_5) \times (\delta_\alpha^\delta\delta_\gamma^\beta + \delta_\alpha^\beta\delta_\gamma^\delta)(\kappa^2\Delta)^2 e^{\kappa^2\Delta}, \tag{21}$$

whereas as $\Delta \to 0$ we, of course, recover the perturbation series. Turning next to the Cayley parameterization one can exploit the result (19) by taking an integral transform

$$V = \frac{1 + \frac{1}{2}\gamma_5 \kappa\phi}{1 - \frac{1}{2}\gamma_5\kappa\phi} = \int_0^\infty e^{-t}(2e^{\gamma_5\kappa\phi t/2} - 1)\,dt$$

$$\therefore \langle V^\beta_\alpha, V'^\delta_\gamma\rangle = \int_0^\infty dt\,dt'\,e^{-(t+t')}\langle(2e^{\gamma_5\kappa\phi t/2} - 1)^\beta_\alpha, (2e^{\gamma_5\kappa\phi' t'/2} - 1)^\delta_\gamma\rangle$$

$$= \int_0^\infty dt\,dt'\,e^{-(t+t')}\begin{pmatrix} 4\langle(e^{\gamma_5\kappa\phi t/2})^\beta_\alpha, (e^{\gamma_5\kappa\phi t'/2})^\delta_\gamma\rangle \\ -3\,1\otimes 1\delta^\beta_\alpha\delta^\delta_\gamma\end{pmatrix}. \quad (22)$$

We shall not belabor the issue by giving the answer (22) in gory detail except to mention that, as with all rational Lagrangians, one meets at the very least incomplete functions like $\int dt\, e^{-t}(1 - \kappa^2\Delta t)^{-1}$, and their derivatives, with their possible inherent ambiguities. By taking other transforms of (19) the reader is equipped to deal with other nonlinear realizations of chiral $SU(3)$.

APPENDIX

For completeness we give a proof of formula (3):

$$J_\nu(\mu; Y) = \int_{Z>0} dZ\,|Z|^\mu e^{-\mathrm{Tr}(ZY)} = \pi^{\frac{1}{2}\nu(\nu-1)}\Gamma^*_\nu(\mu)\,|Y|^{-\mu-\nu}. \quad (3)$$

Since dZ is the invariant measure on the space of Hermitian matrices for $|Y| > 0$, we have on transforming $ZY \to Z$

$$J_\nu(\mu; Y) = |Y|^{-\mu-\nu} J_\nu(\mu; 1). \quad \text{(A1)}$$

Introduce the notation $Z_k = (z_{ij})$, $\nu \geq i, j \geq \nu - k + 1$, and $u_1 = z_{11}$ (real); $v_i = z_{1i}$ ($i = 2, 3, \ldots, \nu$). Expanding by the first row and column,

$$|Z| \equiv |Z_\nu| = [u_1 - Z^{-1}_{\nu-1}(v, \bar{v})]\,|Z_{\nu-1}|, \quad \text{(A2)}$$

where $Z^{-1}_\nu(\,,\,)$ is the (real) quadratic form obtained from the $\nu \times \nu$ matrix (Z^{-1}_ν). By hypothesis on the integration region, $|Z_\nu|$ and $|Z_{\nu-1}|$ are positive. So changing to the variable $w = u_1 - Z^{-1}_{\nu-1}(v, \bar{v})$, we obtain

$$J_\nu(\mu; 1) = \int_{Z_\nu > 0} dZ_\nu\,|Z_\nu|^\mu e^{-\mathrm{Tr}\,Z_\nu}$$
$$= \int_{Z_{\nu-1}>0} dZ_{\nu-1}|Z_{\nu-1}|^\mu e^{-\mathrm{Tr}Z_{\nu-1}}\int_0^\infty dw \iint_{-\infty}^{+\infty} d^2v_2\,d^2v_3\cdots d^2v_\nu \times (w^\mu e^{-w - Z^{-1}_{\nu-1}(v,\bar{v})})$$
$$= \pi^{\nu-1}\Gamma(\mu+1)\int_{Z_{\nu-1}>0} dZ_{\nu-1}\,|Z_{\nu-1}|^\mu\,|Z^{-1}_{\nu-1}|^{-1} e^{-\mathrm{Tr}\,Z_{\nu-1}}$$

$$\text{or } J_\nu(\mu; 1) = \pi^{\nu-1}\Gamma(\mu+1)\,J_{\nu-1}(\mu+1; 1). \quad \text{(A3)}$$

On iterating (A3) with (A1) we obtain (3).

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[5]If one had been dealing only with the propagation of the symmetric field components ϕ, corresponding to the matrices $\lambda^0, \lambda^1, \lambda^3, \lambda^4, \lambda^6, \lambda^8$ of $SU(3)$, then the procedure of Ref. 1 would be relevant and the generating function which replaces (20) is $a(\zeta) = \zeta e^{-c\zeta}[Ei(\zeta) - 2Ei(\zeta/2) + \ln\zeta/4 + \gamma - 2] + e^{\zeta(1/2-c)}[2\zeta - 3)\sinh(\zeta/2) + (2\zeta + 5)\cosh(\zeta/2) + 4]$, a much more complicated result, although also entire in $\zeta = k^2\Delta$.

Generalized Fermi transport in generalized gravitation theories

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If geodesics in space–time can be classified as timelike, null, and spacelike, the affine connection must be of the form $\Gamma^i_{jk} = \{^{\,i}_{jk}\} + 2g^{ia}e_{jka} - (\delta^i_j\delta^a_k + \delta^i_k\delta^a_j - g_{jk}g^{ia})d_a$, with d_a an arbitrary vector and e_{ijk} a tensor satisfying $e_{(ijk)} = e_{[ij]k} = 0$. It is possible to generalize Fermi's law of transport to this affine connection. The requirement that any observer be able to construct and maintain a nonrotating orthogonal space triad along his world line by the bouncing photon experiment implies the Weyl's geometry of paths.

1. INTRODUCTION

Recently,[1] the following result has been proved: Given a metric tensor g_{ij} of a normal hyperbolic type on a differential manifold, the most general symmetric affine connection that defines geodesics which can be classified as timelike, null, and spacelike with respect to that metric is of the form

$$\Gamma^i_{jk} = \{^{\,i}_{jk}\} + 2g^{ia}e_{jka} - (\delta^i_j\delta^a_k + \delta^i_k\delta^a_j - g_{jk}g^{ia})d_a \quad (1)$$

with $\{^{\,i}_{jk}\}$ the Christoffel symbols, d_k an arbitrary vector, and e_{ijk} an arbitrary tensor satisfying

$$e_{(ijk)} = e_{[ij]k} = 0. \quad (2)$$

Assuming (as was in Ref. 1) that standard (atomic) clocks determine the metric and that the world lines of free particles and light rays are timelike and null geodesics, respectively, with respect to Γ^i_{jk}, we obtain a space–time structure which may, in principle, describe a more general gravitational theory than Einstein's (provided, of course, that field equations are available).

The purpose of this paper is to discuss Fermi's law of transport in the generalized model of space–time with Eqs. (1). The physical meaning of Fermi transport was pointed out by Synge (Ref. 2, p. 123): An observer who uses Fermi-transported spatial axes and shoots a photon at a mirror will find that it returns in the same direction (to the first order in the photons' time of travel). An alternative, shorter (but in our opinion not quite rigorous) treatment was given by Pirani.[3] We shall see that in the case of the generalized model this physical requirement again selects a particular transport law for unit vectors orthogonal to a certain (observer's) world line.

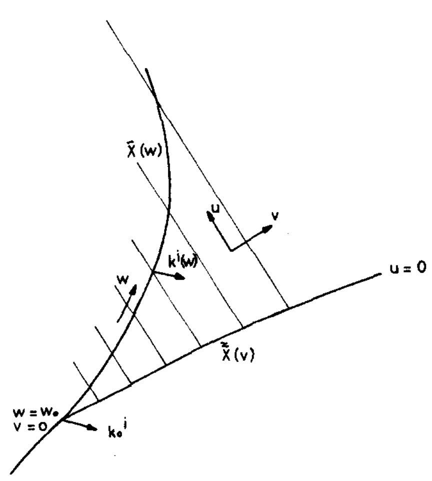

FIG. 1.

Throughout this paper Latin and Greek indices, respectively, take the ranges {0, 1, 2, 3} and {1, 2, 3}, the metric tensor g_{ij} has the signature (+ 1,– 1,– 1,– 1), covariant derivatives with respect to Γ^i_{jk} are denoted by a double stroke (e.g. $g_{ij\|k}$), and the absolute derivative with respect to a parameter p by $\delta/\delta p$. In order to simplify the formulas it is convenient, on occasion, to lower and raise indices using the metric tensor and to denote the scalar product $g_{ij}A^iB^j = A_jB^j$ of any two vectors by (AB): However, it must be kept in mind that covariant differentiation does not commute with raising and lowering of indices. Indeed, an equivalent form of (1) and (2) is

$$g_{ij\|k} = 2g_{ij}d_k + 2e_{ijk}. \quad (3)$$

All functions appearing in this paper are assumed to possess a sufficient number of continuous derivatives.

2. THE GENERALIZED FERMI TRANSPORT

Given a timelike line $\bar{x}(w) \equiv \bar{x}^i(w)$ and two vectors $l^i(w)$ and $m^i(w)$ orthogonal to $W^i(w) \equiv (d\bar{x}^i/dw)\,(w)$, we say that these vector fields are strongly codirectional at $\bar{x}(w_0)$ if $l^i(w_0) = m^i(w_0)$ and $(d/dw)\,(g_{ab}l^a \underset{(\alpha)}{\xi^b})/_{w=w_0} = (d/dw)(g_{ab}m^a \underset{(\alpha)}{\xi^b})/_{w=w_0}$, where $\underset{(\alpha)}{\xi^i}(w)$ are the components of an orthogonal triad in the 3-space orthogonal to $W^i(w)$ along $\bar{x}(w)$. Clearly $l^i(w)$ and $m^i(w)$ are strongly codirectional at $\bar{x}(w_0)$ if and only if $l^i(w_0) = m^i(w_0)$ and $(\delta/\delta w)\, l^i(w_0) = (\delta/\delta w)\, m^i(w_0)$.

Every unit vector k^i_0 at $\bar{x}(w_0)$ which is orthogonal to $W^i(w_0)$, determines a "field of directions of returning light rays" $k^i(w)$, along the half of $\bar{x}(w)$ that consists of events later than $\bar{x}(w_0)$, in accordance with the following construction (illustrated in Fig. 1).

Let $\bar{\bar{x}}(v)$ be the world line of a light ray leaving $\bar{x}(w_0)$ in the direction k^i_0. This means that $\bar{\bar{x}}(0) = \bar{x}(w_0)$ and $p^i_j(w_0)\,(d\bar{\bar{x}}^j/dv)\,(0)$ is proportional to k^i_0, where

$$p^i_j(w) \equiv \delta^i_j - [W(w)W(w)]^{-1}\, W^i(w)W_j(w) \quad (4)$$

is the projection operator on the 3-space orthogonal to $W^i(w)$. $k^i(w)$ is the unit vector at $\bar{x}(w)$, orthogonal to $W^i(w)$, such that the light ray arriving at $\bar{x}(w)$ in its direction intersects $\bar{\bar{x}}(v)$ (at a certain v). Obviously,

$k^i(w)$ is unique in a neighborhood of w_0. We shall see later that $k^i(w) \underset{w\to w_0}{\longrightarrow} k_0^i$ (in the sense of fiber bundles).

A unit vector $n^i(w)$ orthogonal to $W^i(w)$ along $\tilde{x}(w)$ is said to undergo generalized Fermi transport if for every w_0, $n^i(w)$ and the field of directions of returning light rays determined by $n^i(w_0)$ are strongly codirectional at $\tilde{x}(w_0)$. *A priori* there is no evidence that such a vector field exists; however, we shall presently write a transport law which generates such vector fields along every timelike line [Eq. (31) below].

Without any loss of generality, we parametrize the relevant world lines (Fig. 1) so that W^i points to the future and v along $\tilde{\tilde{x}}(v)$ is a special parameter with respect to Γ^i_{jk}: $(\delta/\delta v)\,(d\tilde{\tilde{x}}/dv) = 0$. For every v the function of the variable u, $x = \bar{x}(u, v)$, represents the light ray going from the event $\tilde{\tilde{x}}(v)$ to some event on the line $\tilde{x}(w)$; u is also a special parameter. Thus $\bar{x}(u, v)$ is a parametric representation of a 2-space spanned by a null congruence. We define 2-vector fields on this 2-space:

$$U^i(u, v) \equiv \frac{\partial \bar{x}^i}{\partial u}(u, v), \quad V^i(u, v) = \frac{\partial \bar{x}^i}{\partial v}(u, v); \tag{5}$$

they satisfy the equation

$$\frac{\delta}{\delta u} V^i(u, v) = \frac{\delta}{\delta v} U^i(u, v). \tag{6}$$

According to our parametrization we have $\tilde{x}(w_0) = \tilde{\tilde{x}}(0)$, $\bar{x}(0, v) = \tilde{\tilde{x}}(v)$, and

$$\frac{\delta}{\delta v} V^i(0, v) = 0, \quad (VV) = 0 \text{ along } \tilde{\tilde{x}}(v) \text{ and } V^i(0, v) \text{ points to the future}; \tag{7}$$

$$\frac{\delta}{\delta u} U^i = 0, \quad (UU) = 0 \text{ and } U^i \text{ points to the future}. \tag{8}$$

Obviously, in a neighborhood of $v = 0$, $U^i(0, v)$ is not parallel to $V^i(0, v)$; in particular, $U^i(0, 0)$ is not parallel to $V^i(0, 0)$. Therefore $(UV) > 0$ in a neighborhood of $\bar{x}(0, 0)$.

$\tilde{x}(w)$ is a timelike line in the 2-space $\bar{x}(u, v)$ and can be represented by two functions $u(w)$ and $v(w)$ which satisfy $u(w_0) = v(w_0) = 0$ and $\bar{x}(u(w), v(w)) = \tilde{x}(w)$. As a result we get

$$W^i = u'U^i + v'V^i, \quad u' \equiv \frac{du}{dw}, v' \equiv \frac{dv}{dw} \tag{9}$$

along $\tilde{x}(w)$. The fact that W^i is timelike and points to the future implies $u' > 0$, $v' > 0$, and $2u'v'(UV) + (v')^2(VV) > 0$ in a neighborhood of $w = w_0$.

According to the definitions

$$k_0^i = AP^i_j(w_0)V^j(0, 0), \quad k^i(w) = -BP^i_j(w)U^j(u(w), v(w)), \tag{10}$$

where A and B are positive scalars chosen so as to make k_0^i and k^i unit vectors.

It is possible now to achieve the final results by a direct calculation. But we are still at liberty to normalize the special parameters u and v without any loss of generality and the parameter w along $\tilde{x}(w)$ without essential loss of generality. In order to reduce the complexity of the formulas we choose the following normalization:

$$(WW) = 1, \quad (WV) = 1 \text{ at } \tilde{x}(w_0), \quad (UV) = 2 \text{ along } \tilde{x}(w). \tag{11}$$

This means, in particular, that we take $dw = ds$ along $\tilde{x}(w)$. Equations (9) and (11) [with the aid of (7) and (8)] imply

$$4u'v' + (v')^2(VV) = 1 \tag{12}$$

along $\tilde{x}(w)$ and

$$v'(w_0) = u'(w_0) = \tfrac{1}{2}. \tag{13}$$

Equation (10) now takes the form

$$k_0^i = \tfrac{1}{2}V^i(0, 0), \; -\tfrac{1}{2}U^i(0, 0), \tag{14}$$

$$k^i = v'V^i - [(2v')^{-1} - u']U^i \tag{15}$$

along $\tilde{x}(w)$.

It is now easily seen that $k^i(w_0) = k_0^i$.

The last step consists in differentiating Eq. (15) with respect to w at w_0. We have, of course,

$$\frac{\delta}{\delta w} = u'\frac{\delta}{\delta u} + v'\frac{\delta}{\delta v} \tag{16}$$

for any function of u and v. Using (6)–(8), (13), (15), and (16) we obtain

$$\frac{\delta k^i}{\delta w}(w_0) = [u''(w_0) + 2v''(w_0)]U^i(0, 0) + v''(w_0)V^i(0, 0). \tag{17}$$

Finally we want to express $(\delta k^i/\delta w)\,(w_0)$ in terms of $k^i(w_0)$ and covariant derivatives of W^i at w_0. Equations (9), (13), and (14) imply [at $\tilde{x}(w_0)$]

$$k^i = \tfrac{1}{2}(-U^i + V^i), \quad W^i = \tfrac{1}{2}(U^i + V^i), \tag{18}$$

$$U^i = -k^i + W^i, \quad V^i = k^i + W^i. \tag{19}$$

Hence [at $\tilde{x}(w_0)$]

$$\frac{\delta k^i}{\delta w} = pk^i + qW^i, \qquad p = -(u'' + v''), \quad q = u'' + 3v''. \tag{20}$$

Differentiating Eq. (12) with respect to w we obtain [at $\tilde{x}(w_0)$]

$$u'' + v'' = -\frac{1}{8}\frac{d}{dw}(VV). \tag{21}$$

Equation (9) implies [at $\tilde{x}(w_0)$]

$$\frac{\delta W^i}{\delta w} = u''U^i + v''V^i + \tfrac{1}{2}\frac{\delta U^i}{\delta v},$$

and a scalar product of $k^i(w_0)$ with this equation leads to the result

$$-u'' + v'' = \frac{1}{4}\left(V\frac{\delta U}{\delta v}\right) - \frac{1}{4}\left(U\frac{\delta U}{\delta v}\right) - \left(k\frac{\delta W}{\delta w}\right). \tag{22}$$

Substituting from (21) and (22) into (20) we obtain

$$p = \frac{1}{8}\frac{d}{dw}(VV), \quad q = \frac{1}{4}\left(V\frac{\delta U}{\delta v}\right) - \frac{1}{4}\left(U\frac{\delta U}{\delta v}\right) - \frac{1}{4}\frac{d}{dw}(VV) - \left(k\frac{\delta W}{\delta w}\right). \tag{23}$$

Equations (3), (6), (7), (13), and (16) imply [at $\tilde{x}(w_0)$]

$$\frac{d}{dw}(VV) = 2e_{abc}V^aV^bW^c + \left(V\frac{\delta U}{\delta v}\right). \tag{24}$$

Differentiating $(UV) = 2$ [Eq. (11)] with respect to w and using Eqs. (3), (6), (7), (8), (13), (16), and (18) we obtain [at $\tilde{x}(w_0)$]

$$\left(V\frac{\delta U}{\delta v}\right) = -\left(U\frac{\delta U}{\delta v}\right) - 8d_aW^a - 4e_{abc}V^aU^bW^c. \tag{25}$$

Differentiation of $(UU) = 0$ [Eq. (8)] with respect to v gives

$$\left(U\frac{\delta U}{\delta v}\right) = -e_{abc}U^aU^bV^c. \tag{26}$$

Substituting from (24)–(26) into (23), we obtain

$$p = -d_aW^a + \tfrac{1}{8}e_{abc}U^aU^bV^c - \tfrac{1}{2}e_{abc}V^aU^bW^c + \tfrac{1}{4}e_{abc}V^aV^bW^c;$$
$$q = \tfrac{1}{4}e_{abc}U^aU^bV^c - \tfrac{1}{2}e_{abc}V^aV^bW^c - \left(k\frac{\delta W}{\delta w}\right). \tag{27}$$

Replacing every U^a and V^a appearing in (27) by the expressions of Eq. (19) and making use of the symmetries of the tensor e_{abc} [Eq. (2)] we obtain the final desired expression for $(\delta k^i/\delta w)(w_0)$. In accordance with this result and with the previous discussion we may say that a unit vector $n^i(w)$ orthogonal to $W^i(w)$ along $\bar{x}(w)$ undergoes generalized Fermi transport if and only if

$$\frac{\delta n^i}{\delta w} = (e_{abc}n^an^bW^c - d_aW^a)n^i + \left[e_{abc}W^aW^bn^c - \left(n\frac{\delta W}{\delta w}\right)\right]W^i. \tag{28}$$

[The abrupt change in notation (from k^i to n^i) is to indicate that whereas k^i satisfied condition (28) only at $\bar{x}(w_0)$, any n^i that undergoes generalized Fermi transport does so along the curve $x(w)$.]

Synge (in a private communication) has given the following alternative and shorter derivation of (28) from (20): Since by construction $(WW) = 1$, $(kk) = -1$, and $(kW) = 0$ along $\bar{x}(w)$, Eq. (20) $(\delta k^i/\delta w = pk^i + qW^i)$ implies at $\bar{x}(w_0)$

$$\pi = -\left(k\frac{\delta k}{\delta w}\right), \quad q = \left(W\frac{\delta k}{\delta w}\right). \tag{29}$$

From the equations $(d/dw)(kk) = 0$ and $(d/dw)(kW) = 0$ we have

$$-\left(k\frac{\delta k}{\delta w}\right) = \frac{1}{2}g_{ab\|c}k^ak^bW^c,$$
$$\left(W\frac{\delta k}{\delta w}\right) = -g_{ab\|c}k^aW^bW^c - \left(k\frac{\delta W}{\delta w}\right). \tag{30}$$

Substituting (30) into (29) and (20) and making use of Eqs. (2) and (3) lead immediately to (28).

In the case that w along $\bar{x}(w)$ is not the metrical length (in the generalized model of space–time s is not the only natural parameter along every timelike line), it easily comes out that a unit vector $n^i(w)$ orthogonal to $W^i(w)$ [$\equiv (d\bar{x}^i/dw)(w)$] undergoes generalized Fermi transport if and only if

$$\frac{\delta n^i}{\delta w} = (e_{abc}n^an^bW^c - d_aW^a)n^i + (WW)^{-1}\left[e_{abc}W^aW^bn^c - \left(n\frac{\delta W}{\delta w}\right)\right]W^i. \tag{31}$$

This equation is not linear in n^i.

We want to emphasize that the last equation is the necessary and sufficient condition for a *given* field of unit vectors orthogonal to W^i to be strongly codirectional at every event with the field of the directions of the returning light rays determined by the member of the given field at this event. The question now arises as to whether this equation, as a transport law for vectors, retains the unit length of an arbitrary $n^i(w)$ and preserves the orthogonality relation between $W^i(w)$ and $n^i(w)$. The answer is that it does. For suppose that the field $n^i(w)$ along $\bar{x}(w)$ satisfies (31). Then, via (2), we obtain

$$\frac{d}{dw}(nW) = (e_{abc}n^an^bW^c + d_aW^a)(nw);$$
$$\frac{d}{dw}(nn) = 2(WW)^{-1}\left[e_{abc}W^aW^bn^c - \left(n\frac{\delta W}{\delta w}\right)\right](nW) + 2e_{abc}n^an^bW^c(nn) + 2e_{abc}n^an^bW^c.$$

The first equation implies that if (nW) vanishes at one event then it vanishes along the whole line. And if, in addition, $(nn) = -1$ at one event, then the second equation ensures that $(nn) = -1$ along the whole line. Therefore, (31) is indeed a transport law for unit vectors orthogonal to a certain timelike line, and we shall call this equation the generalized Fermi transport law.

3. CONSERVATION OF SCALAR PRODUCTS BETWEEN FERMI TRANSPORTED VECTORS AND THE WEYL'S GEOMETRY OF PATHS

The generalized Fermi transport may be considered as a transport law for spatial axes along an observer's world line if it preserves scalar products (or at least the orthogonality of vectors). Let $n^i(w)$ and $m^i(w)$ be two unit vectors orthogonal to W^i along $\bar{x}(w)$, subjected to the generalized Fermi transport (31). Via (3), (31), and the concluding remarks of the preceding section we get

$$\frac{d}{dw}(nm) = 2e_{abc}n^am^bW^c + (nm)(e_{abc}n^an^bW^c + e_{abc}m^am^bW^c). \tag{32}$$

This equation implies that if the generalized Fermi transport preserves the orthogonality relation between vectors, then

$$e_{abc}n^am^bW^c = 0 \tag{33}$$

for every three orthogonal vectors n^a, m^a, W^a such that W^a is timelike. A cumbersome but straightforward calculation, using a system of coordinates in which $g_{ij} = \mathrm{diag}(+1, -1, -1, -1)$ at one event, shows that (33) and (2) imply

$$e_{ijk} = g_{ij}e_k - \tfrac{1}{2}g_{ki}e_j - \tfrac{1}{2}g_{jk}e_i, \tag{34}$$

where e_k is an arbitrary covariant vector, and (34) in turn implies $(d/dw)(nm) = 0$, even if n^i and m^i are not orthogonal to each other, as is easily seen by a direct substitution of (34) into (32). Therefore, a necessary and sufficient condition for the generalized Fermi transport to preserve the scalar product or (at least) the orthogonality relation between vectors is that e_{ijk} be of the form (34); d_k is still arbitrary. And in this case the transport law can be further generalized to an arbitrary vector A^i (not necessarily of unit length and orthogonal to W^i) in the form

$$\frac{\delta A^i}{\delta w} = -(e_aW^a + d_aW^a)A^i + \left[e_aA^a - (WW)^{-1}\left(A\frac{\delta W}{\delta w}\right)\right]W^i + (WW)^{-1}(AW)\frac{\delta W^i}{\delta w}. \tag{35}$$

This is the generalized Fermi–Walker transport (Ref. 2, p. 13), and it is linear in A^i.

The projective transformation $\Gamma^i_{jk} \to \Gamma^i_{jk} + \delta^i_j \psi_k + \delta^i_k \psi_j$, where ψ_i is an arbitrary covariant vector, is the most general change of an affine connection that preserves the geodesics.[4] Since

$$\delta^i_j \psi_k + \delta^i_k \psi_j \equiv -2 g^{ia} e'_{jka} + 2(\delta^i_j \delta^a_k + \delta^i_k \delta^a_j - g_{jk} g^{ia}) \psi_a,$$

where $e'_{jka} = \frac{1}{2} g_{aj} \psi_k + \frac{1}{2} g_{ak} \psi_j - g_{jk} \psi_a$, a projective change does not spoil form (1) of the affine connection, nor does it spoil the form (34) of e_{ijk}, if e_{ijk} has that form. In the latter case, a projective change with $\psi_i = -e_i$ transforms the Γ^i_{jk} into

$$\Gamma^i_{jk} = \left\{ {i \atop jk} \right\} - (\delta^i_j \delta^a_k + \delta^i_k \delta^a_j - g_{jk} g^{ia})(d_a - 2e_a).$$

We recognize here the affine connection of Weyl's theory of gravitation and electromagnetism. Thus we have proved that the Weyl's geometry of paths follows from the requirement that the generalized Fermi transport preserve scalar products.

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Linear adiabatic invariants and coherent states

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The Born–Fock adiabatic theorem is extended to all orders for some quadratic quantum systems with finitely or infinitely degenerate energy spectra. A prescription is given for obtaining adiabatic invariants to any order. For any quadratic quantum system with N degrees of freedom there are $2N$ linear adiabatic invariant series, which correspond to the $2N$ exact invariants. The exact quantum mechanical solution for any nonstationary quadratic quantum system is also constructed by making use of the coherent-state representation: The Green's function, coherent states, transition amplitudes and probabilities and their generating functions are obtained explicitly. Two particular systems, the N-dimensional time-dependent general oscillator and charged particle motion in a varying and uniform electromagnetic field, are considered in greater detail as examples.

I. INTRODUCTION

Recently there has been renewed interest in the subject of exact and adiabatic invariants for both classical and quantum systems. The main purpose of this paper is to find all the linear integrals of motion of an arbitrary time-dependent quadratic quantum system and to construct adiabatic invariants from the exact solutions by a method of expansion. Lewis and Riesenfeld[1] have developed the method of time-dependent invariants and applied it to classical and quantum oscillators and to charged particle motion in a uniform electromagnetic field. Lewis's treatment of the harmonic oscillator was extended to general linear and nonlinear classical oscillators by Symon,[2] who gave a prescription for obtaining a quadratic adiabatic invariant as a power series to any order in the variation of the coefficients. Earlier Kruskal[3] proposed a method for obtaining quadratic adiabatic invariants of the action type $I = \oint p\,dq$, for classical systems, all solutions of which are nearly periodic. By successive application of Kruskal's theory one can obtain Γ invariants, where Γ is the number of the system periodicities and $\Gamma \le N$, N being the number of the degrees of freedom. Kruskal's method was generalized by Stern[4] for constructing new invariants, which in specific cases coincide with I. Namara and Whiteman[5] gave another method for the construction of adiabatic invariants by expanding the Poisson brackets in series. The problem of adiabatic invariants is discussed in Ref. 6. In this paper we suggest that for any system there must be $2N$ adiabatic invariants, which correspond to the $2N$ independent exact invariants. In the case of quadratic systems these invariants are linear with respect to the coordinates q_j and momenta p_j, and we construct them here explicitly. Any other invariant can be built up by means of linear ones. We have constructed the $2N$ invariants for quantum systems and they certainly hold for classical systems too.

The problem of adiabatic invariance in quantum mechanics has been treated by many authors.[7-11] Born and Fock[7] proved adiabatic invariance to first-order in the adiabatic parameter for quantum systems with a nondegenerate energy spectrum. An extension of this theorem to all orders was made by Lenard[8] for those quantum systems which have a finite number of nondegenerate states. Dyhne[9] considered the quantum oscillator and charged particle motion in a nonuniform magnetic field in the adiabatic approximation and showed the transition amplitudes to be exponentially small. Some adiabatic theorems in quantum mechanics were proved by Young and Deal.[10] In Ref. 11 the S matrix of the quantum oscillator is expanded in asymptotic series. In this paper we demonstrate the validity of the Born–Fock theorem to all orders for quadratic quantum systems.

All $2N$ adiabatic invariants are also shown to be constant to all orders. The familiar adiabatic invariants, i.e., the ratio of energy to frequency (action) of the harmonic oscillator and the magnetic moment of a particle in an electrogmagnetic field can easily be expressed as quadratic invariants in terms of the linear ones and shown to be also constant to all orders in the quantum case as well as in the classical case. The constancy of the magnetic moment in all orders for the classical particle was derived by Kruskal,[12] and Kulsrud[13] proved the same for the ratio of energy to frequency of the classical oscillator. The total change of the action adiabatic invariant of the one-dimensional classical oscillator was calculated by Dyhne.[9] For the quantum oscillator this was done in Ref. 14. We give here exact formulas for the changes of all linear and quadratic adiabatic invariants of the N-dimensional general harmonic oscillator. For a charged particle, moving in a uniform electromagnetic field, and for the N-dimensional oscillator, this was done in Ref. 15.

The adiabatic invariants are obtained by expanding the exact ones in asymptotic series in the time derivatives of the coefficients of the Hamiltonian. The exact time-dependent invariants of quadratic quantum systems can be easily derived in terms of the solutions of linear differential equations. If the exact solutions of these equations are not known (as is the case, in general, as we shall see), one can always solve them recursively and use the adiabatic invariants.

So it is of considerable interest to have a method for obtaining adiabatic invariants and to investigate the accuracy of their conservation. By using the exact linear invariants and the coherent state representation[16] it is easy to construct the solution of the Schrödinger equation for any quadratic system. Following the method of Refs. 15 and 17 we solve this problem in Sec. II, obtaining explicit formulas for the coherent states, Green's function, and transition amplitudes and probabilities and their generating functions. Transition amplitudes connecting any initial energy eigenstate to the final one are expressed in terms of Hermite polynomials of $2N$ variables.[18] We consider in greater detail some systems, where the solution of the wave equation can be expressed in terms of the solutions of a simple and familiar equation, i.e., the equation of motion of the classical oscillator. The problem of adiabatic invariants is treated in Sec. III.

II. N-DIMENSIONAL TIME-DEPENDENT QUADRATIC SYSTEM. EXACT SOLUTION

A. Coherent states and Green's function

We consider a quantum system whose Hamiltonian is a general quadratic form with respect to the coordinates q_j and momenta p_j, $j = 1,2,\ldots,N$ ($h = c = 1$)

$$H(t) = B_{\alpha,\beta}(t)Q_\alpha Q_\beta + C_\alpha(t)Q_\alpha, \quad \alpha,\beta = 1,2,\ldots,2N \tag{1}$$

where $Q_j = p_j$, $Q_{N+j} = q_j$, and the Hermitian matrix $B(t)$ and the real vector $\mathbf{C}(t)$ are arbitrary functions of time. Hereafter quadratic forms of the type (1) will be written as

$$H = \mathbf{Q}B\mathbf{Q} + \mathbf{CQ}. \tag{1a}$$

The range of the Latin indices is $1,2,\ldots,N$, and the Greek indices run over $1,2,\ldots,2N$. The harmonic oscillator and the motion of a charged particle in a uniform electromagnetic field are the most familiar particular cases of (1). The time-dependent quantum oscillator was thoroughly examined by Husimi,[19] and later many authors[1,9,11,14,15,20] have treated different aspects of the problem. Coherent states for nonstationary quadratic systems were first introduced in Ref. 15 and used for calculations in the problems of the N-dimensional oscillator and charged oscillators in uniform electromagnetic fields.[15,17,21] Recently Holz[21] constructed coherent states and calculated transition amplitudes between them for a system of the type (1) with

$$B(t) = \begin{pmatrix} I & a(t) \\ \tilde{a}(t) & b(t) \end{pmatrix}, \tag{2}$$

$a(t)$ and $b(t)$ being $N \times N$ real matrices.

In accordance with the suggestion in Ref. 15 we look for $2N$ exact linear invariants of the form

$$I_\alpha(t) = \Lambda_{\alpha,\beta}(t)Q_\beta + \delta_\alpha(t), \tag{3}$$

or, in matrix form,

$$\mathbf{I}(t) = \Lambda(t)\mathbf{Q} + \boldsymbol{\delta}(t), \tag{3'}$$

where the matrix $\Lambda(t)$ and vector $\boldsymbol{\delta}(t)$ are defined in accordance with the requirement

$$\frac{\partial}{\partial t}\mathbf{I}(t) - i[\mathbf{I}(t), H] = 0, \tag{4}$$

which leads to the following differential equations

$$\dot{\Lambda} = \Lambda R(t), \tag{5a}$$

$$\dot{\boldsymbol{\delta}} = i\Lambda\sigma_2\mathbf{C}(t), \tag{5b}$$

the two $2N \times 2N$ matrices R and σ_2 being defined as

$$R = i\sigma_2[B(t) + B^*(t)], \quad \sigma_2 = i\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}. \tag{6}$$

We choose the initial conditions

$$\Lambda(0) = I, \quad \boldsymbol{\delta}(0) = 0 \tag{7}$$

and write the solutions of (5) as

$$\Lambda(t) = \hat{T}\exp\left(\int_0^t dt_1 R(t_1)\right), \tag{8a}$$

$$\boldsymbol{\delta}(t) = i\int_0^t \Lambda(t_1)\sigma_2 C(t_1)dt_1, \tag{8b}$$

$\hat{T}$ standing for the antichronological product. The normalized solution $\Lambda(t)$ exists for any continuous $R(t)$, i.e., for continuous $B(t)$.[22] By virtue of (7) we have the commutators

$$[I_\alpha(0), I_\beta(0)] = [Q_\alpha, Q_\beta] = (\sigma_2)_{\alpha,\beta}, \tag{9}$$

and remembering that the evolution of any Heisenberg operator is $I(t) = S^{-1}I(0)S$, we derive

$$[I_\alpha(t), I_\beta(t)] = (\sigma_2)_{\alpha,\beta}, \tag{10}$$

which imposes upon Λ the relation

$$\Lambda\sigma_2\tilde{\Lambda} = \sigma_2, \tag{11}$$

$\tilde{\Lambda}$ being the transpose of Λ. The commutation relations (10) are invariant under the transformation $\mathbf{I}' = C\mathbf{I}$, where C is a symplectic matrix. This corresponds to another choice of initial conditions for Λ and $\boldsymbol{\delta}$ or to a canonical transformation in phase space. It is clear that (3) is also a canonical transformation.

In order to apply our method[15] we introduce, instead of $I_\alpha(t)$, lowering and raising operators $A_j(t), A_j^\dagger(t)$:

$$[A_i(t), A_j^\dagger(t)] = \delta_{i,j}, \quad i,j = 1,2,\ldots,N \tag{12}$$

in accordance with the formulas

$$A_j(t) = (1/\sqrt{2})[iI_j(t) + I_{N+j}(t)]. \tag{13}$$

We rewrite (13) in the form

$$A_j = \frac{1}{\sqrt{2}}[(\lambda_p)_{j,k}p_k + (\lambda_q)_{j,k}q_k + \Delta_j], \tag{14}$$

where

$$\Delta_j = i\delta_j + \delta_{N+j},$$

$$\lambda_p = \lambda_3 + i\lambda_1, \lambda_q = i\lambda_2 + \lambda_4, \quad \Lambda \equiv \begin{pmatrix} \lambda_1 & \lambda_2 \\ \lambda_3 & \lambda_4 \end{pmatrix}.$$

Further we follow Ref. 15, and for this reason the details of calculations are omitted. Coherent states $|\boldsymbol{\alpha};t\rangle$, $\boldsymbol{\alpha} = (\alpha_1,\ldots,\alpha_N)$, with α_j being complex numbers and

$$A_j(t)|\boldsymbol{\alpha}_j;t\rangle = \alpha_j|\boldsymbol{\alpha};t\rangle, \quad \left(i\frac{\partial}{\partial t} - H\right)|\boldsymbol{\alpha};t\rangle = 0 \tag{15}$$

are obtained as an exponential of a quadratic

$$|\boldsymbol{\alpha};t\rangle = \Pi^{-N/4}\exp[\sigma(t) + \boldsymbol{\nu}(t)\boldsymbol{q} - \tfrac{1}{2}\boldsymbol{q}\mu(t)\boldsymbol{q}], \tag{16}$$

where

$$\mu = i\lambda_p^{-1}\lambda_q, \quad \boldsymbol{\nu} = -i\lambda_p^{-1}\boldsymbol{\Delta} + (1/\sqrt{2})(\lambda_q^\dagger - \lambda_p^{-1}\lambda_q\lambda_p^\dagger)\boldsymbol{\alpha}, \tag{17a}$$

$$\sigma = \Phi(t) - \tfrac{1}{2}|\boldsymbol{\alpha}|^2 + (1/\sqrt{2})(\boldsymbol{\Delta}^* - \boldsymbol{\Delta}\tilde{\lambda}_p^{-1}\lambda_p^\dagger)\boldsymbol{\alpha} + \tfrac{1}{4}i\boldsymbol{\alpha}(\lambda_p^*\lambda_p^{-1}\lambda_q\lambda_p^\dagger - \lambda_q^*\lambda_p^\dagger)\boldsymbol{\alpha}, \tag{17b}$$

and

$$\Phi(t) = \int_0^t dt_1[-Sp(b_2 + b_1\lambda_p^{-1}\lambda_q) + i\boldsymbol{\Delta}\tilde{\lambda}_p^{-1}b_1\lambda_p^{-1}\boldsymbol{\Delta} + i\mathbf{c}_1\lambda_p^{-1}\boldsymbol{\Delta}]. \tag{18}$$

Here we introduce the notations

$$B = \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix}, \quad \mathbf{C} = \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{pmatrix}, \tag{19}$$

where b_1, b_2, b_3 and b_4 are $N \times N$ matrices and $\mathbf{c}_1$ and $\mathbf{c}_2$ are N vectors.

For convenience we rewrite $|\boldsymbol{\alpha}; t\rangle$ in the form

$$|\boldsymbol{\alpha}; t\rangle = |\mathbf{0}; t\rangle \exp(-\tfrac{1}{2}|\alpha|^2 + \mathbf{s}\boldsymbol{\alpha} - \tfrac{1}{2}\boldsymbol{\alpha} w \boldsymbol{\alpha}), \quad (20)$$

where

$$w = \tfrac{1}{2} i(\lambda_q^* \lambda_p^\dagger - \lambda_p^* \lambda_p^{-1} \lambda_q \lambda_p^\dagger), \qquad \mathbf{s} = (1/\sqrt{2})(\Delta^* - \lambda_p^* \lambda_p^{-1}\Delta + \lambda_q^* q - \lambda_p^* \lambda_p^{-1} \lambda_q q) \quad (21)$$

and the vacuum

$$|\mathbf{0};\rangle = \pi^{-N/4} \exp[-\tfrac{1}{2}\mathbf{q}\mu\mathbf{q} - i\mathbf{q}\lambda_p^{-1}\Delta + \Phi(t)], \qquad A_j(t)|\mathbf{0}; t\rangle = 0. \quad (22)$$

Coherent states $|\boldsymbol{\alpha}; t\rangle$ describe the most classical states of quadratic quantum systems in a manner similar to that for the oscillator.[15,17] Stoler[23] has recently shown that all minimum uncertainty packets are equivalent to coherent states. The eigenvalues α_j of the invariants A_j are connected with the coordinates of the initial point in the phase space, where the classical motion started.

Formula (20) shows that the eigenstates of the quadratic invariants $A_j^\dagger A_j$ are given by the formula

$$|\mathbf{n}; t\rangle = (n_1! \cdots n_N!)^{-1/2} |\mathbf{0}; t\rangle H_{\mathbf{n}}(\tilde{w}^{-1}s), \quad (23)$$

where $\mathbf{n} = (n_1, \ldots, n_N)$, n_j being positive integers, and $H_{\mathbf{n}}(\mathbf{x})$ are Hermite polynomials of N variables.[18]

Green's function is obtained as

$$G(\mathbf{q}_2, t_2; \mathbf{q}_1, t_1) = 2^N |\mathbf{0}; 2\rangle\langle \mathbf{0}; 1| (\det P)^{-1/2} \exp(\tfrac{1}{2}\mathbf{l}P\mathbf{l}), \quad (24)$$

where P is a $2N \times 2N$ matrix

$$P = \begin{pmatrix} 2 + w(2) + w^*(1) & i[w(2) - w^*(1)] \\ i[w(2) - w^*(1)] & 2 - w(2) - w^*(1) \end{pmatrix} \quad (24a)$$

and $\mathbf{l}$ is $2N$ vector

$$\mathbf{l} = \begin{pmatrix} s(2) + s^*(1) \\ is(2) - is^*(1) \end{pmatrix}. \quad (24b)$$

The $N \times N$ matrices $w(2)$ and $w(1)$ and the N vectors $s(2)$ and $s(1)$ are defined by formulas (21) for $\mathbf{q}_2, t_2$ and $\mathbf{q}_1, t_1$, respectively. We have used the known Gaussian integral

$$\int \exp(-\tfrac{1}{2}\mathbf{x}a\mathbf{x} + \mathbf{b}\mathbf{x}) dx_1 \cdots dx_N = (2\pi)^N (\det a)^{-1/2} \exp(\tfrac{1}{2}\mathbf{b}a^{-1}\mathbf{b}). \quad (25)$$

The derivation of the Green's function by means of coherent states [Gaussian integral (25)] is completely equivalent to the calculation of the corresponding Feynman path integral; but, in our opinion, the former is more convenient.

B. Transition amplitudes and probabilities and their generating functions

The coherent states having been constructed, all the transition amplitudes can be obtained explicitly in a straightforward manner. Let the Hamiltonian (1) be stationary in the remote past and the remote future. More precisely let us suppose

$$B(t) = \text{const}, \quad \mathbf{C}(t) = 0 \text{ for } t \le 0 \text{ and } t \to \infty. \quad (26)$$

Under these conditions as $t \to \pm\infty$ there exist initial $|\boldsymbol{\alpha}; in\rangle$ and final $|\beta; f\rangle$ coherent states and initial $|\mathbf{n}; in\rangle$ and final $|\mathbf{m}; f\rangle$ discrete spectra and the problem of transitions between them can be solved. It must be noted that, in general, the initial (or final) discrete spectrum $|\mathbf{n}; in\rangle$ does not coincide with the energy spectrum as in the case of the oscillator and a charged particle in an electromagnetic field. For example, the free motion of a particle

$$H = \tfrac{1}{2}p^2, \quad B = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix} \quad (27)$$

and the inverse oscillator

$$H = \tfrac{1}{2}(p^2 - q^2), \quad B = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \quad (28)$$

do not possess discrete energy spectra although the discrete states (23) exist. The initial and final states are constructed by means of the corresponding lowering and raising operators in the same manner as the states $|\boldsymbol{\alpha}; t\rangle$ and $|\mathbf{n}; t\rangle$ are built up by means of the invariants (13).

Evaluating the corresponding Gaussian integral and taking into account the fact that $|\alpha; t\rangle$ is the generating function of the states $|\mathbf{n}; t\rangle$, we obtain the transition amplitudes (29) and (32):

$$\langle \beta; f | \boldsymbol{\alpha}; t\rangle = \langle \mathbf{0}; f | \mathbf{0}; t\rangle \exp[-\tfrac{1}{2}(|\boldsymbol{\alpha}|^2 + |\beta|^2) + \mathbf{S}\boldsymbol{\zeta} - \tfrac{1}{2}\boldsymbol{\zeta}W\boldsymbol{\zeta}], \quad (29)$$

where $\boldsymbol{\zeta}$ and $\mathbf{S}$ are the $2N$ vectors

$$\boldsymbol{\zeta} = \begin{pmatrix} \boldsymbol{\alpha} \\ \beta \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \boldsymbol{\rho} - \frac{1}{2} i\tau(\tilde{\mu}_1 + \mu_1)\lambda_p^{-1}\Delta \\ -\frac{1}{2} i\tau_f^*(\tilde{\mu}_1 + \mu_1)\lambda_p^{-1}\Delta \end{pmatrix} \quad (30)$$

and W is a $2N \times 2N$ matrix

$$W = \begin{pmatrix} w - \tau\mu_1\tilde{\tau} & -\tau\mu_1\tau_f^\dagger \\ -\tau_f^*\mu_1\tilde{\tau} & w_f^* - \tau_f^*\mu_1\tau_f^\dagger \end{pmatrix}. \quad (31)$$

We have introduced the notations

$$\mu_1 = (\mu + \mu_f^*)^{-1}, \quad \boldsymbol{\rho} = (1/\sqrt{2})(\Delta^* - \lambda_p^*\lambda_p^{-1}\Delta), \quad \tau = (1/\sqrt{2})(\lambda_q^* - \lambda_p^*\tilde{\lambda}_q\tilde{\lambda}_p^{-1}),$$

where the subscript f stands for "final":

$$\langle \mathbf{m}; f | \mathbf{n}; t\rangle = (n_1! \cdots n_N! m_1! \cdots m_N!)^{-1/2} \times \langle \mathbf{0}; f | \mathbf{0}; t\rangle H_{\mathbf{M}}(\tilde{W}^{-1}S), \quad (32)$$

where

$$\mathbf{M} = (n_1, \ldots, n_N, m_1, \ldots, m_N).$$

The solution $\Lambda(t)$ for constant R, as is the case when $t \le 0$ and $t \to \infty$, is given by

$$\Lambda(t) = e^{Rt}. \quad (33)$$

One can also obtain the generating function $\varphi(u, v)$ of the transition probabilities $|\langle \mathbf{m}; f | \mathbf{n}; t\rangle|^2$ by computing the Gaussian integral

$$\varphi(u, v) = \pi^{-2N} \int d^2 d_1 \cdots d^2 d_N d^2\beta_1 \cdots d^2\beta_N \times \langle \beta; f | \boldsymbol{\alpha}; t\rangle\langle v^*\boldsymbol{\alpha}; t | u\beta; f\rangle, \quad (34)$$

where u and v are diagonal matrices

$$u = \mathrm{diag}(u_1, u_2, \ldots, u_N), \quad v = \mathrm{diag}(v_1, v_2, \ldots, v_N); \quad |u_j| = |v_j| = 1. \tag{34'}$$

Formula (34) results in

$$\varphi(u,v) = 2^{2N}|\langle 0; f|0;t\rangle|^2(\det\mathcal{P})^{-1/2}\exp(\tfrac{1}{2}\mathbf{L}\mathcal{P}\mathbf{L}), \tag{35}$$

where

$$\mathcal{P} = \begin{pmatrix} 2+E & D \\ 0 & 2+F \end{pmatrix} + \begin{pmatrix} V\sigma_3 & 0 \\ 0 & U\sigma_3 \end{pmatrix} \times \begin{pmatrix} \sigma_3 E^*\sigma_3 & \sigma_3 D^*\sigma_3 \\ 0 & \sigma_3 F^*\sigma_3 \end{pmatrix}\begin{pmatrix} V\sigma_3 & 0 \\ 0 & U\sigma_3 \end{pmatrix}; \tag{35'}$$

$$E = \begin{pmatrix} w_1 & iw_1 \\ iw_1 & -w_1 \end{pmatrix}, \quad D = \begin{pmatrix} w_2 + \tilde{w}_3 & i(w_2 + \tilde{w}_3) \\ -i(w_2 + \tilde{w}_3) & -w_2 - \tilde{w}_3 \end{pmatrix}, \quad F = \begin{pmatrix} w_4 & iw_4 \\ iw_4 & -w_4 \end{pmatrix}, \tag{35''}$$

$$U = \begin{pmatrix} u & 0 \\ 0 & u \end{pmatrix}, \quad V = \begin{pmatrix} v & 0 \\ 0 & v \end{pmatrix}, \quad \mathbf{L} = \begin{pmatrix} (1+v)\mathbf{s}_1 \\ (1-v)\mathbf{s}_1 \\ (1+u)\mathbf{s}_2 \\ (1-u)\mathbf{s}_2 \end{pmatrix}. \tag{35'''}$$

Here the $N \times N$ matrices w_i, $i = 1, \ldots, 4$ and the N vectors s_i, $i = 1, 2$ are defined by means of the matrix W and the vector $\mathbf{S}$ as

$$W = \begin{pmatrix} w_1 & w_2 \\ w_3 & w_4 \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \mathbf{s}_1 \\ \mathbf{s}_2 \end{pmatrix}. \tag{36}$$

The following relation holds

$$\varphi(u,v) = \sum_{\substack{n_j=0 \\ m_j=0}}^{\infty} |\langle \mathbf{m}; f|\mathbf{n}; t\rangle|^2 u_1^{m_1}\ldots u_N^{m_N} \cdot v_1^{n_1}\ldots v_N^{n_N}. \tag{37}$$

C. Some special cases of interest

We have derived the exact solution for any time-dependent quadratic quantum system in terms of the solution $\Lambda(t)$ of the matrix differential equation (5). We know the formal solution of this equation, namely the antichronological exponential (8). But in practice this exponential is far from being useful for calculations, and it is of interest to point out the cases when the matrix equation (5) can be reduced to a simpler differential equation. One can point out three particular cases when Eq. (5) is equivalent to a very familiar equation, namely the equation of motion of the classical harmonic oscillator.

$$\ddot{\epsilon} + \Omega^2(t)\epsilon = 0. \tag{38}$$

1. N-dimensional oscillator

The simplest case is of course the case of the pure quadratic Hamiltonian, i.e., of the matrix $B(t)$ diagonal. This is the case of the N-dimensional oscillator which was treated in Ref. 15. The case when external forces are present (forced oscillator) is considered in Ref. 17. The solution of the wave equation in the case of $B(t)$ being diagonal is factorized, every factor being expressed in terms of its function $\epsilon_j(t)$, $j = 1, \ldots, N$. The functions $\Omega_j(t)$ in this case are simply the frequencies of the oscillator.

2. General forced oscillator

There is one more case when the solution is fully factorized and expressed in terms of the functions $\epsilon_j(t)$. Let the symmetric matrix $B(t)$ be of the form

$$B(t) = \begin{pmatrix} a(t) & b(t) \\ \tilde{b}(t) & c(t) \end{pmatrix}, \tag{39}$$

where the $N \times N$ matrices $a, b,$ and c are diagonal. The Hamiltonian (1) takes the form of the general forced oscillator

$$H = \tfrac{1}{2}\sum_{j=1}^{N}\{a_j(t)p_j^2 + b_j(t)[p_j, q_j]_+ + c_j(t)q_j^2 + d_j(t)p_j + e_j(t)q_j\}, \tag{40}$$

where $a_j, b_j, c_j, d_j,$ and e_j are arbitrary functions of time.

The N non-Hermitian linear invariants of the type (14) are

$$A_j(t) = i(a_j/2)^{1/2}\{\epsilon_j p_j + (1/a_j)(\epsilon_j b_j - \dot{\epsilon}_j - \tfrac{1}{2}(\dot{a}_j/a_j)\epsilon_j)q_j\} + \delta_j(t), \tag{41}$$

where

$$\delta_j(t) = i2^{-3/2}\int_0^t \sqrt{a_j}\left[\frac{d_j}{a_j}\left(\epsilon_j b_j - \dot{\epsilon}_j - \frac{1}{2}\frac{\dot{a}_j}{a_j}\epsilon_j\right) - \epsilon_j e_j\right]dt \tag{41'}$$

and ϵ_j are solutions of the equations

$$\ddot{\epsilon}_j + \Omega_j^2(t)\epsilon_j = 0, \tag{42}$$

$$\Omega_j^2 = a_j c_j + b_j\frac{\dot{a}_j}{a_j} + \frac{1}{2}\frac{\ddot{a}_j}{a_j} - \frac{3}{4}\frac{\dot{a}_j^2}{a_j^2} - b_j^2 - \dot{b}_j. \tag{42'}$$

Condition (11) reduces to the requirement

$$\epsilon_j = |\epsilon_j|\exp\left(i\int_0^t \frac{dt}{|\epsilon_j|^2}\right). \tag{43}$$

Further, we give the results only, dropping the subscript $j = 1, \ldots, N$, since all the formulas are factorized.

The coherent states are

$$|\alpha; t\rangle = |0; t\rangle \exp[-\tfrac{1}{2}|\alpha|^2 + (2/a)^{1/2}\alpha q/\epsilon + (\delta^* + \delta\epsilon^*/\epsilon)\alpha - \alpha^2\epsilon^*/2\epsilon] \tag{44}$$

and the vacuum $|0; t\rangle$ is

$$|0;t\rangle = [\epsilon(\pi a)^{\frac{1}{2}}]^{-1/2}\exp\left[\frac{1}{2}\phi + \frac{i}{2a}\left(\frac{\dot{\epsilon}}{\epsilon} + \frac{\dot{a}}{2a} - b\right)q^2 - \left(\frac{2}{a}\right)^{1/2}\frac{\delta}{a}q\right],$$

$$\phi = \int_0^t \left[\frac{2i\delta^2}{\epsilon^2} + \left(\frac{2}{a}\right)^{1/2}\frac{\delta d}{\epsilon}\right]dt. \tag{45}$$

The explicit form (44) of the coherent states $|\alpha; t\rangle$ having been obtained, the rest of the formulas [(23)–(37)] can be easily derived. The eigenstates of the operator $A^\dagger A$ take the form

$$|n;t\rangle = |0;t\rangle \frac{(\epsilon^*/2\epsilon)^{n/2}}{\sqrt{n!}} H_n(x), \quad x = \frac{q}{|\epsilon|\sqrt{a}} + \frac{\epsilon\delta^* + \epsilon^*\delta}{|\epsilon|\sqrt{2}}, \tag{46}$$

$H_n(x)$ being the usual Hermite polynomial. The transition amplitudes, calculated under conditions (26) (which now read $e = d = 0$ and $a, b,$ and $c =$ const for $t \le 0$ and $t \to \infty$) are

$$\begin{aligned}\langle\beta;f|\alpha;t\rangle &= \langle 0;f|0;t\rangle \exp[-\tfrac{1}{2}(|\alpha|^2 + |\beta|^2)] \\ &\times \exp\{(1/\xi)[\eta^*\alpha^2/2 + \alpha\beta^* \\ &+ (\xi\delta^* - \eta^*\delta)\alpha - \delta\beta^* - \eta\beta^{*2}/2]\},\end{aligned} \tag{47}$$

$$\langle m;f|n;t\rangle = (n!m!)^{-1/2}\langle 0;f|0;t\rangle H_{n,m}(x_1, x_2), \tag{48}$$

where δ is given by formula (41′),

$$x_1 = \delta - \eta\delta^*/\xi^*, \quad x_2 = -\delta^*/\xi^*$$

and the quantities ξ and η are defined in terms of ϵ and $\dot\epsilon$ as

$$\xi = \tfrac{1}{2}\exp(-i\Omega_f t)\left\{-i\dot\epsilon\left(\frac{a_f}{a\Omega_f}\right)^{1/2} + \epsilon\left[i\left(b - \frac{\dot a}{2a}\right)\left(\frac{a_f}{a\Omega_f}\right)^{1/2} + \left(\frac{a}{a_f}\right)^{1/2}\left(\sqrt{\Omega_f} - \frac{ib}{\sqrt{\Omega_f}}\right)\right]\right\}, \tag{49}$$

$$\eta = \tfrac{1}{2}\exp(i\Omega_f t)\left\{-i\dot\epsilon\left(\frac{a_f}{a\Omega_f}\right)^{1/2} + \epsilon\left[i\left(b - \frac{\dot a}{2a}\right)\left(\frac{a_f}{a\Omega_f}\right)^{1/2} - \left(\frac{a}{a_f}\right)^{1/2}\left(\sqrt{\Omega_f} + \frac{ib}{\sqrt{\Omega_f}}\right)\right]\right\}, \tag{49′}$$

the subscript f standing for "final."

The following identities hold

$$|\xi|^2 - |\eta|^2 = 1, \tag{50}$$

$$\epsilon = (a_f/a\Omega_f)^{1/2}[\xi\exp(i\Omega_f t) - \eta\exp(-i\Omega_f t)]. \tag{51}$$

In the final region $t \to \infty$ the quantities ξ and η become constant and can be related to the amplitudes of the reflected and transmitted waves for a particle which encounters an effective potential barrier defined by the function $\Omega(t)$. The amplitudes (47) and (48) also become constant as $t \to \infty$. If the external forces $d(t) = e(t) \equiv 0$, i.e., $\delta(t) \equiv 0$, formulas (47) and (48) coincide with those of the N-dimensional oscillator, the only difference being in the definition of the parameters ξ and η.

We do not reproduce the formulas for the Green's function (24) and for the generating function (35) in terms of the function $\epsilon(t)$, since this is trivial after $|\alpha;t\rangle$ and $\langle\beta;f/\alpha;t\rangle$ have been obtained explicitly.

3. Charge in fields

The third case where we succeeded in expressing the exact solution in terms of a function $\epsilon(t)$, which obeys the classical equation (38), is that of charged particle motion in a uniform electromagnetic field. The matrix $B(t)$ is of the form (39); this time $a(t)$ and $c(t)$ being diagonal and $b(t)$ antidiagonal. For example, the motion of a particle in a uniform magnetic field is described by ($M = 1$)

$$B = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{2}\omega \\ 0 & 1 & \frac{1}{2}\omega & 0 \\ 0 & \frac{1}{2}\omega & \frac{1}{4}\omega^2 & 0 \\ \frac{1}{2}\omega & 0 & 0 & \frac{1}{4}\omega^2 \end{pmatrix}, \tag{52}$$

where ω is the Lamor frequency $\omega = e\mathcal{H}$. The solution of the Schrödinger equation in this case is not factorized: The two linear invariants of the type (41) depend simultaneously on all the momenta and coordinates ($p_x, p_y, x,$ and y for the motion in the xy plane). The details of the solution are given in Refs. 15 and 17.

It is of interest to note that in the general case of the matrix $B(t)$ being crossdiagonal, i.e., $a(t)$ and $c(t)$ in (39) diagonal and $b(t)$ antidiagonal, the solution is "half" factorized. This case will be considered elsewhere.

In the cases listed above the discrete spectra $|\mathbf{n};t\rangle$ coincide with the initial energy spectra if the following initial conditions are chosen for constant Ω:

$$\epsilon = \exp(i\Omega t), \quad \dot\epsilon = i\Omega\epsilon. \tag{53}$$

For example, if the coefficients of the Hamiltonian (40) are constant [and $d(t) = e(t) \equiv 0$] the following formula holds:

$$H = \sum_{j=1}^{N} \Omega_j \left(A_j^\dagger A_j + \frac{1}{2}\right). \tag{54}$$

It is worth recalling the invariance of quantum mechanics under rotations in the coordinate space. One may use rotations in order to reduce the matrix $B(t)$, if possible, to a simpler form, say to that for (40), or diagonalize it.

III. ADIABATIC INVARIANTS

In the previous section we have constructed all the linear integrals of motions $A_j(t)$ for any quadratic quantum system and then used these invariants for obtaining explicit formulas for the exact solution. Attractive as these results may seem at first sight, there is, however, one difficulty: The point is that the exact invariants are expressed in terms of the solutions of linear differential equations (5) or (38) but neither (5) nor (38) can be solved exactly for every $R(t)$ or $\Omega(t)$. For constant R or Ω the exact solutions of these equations are known and thus the exact (time-dependent) invariants and the solution of the Schrödinger equation are known for stationary quadratic Hamiltonians. It is of interest then to look for approximate invariants whose total changes vanish together with the rate of change of the coefficients of the Hamiltonian. Such approximate invariants are known as adiabatic invariants. The exact invariants being obtained explicitly in terms of the solutions of differential equations, the adiabatic invariants can be easily derived by expanding the exact formulas in series in the time-derivatives of the coefficients of the Hamiltonian. For this purpose Eq. (5) or (38) is to be solved recursively, and then this recursive solution is to be substituted in the formulas of the exact invariants. In this paper we consider the adiabatic invariants for those quadratic systems whose exact solution is expressed in terms of the function $\epsilon(t)$. These systems are described in Sec. IIC. We also assume that the external forces vanish. The adiabatic invariance of the general system (1) will be considered elsewhere.

We let the coefficients of the Hamiltonian start varying at $t = 0$ and become constant again as $t \to \infty$.

In order to introduce the adiabatic parameter, we let the

Hamiltonian depend on time through a small parameter

$$H = H(\tau), \quad \tau = \theta t. \tag{55}$$

Then the small θ corresponds to small time-derivatives $d/dt = \theta d/d\tau$.

The equations for the functions $\epsilon_j(t)$ become

$$\theta^2\epsilon'' + \Omega^2(\theta,\tau)\epsilon = 0, \tag{56}$$

where $\epsilon' = d\epsilon/d\tau$.

We first consider the adiabatic invariants of the general oscillator (40). Since the solution in this case is fully factorized we drop the subscript $j = 1, 2, \ldots, N$. The "frequency" Ω is

$$\Omega^2 = \Omega_0^2(\tau) + \theta\Omega_1^2(\tau) + \theta^2\Omega_2^2(\tau), \tag{57}$$

where

$$\Omega_0^2 = ac - b^2, \quad \Omega_1^2 = b^2a'/a - b', \quad \Omega_2^2 = a''/2a - \tfrac{3}{4}(a'/a)^2. \tag{57'}$$

In accordance with (43) we anticipate that

$$\epsilon(\tau,\theta) = |\epsilon(\tau,\theta)| \exp\left(\frac{i}{\theta}\int_0^\tau \frac{d\tau}{|\epsilon|^2}\right), \tag{58}$$

where $|\epsilon(\tau,\theta)|$ can be developed as asymptotic series in

$$|\epsilon(\tau,\theta)| = |\epsilon(\tau)|_0 + \theta|\epsilon(\tau)|_1 + \cdots. \tag{59}$$

The lowest-order terms are

$$|\epsilon|_0 = \Omega_0^{-1/2}, \quad |\epsilon|_1 = -\tfrac{1}{4}\Omega_1^2\Omega_0^{-5/2}. \tag{60}$$

the mth order reads

$$|\epsilon|_m\Omega_0 + |\epsilon|_{m-1}\Omega_1^2 + |\epsilon|_{m-2}\Omega_2^2 + |\epsilon|''_{m-2} - s_m = 0, \quad m = 3, 4, \ldots, \tag{61}$$

where s_m are defined by means of the expansion

$$|\epsilon|^{-3} = s_0(\tau) + \theta s_1(\tau) + \cdots. \tag{61'}$$

Suppose that the coefficients a, b, and c of the Hamiltonian (40) have n continuous derivatives and that these n derivatives are zero in the final region $t \to \infty$. Then we easily derive from (61) and (61a) that in the final region

$$|\epsilon|_0 = (\Omega_0^f)^{-1/2}, \quad |\epsilon|_k = 0, \quad k = 1, 2, \ldots, n. \tag{62}$$

By substituting (59) in formula (41) for the exact invariants, one can get the adiabatic invariance series and the linear adiabatic invariants to any order in θ. The zero-order adiabatic invariants are

$$A_0 = i\left(\frac{a}{2}\right)^{1/2} \exp\left[\frac{i}{\theta}\int_0^\tau d\tau\Omega_0(\tau)\right] \times \left[\frac{1}{\sqrt{\Omega_0}}p + \frac{1}{a}\left(\frac{B}{\sqrt{\Omega_0}} - i\sqrt{\Omega_0}\right)q\right]. \tag{63}$$

In the final region one has, by virtue of (62),

$$A = A_0 + O(\theta^{n+1}), \tag{64}$$

which means that the adiabatic invariants A_0 are conserved to the $(n+1)$th order in θ. The same conclusion can be made if one calculates the relative changes ΔA_0. We give formulas in the cases of coherent states $|\alpha; t\rangle$ and discrete states $|n; t\rangle$, respectively;

$$\text{(a)} \quad \Delta_{A_0} = \xi^* - 1 - \eta\alpha^*/\alpha, \tag{65}$$

$$\text{(b)} \quad \langle n; t\to\infty|A_0|n; t\to\infty\rangle = 0. \tag{66}$$

Here the constant parameters ξ and η are defined by means of formulas (49) and (49') for $t \to \infty$. Using (62) we obtain the asymptotic series for ξ and η as

$$\xi = \xi_0 + O(\theta^{n+1}), \quad \eta = O(\theta^{n+1}), \tag{67}$$

where

$$\xi_0 = \exp\left(\frac{i}{\theta}\int_0^\tau d\tau(\Omega_0 - \Omega_0^f)\right). \tag{68}$$

We observe that

$$\Delta_{A_0} = O(\theta^{n+1}), \tag{69}$$

i.e., the adiabatic invariants A_0 are conserved to the $(n+1)$th order in θ.

It is of interest to consider the evolution of the quadratic adiabatic invariant

$$I_0 = \sum_{j=1}^N \left(A_{0,j}^\dagger A_{0,j} + \frac{1}{2}\right), \tag{70}$$

which is analogous to the classical adiabatic invariant E/Ω. In the states $|n; t\rangle$ one has

$$\Delta_{I_0} = \sum_{j=1}^N 2|\eta_j|^2(2n_j + 1)\left(\sum_{j=1}^N (2n_j + 1)\right)^{-1}. \tag{71}$$

By virtue of (67) we get that I_0 conserves to the $2(n+1)$th order.

By substituting the asymptotic series (59) in formulas (44)–(48) of the exact solution one can obtain an approximate solution to any desired order in θ, in particular, one can obtain the adiabatic Green's function. The transition amplitudes (47) and (48) can be easily expanded in ξ and η, and by using (67) one can obtain the adiabatic transition amplitudes. We give the expansion of the energy distribution $|\langle m; f|n; t\rangle|^2$ in the case, where external forces $d(t) = e(t) \equiv 0$ ($\delta \equiv 0$ in formulas of the transitions):

$$|\langle m; f|n; t\rangle|^2 = \prod_{j=1}^N (n_j^{(1)})! R_i^{k_j} [2^{2k_j} k_j! (n_j^{(2)})!]^{-1} \times \left[1 - \left(1 + \frac{n_j^{(2)}(1 + n_j^{(1)})}{1 + k_j}\right)\frac{R_j}{2} + \cdots\right], \tag{72}$$

$$|\langle n; f|n; t\rangle|^2 = \prod_{j=1}^N \left[1 - \tfrac{1}{2}(n_j^2 + n_j + 1)R_j + \cdots\right], \tag{72'}$$

where

$$R_j = |\eta_j/\xi_j|^2, \quad k_j = \tfrac{1}{2}(|n_j - m_j|), \quad n_j^{(1)} = \max(n_j, m_j), \quad n_j^{(2)} = \min(n_j, m_j). \tag{73}$$

Formulas (72) and (72') show the validity of the adiabatic invariance to the $2(n+1)$the order in θ. The parameter R may be treated as a reflection coefficient of a particle from the one-dimensional effective potential, defined by $\Omega(t)$[9,15]. Thus the reflection coefficient is an amount of $2(n+1)$th order in the adiabatic parameter θ.

The above treatment of the N-dimensional general oscillator certainly holds for the usual N-dimensional oscillator, since the latter is a particular case of (40) ($a \equiv 1, B = d = e \equiv 0$).

In the case of a charged particle in electromagnetic field we have to consider, instead of (56), the equation

$$\theta^2\epsilon'' + \Omega^2(\tau)\epsilon = 0. \tag{74}$$

By considering Eq. (74) in a manner similar to that for (56), one can obtain the same adiabatic results concerning the linear and quadratic adiabatic invariants and the distribution over energy. [The asymptotic expansion of the solution $\epsilon(\tau,\theta)$ of Eq. (74) contains only even powers of θ.[13]] In terms of the corresponding ξ and η all formulas are given in Ref. 15. We will mention here the conservation of the magnetic moment μ to the $2(n+1)$th order in θ. Indeed, the magnetic moment μ can be expressed in terms of the linear adiabatic invariants as

$$\mu = (e/M)A_0^\dagger A_0, \tag{75}$$

and we have seen that quadratic adiabatic invariants $A_0^\dagger A_0$ are constant to the $2(n+1)$ the order in θ. Formula (75) follows from the classical relation $\phi = (2\pi M/e)\mu$ between the magnetic moment and the magnetic flux ϕ through the circular path. The magnetic flux ϕ is proportional to $A_0^\dagger A_0$.

Adiabatic aspects of the solution of Eq. (74) were treated by Kulsrud[13] and Chandrasekhar.[24] In this paper we applied Kulsrud's method to Eq. (56). Chandrasekhar's method was recently[25] shown to be equivalent to that of Kulsrud.

The quantum systems considered above have finitely (the N-dimensional oscillator) and infinitely (the charge in an electromagnetic field) degenerate energy spectra. If the Hamiltonians depend analytically on the time, then adiabatic invariants are constant to all orders in the adiabatic parameter θ.

IV. CONCLUDING REMARKS

In conclusion we note that by means of N linear invariants A_j one can construct the Lie algebra of $U(N,1)$ and establish that the dynamical symmetry of any quadratic system with N degrees of freedom can be described by the noncompact group $U(N,1)$. Since the commutation relations are the same both for the exact and the adiabatic invariants, one may use the latter for the contraction of $U(N,1)$. Thus the symmetry properties of the adiabatic solution coincide with those of the exact solution.

The connection of coherent states with noncompact groups was studied recently by Barut and Girardello.[26] This connection makes obvious the possibility of using noncompact groups for classical mechanics. Coherent states exist for nonquadratic quantum systems too. It is of interest to consider the quasiclassical approximation (i.e., large quantum numbers) of the exact formulas, obtained in this paper.

The results of this paper can be generalized to quadratic quantum systems with an infinite number of degrees of freedom ($N \to \infty$).

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A formula for the pressure in statistical mechanics

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A new expression for the pressure in terms of irreducible distribution functions is given. A derivation for both the classical and quantum mechanical case and a brief discussion of the limits of validity of the formula are given.

1. INTRODUCTION

In statistical mechanics the pressure of a simple fluid in equilibrium is usually obtained by calculating the partition function and taking its logarithmic derivative with respect to the volume. In this paper we shall express the pressure in a different way (in terms of irreducible distribution functions, to be defined below). The resulting expression [formula (2.8)], which we thought to be new, turned out to have been, implicitly at least, contained in a paper by Green.[1] We owe this information to the referee, and we are grateful to him for having drawn our attention to Green's interesting paper.

Although our derivation is closely related to that of Green's, it seems to be somewhat more direct and streamlined.

Also while we do not see any immediate applications, the result is simple and could perhaps be of interest for formal considerations.

We begin our discussion by finding an expression for the probability $P(\Omega)$ that, in the thermodynamic limit, a macroscopic region Ω (contained in V) is free of particle. By a "macroscopic" volume we mean one the dimensions of which are very much larger than any characteristic length associated with the fluid (size of molecules, intermolecular distance, correlation length, etc., etc.). Let the system have N particles and volume V. Call $P_{N,V}(\mathbf{r}_1,\ldots,\mathbf{r}_N)d\mathbf{r}_1\ldots d\mathbf{r}_N$ the probability that a particle is in $d\mathbf{r}_1$ around $\mathbf{r}_1,\ldots,$ in $d\mathbf{r}_N$ around $\mathbf{r}_N$. Then, before we take the thermodynamic limit, the probability $P_{N,V}(\Omega)$ of finding no particles in Ω is

$$P_{N,V}(\Omega)=\int\cdots\int P_{N,V}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\prod_{j=1}^{N}[1-\theta_\Omega(\mathbf{r}_j)]\times d\mathbf{r}_1\cdots d\mathbf{r}_N. \quad (1.1)$$

Here $\theta_\Omega(\mathbf{r})$ is the characteristic function of Ω, i.e.,

$$\begin{aligned}\theta_\Omega(\mathbf{r})&=1, \quad \mathbf{r} \text{ in } \Omega,\\ &=0, \quad \mathbf{r} \text{ not in } \Omega.\end{aligned} \quad (1.2)$$

Multiplying out the product in (1.1), we obtain

$$P_{N,V}(\Omega)=1-A_1+A_2-A_3+\cdots, \quad (1.3)$$

$$\begin{aligned}A_1&=N\int_\Omega d\mathbf{r}_1\int_V d\mathbf{r}_2\cdots d\mathbf{r}_N P_{N,V}(\mathbf{r}_1,\ldots\mathbf{r}_N)\\ A_2&=\frac{N(N-1)}{2!}\int_\Omega d\mathbf{r}_1 d\mathbf{r}_2\int_V d\mathbf{r}_3\cdots d\mathbf{r}_N P_{N,V}(\mathbf{r}_1,\ldots,\mathbf{r}_N),\\ &\vdots \qquad\qquad (1.4)\\ A_l&=\frac{N!}{(N-l)!\,l!}\int_\Omega d\mathbf{r}_1\cdots d\mathbf{r}_l\int_V d\mathbf{r}_{l+1}\cdots d\mathbf{r}_N P_{N,V}(\mathbf{r}_1,\ldots,\mathbf{r}_N).\end{aligned}$$

(This is the usual inclusion–exclusion lemma of probability theory.)

The l-particle distribution function is defined, as usual,[2] by

$$n_l(\mathbf{r}_1,\ldots,\mathbf{r}_l)=\frac{N!}{(N-l)!}\int_V d\mathbf{r}_{l+1}d\mathbf{r}_{l+2}\cdots d\mathbf{r}_N \times P_{N,V}(\mathbf{r}_1,\ldots,\mathbf{r}_N). \quad (1.5)$$

The n_l have a thermodynamic limit $\bar{n}_l$, and this is now assumed to be taken. Using (1.5) and (1.4), we have

$$P(\Omega)=1-\frac{1}{1!}\int_\Omega d\mathbf{r}_1\bar{n}_1(\mathbf{r}_1)+\frac{1}{2!}\int_\Omega d\mathbf{r}_1 d\mathbf{r}_2\bar{n}_2(\mathbf{r}_1,\mathbf{r}_2)-\cdots. \quad (1.6)$$

We now introduce the *irreducible l-particle distribution functions* $\bar{\chi}_l$ (cluster functions) as follows[3]:

$$\begin{aligned}\bar{n}_1(\mathbf{r}_1)&\equiv\bar{\chi}_1(\mathbf{r}_1),\\ \bar{n}_2(\mathbf{r}_1,\mathbf{r}_2)&\equiv\bar{\chi}_2(\mathbf{r}_1,\mathbf{r}_2)+\bar{\chi}_1(\mathbf{r}_1)\bar{\chi}_1(\mathbf{r}_2),\\ \bar{n}_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)&\equiv\bar{\chi}_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)+\bar{\chi}_1(\mathbf{r}_1)\bar{\chi}_2(\mathbf{r}_2,\mathbf{r}_3)\\ &\quad+\bar{\chi}_1(\mathbf{r}_2)\bar{\chi}_2(\mathbf{r}_1,\mathbf{r}_3)+\bar{\chi}_1(\mathbf{r}_3)\bar{\chi}_2(\mathbf{r}_1,\mathbf{r}_2)\\ &\quad+\bar{\chi}_1(\mathbf{r}_1)\bar{\chi}_1(\mathbf{r}_2)\bar{\chi}_3(\mathbf{r}_3),\end{aligned} \quad (1.7)$$

and so on.

The relationship between the $\bar{n}_l$ and the $\bar{\chi}_l$ may be expressed in terms of the well-known identity[4]

$$1+\sum_{l=1}^{\infty}\frac{t^l}{l!}\int_\Omega d\mathbf{r}_1\cdots d\mathbf{r}_l\bar{n}_l(\mathbf{r}_1,\ldots,\mathbf{r}_l)=\exp\left(\sum_{l=1}^{\infty}\frac{t^l}{l!}\int_\Omega d\mathbf{r}_1\cdots d\mathbf{r}_l\bar{\chi}_l(\mathbf{r}_1,\ldots,\mathbf{r}_l)\right). \quad (1.8)$$

In (1.8), t is arbitrary, but it assumed that the series involved in (1.8) converge. Choosing $t=-1$, the left-hand side of (1.8) becomes the right-hand side of (1.6), so that we finally have

$$P(\Omega)=\exp\left(\sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\int_\Omega\bar{\chi}_l(\mathbf{r}_1,\ldots,\mathbf{r}_l)d\mathbf{r}_1\cdots d\mathbf{r}_l\right). \quad (1.9)$$

2. CLASSICAL CASE

In the case of classical statistical mechanics $P_{N,V}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is given by

$$P_{N,V}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\exp[-\beta\phi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N)]\Big/\int_V\exp(-\beta\phi_N)d\mathbf{r}_1\cdots d\mathbf{r}_N, \quad (2.1)$$

where $\beta=1/kT$ and $\phi_N(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is the potential of the intermolecular forces. Therefore,

$$P_{N,V}(\Omega)=\int_{V-\Omega}\exp(-\beta\phi_N)d\mathbf{r}_1\cdots d\mathbf{r}_N\Big/\int_V\exp(-\beta\phi_N)d\mathbf{r}_1\cdots d\mathbf{r}_N. \quad (2.2)$$

Now in classical statistics the partition function is given by

$$Z_N \frac{1}{N!} \lambda^{3N} \int_V \exp(-\beta\phi_N) d\mathbf{r}_1 \cdots d\mathbf{r}_N = \exp[-\beta F_N(V)], \tag{2.3}$$

where $\lambda \equiv h/\sqrt{2\pi mkT}$ and $F_N(V)$ is the Helmholz free energy for N particles in the domain V. Therefore, since Ω is a macroscopic domain, so is V-Ω, and we must have

$$P_{N,V}(\Omega) = e^{+\beta[F_N(V)-F_N(V-\Omega)]}. \tag{2.4}$$

Now we are going to the thermodynamic limit, so we may assume $\Omega \ll V$. Expanding and using the usual formula for the pressure

$$p = -\left(\frac{\partial F_N(V)}{\partial V}\right)_T, \tag{2.5}$$

we have at once

$$P(\Omega) = e^{-\beta p \Omega}. \tag{2.6}$$

Comparing (2.6) with (1.9), we see that

$$\beta p \Omega = \sum_{l=1}^{\infty} \frac{(-1)^{l+1}}{l!} \int_\Omega \overline{\chi}_l(\mathbf{r}_1, \ldots, \mathbf{r}_l) d\mathbf{r}_1 \cdots d\mathbf{r}_l. \tag{2.7}$$

Since Ω is a macroscopic volume, arbitrarily large, we may also write

$$\beta p = \lim_{\Omega\to\infty} \frac{1}{\Omega} \sum_{l=1}^{\infty} \frac{(-1)^{l+1}}{l!} \int_\Omega \overline{\chi}_l(\mathbf{r}_1, \ldots, \mathbf{r}_l) d\mathbf{r}_1 \cdots d\mathbf{r}_l. \tag{2.8}$$

This is the originally mentioned new formula for the pressure. It depends only on the assumption of the convergence of the series on the right-hand side of (2.8).

Although the above argument is both appealing and convincing, it is not entirely rigorous. Hidden somewhat in the derivation is the fact that we are dealing with a double limit

$$\lim_{\Omega\to\infty} \lim_{V\to\infty} (1/\Omega) \log P_{N,V}(\Omega)$$

so that as $V \to \infty$ the volume Ω cannot be really considered to be macroscopic.

In the Appendix we sketch a proof, valid, however, only for low densities.

3. QUANTUM MECHANICAL CASE

For quantum statistical mechanics there is no formula for $P_{N,V}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ of the same simplicity as (2.1). $P_{N,V}$ depends on the wavefunctions, which in turn depend in detail on the domain V. We may, however, proceed as follows. Using the grand partition function, we have

$$P_{\bar{N},V}(\Omega) = \sum_N e^{\beta\mu N} \sum_i e^{-\beta E_i^{N,V}} \int_{V-\Omega} |\psi_i^{N,V}|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N \Big/ \sum_N e^{\beta\mu N} \sum_i e^{-\beta E_i^{N,V}}, \tag{3.1}$$

where μ is the chemical potential and $\psi_i^{N,V}$ and $E_i^{N,V}$ are the normalized wavefunctions and energy eigenvalues of N particles in the domain V, interacting via the potential $\phi_N(\mathbf{r}_1, \ldots, \mathbf{r}_N)$. $\bar{N}$ is the mean number of particles, determined from μ and the grand partition function in the usual way:

$$\bar{N} = +\left(\frac{\partial}{\partial\mu} \log\left(\sum_N e^{\beta\mu N} e^{-\beta E_i^{N,V}}\right)\right)_{T,V}. \tag{3.2}$$

Define[5] the "Slater sum"

$$W_{N,V}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = N!\lambda^{3N} \sum_i e^{-\beta E_i^{N,V}} |\psi_i^{N,V}|^2 \tag{3.3}$$

so that

$$P_{N,V}(\Omega) = \sum_N e^{\beta\mu N} \frac{1}{N!\lambda^{3N}} \int_{V-\Omega} W_{N,V} d\mathbf{r}_1 \cdots d\mathbf{r}_N \Big/ \sum_N e^{\beta\mu N} \frac{1}{N!\lambda^{3N}} \int_V W_{N,V} d\mathbf{r}_1 \ldots d\mathbf{r}_N. \tag{3.4}$$

We now express $W_{N,V}$ in terms of the cluster functions[6]

$$\begin{aligned} W_{1,V}(\mathbf{r}_1) &\equiv U_{1,V}(\mathbf{r}_1), \\ W_{2,V}(\mathbf{r}_1, \mathbf{r}_2) &\equiv U_{2,V}(\mathbf{r}_1, \mathbf{r}_2) + U_{1,V}(\mathbf{r}_1)U_{2,V}(\mathbf{r}_2), \\ W_{3,V}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) &= U_{3,V}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) + U_{1,V}(\mathbf{r}_1)U_{2,V}(\mathbf{r}_2, \mathbf{r}_3) \\ &\quad + U_{1,V}(\mathbf{r}_2)U_{2,V}(\mathbf{r}_1, \mathbf{r}_3) + U_{1,V}(\mathbf{r}_3)U_{2,V}(\mathbf{r}_1, \mathbf{r}_2) \\ &\quad + U_{1,V}(\mathbf{r}_1)U_{1,V}(\mathbf{r}_2)U_{1,V}(\mathbf{r}_3) \end{aligned} \tag{3.5}$$

and so forth. Using (3.5), one easily sees[7]

$$\frac{1}{N!} \int_V W_{N,V}(\mathbf{r}_1, \ldots, \mathbf{r}_N) d\mathbf{r}_1 \cdots d\mathbf{r}_N = \sum_{m=0,1,\ldots,\infty} \frac{[a_1(V)]^{m_1}}{m_1!} \frac{[a_2(V)]^{m_2}}{m_2!} \cdots \frac{[a_l(V)]^{m_l}}{m_l!} \times \cdots \left(\sum_1^\infty m_l l = N\right), \tag{3.6}$$

where

$$a_l(V) \equiv \frac{1}{l!} \int_V d\mathbf{r}_1 \cdots d\mathbf{r}_l U_{l,V}(\mathbf{r}_1, \ldots, \mathbf{r}_l). \tag{3.7}$$

The identical combinatorial argument gives

$$\frac{1}{N!} \int_{V-\Omega} W_{N,V}(\mathbf{r}_1, \ldots, \mathbf{r}_N) d\mathbf{r}_1 \cdots d\mathbf{r}_N = \sum_{m_l=0,1,2,\ldots,\infty} \frac{[a_1(V,\Omega)]^{m_1}}{m_1!} \cdots \frac{[a_l(V,\Omega)]^{m_l}}{m_l!} \times \cdots \left(\sum_1^\infty l m_l = N\right), \tag{3.8}$$

where

$$a_l(V,\Omega) \equiv \frac{1}{l!} \int_{V-\Omega} d\mathbf{r}_1 \cdots d\mathbf{r}_l U_{l,V}(\mathbf{r}_1, \ldots, \mathbf{r}_l). \tag{3.9}$$

Putting (3.6) and (3.8) into (3.4), one has

$$P_{N,V}(\Omega) = \sum_{m_i=0}^{\infty} \frac{z^{m_1}[a_1(V,\Omega)]^{m_1}}{m_1!} \frac{z^{2m_2}[a_2(V,\Omega)]^{m_2}}{m_2!} \cdots \Big/ \sum_{m_i=0}^{\infty} \frac{z^{m_1}[a_1(V)]^{m_1}}{m_1!} \frac{z^{2m_2}[a_2(V)]^{m_2}}{m_2!} \cdots = \exp\left(\sum_{l=1}^{\infty} [a_l(V,\Omega) - a_l(V)] z^l\right), \tag{3.10}$$

where the fugacity z is defined by

$$z = e^{\beta\mu}/\lambda^3. \tag{3.11}$$

We shall now express the a_l in terms of the cluster integrals b_l which are defined as the thermodynamic limit of

$$b_l(V) = \frac{1}{Vl!} \int_V U_{l,V}(\mathbf{r}_1, \ldots, \mathbf{r}_l) d\mathbf{r}_1 \cdots d\mathbf{r}_l. \tag{3.12}$$

This limit may be written (because of the cluster property[6] of the $U_{l,V}$)

$$\bar{b}_l = \frac{1}{l!}\int_{\text{all space}} d\mathbf{r}_2\cdots d\mathbf{r}_l U_{l,\infty}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_l). \quad (3.13)$$

Therefore for large V, $V-\Omega$

$$a_l(V) = V\bar{b}_l, \quad a_l(V-\Omega)\bar{b}_l \quad (3.14)$$

and, using (3.10) and the standard expression for the pressure,[7]

$$P(\Omega) = \exp\left(-\Omega\sum_{l=1}^{\infty}\bar{b}_l z^l\right) = \exp(-\beta p\Omega). \quad (3.15)$$

Finally, comparison of (3.15) and (2.6) shows that once again we obtain the formula (2.8) for the pressure.

The derivation in this case apparently assumes more than in the classical case; we require the convergence of the fugacity expression for the pressure in terms of the cluster integrals. There is no reason to expect this if a phase transition takes place (for example, gas-liquid or Einstein–Bose). Indeed, it is possible to calculate the right-hand side of (2.8) for an ideal Bose-Einstein gas. The result is (2.8) above the transition temperature, while below the transition temperature[8]

$$\lim_{\Omega\to\infty}\frac{1}{\Omega}\sum_{l=1}^{\infty}\frac{(-1)^{l+1}}{l!}\int_\Omega \bar{\chi}_l(\mathbf{r}_1,\ldots,\mathbf{r}_l)\,d\mathbf{r}_1\cdots d\mathbf{r}_l = \beta p_c + \rho - \rho_c, \quad (3.16)$$

where ρ is the density N/V and ρ_c is the density at the critical temperature. Therefore (2.8) is not true in general. We suspect, however, that it might be valid in a single phase region of the fluid.

APPENDIX

The cluster functions $\bar{\chi}_s(\mathbf{r}_1,\ldots,\mathbf{r}_s;\rho)$ depend, of course, on the density ρ ($=1/v$, where v is the specific volume), and, as is well known,

$$\frac{1}{v} = \rho = \bar{\chi}_1(\mathbf{r},\rho) = \sum_{l=1}^{\infty} l\bar{b}_l z^l \quad (\text{A1})$$

relates density to fugacity, where we also have the familiar formula for the pressure

$$\frac{p}{kT} = \sum_{l=1}^{\infty}\bar{b}_l z^l. \quad (\text{A2})$$

We can now express the $\bar{\chi}_s(\mathbf{r}_1,\ldots,\mathbf{r}_s;\rho)$ as functions of fugacity z, and, following Uhlenbeck and Ford[2], we define the quantities $\bar{b}_l(\mathbf{r}_1,\ldots,\mathbf{r}_s)$ as coefficients in the power series expansion of $\bar{\chi}_s(\mathbf{r}_1,\ldots,\mathbf{r}_s;\rho)$:

$$\bar{\chi}_s(\mathbf{r}_1,\ldots,\mathbf{r}_s;\rho) = \sum_{l=s}^{\infty}\bar{b}_l(\mathbf{r}_1,\ldots,\mathbf{r}_s)z^l. \quad (\text{A3})$$

That such an expansion is valid at least for sufficiently small z requires, of course, proof. While we are unable to supply a precise reference to such a proof, we have no doubt that the present status of the rigorous foundations of classical statistical mechanics (for equilibrium) is such that under suitable restrictions on the interaction potential the expansion can be indeed justified.

We now use the formula

$$\lim_{\Omega\to\infty}\frac{1}{\Omega}\int_\Omega\cdots\int_\Omega \bar{b}_l(\mathbf{r}_1,\ldots,\mathbf{r}_s)\,d\mathbf{r}_1\cdots d\mathbf{r}_s = \frac{l!}{(l-s)!}\bar{b}_l \quad (\text{A4})$$

(see Uhlenbeck and Ford[2]) and hence (allowing for an interchange of the limiting processes)

$$\begin{aligned}\lim_{\Omega\to\infty}\frac{1}{\Omega}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_\Omega\cdots\int_\Omega \bar{\chi}_n(\mathbf{r}_1,\ldots,\mathbf{r}_n;\rho)\,d\mathbf{r}_1\cdots d\mathbf{r}_n &= \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\sum_{l=n}^{\infty}\frac{l!}{(l-n)!}\bar{b}_l z^l \\ &= \sum_{n=1}^{\infty}(-1)^n\sum_{l=n}^{\infty}\binom{l}{n}\bar{b}_l z^l \\ &= \sum_{l=1}^{\infty}\bar{b}_l z_0^l\sum_{n=1}^{l}(-1)^n\binom{l}{n} = -\sum_{l=1}^{\infty}\bar{b}_l z^l = -\frac{p}{kT}. \end{aligned} \quad (\text{A5})$$

Use has been made of the fact that

$$\sum_{n=1}^{l}(-1)^n\binom{l}{n} = -1.$$

Formally the proof is also applicable to the quantum mechanical case provided (A4) can be justified (Uhlenbeck and Ford prove it only in the classical case) as well as the expansion (A3).

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[1] Melville Green, "Some Applications of the Generating Functional of the Molecular Distribution Functions." in *Lectures in Theoretical Physics* (Interscience, New York, 1960), Vol. 3.

[2] See, e.g., G. E. Uhlenbeck and G. W. Ford, "The Theory of Linear Graphs with Applications to the Theory of Virial Development of the Properties of Gases," in *Studies in Statistical Mechanics* (North-Holland, Amsterdam, 1962), pp. 123–211, in particular formula (37) on p. 139. Although the discussion is classical, the definitions are identical in the quantum case.

[3] Reference 2, p. 143.

[4] This formula is best known in a somewhat different context, but the simple combinatorial principle on which it is based is, of course, quite general.

[5] J. de Boer, Rep. Prog. Phys. **12**, 305 (1948), esp. p. 332.

[6] Reference 5, p. 336.

[7] Reference 5, p. 337.

[8] This formula has been derived by J. W. Cannon, oral communication.

Generalized isoperimetric inequalities*

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New inequalities for certain Green's functions are given. They may be interpreted physically in many ways, for example, as applying to the quantum mechanical motion of a particle in a potential or to diffusion in the presence of absorbers. These inequalities involve a symmetrization process very closely related to Steiner symmetrization used in the theory of isoperimetric inequalities. The usual geometrical and physical isoperimetric inequalities are very special cases of our general inequality (3.9), arising when the potential is taken to be a characteristic function of a bounded domain and the "time" in the Green's function is allowed to get very large or very small.

1. INTRODUCTION

The classical isoperimetric inequality (known already to the Greeks) states that, of all curves with given perimeter, the circle has the largest area. Similarly, of all solids with a given surface area, the sphere has the largest volume. To these (and other) purely geometrical "isoperimetric" inequalities, some of a more physical nature have been added.[1] For example, Lord Rayleigh conjectured (in 1877) that, of all membranes with a given area and fixed boundary, the circular one has the minimum lowest natural frequency. This was not fully proved for about 50 years. Again, Poincaré (1903) stated and gave a partial proof of the conjecture that of all solids with a given volume the sphere has the minimum electrostatic capacity. (This was not fully proved until 1930, by G. Szegö.)

Now the circle is the most symmetrical of all domains in the plane. J. Steiner (in 1836) invented a geometric operation (which we shall call "Steiner symmetrization") which increases the symmetry of any domain. In the plane, it preserves area and does not increase the length of the boundary of a domain. We shall describe this process in detail below, but mention at this point that Steiner symmetrization never increases the lowest natural frequency of a membrane or the electrostatic capacity of a solid. (These and other similar results were first proved[1] by Pólya and Szegö.) Such results represent a very considerable generalization of the classic isoperimetric inequalities.

In this paper we shall be concerned with a still greater generalization of these ideas. There are essentially two new elements in this generalization. The first is that instead of just a quantity like the lowest natural frequency of a membrane, the entire Green's function is involved. The second is that the inequalities involve a *function* rather than a *domain*, the domain type of results arising when the function involved is specialized to a characteristic function of the domain. As an example of what our results are like, consider a particle (in two dimensions) interacting with a potential $\phi(x,y)$. If the potential approaches infinity at infinity, the allowed energy states will be discrete, with energies $\epsilon_0, \epsilon_1, \epsilon_2, \cdots$. (We use quantum mechanical language only for convenience; we are really considering the spectra of certain differential operators.) Let us define the "partition function" $Z(t)$ by (t is a real positive parameter)

$$Z(t) = \sum_{j=0}^{\infty} e^{-t\epsilon_j}. \tag{1.1}$$

(It is a certain integral over the Green's function for the system.) Let the potential $\phi(x,y)$ be replaced by a "Steiner symmetrized" potential $\phi^*(x,y)$, the exact definition of which will be given later. Call the corresponding energy levels ϵ_j^*, and the corresponding partition function $Z^*(t)$. Then, for this case, our inequality takes the form

$$Z(t) \le Z^*(t). \tag{1.2}$$

Now suppose $\phi(x,y)$ is taken to be zero inside a certain domain D and infinite outside D. The "Steiner symmetrized" potential $\phi^*(x,y)$ will be zero in a domain D^* and infinite outside D^*, and in fact D^* will be the Steiner symmetrization of the domain D. Clearly, apart from constants all of which may be absorbed into t, the ϵ_j are the squares of the natural frequencies of a uniform membrane having the shape of D with fixed boundary. By letting t approach infinity, only the ϵ_0 contributes and (1.2) may be written

$$e^{-\epsilon_0 t} \le e^{-\epsilon_0^* t},$$

or

$$\epsilon_0^* \le \epsilon_0. \tag{1.3}$$

This is just Pólya and Szegö's generalization of Rayleigh's conjecture. On the other hand, when t is small, the leading terms of $Z(t)$ are given by[2] (in suitable units)

$$Z(t) = \frac{\Omega(D)}{2\pi t} - \frac{L(D)}{4}\frac{1}{(2\pi t)^{1/2}}, \tag{1.4}$$

where $\Omega(D)$ is the area of the domain D and $L(D)$ is the length of its boundary. Similarly

$$Z^*(t) = \frac{\Omega(D^*)}{2\pi t} - \frac{L(D^*)}{4}\frac{1}{(2\pi t)^{1/2}}. \tag{1.5}$$

Since $\Omega(D) = \Omega(D^*)$, (1.2) becomes

$$L(D) \ge L(D^*), \tag{1.6}$$

which is just Steiner's generalization of the classic isoperimetric inequality.

That is, the usual Steiner type of isoperimetric inequalities are just extreme specializations of (1.2).

The outline of this paper is as follows. In Sec. 2, the basic method is outlined and our general inequality is given for one-dimensional systems. (Unlike the situation for the usual isoperimetric inequalities, there are nontrivial results in one dimension.) Some limiting cases (large and small "time") are discussed. In Sec. 3, the results are generalized to higher dimensionality, and our basic result is the inequality (3.9). This is essentially an extension of the results of Pólya and Szegö on Steiner symmetrization of domains to certain differential operators. (We do not discuss in this paper similar extensions of other symmetrization processes such as circular and spherical symmetrization,[1] which we shall report on elsewhere.) In Appendix A, some very simple illustrative examples are given. Finally, in Appendix B, a further kind of generalization is indicated in a very simple case.

2. ONE DIMENSION

In this paper we shall use the language of quantum mechanics as a natural and convenient physical setting for our results, though they can just as well be expressed in terms of heat conduction, diffusion or the formal properties of certain differential operators. We begin the discussion by considering a one-dimensional particle of unit mass interacting with a potential $\phi(x)$ which approaches infinity as $|x|$ approaches infinity. Such a particle has a Hamiltonian operator[3]

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \phi(x) \tag{2.1}$$

(units such that $\hbar = 1$) and (normalized) characteristic functions and values given by

$$H\psi_j(x) = \epsilon_j \psi_j(x). \tag{2.2}$$

The *Green's function* $G(x,t|x')$ is defined by

$$HG(x,t|x') + \frac{\partial G(x,t|x')}{\partial t} = 0 \quad (t > 0) \tag{2.3}$$

with

$$\lim_{t\to 0} G(x,t|x') = \delta(x - x'), \tag{2.4}$$

$\delta(x)$ being the usual Dirac delta function. There are many formal representations of the Green's function, the most familiar of which is

$$G(x,t|x') = \sum_j e^{-\epsilon_j t}\psi_j(x)\psi_j(x'). \tag{2.5}$$

Now G may also be written as a path (or Wiener) integral[4]

$$G(x,t|x') = \lim_{n\to\infty} \int_{-\infty}^{\infty} dx_2 dx_3 \cdots dx_{n-1} \times P(x - x_2) e^{-\Delta_n \phi(x_2)} P(x_2 - x_3) e^{-\Delta_n \phi(x_3)} \times \cdots P(x_{n-1} - x') e^{-\Delta_n \phi(x')}, \tag{2.6}$$

where

$$\Delta_n \equiv t/(n-1), \qquad P(x) \equiv (2\pi\Delta_n)^{-1/2} e^{-x^2/2\Delta_n}. \tag{2.7}$$

Let us consider the quantity

$$I \equiv \int_{-\infty}^{\infty} dx\,dx'\, G(x,t|x')\,\Gamma(x' - x)\gamma(x) = \lim_{n\to\infty} \int_{-\infty}^{\infty} dx_1 dx_2 \cdots dx_n P(x_1 - x_2) e^{-\Delta_n \phi(x_2)} \cdots P(x_{n-1} - x_n) e^{-\Delta_n \phi(x_n)} \Gamma(x_n - x_1)\gamma(x_1), \tag{2.8}$$

where Γ, γ are real nonnegative quantities. We shall make use of the following inequality, which is the crux of our entire discussion. Let $H^{(j)}(x), F^{(j)}(x)$ be real valued nonnegative functions of x which go to zero as $|x|$ approaches infinity sufficiently rapidly so that all the following integrals exist. Define $[H^{(j)}(x)]^*$ as the *symmetrically decreasing rearrangement*[5] of $H^{(j)}(x)$. Then

$$\int_{-\infty}^{\infty} dx_1 \ldots dx_n H^{(1)}(x_1 - x_2) H^{(2)}(x_2 - x_3) \ldots \times H^{(n)}(x_n - x_1) F^{(1)}(x_1) F^{(2)}(x_2) \ldots F^{(n)}(x_n) \le \int_{-\infty}^{\infty} dx_1 \ldots dx_n [H^{(1)}(x_1 - x_2)]^* \ldots \times [H^{(n)}(x_n - x_1)]^* [F^{(1)}(x_1)]^* \ldots [F^{(n)}(x_n)]^*. \tag{2.9}$$

This theorem exists in the literature[6] for $n = 2$. A formal proof for arbitrary n (by R. Friedberg and myself) has been constructed, and will be published elsewhere. Intuitively, however, the theorem has an almost trivial interpretation. Let the real axis be uniformly covered with particles at concentration C. Further, let $H^{(1)}(x_1 - x_2)dx_2$ be the probability that a particle initially at x_1 finds itself after one interval of time between x_2 and $x_2 + dx_2$. Similarly, let $H^{(2)}$ represent the same probability, the "jump" taking place during the second interval of time, etc., etc. Let $F^{(2)}(x_2)$ be the probability that a particle at x_2 survives absorption before it jumps to x_3 (in the second interval), $F^{(3)}(x_3)$ be the probability that a particle at x_3 survives absorption before it jumps to x_4 (in the third interval), etc., etc. Then

$$l(C\,dx_1) \int_{-\infty}^{\infty} H^{(1)}(x_1 - x_2) F^{(2)}(x_2) H^{(2)}(x_2 - x_3) F^{(3)}(x_3) \ldots \times H^{(n)}(x_n - x_1) F^{(n+1)}(x_1) dx_2 \ldots dx_n$$

represents the number of particles which start in the interval dx_1 around x_1 and end after n jumps within the (very small) interval l around x_1. The total number of particles returning to within l of this starting point (l very small) is therefore [defining $F^{(n+1)}(x)$ as $F^{(1)}(x)$]

$$Cl \int_{-\infty}^{\infty} dx_1 \ldots dx_n H^{(1)}(x_1 - x_2) \ldots \times H^{(n)}(x_n - x_1) F^{(1)}(x_1) \ldots F^{(n)}(x_n),$$

which is proportional to the left-hand side of (2.9). Now it is intuitively obvious why (2.9) is valid: The right-hand side of (2.9) is proportional to the same probability with the absorbing material rearranged to increase as we go away from the origin, and the jumping probabilities rearranged to favor short jumps. That is, for the particles which survive anyway (those near the origin), the short jumps are favored, tending to keep them in the region of high survival, so that in the end more survive.

Accepting (2.9), we apply it to (2.8). Since $P(x)$ is already a symmetrically decreasing function,

$$[P(x)]^* = P(x). \tag{2.10}$$

Further, if for $j = 2, \ldots, n$

$$F^{(j)}(x) \equiv e^{-\Delta_n \phi(x)}, \tag{2.11}$$

then

$$[F^{(j)}(x)]^* = e^{-\Delta_n *[\phi(x)]} \tag{2.12}$$

where $*[\phi(x)]$ is the symmetrically increasing rearrangement of $\phi(x)$.[7] Therefore, (2.9) tells us

$$\int_{-\infty}^{\infty} G(x,t|x')\Gamma(x' - x)\gamma(x)\,dx\,dx' \le \int G^*(x,t|x')[\Gamma(x' - x)]^*[\gamma(x)]^* dx\,dx', \tag{2.13}$$

where $G^*(x,t|x')$ is the Green's function for the "symmetrized" Hamiltonian

$$H^* \equiv \frac{1}{2}\frac{d^2}{dx^2} + *[\phi(x)]. \tag{2.14}$$

Note added in proof: We should mention that (2.9) may be used to obtain more general inequalities than (2.13). For example, we have at once

$$\int G(x_1, t_1|x_1')\Gamma_1(x_1' - x_2)\gamma_1(x_2)G(x_2, t_2|x_2')\Gamma_2(x_2' - x_3)\gamma_2(x_3) \times \cdots G(x_m, t_m|x_m')\Gamma_m(x_m' - x_1)\gamma_m(x_1) \leq \int G^*\Gamma_1^*\gamma_1^*G^*\Gamma_2^*\gamma_2^*\cdots G^*\Gamma_m^*\gamma_m^*, \tag{2.13'}$$

where the arguments of the various functions in the second line are the same as the corresponding ones in the first line. We have found no immediate applications for these more complex inequalities, and have therefore left them out in the discussions of this paper.

(A method of obtaining the various rearranged functions, along with some elementary examples, is found in Appendix A.) The inequality (2.13) is the basic result of this section. Some special cases however are of particular interest:

(a) Letting $\Gamma(x' - x)$ approach the Dirac δ function $\delta(x' - x)$ and $\gamma(x)$ approach unity, we obtain (since both of these are symmetric and not increasing)

$$\int_{-\infty}^{\infty} G(x, t|x)dx \leq \int G^*(x, t|x)dx. \tag{2.15}$$

Using (2.5), we see that this becomes an inequality for the partition function, i.e.,

$$\sum_j e^{-\epsilon_j t} \leq \sum_j e^{-\epsilon_j^* t}, \tag{2.16}$$

where

$$H^*\psi_j^* = \epsilon_j^*\psi_j^* \tag{2.17}$$

define the normalized characteristic functions ψ_j^* and characteristic values ϵ_j^* of H^*.

(b) Letting both Γ and γ approach unity, we obtain

$$\int_{-\infty}^{\infty} G(x, t|x')dxdx' \leq \int G^*(x, t|x')dxdx'. \tag{2.18}$$

Again, by using (2.5), this becomes

$$\sum_j e^{-\epsilon_j t}\left(\int_{-\infty}^{\infty}\psi_j(x)dx\right)^2 \leq \sum_j e^{-\epsilon_j^* t}\left(\int_{-\infty}^{\infty}\psi_j^*(x)dx\right)^2. \tag{2.19}$$

(c) By letting Γ and γ both approach δ functions,

$$\Gamma(x) = \delta(x - a), \quad \gamma(x) = \delta(x - b),$$
$$[\Gamma(x)]^* = \delta(x), \quad [\gamma(x)]^* = \delta(x),$$

(2.13) becomes

$$G(b, t|a + b) \leq G^*(0, t|0)$$

or

$$G(x, t|x') \leq G^*(0, t|0) \tag{2.20}$$

since a and b are arbitrary. The inequality (2.20) gives a general upper bound on the Green's function at arbitrary x, x' in terms of the Green's function for the "symmetrized" Hamiltonian at the origin.

We conclude this section with a discussion of two limiting cases:

(1) *t very large:* In this case the essential result comes from (2.16) which tells us

$$\epsilon_0^* \leq \epsilon_0. \tag{2.21}$$

That is, our inequality provides a *lower bound* on the lowest eigenvalue of H. This may prove of use since the usual variational principle (Rayleigh-Ritz principle) provides a convenient upper bound, and then (2.21) enables us to bracket ϵ_0.

(2) *t very small:* For this case the leading term of the Green's function is trivially obtained by the method of Kac.[4] The result is

$$G(x, t|x') = \frac{e^{-(x-x')^2/2t}}{(2\pi t)^{1/2}}\, e^{-t\phi(x)}. \tag{2.22}$$

[$\phi(x)$ may be replaced by $\phi(x')$ in this expression, since first factor is essentially $\delta(x - x')$ for small t.] Similarly,

$$G^*(x, t|x') = \frac{e^{-(x-x')^2/2t}}{(2\pi t)^{1/2}}\, e^{-t*[\phi(x)]}. \tag{2.23}$$

By using (2.22) and (2.23), (2.13) becomes

$$\int_{-\infty}^{\infty} dxdx'\, \frac{e^{-(x-x')^2/2t}}{(2\pi t)^{1/2}}\, \Gamma(x' - x)\gamma(x) \leq \int_{-\infty}^{\infty} dxdx'\, \frac{e^{-(x-x')^2/2t}}{(2\pi t)^{1/2}}\, e^{-t*[\phi(x)]}\,\Gamma^*(x' - x)\gamma^*(x). \tag{2.24}$$

If $\Gamma, \Gamma^*, \gamma, \gamma^*$ are smooth enough, (2.24) becomes

$$\Gamma(0)\int_{-\infty}^{\infty} dx\; e^{-t\phi(x)}\gamma(x) \leq \Gamma^*(0)\int_{-\infty}^{\infty} dx\; e^{-t*[\phi(x)]}\gamma^*(x). \tag{2.25}$$

The result is an immediate consequence of a well-known rearrangement inequality,[8]

$$\int_{-\infty}^{\infty}\sigma(x)\gamma(x)dx \leq \int_{-\infty}^{\infty}\sigma^*(x)\gamma^*(x)dx \tag{2.26}$$

since $\Gamma^*(0) \geq \Gamma(0)$. [$\Gamma^*(0)$ being the maximum value of the function $\Gamma(x)$.]

If we wish to calculate the "partition function" from (2.15), (2.22) and (2.23) are inadequate. They become

$$G(x, t|x) = e^{-t\phi(x)}/(2\pi t)^{1/2}, \tag{2.22'}$$

$$G^*(x, t|x) = e^{-t*[\phi(x)]}/(2\pi t)^{1/2}, \tag{2.23'}$$

which, because of the equimeasurability of ϕ and $*[\phi]$, reduce (2.15) to a trivial equality. Again, the next term of $G(x, t|x)$ is easily obtained by the method of Kac[4] (it is essentially the first quantum correction to the "classical" partition function obtained by Wigner and Kirkwood), and yields

$$\int_{-\infty}^{\infty} G(x, t|x)dx = \frac{1}{(2\pi t)^{1/2}} \times \left[\int_{-\infty}^{\infty} dx\; e^{-t\phi} - \frac{t^3}{24}\int_{-\infty}^{\infty} dx\left(\frac{d\phi(x)}{dx}\right)^2 e^{-t\phi}\right]. \tag{2.27}$$

Making use of (2.15), we have

$$\int_{-\infty}^{\infty} dx\left(\frac{d\phi}{dx}\right)^2 e^{-t\phi} \geq \int_{-\infty}^{\infty} dx\left(\frac{d*[\phi]}{dx}\right)^2 e^{-t*[\phi]}. \tag{2.28}$$

It is not difficult to prove this inequality directly for arbitrary nonnegative t.

3. HIGHER DIMENSIONS

We shall now consider a particle moving in a three-dimensional Euclidian space [a point of which is specified by $\mathbf{r} = (x,y,z)$], under the influence of a potential $\phi(\mathbf{r})$. (Everything we say in this section applies to the case of a d-dimensional Euclidian space with only trivial changes.) It is assumed that $\phi(\mathbf{r})$ goes to infinity as $|\mathbf{r}|$ does. The Hamiltonian is

$$H = -\tfrac{1}{2}\nabla^2 + \phi(\mathbf{r}), \tag{3.1}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \tag{3.2}$$

Again, the Green's function $G(\mathbf{r},t|\mathbf{r}')$ is defined by

$$HG(\mathbf{r},t|\mathbf{r}') + \frac{\partial G(\mathbf{r},t|\mathbf{r}')}{\partial t} = 0 \quad (t>0) \tag{3.3}$$

and

$$\lim_{t\to 0} G(\mathbf{r},t|\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{3.4}$$

The Wiener integral representation of the Green's function is

$$G(\mathbf{r},t|\mathbf{r}') = \lim_{n\to\infty}\int dr_2\cdots dr_{n-1}\tilde{P}(\mathbf{r}-\mathbf{r}_2)e^{-\Delta_n\phi(\mathbf{r}_2)} \times \tilde{P}(\mathbf{r}_2-\mathbf{r}_3)e^{-\Delta_n\phi(\mathbf{r}_3)}\cdots\tilde{P}(\mathbf{r}_{n-1}-\mathbf{r}')e^{-\Delta_n\phi(\mathbf{r}')}, \tag{3.5}$$

where

$$\tilde{P}(\mathbf{r}) \equiv e^{-\mathbf{r}^2/2\Delta_n}/(2\pi\Delta_n)^{3/2} \tag{3.6}$$

and all integrals on any coordinate are to be taken from $-\infty$ to $+\infty$ unless otherwise stated.

Introducing nonnegative functions $\Gamma(\mathbf{r}), \gamma(\mathbf{r})$, we have

$$\int G(\mathbf{r},t|\mathbf{r}')\Gamma(\mathbf{r}'-\mathbf{r})\gamma(\mathbf{r})d\mathbf{r}d\mathbf{r}' = \lim_{n\to\infty}\int d\mathbf{r}_1\ldots d\mathbf{r}_n\tilde{P}(\mathbf{r}_1-\mathbf{r}_2)e^{-\Delta_n\phi(\mathbf{r}_2)}\ldots \times\tilde{P}(\mathbf{r}_{n-1}-\mathbf{r}_n)e^{-\Delta_n\phi(\mathbf{r}_n)}\Gamma(\mathbf{r}_n-\mathbf{r}_1)\gamma(\mathbf{r}_1). \tag{3.7}$$

Now suppose we consider an arbitrary direction in space, and choose one of the coordinates (say z) to be along it. By writing $\mathbf{r} = (\boldsymbol{\rho}, z)$, (3.7) becomes

$$\int G(\mathbf{r},t|\mathbf{r}')\Gamma(\mathbf{r}'-\mathbf{r})\gamma(\mathbf{r})d\mathbf{r}d\mathbf{r}' = \lim_{n\to\infty}\int d\boldsymbol{\rho}_1\cdots d\boldsymbol{\rho}_n\int dz_1\cdots dz_n \times\tilde{P}(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2,z_1-z_2)e^{-\Delta_n(\boldsymbol{\rho}_2,z_2)}\ldots \times\tilde{P}(\boldsymbol{\rho}_{n-1}-\boldsymbol{\rho}_n,z_{n-1}-z_n)e^{-\Delta_n\phi(\boldsymbol{\rho}_n,z_n)} \times\Gamma(\boldsymbol{\rho}_n-\boldsymbol{\rho}_1,z_n-z_1)\gamma(\boldsymbol{\rho}_1,z_1). \tag{3.8}$$

Holding $\boldsymbol{\rho}_1,\ldots,\boldsymbol{\rho}_n$ fixed, we can apply (2.9) to the z integrations. Exactly the same reasoning as in the previous section now leads to the fundamental result of this paper

$$\int G(\mathbf{r},t|\mathbf{r}')\Gamma(\mathbf{r}'-\mathbf{r})\gamma(\mathbf{r})d\mathbf{r}d\mathbf{r}' \le \int G_z^*(\mathbf{r},t|\mathbf{r}')[\Gamma(\mathbf{r}'-\mathbf{r})]_z^*[\gamma(\mathbf{r})]_z^*d\mathbf{r}d\mathbf{r}', \tag{3.9}$$

where $[\Gamma(\mathbf{r})]_z^*, [\gamma(\mathbf{r})]_z^*$ are the *symmetrically decreasing rearrangements* of Γ and γ viewed as functions of z (x,y held fixed). $G_z^*(\mathbf{r},t|\mathbf{r}')$ is the Green's function for the Hamiltonian

$$[H]_z^* \equiv -\tfrac{1}{2}\nabla^2 + {}_z^*[\phi(\mathbf{r})], \tag{3.10}$$

where ${}_z^*[\phi(\mathbf{r})]$ is the *symmetrically increasing rearrangement* of $\phi(\mathbf{r})$ viewed as a function of z for fixed x,y.

Specializing Γ and γ as in the previous section, we obtain the interesting special cases

(a) $$\sum_j e^{-\epsilon_j t} \le \sum_j e^{-[\epsilon_j]_z^* t}, \tag{3.11}$$

(b) $$\sum_j e^{-\epsilon_j t}\left(\int\psi_j(\mathbf{r})d\mathbf{r}\right)^2 \le \sum_j e^{-[\epsilon_j]^* t}\left(\int[\psi_j(\mathbf{r})]_z^* d\mathbf{r}\right)^2, \tag{3.12}$$

(c) $$G(\mathbf{r},t|\mathbf{r}') \le G_z^*(0,t|0), \tag{3.13}$$

where

$$[H]_z^*[\psi_j]_z^* = [\epsilon_j]_z^*[\psi_j]_z^* \tag{3.14}$$

and the wavefunctions are chosen normalized.

The relationship of (3.9) to the process of "Steiner symmetrization" may be seen as follows. Choose the potential $\phi(\mathbf{r})$ to be zero if $\mathbf{r}$ is a point of some bounded domain D and infinite if it is not. Then the characteristic values and functions of H are given by

$$-\tfrac{1}{2}\nabla^2\psi_i = \epsilon_i\psi_i \quad (\mathbf{r}\text{ in }D), \tag{3.15}$$

$$\psi_i = 0 \quad (\mathbf{r}\text{ not in }D) \tag{3.16}$$

and

$$\psi_i = 0 \quad (\mathbf{r}\text{ on the boundary of }D). \tag{3.17}$$

What is the potential ${}_z^*[\phi(\mathbf{r})]$? It must satisfy the condition[5] (for "arbitrary" W such that the integral converges)

$$\int_{-\infty}^{\infty}W(\phi(\mathbf{r}))dz = \int_{-\infty}^{\infty}W({}_z^*[\phi(\mathbf{r})])dz \tag{3.18}$$

and be a nondecreasing function of $|z|$. For convergence we must assume $W(\infty)$ is zero and $W(0)$ finite. Then the left-hand side of (3.18) is just $W(0)l(x,y)$, where $l(x,y)$ is the length of the intersection of a line parallel to the z axis and passing through the point $(x,y,0)$, with the domain D. Let us define a domain D_z^* by the following conditions:

(a) D_z^* is symmetric with respect to the plane $z=0$.

(b) Any straight line perpendicular to the plane $z=0$ which intersects one of the domains D and D_z^* also intersects the other, and these intersections have the same length.

(c) The intersection with D_z^* consists of just one line segment (the intersection with D could consist of several segments), which, because of (a), is bisected by the plane $z=0$.

Now choosing ${}_z^*[\phi(\mathbf{r})]$ to be zero if $\mathbf{r}$ is in the interior of D_z^* and infinite otherwise, we see at once that (3.18) is satisfied [because of (b)] and that it is a symmetric increasing function of z because of (a) and (c). Thus the characteristic value problem for $[H]_z^*$ is

$$-\tfrac{1}{2}\nabla^2[\psi_j]_z^* = [\epsilon_j]_z^*[\psi_j]_z^* \quad (\mathbf{r}\text{ in }D_z^*), \tag{3.19}$$

$$[\psi_j]_z^* = 0 \quad (\mathbf{r}\text{ not in }D_z^*), \tag{3.20}$$

and

$$[\psi_j]_z^* = 0 \quad (\mathbf{r}\text{ on the boundary of }D_z^*). \tag{3.21}$$

The domain D_z^* satisfies exactly the definition[9] for the Steiner symmetrization of the domain D with respect to a plane $z = 0$. Choosing to apply this to (3.11) for very large t, we obtain the result of Pólya and Szegö[1] (mentioned in the introduction for the two-dimensional case) that Steiner symmetrization decreases the lowest natural frequency of a vibrating fluid confined to a domain D, with Dirichlet boundary conditions on the boundary of D. The inequality (3.9) may be thought of as a generalization of their results.

We also mention that if we integrate (3.12) over t from zero to infinity and consider the two-dimensional case, the left-hand side of (3.12) becomes (apart from a factor of 4) the *torsional rigidity* of the domain D (Pólya and Szegö, Ref. 1, p. 106) and the right-hand side becomes the torsional rigidity of the Steiner symmetrized domain. Therefore, we have shown that Steiner symmetrization increases the torsional rigidity, a result first proved by Pólya in 1948.

The symmetrization process leading to (3.9) may be applied again to some other direction (rather than the z direction). By continuing this procedure with respect to "all possible directions"[10] we will finally obtain

$$\int G(\mathbf{r}, t|\mathbf{r}')\Gamma(\mathbf{r}' - \mathbf{r})\gamma(\mathbf{r})d\mathbf{r}d\mathbf{r}' \leq \int G_s^*(\mathbf{r}, t|\mathbf{r}')\Gamma_s^*(\mathbf{r} - \mathbf{r}')\gamma_s^*(\mathbf{r})d\mathbf{r}d\mathbf{r}', \quad (3.22)$$

where $\Gamma_s^*(\mathbf{r})$ and $\gamma_s^*(\mathbf{r})$ are rearrangements of Γ and γ which are nonincreasing functions of $|\mathbf{r}|$ alone. $G_s^*(\mathbf{r}, t|\mathbf{r}')$ is the Green's function for the Hamiltonian

$$[H]_s^* = -\tfrac{1}{2}\nabla^2 + {}_s^*[\phi(\mathbf{r})], \quad (3.23)$$

where ${}_s^*[\phi(\mathbf{r})]$ is the rearrangement of $\phi(\mathbf{r})$ which is a nondecreasing function of $|\mathbf{r}|$ alone. Therefore, upper bounds of the form (3.22) may be obtained by solving a problem with spherical symmetry. (A method for finding these spherically symmetric rearrangements along with some elementary examples is found in Appendix A.)

Finally, we conclude by discussing two limiting cases:

(1) *t very large:* Once more the essential result comes from (3.11), which tells us

$$[\epsilon_0]_s^* \leq [\epsilon_0]_z^* \leq \epsilon_0, \quad (3.24)$$

Again providing, in principle, lower bounds for the ground state energy.[11]

(2) *t very small:* Just as in the one-dimensional case the leading and first correction term to the partition function may be written

$$\int G(\mathbf{r}, t|\mathbf{r})d\mathbf{r} = \frac{1}{(2\pi t)^{3/2}}\left(\int d\mathbf{r} e^{-t\phi(\mathbf{r})} - \frac{t^3}{24}\int d\mathbf{r}[\nabla\phi(\mathbf{r})]^2 e^{-t\phi(\mathbf{r})}\right), \quad (3.25)$$

which with (3.11) yields

$$\int d\mathbf{r}(\nabla\phi)^2 e^{-t\phi} \leq \int d\mathbf{r}[\nabla {}_z^*(\phi)]^2 e^{-t\,{}_z^*(\phi)}. \quad (3.26)$$

It is not difficult to prove this inequality directly for all positive t. Comparing these results with those mentioned for the vibrations of a membrane [(1.4), (1.5), (1.6)], we see that the inequality (3.26) is the analog (for a smooth potential) of the isoperimetric inequality stating that the Steiner symmetrization decreases the surface area, while leaving the volume unchanged [the unchanged volume corresponding to the fact that ϕ and ${}_z^*(\phi)$ are equimeasurable].

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APPENDIX A

In this appendix, pedagogic in intent, we indicate how the various rearrangements of the functions required in this paper may be carried out, and give some elementary examples.

1. Symmetrically decreasing rearrangements

Suppose $f(x)$ is a nonnegative function which approaches zero as $|x|$ approaches infinity, and we want its symmetrically decreasing rearrangement $f^*(x)$. Instead of the general condition (arbitrary W) mentioned in Footnote 5, it is sufficient to require, for equimeasurability, that for arbitrary real $y > 0$

$$\int_{-\infty}^{\infty} dx\ \theta(f(x) - y) = \int_{-\infty}^{\infty} dx\ \theta(f^*(x) - y) \quad (A1)$$

where $\theta(u)$ is the usual step function

$$\theta(u) = 1, \quad u \geq 0, \qquad = 0, \quad u < 0. \quad (A2)$$

This is intuitively clear, but purely formally we may differentiate (A1) with respect to y and obtain

$$\int_{-\infty}^{\infty} dx\ \delta(y - f(x)) = \int_{-\infty}^{\infty} dx\ \delta(y - f^*(x)). \quad (A3)$$

Multiplying both sides of (A3) by $W(y)$, integrating over y, and interchanging the order of integration, we have at once

$$\int_{-\infty}^{\infty} W(f(x))dx = \int_{-\infty}^{\infty} W(f^*(x))dx. \quad (A4)$$

This is just the condition that f^* be a rearrangement of f.

The integrals in (A1) have the following significance: The left-hand side is the length of the intervals on the x axis for which $f(x) \geq y$. Call the solutions (in increasing order) of

$$f(x) = y \quad (A5)$$

$x_1, x_2, \ldots, x_{2n}$. Then $f(x) > y$ for $x_1 < x < x_2$, $x_3 < x < x_4$, etc., etc. The left-hand side of (A1) is just $x_2 - x_1) + (x_4 - x_3) + \ldots + (x_{2n} - x_{2n-1})$. On the other hand, since $f^*(x)$ is a symmetrical nonincreasing function of x, the equation

$$f^*(x) = y \quad (A6)$$

has only two solutions $x = \pm u(y)$ $(u > 0)$ so that (A1) becomes

$$(x_2 - x_1) + (x_4 - x_3) + \ldots = 2u. \quad (A7)$$

Substituting $y = f^*(u)$ into the left-hand side of (A7), we obtain an equation for $f^*(u)$ $(u > 0)$. If there are regions of finite length on the x axis for which (A5) is satisfied for a particular y [i.e. flat portions of the curve $y = f(x)$], then the x_i are determined by the end points of these regions. The curve $y = f^*(x)$ will also have flat portions of the same length at this particular y, and u means the largest root of $f^*(x) = y$.

We consider several elementary examples

$$\text{(i)}\quad \begin{aligned} f(x) &= ce^{x/b}, \quad x<0,\\ &= ce^{-x/a}, \quad x>0, \end{aligned} \qquad a,b,c>0, \tag{A8}$$

$$\begin{aligned} &x_1 = b\log(y/c), \quad x_2 = -a\log(y/c),\\ &x_2 - x_1 = -(a+b)\log y/c = 2u,\\ &f^*(u) = ce^{-2u(a+b)}, \quad u>0.\\ &f^*(u) = ce^{-2|u|/(a+b)}, \end{aligned} \tag{A9}$$

$$\text{(ii)}\quad \begin{aligned} f(x) &= f_1, \quad a_1 < x < b_1,\\ &= f_2, \quad a_2 < x < b_2,\\ &\;\cdot\\ &\;\cdot\\ &\;\cdot\\ &= f_n, \quad a_n < x < b_n,\\ &= 0, \quad \text{otherwise,} \end{aligned} \qquad f_1 > f_2 > f_3 \ldots > f_n > 0. \tag{A10}$$

Call $b_i - a_i = l_i$. Then clearly $(x>0)$

$$\begin{aligned} f^*(x) &= f_1 \quad 0 < x < l_1/2\\ &= f_2 \quad l_1/2 < x < (l_1 + l_2)/2\\ &\;\cdot\\ &\;\cdot\\ &\;\cdot\\ &= f_n, \quad (l_1 + \ldots + l_{n-1})/2\\ &\qquad < x < (l_1 + l_2 + \ldots + l_n)/2,\\ &= 0, \quad x > (l_1 + l_2 + \ldots + l_n)/2. \end{aligned} \tag{A11}$$

2. Symmetrically increasing rearrangements

Suppose we have a function $g(x)$ which approaches infinity as $|x|$ approaches infinity, and we want its symmetrically increasing rearrangement $^*g(x)$. Again, it is sufficient for equimeasurability to require

$$\int_{-\infty}^{\infty} dx\ \theta(y - g(x)) = \int_{-\infty}^{\infty} dx\ \theta(y - {}^*g(x)). \tag{A12}$$

The left-hand side of (A12) is the length of the intervals on the x axis for which $g(x) \le y$. Calling the roots of $g(x) = y$, $x_1, \ldots, x_{2n}$, again, and the roots of $^*g(x) = y$ $\pm u$ $(u>0)$, $^*g(u)$ is determined by

$$[(x_2 - x_1) + \cdots + (x_{2n} - x_{2n-1})] = 2u. \tag{A13}$$

Again, when there are flat portions to the curve $y = g(x)$, a little care must be exercised. Elementary examples are the following:

$$\text{(iii)}\quad \begin{aligned} g(x) &= A(x/a - a/x)^2, \quad x>0,\\ &= \infty, \quad x<0. \end{aligned}$$

Direct calculation gives $x_1 = \frac{1}{2}a[-\alpha + (\alpha^2+4)^{1/2}]$, $x_2 = \frac{1}{2}a[\alpha + (\alpha^2+4)^{1/2}]$, $\alpha \equiv (y/A)^{1/2}$. Therefore, $x_2 - x_1 = a\alpha = 2u$. Substituting $y = {}^*g(u)$, we obtain

$$^*g(u) = 4Au^2. \tag{A14}$$

$$\text{(iv)}\quad \begin{aligned} g(x) &= 0, \quad \text{in the nonoverlapping intervals}\\ &\qquad (a_1,b_1),(a_2,b_2),\ldots,(a_n,b_n),\\ &= \infty, \quad \text{otherwise,} \end{aligned} \tag{A15}$$

$$\begin{aligned} ^*g(x) &= 0, \quad -L/2 < x < L/2,\\ &= \infty, \quad \text{otherwise,} \end{aligned} \tag{A16}$$

where

$$L = \sum_{i=1} l_i, \tag{A17}$$

$$l_i = b_i - a_i. \tag{A18}$$

3. Symmetrically decreasing spherically symmetric rearrangements

Just as in (1) we need only require

$$\int d\mathbf{r}\ \theta(f(\mathbf{r}) - v) = \int d\mathbf{r}\ \theta([f(\mathbf{r})]_s^* - v), \tag{A19}$$

where $f(\mathbf{r})$ is a nonnegative function which approaches zero as $|\mathbf{r}|$ approaches infinity and $v>0$. Again, the left-hand side of (A19) is the volume $\Omega(v)$ occupied by the set of all points satisfying $f(\mathbf{r}) \ge v$. The right-hand side is given by $(4\pi/3)r(v)$ is the largest solution of

$$[f(r(v))]_s^* = v. \tag{A20}$$

Therefore, we obtain as the equation for $[f(r)]_s^*$

$$\Omega(f(r)]_s^*) = \tfrac{4}{3}\pi r^3. \tag{A21}$$

An elementary example is

(v) $f = F\left(\left[\sum_{\alpha,\beta} A_{\alpha\beta}x_\alpha x_\beta\right]^{1/2}\right)$, where $A_{\alpha\beta}$ is a real symmetric positive definite matrix and $F(\tau)$ is a monotonically decreasing function of τ. The volume Ω is easily calculated by transforming to principal axes, and we find at once that

$$[f(r)]_s^* = F(\det A)^{1/6} r), \tag{A22}$$

where $\det A$ is the determinant of the matrix A.

4. Symmetrically increasing spherically symmetric rearrangements

If $g(\mathbf{r})$ is a function which approaches infinity when $|\mathbf{r}|$ approaches infinity, the same reasoning as in the previous section tells us the $^*_s[g(r)]$ is given by

$$\tilde{\Omega}(^*_s[g(r)]) = \tfrac{4}{3}\pi r^3, \tag{A23}$$

where $\tilde{\Omega}(v)$ is the volume occupied by the set of all points satisfying $g(\mathbf{r}) \le v$.

Examples:

(vi) $g = G((A_{\alpha\beta}x_\alpha x_\beta)^{1/2})$ [see (v)], where $G(\tau)$ is a monotonically increasing function of τ. Then

$$^*_s[g(r)] = G((\det A)^{1/6} r). \tag{A24}$$

(vii) $g(\mathbf{r}) = \dfrac{|x|}{a} + \dfrac{|y|}{b} + \dfrac{|z|}{c}$, $\quad a, b, c$, positive,

$$\tilde{\Omega}(v) = \int d\mathbf{r}\ \theta(g(\mathbf{r}) - v) = \int r^2 dr d\omega\ \theta(rq(\theta,\phi) - v),$$

where

$$q(\theta,\phi) = \frac{|\cos\theta\cos\phi|}{a} + \frac{|\cos\theta\sin\phi|}{b} + \frac{|\sin\theta|}{c}$$

and $d\omega = \sin\theta\, d\theta d\phi$. Therefore,

$$\tilde{\Omega}(v) = \frac{4\pi}{3} v^3\ \overline{\frac{1}{q^3}}, \qquad \overline{\frac{1}{q^3}} \equiv \frac{1}{4\pi}\int d\omega\ \frac{1}{q^3}.$$

Finally, then

$$\overset{*}{_s}[g(r)] = \frac{r}{(1/q^3)^{1/3}}. \tag{A25}$$

Some of the examples of this appendix have been used to check our fundamental inequalities. Others, simple as they are, give rise to interesting inequalities. Thus, if the $g(x)$ of (iii) is used as a potential, the energy levels and wavefunctions are known.[12] The energy levels are

$$\epsilon_j = (8A/a^2)^{1/2}\{j + \tfrac{1}{2} + \tfrac{1}{4}[(8Aa^2+1)^{1/2} - (8Aa^2)^{1/2}]\},\quad j = 0,1,\cdots. \tag{A26}$$

Since $*g$ is an harmonic oscillator potential, the levels are

$$\epsilon_j^* = (8A/a^2)^{1/2}(j + \tfrac{1}{2}). \tag{A27}$$

Therefore, $\epsilon_j > \epsilon_j^*$ for all j, and the partition function inequality is trivially satisfied.

Another easily calculable case is when the potential is chosen to be

$$\phi = \tfrac{1}{2}A_{\alpha\beta}x_\alpha x_\beta, \tag{A28}$$

where $A_{\alpha\beta}$ is a positive definite matrix. By (A24)

$$\overset{*}{_s}[\phi] = \tfrac{1}{2}(\det A)^{1/3}r^2. \tag{A29}$$

The characteristic values of H are

$$\epsilon_{n_1n_2n_3} = \sum_{i=1}(A_i)^{1/2}(n_i + \tfrac{1}{2}),\quad n_i = 0,1,2,\ldots, \tag{A30}$$

where the A_i are the characteristic values of $A_{\alpha\beta}$. The characteristic values of $[H]_s^*$ are

$$[\epsilon_{n_1n_2n_3}]_s^* = (\det A)^{1/6}(n_1 + n_2 + n_3 + \tfrac{3}{2}). \tag{A31}$$

Computing the partition function, we easily obtain

$$\sum \exp(-\epsilon_{n_1n_2n_3}t) = \prod_i \frac{1}{2\sinh[(A_i)^{1/2}t/2]}$$
$$\sum \exp(-[\epsilon_{n_1n_2n_3}]_s^* t) = \left(\frac{1}{2\sinh[(\det A)^{1/6}t/2]}\right)^3. \tag{A32}$$

The inequality (3.11) now reads

$$\prod_i \frac{1}{2\sinh[A_i)^{1/2}t/2]} \le \left(\frac{1}{2\sinh[(\det A)^{1/6}t/2]}\right)^3 \tag{A33}$$

This is easily proved directly, making use of the fact that log (sinhτ) is an increasing convex function of τ for $\tau > 0$. Similarly both sides of (3.12) are easily calculable, and the result is again not difficult to prove directly.

Finally, we mention a simple example where the resulting inequality is not so obvious. If the potential is given by (A15), the symmetrically increasing rearrangement is given by (A16). Again, it is trivial to compute the characteristic values and functions for both H and H^*. This gives for (3.11) and (3.12)

$$\sum_{r=1}^{\infty}\sum_{i=1}^{n} e^{-\pi^2tr^2/(2l_i^2)} \le \sum_{r=1}^{\infty}\exp[-\pi^2tr^2/2(l_1 + l_2 + \cdots + l_n)^2] \tag{A34}$$

and

$$\sum_{r\ \mathrm{odd}}\left(\sum_{i=1}\frac{8l_i}{r^2\pi^2}e^{-(\pi^2tr^2)/(2l_i^2)}\right) \le \sum_{r=1}\frac{8(l_1 + l_2 + \ldots + l_n)}{r^2\pi^2} \times \exp[-\pi^2tr^2/2(l_1 + l_2 + \ldots + l_n)^2], \tag{A35}$$

which are interesting inequalities among theta functions.

APPENDIX B

The results of Sec. 3 may easily be extended in the following way. Suppose the "kinetic energy" term $\mathbf{p}^2/2$ $[p_\alpha \equiv (1/i)(\partial/\partial x_\alpha),\ (x_1,x_2,x_3) \equiv (x,y,z)]$ is replaced by the more general expression

$$K(\mathbf{p}) = \tfrac{1}{2}(M^{-1})_{\alpha\beta}p_\alpha p_\beta, \tag{B1}$$

where $(M_{\alpha\beta})$ is a real constant symmetric positive definite matrix. This type of differential operator arises in the study of heat flow in crystals $(M^{-1})_{\alpha\beta}$ is then proportional to the heat conductivity tensor) or in the study of electronic states in semiconductors [where $(M_{\alpha\beta})$ is the "effective mass tensor"]. The only change which this makes in (3.5) is that $\tilde{P}(\mathbf{r})$ is replaced by

$$\tilde{P}(\mathbf{r}) = \frac{1}{(2\pi\Delta_n)^{3/2}}(\det M)^{1/2}\exp - M_{\alpha\beta}x_\alpha x_\beta/(2\Delta_n) \tag{B2}$$

as a simple calculation shows. To apply the inequality (2.9), we must find the symmetrically decreasing rearrangement of $\tilde{P}(r)$ [as given by (B2)] regarded as a function of z (i.e., x_3). Call this $[\tilde{P}(\mathbf{r})]_z^*$. Writing

$$M_{\alpha\beta}x_\alpha x_\beta = M_{33}z^2 + 2(M_{3a}x_a)z + M_{ab}x_a x_b \tag{B3}$$

(where a, b take on the values 1, 2), we can complete the square

$$M_{\alpha\beta}x_\alpha x_\beta = M_{33}(z + M_{3a}x_a/M_{33}) + M_{ab}x_a x_b - (M_{3a}x_a)^2/M_{33}. \tag{B4}$$

Therefore, as we see at once from the definition given in Footnote 5,

$$[\tilde{P}(\mathbf{r})]_z^* = \frac{1}{(2\pi\Delta_n)^{3/2}}(\det M)^{1/2} \times \exp\left[-\frac{1}{2}\Delta_n\left(M_{33}z^2 + M_{ab}x_a x_b - \frac{(M_{3a}x_a)^2}{M_{33}}\right)\right]$$
$$= \frac{1}{(2\pi\Delta_n)^{3/2}}[\det(M_z^*)]^{1/2}\exp\left(-\frac{1}{2}\Delta_n(M_z^*)_{\alpha\beta}x_\alpha x_\beta\right). \tag{B5}$$

In (B5), $(M_z^*)_{\alpha\beta}$ is the matrix

$$(M_z^*)_{33} = M_{33},\quad (M_z^*)_{3a} = (M_z^*)_{a3} = 0,$$
$$(M_z^*)_{ab} = M_{ab} - (1/M_{33})M_{3a}M_{3b}, \tag{B6}$$

and we have made use of the fact that

$$\det(M_z^*) = \det M. \tag{B7}$$

Since (B5) is exactly of the form (B2), all the reasoning of Sec. 3 goes through without any modification, and we are led to the following result: (3.9) is still valid if $G_z^*(\mathbf{r},t|\mathbf{r}')$ is the Green's function corresponding to the Hamiltonian

$$[H]_z^* = \tfrac{1}{2}([M_z^*]^{-1})_{\alpha\beta}p_\alpha p_\beta + \overset{*}{_z}[\phi(\mathbf{r})]. \tag{B8}$$

The symmetrization process leading to (B8), may be applied now to some other direction. By continuing the process for "all possible directions," we must finally obtain the result that $\tilde{P}(\mathbf{r})$ and $\phi(\mathbf{r})$ are replaced by $[\tilde{P}(\mathbf{r})]_s^*$ and ${}_s^*[\phi(\mathbf{r})]$. Using (v) of Appendix A, we have at once that

$$[\tilde{P}(\mathbf{r})]_s^* = \frac{1}{(2\pi\Delta_n)^{3/2}} (\det M)^{1/2} e^{-(1/2\Delta_n)(\det M)^{1/3} r^2}. \tag{B9}$$

Therefore (3.22) is still valid if $G_s^*(\mathbf{r}, t|\mathbf{r}')$ is the Green's function corresponding to the Hamiltonian

$$[H]_s^* = \tfrac{1}{2}(\det M)^{-1/3} p^2 + {}_s^*[\phi(r)]. \tag{B10}$$

If we take as an example ϕ given by (A28), H becomes the general Hamiltonian for small oscillations,

$$H = \tfrac{1}{2}(M^{-1})_{\alpha\beta} p_\alpha p_\beta + \tfrac{1}{2} A_{\alpha\beta} x_\alpha x_\beta \tag{B11}$$

and

$$[H]_s^* = \tfrac{1}{2}(\det M)^{-1/3} p^2 + \tfrac{1}{2}(\det A)^{1/3} r^2. \tag{B12}$$

For this case everything is calculable and, as in Appendix A, the partition function inequality may be verified by well-known inequalities.

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[1]An invaluable reference in this field is G. Pólya and G. Szegö, *Isoperimetric Inequalities in Mathematical Physics* (Princeton U. P., Princeton, N. J., 1951).

[2]See, for example, M. Kac, Am. Math. Monthly **73**, 1 (1966).

[3]The type of result which we shall obtain is easily generalized to time-dependent Hamiltonians, more complicated kinetic energy terms, and potentials which approach zero at infinity (in which case scattering theory is involved). We limit our discussion here in the interest of simplicity. However, the generalization to a higher number of dimensions forms an important part of this work. A generalization to a slightly more complex kinetic energy expression is given in Appendix B.

[4]M. Kac, *Probability and Related Topics in Physical Science* (Interscience, New York, 1959), Vol. I, pp. 161ff.

[5]G. H. Hardy, J. E. Littlewood, and G. Pólya, *Inequalities* (Cambridge U. P., London and New York, 1952), 2nd ed., pp. 276ff. Intuitively, a rearrangement $F_R(x)$ of a function $F(x)$ means that $F_R(x)$ takes on the same values as $F(x)$, but at different locations. That is, for "arbitrary" W (such that the integral converges) $\int_{-\infty}^{\infty} W(F(x))dx = \int_{-\infty}^{\infty} W(F_R(x))dx$. The symmetrically decreasing rearrangement is the $F_R(x)$ which is a nonincreasing function of $|x|$, where the origin is chosen arbitrarily. Functions which are rearrangements of each other are also said to be *equimeasurable*.

[6]Reference 5, pp. 279ff.

[7]That is, that rearrangement of $\phi(x)$ which is a nondecreasing function of $|x|$. This is obvious since the definition mentioned in Footnote 5 tells us that $\exp\{-\Delta_n{}^*[\phi(x)]\}$ is a rearrangement of $F^{(j)}(x)$, and it is a symmetrically decreasing function.

[8]Reference 5, pp. 278ff.

[9]Reference 1, p. 5.

[10]There is a limiting process here which certainly requires a little justification. However, in keeping with the spirit of this paper, we are trying to obtain results rather than be rigorous.

[11]An upper bound on ϵ_0(say $\epsilon_0{}'$) is found from the Rayleigh–Ritz principle. If we take as the trial function one which is spherically symmetric, it is very easy to see that lowest value of $\epsilon_0{}'$ (within this class of functions) is just the ground state energy of a particle in a spherically symmetric potential $\bar{\phi}(r)$ obtained by averaging $\phi(\mathbf{r})$ over direction for a given $|\mathbf{r}|$. Therefore, ϵ_0 lies between the lowest energies of two problems with spherically symmetric potentials.

[12]I. I. Goldman *et al.*, *Problems in Quantum Mechanics* (Academic, New York, 1960), p. 63.

A discrete version of the inverse scattering problem

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A discrete version of the inverse scattering problem is considered. The Schrödinger equation with a potential is replaced by a difference equation. The problem is to determine the coefficients given the phase shift. Application is mainly pedagogical. The motivation for the principal steps becomes obvious and the mathematics is elementary. At any stage one can pass, by a limiting procedure, to the usual Schrödinger problem—and reobtain the classical results.

1. INTRODUCTION

The inverse scattering problem in quantum mechanics can be stated as follows.

We are given that $\psi(E;x)$, $0 \le x < \infty$, satisfies the (Schrödinger) equation

$$\frac{1}{2}\frac{d^2\psi(E;x)}{dx^2} - q(x)\psi(E;x) = -E\psi(E;x) \tag{1.1}$$

and the boundary conditions

$$\psi(E;0) = 0, \quad \psi'(E;0) = 1, \tag{1.2}$$

and [assuming that the potential $q(x)$ is suitably behaved] for $E > 0$ is asymptotically proportional to

$$\sin[\sqrt{2E}x + \delta(E)], \quad x \to \infty. \tag{1.3}$$

If the phase shifts $\delta(E)$ are known for all $E > 0$, can one determine the potential $q(x)$?

If the potential is such that there are no bound states, the answer is in the affirmative, but if there are bound states

$$\psi(E_i;x), \quad E_i < 0, \tag{1.4}$$

then, in addition to $\delta(E)$, one must know the E_i and the normalization constants

$$C_i = \int_0^\infty \psi^2(E_i;x)\,dx. \tag{1.5}$$

This problem has been extensively discussed in the literature, and an excellent exposition can be found, e.g., in the recent book by Newton.[1]

The solution is achieved in two separate steps:

(a) From the knowledge of $\delta(E)$, E_i, and C_i, one constructs the spectral function $\rho(E)$ for the operator

$$\tfrac{1}{2}D^2 - q(x)$$

(this was first done by Jost and Kohn[2]).

(b) Having found $\rho(E)$, one constructs the potential by an elegant procedure due to Gel'fand and Levitan.[3]

The details are intricate and the presentation (especially of (b)] not easily motivated. Remarkably enough, this is not the case if one considers the discrete version of the problem. Nearly everything becomes so transparent as to border on the trivial, at the same time throwing considerable light on the theory.

Since our purpose in writing this paper is largely pedagogical, we do not strive for optimal conditions, thus sacrificing generality for the sake of simplicity and clarity.

2. A DISCRETE VERSION OF THE GEL'FAND-LEVITAN PROCEDURE

The obvious discretized version of (1.1) is

$$\tfrac{1}{2}[\psi(E;(n+1)\Delta) - 2\psi(E;n\Delta) + \psi(E;(n-1)\Delta]/\Delta^2 + [E - q(n\Delta)]\psi(E;n\Delta) = 0, \tag{2.1}$$

but it turns out that the discussion can be greatly simplified if instead of (2.1) we take

$$\tfrac{1}{2}\psi(E;(n+1)\Delta) + \tfrac{1}{2}\psi(E;(n-1)\Delta) = (1 - E\Delta^2)\,e^{\Delta^2 q(n\Delta)}\psi(E;n\Delta), \tag{2.2}$$

which in the limit $\Delta \to 0$ also goes over into the Schrödinger equation (1.1).

Setting

$$\lambda = 1 - E\Delta^2, \tag{2.3}$$

$$v(n) = \Delta^2 q(n\Delta), \tag{2.4}$$

and

$$\phi(\lambda;n) = e^{v(n)/2}\,\psi(E;n\Delta), \tag{2.5}$$

we see that (2.2) can be rewritten in the equivalent form

$$\tfrac{1}{2}e^{-[v(n)+v(n+1)]/2}\,\phi(\lambda;n+1) + \tfrac{1}{2}e^{-[v(n-1)+v(n)]/2}\,\phi(\lambda;n-1) = \lambda\phi(\lambda;n), \tag{2.6}$$

which in matrix notation becomes

$$A\phi = \lambda\phi, \tag{2.7}$$

where the symmetric matrix A is tridiagonal, and its (m,n) element $a_{m,n}$ $(m,n \ge 1)$ is given by the formula

$$a_{m,n} = \tfrac{1}{2}e^{-[v(m)+v(n)]/2}(\delta_{m,n+1}). \tag{2.8}$$

For future convenience we shall set

$$v(0) = 0.$$

The boundary condition $\phi(\lambda;0) = 0$ is automatic, and we take

$$\phi(\lambda;1) = 1 \tag{2.9}$$

rather than $\phi(\lambda;1) = \Delta$ as the other boundary condition.[4] Let $\mathring{A}$ be the matrix corresponding to $v(n) \equiv 0$, i.e.,

$$\mathring{a}_{mn} = \tfrac{1}{2}(\delta_{m,n-1} + \delta_{m,n+1}). \tag{2.10}$$

In this case

$$\mathring{\phi}(\lambda;n) = \frac{[\lambda + (\lambda^2-1)^{1/2}]^n - [\lambda - (\lambda^2-1)^{1/2}]^n}{2(\lambda^2-1)^{1/2}} \tag{2.11}$$

satisfies the recursion

$$\tfrac{1}{2}\mathring{\phi}(\lambda;n+1)+\tfrac{1}{2}\mathring{\phi}(\lambda;n-1)=\lambda\mathring{\phi}(\lambda;n), \tag{2.12}$$

and the spectral distribution $\sigma(\lambda)$ is given by the well-known formula

$$\sigma(\lambda)=\begin{cases}0, & \lambda<-1,\\ \frac{2}{\pi}\int_{-1}^{\lambda}\surd(1-\mu^2)^{1/2}\,d\mu, & -1<\lambda<1,\\ 1, & \lambda>1.\end{cases} \tag{2.13}$$

Let the spectral distribution of A be $\rho(\lambda)$, so that

$$\int \phi(\lambda;m)\phi(\lambda;n)d\rho(\lambda)=\delta_{mn}, \tag{2.14}$$

$$\int \lambda\phi(\lambda;m)\phi(\lambda;n)d\rho(\lambda)=a_{mn}, \tag{2.15}$$

and in fact

$$\int \lambda^r\phi(\lambda;m)\phi(\lambda;n)d\rho(\lambda)=a_{mn}^{(r)}, \tag{2.15$'$}$$

where $a_{mn}^{(r)}$ is the (m,n) element of A^r.

Since the $\phi(\lambda;n)$ are polynomials, they are *the* orthogonal polynomials (properly normalized) with respect to the weight $\rho(\lambda)$.

The inverse problem is now almost trivial because given $\rho(\lambda)$ we can determine the orthonormal polynomials with respect to ρ and then calculate $a_{n,n+1}$. There are two important points which remain. The first is that since

$$a_{n,n+1}=\tfrac{1}{2}e^{-[v(n)+v(n+1)]/2} \tag{2.16}$$

is positive, one must be sure that the orthonormal polynomials are such that

$$\int \lambda\phi(\lambda;n)\phi(\lambda;n+1)d\rho(\lambda)>0. \tag{2.17a}$$

That this condition can indeed be fulfilled will become apparent in the sequel. The second point is that ρ cannot be prescribed quite arbitrarily, since we must have

$$a_{nn}=\int \lambda\phi^2(\lambda;n)d\rho(\lambda)=0. \tag{2.17b}$$

We must therefore impose an *a priori* condition on ρ to insure (2.17b). The simplest such condition is that

$$\rho(-\lambda)=1-\rho(\lambda), \tag{2.17$'$}$$

which insures that the orthogonal polynomials are either even or odd and hence (2.17b). From now on (2.17′) will be assumed.

Given ρ, we imitate the Gel'fand–Levitan procedure by seeking the orthonormal polynomials in the form

$$\phi(\lambda;n)=K(n,n)\mathring{\phi}(\lambda;n)+\sum_{m=1}^{n-1}K(n,m)\phi(\lambda;m). \tag{2.18}$$

The polynomial $\phi(\lambda;n)$, which is of degree $n-1$, is orthogonal to every polynomial of degree lower than $n-1$ and hence to every $\mathring{\phi}(\lambda;m)$ for $m<n$.

Thus, orthogonality conditions are equivalent to

$$\int \phi(\lambda;n)\mathring{\phi}(\lambda;m)d\rho(\lambda)=0,\quad m<n, \tag{2.19}$$

and setting

$$q(m,l)=\int \mathring{\phi}(\lambda;m)\mathring{\phi}(\lambda;l)d(\rho(\lambda)-\sigma(\lambda)), \tag{2.20}$$

we see that (2.19) can be rewritten in the form

$$0=K(n,n)q(n,m)+K(n,m)+\sum_{l=1}^{n-1}K(n,l)q(l,m),\quad n>m, \tag{2.21}$$

which is strongly reminiscent of the Gel'fand–Levitan equations.

The normalization condition

$$\int \phi^2(\lambda;n)d\rho(\lambda)=1 \tag{2.22}$$

is equivalent to the condition

$$K(n,n)\int \phi(\lambda;n)\mathring{\phi}(\lambda;n)d\rho(\lambda)=1, \tag{2.23}$$

which upon using (2.18) and (2.20) becomes

$$\frac{1}{K(n,n)}=K(n,n)[1+q(n,n)]+\sum_{l=1}^{n-1}K(n,l)q(l,n). \tag{2.24}$$

Setting

$$\kappa(n,m)=[K(n,m)]/[K(n,n)],\quad m<n, \tag{2.25}$$

we see that Eqs. (2.21) can be written in the form

$$0=q(n,m)+\kappa(n,m)+\sum_{l=1}^{n-1}\kappa(n,l)q(l,m), \tag{2.26}$$

and these equations constitute a system of $n-1$ linear equations from which $\kappa(n,m), 1\le m\le n-1$, are (uniquely) determined.

The normalization condition (2.24) now assumes the form

$$\frac{1}{K^2(n,n)}=1+q(n,n)+\sum_{l=1}^{n-1}\kappa(n,l)q(l,n), \tag{2.27}$$

and serves the sole purpose of determining $K(n,n)$.

Since $K^2(n,n)$ is involved, there is an ambiguity in sign, and keeping in mind the fundamental recursion (2.6) [which implies that the leading coefficient of $\phi(\lambda;n)$, which is $K(n,n)$, must be positive], we are *compelled* to choose the plus sign.

Finally,

$$\begin{aligned}a_{n,n+1}&=\int \lambda\phi(\lambda;n)\phi(\lambda,n+1)d\rho(\lambda)\\&=K(n,n)\int \lambda\mathring{\phi}(\lambda;n)\phi(\lambda,n+1)d\rho(\lambda),\end{aligned}$$

and since

$$\lambda\mathring{\phi}(\lambda;n)=\tfrac{1}{2}\mathring{\phi}(\lambda;n-1)+\tfrac{1}{2}\mathring{\phi}(\lambda;n+1),$$

we obtain [using (2.23) with $(n+1)$ instead of n]

$$\begin{aligned}a_{n,n+1}&=\tfrac{1}{2}K(n,n)\int \mathring{\phi}(\lambda;n+1)\phi(\lambda;n+1)d\rho(\lambda)\\&=\frac{1}{2}\,\frac{K(n,n)}{K(n+1,n+1)},\end{aligned} \tag{2.28}$$

or equivalently

$$\tfrac{1}{2}[v(n)+v(n+1)]=\log K(n+1,n+1)-\log K(n,n). \tag{2.29}$$

Equation (2.29) does not in general determine $v(n)$, but if, e.g., it is known that

$$\lim_{n\to\infty}v(n)=0, \tag{2.30}$$

then, in fact, v becomes uniquely determined.

To see this, note that

$$\tfrac{1}{2}[v(1) \pm v(n+1)] = \sum_{r=1}^{n} (-1)^{r+1} \log \frac{K(r+1,r+1)}{K(r,r)},$$

and hence

$$\tfrac{1}{2}v(1) = \sum_{r=1}^{\infty} (-1)^{r+1} \log \frac{K(r+1,r+1)}{K(r,r)}, \qquad (2.31)$$

where the convergence of the series in (2.31) is a consequence of (2.30). Conversely, if the series in (2.31) converges, then (2.30) follows.

While it does not seem to be easy to give simple conditions on ρ to insure (2.30), it is clear that if ρ and σ are sufficiently close, then (2.30) will be satisfied.

3. REMARKS AND AN EXAMPLE

1. If we consider (2.18) for $-1 < \lambda < 1$ (which in view of $\lambda = 1 - E\Delta^2$ implies that $E > 0$), and set

$$\lambda \cos\theta,$$

we obtain

$$\mathring{\phi}(\lambda; m) = (\sin m\theta)/(\sin\theta),$$

where $\theta = \arccos\lambda = \arccos(1 - E\Delta^2)$, so that for small Δ (and fixed E) we have

$$\theta = \Delta\sqrt{2E} + O(\Delta^2).$$

Thus

$$\Delta\phi(E; n\Delta) \sim K(n,n)\Delta \frac{\sin n\Delta\sqrt{2E}}{\sin\Delta\sqrt{2E}} + \Delta \sum_{m=1}^{n-1} K(n,m) \frac{\sin m\Delta\sqrt{2E}}{\sin\Delta\sqrt{2E}}, \qquad (3.1)$$

and from (2.29) it follows on the assumption of convergence of the series

$$\sum_{n=1}^{\infty} v(n)$$

that $\log K(n,n)$ approaches a finite limit as $n \to \infty$. It thus appears that in the limit

$$\Delta \to 0, \quad n\Delta = x$$

(3.1) should go over into

$$\psi(E;x) = \alpha \frac{\sin x\sqrt{2E}}{\sqrt{2E}} + \int_0^x K(x,\xi) \frac{\sin\xi\sqrt{2E}}{\sqrt{2E}}\, d\xi, \qquad (3.2)$$

and that $\alpha = 1$ if the boundary condition $\psi'(E;x) = 1$ is to be satisfied.

Formula (3.2) (with $\alpha = 1$) is, of course, the basic representation of the Gel'fand–Levitan theory.

2. If we consider a simple random walk (with equiprobable ± 1 steps) and denote by $s_0, s_1, \cdots$ the consecutive displacements, we have by definition of the mathematical expectation that

$$E\left\{\exp -\left(\sum_{k=0}^{r} v(s_k)\right); s_0 > 0, s_1 > 0, \ldots, s_{r-1} > 0 \mid s_r = s > 0\right\}$$
$$= \sum_{s_1>0, s_2>0, \ldots, s_{N-1}>0} \exp\left(-\sum_{k=0}^{r} v(s_k)\right) \times P(s_0|s_1)P(s_1|s_2)\cdots P(s_{r-1}|s),$$

where $P(x|y)$ is the transition probability to go from x to y, which in our case is given by the formula

$$P(x|y) = \tfrac{1}{2}\delta(x, y-1) + \tfrac{1}{2}\delta(x, y+1),$$

and δ is the Kronecker symbol.

It thus follows that

$$E\left\{\exp\left(-\sum_{k=0}^{r} v(s_k)\right); s_0 > 0, s_1 > 0, \ldots, s_{r-1} > 0 \mid s_r = s > 0\right\} = e^{-[v(s_0)+v(s)]/2}\, a_{s_0 s}^{(r)}, \quad r \geq 1, \qquad (3.3)$$

where $a_{s_0 s}^{(r)}$ is the (s_0, s) element of A^r, A being the matrix defined by (2.8).

Using the spectral representation, we can rewrite (3.3) in the form

$$E\left\{\exp\left(-\sum_{k=0}^{r} v(s_k)\right); s_0 > 0, s_1 > 0, \ldots, s_{r-1} > 0 | s_r = s > 0\right\} = e^{-[v(s_0)+v(s)]/2} \int \lambda^r \phi(\lambda; s_0)\phi(\lambda; s)\, d\rho(\lambda). \qquad (3.4)$$

Setting $s_0 = s = 1$, we obtain [in view of the normalization $\phi(\lambda; 1) = 1$]

$$\int \lambda^r d\rho(\lambda) = e^{-v(1)} E\left\{\exp\left(-\sum_{k=1}^{r-1} v(s_k)\right); s_1 > 0, \ldots, s_{r-1} > 0 \mid s_r = 1\right\}, \qquad (3.5)$$

which connects the moments of $\rho(\lambda)$ with the "potential" $v(n)$.

3. To illustrate the theory, we shall work out an example which is an analog of an example worked out by Gel'fand and Levitan.

Let

$$d\rho(\lambda) = \alpha d\sigma(\lambda) + \tfrac{1}{2}(1-\alpha)\delta(\lambda - \bar{\lambda})d\lambda + \tfrac{1}{2}(1-\alpha)\delta(\lambda + \lambda)d\lambda, \qquad (3.6)$$

where $0 < \alpha \leq 1$ and $\bar{\lambda} > 1$.

We have

$$q(l,m) = \int \mathring{\phi}(\lambda; l)\mathring{\phi}(\lambda; m)\, d(\rho(\lambda) - \sigma(\lambda)) = -(1-\alpha)\delta_{l,m} + \tfrac{1}{2}(1-\alpha) \times [1 + (-1)^{l+m}]\mathring{\phi}(\bar{\lambda}; l)\mathring{\phi}(\bar{\lambda}; m). \qquad (3.7)$$

Equations (2.26) become

$$0 = \alpha\kappa(n,m) + \tfrac{1}{2}(1-\alpha)[1 + (-1)^n]\mathring{\phi}(\bar{\lambda}; n)\mathring{\phi}(\bar{\lambda}; m) + (1-\alpha)\mathring{\phi}(\bar{\lambda}; m) \sum_{\substack{l \text{ even} \\ 1<l<n-1}} \kappa(n,l)\mathring{\phi}(\lambda; l) \qquad (3.8a)$$

if m is even and

$$0 = \alpha\kappa(n,m) + \tfrac{1}{2}(1-\alpha)[1 - (-1)^n]\mathring{\phi}(\bar{\lambda}; n)\mathring{\phi}(\bar{\lambda}; m) + (1-\alpha)\mathring{\phi}(\lambda; m) \sum_{\substack{l \text{ odd} \\ 1<l<n-1}} \kappa(n,l)\phi(\bar{\lambda}; l) \qquad (3.8b)$$

if m is odd.

It is now quite easy to obtain

$$\kappa(n,m) = -\tfrac{1}{2}[1 + (-1)^n](1-\alpha)\mathring{\phi}(\bar{\lambda}; m)\mathring{\phi}(\bar{\lambda}; n) \times\left[\alpha + (1-\alpha) \sum_{\substack{l<n-1 \\ l \text{ even}}} \mathring{\phi}^2(\bar{\lambda}; l)\right]^{-1} \qquad (3.9a)$$

for m even and

$$\kappa(n,m) = \tfrac{1}{2}[1-(-1)^n](1-\alpha)\mathring{\phi}(\bar\lambda;m)\mathring{\phi}(\bar\lambda;n) \times\Big[\alpha + (1-\alpha)\sum_{\substack{l<n-1\\ l\ \mathrm{odd}}} \mathring{\phi}^2(\bar\lambda;l)\Big]^{-1} \tag{3.9b}$$

for m odd I_n particular, it follows that $\kappa(n,m) = 0$ if n and m are of different parity.

Finally, substituting into (2.27) we get

$$\frac{1}{K^2(n,n)} = \alpha\left\{1 + (1-\alpha)\frac{\mathring{\phi}^2(\bar\lambda;n)}{\alpha + (1-\alpha)\sum_{\substack{m\le n-1\\ m\ \mathrm{even}}}\mathring{\phi}^2(\bar\lambda;m)}\right\} \tag{3.10a}$$

if n is odd.

If n is even and similarly

$$\frac{1}{K^2(n,n)} = \alpha\left\{1 + (1-\alpha)\frac{\mathring{\phi}^2(\bar\lambda;n)}{\alpha + (1-\alpha)\sum_{\substack{m\le n-1\\ m\ \mathrm{odd}}}\mathring{\phi}^2(\bar\lambda;m)}\right\}. \tag{3.10b}$$

It is not difficult to convince oneself that, to pass to the continuous limit, one should put

$$\lambda = 1 + \bar\epsilon\Delta^2, \qquad (\bar\epsilon = -\bar E) \tag{3.11}$$

and

$$\alpha = 1 - c\Delta^3, \qquad c > 0. \tag{3.12}$$

One then obtains by a straightforward calculation that

$$K(x,x) = -c\,\sinh^2 x\sqrt{2\bar\epsilon}\Big/\Big(2\epsilon + c\int_0^x \sinh^2\xi\sqrt{2\bar\epsilon}\,d\xi\Big) \tag{3.13}$$

4. DETERMINATION OF SPECTRAL DENSITIES

To simplify the discussion, we shall assume from now on that

$$v(n) = 0 \quad \text{for } n > n_0, \tag{4.1}$$

so that for sufficiently large n

$$\phi(\lambda;n) = \alpha(\lambda)[\lambda + (\lambda^2-1)^{1/2}]^n + \beta(\lambda)[\lambda\ (\lambda^2-1)^{1/2}]^n. \tag{4.2}$$

For $-1 < \lambda < 1$, we can set

$$\lambda = \cos\theta$$

and rewrite (4.2) in the form

$$\phi(\theta;n) = A(\theta)e^{in\theta} + B(\theta)e^{-in\theta}. \tag{4.3}$$

From the normalization condition

$$\int \phi^2(\lambda;n)\,d\rho(\lambda) = 1,$$

it follows that

$$\int_1^\infty \phi^2(\lambda;n)\,d\rho(\lambda) \le 1,$$

and dividing by λ^{2n} and letting $n\to\infty$, one obtains

$$\int_1^\infty \alpha^2(\lambda)\,d\rho(\lambda) = 0,$$

so that $\alpha(\lambda) = 0$ at every point of increase of ρ for $\lambda > 1$. Similarly, $\beta(\lambda) = 0$ at every point of increase of $\rho(\lambda)$ for $\lambda < -1$.

In other words, if $\lambda > 1$ ($\lambda < -1$) is a point in the spectrum, then $\alpha(\lambda) = 0$ [$\beta(\lambda) = 0$].

All this is merely to confirm that eigenfunctions must be bounded.

The question whether there are bound states can be approached as follows.

For $\lambda > 1$ the only candidates for bound states are, for sufficiently large n, of the form

$$\phi(\lambda;n) = \beta(\lambda)[\lambda - (\lambda^2-1)^{1/2}]^n,$$

and since ϕ and ψ are identical for large n {they differ only by a factor $\exp[v(n)/2]$, and hence not at all when $v(n) = 0$}, we also have (for sufficiently large n)

$$\psi(\lambda;n) = \beta(\lambda)[\lambda - (\lambda^2-1)^{1/2}]^n.$$

If we now use repeatedly the recursion

$$\psi(\lambda;n-1) = -\psi(\lambda;n+1) + 2\lambda e^{v(n)}\psi(\lambda;n), \tag{4.4}$$

we ultimately arrive at the formula

$$\psi(\lambda;0) = \beta(\lambda)P(\lambda - (\lambda^2-1)^{1/2}), \tag{4.5}$$

where $P(z)$ is a polynomial [of degree $2n_0$ if $v(n_0) \ne 0$]. In deriving (4.5), repeated use is made of the identity

$$2\lambda = \lambda - (\lambda^2-1)^{1/2} + [\lambda - (\lambda^2-1)^{1/2}]^{-1}.$$

Similarly, for $\lambda < -1$ we have

$$\psi(\lambda;0) = \alpha(\lambda)P(\lambda - (\lambda^2-1)^{1/2}), \tag{4.6}$$

where P is the same polynomial as in (4.5) and where in deriving (4.6) we use repeatedly the identity

$$2\lambda = \lambda + (\lambda^2-1)^{1/2} + [\lambda + (\lambda^2-1)^{1/2}]^{-1}.$$

It is now apparent that to each root of $P(z)$ which lies inside the unit circle there corresponds a bound state, and vice versa. These roots (if any) are real, and since $P(z)$ can be seen to be of the form $Q(z^2)$,[5] they come in positive–negative pairs.

In the Appendix, we also prove that the real roots are all simple.

Let us assume now that $-1 \le \lambda \le 1$, and set

$$\lambda = \cos\theta.$$

Let us also define $\psi_+(\theta;n)$ and $\psi_-(\theta;n)$ as the solutions of the recursion

$$\tfrac12\psi(\lambda;n-1) + \tfrac12\psi(\lambda;n+1) = \lambda e^{v(n)}\psi(\lambda;n), \tag{4.7}$$

which for sufficiently large n are given by the equations

$$\psi_\pm(\theta;n) = e^{\pm in\theta}. \tag{4.8}$$

It is clear from the definition of the polynomial $P(z)$ that we have

$$\psi_\pm(\theta;0) = P(e^{\pm i\theta}). \tag{4.9}$$

Consider now

$$\psi(\theta;n) = e^{-v(n)/2}\phi(\theta;n), \tag{4.10}$$

which is the solution of (4.7) satisfying the boundary conditions

$$\psi(\theta;0) = 0, \qquad \psi(\theta;1) = e^{-v(1)/2} \tag{4.11}$$

[the second boundary condition is merely a consequence of the boundary condition $\phi(\lambda;1)=1$].

Since every solution of a second-order recursion is a linear combination of any two independent solutions, we have

$$\psi(\theta;n)=A(\theta)\psi_+(\theta;n)+B(\theta)\psi_-(\theta;n), \tag{4.12}$$

and by (4.11) and (4.9) we conclude that

$$0=A(\theta)P(e^{i\theta})+B(\theta)P(e^{-i\theta}). \tag{4.13}$$

Now, if $\psi_1(\lambda;n)$ and $\psi_2(\lambda;n)$ are two solutions of (4.7), i.e., if

$$\tfrac{1}{2}\psi_1(\lambda;n-1)+\tfrac{1}{2}\psi_1(\lambda;n+1)=\lambda e^{v(n)}\psi_1(\lambda;n),$$
$$\tfrac{1}{2}\psi_2(\lambda;n-1)+\tfrac{1}{2}\psi_2(\lambda;n+1)=\lambda e^{v(n)}\psi_2(\lambda;n),$$

then, multiplying the first equation by $\psi_2(\lambda;n)$, the second by $\psi_1(\lambda;n)$, and subtracting, we obtain that for all[6] n

$$\psi_1(\lambda;n-1)\psi_2(\lambda;n)-\psi_2(\lambda;n-1)\psi_1(\lambda;n)$$
$$=\psi_1(\lambda;n)\psi_2(\lambda;n+1)-\psi_2(\lambda;n)\psi_1(\lambda;n+1),$$

or, equivalently,

$$\psi_1(\lambda;0)\psi_2(\lambda;1)-\psi_2(\lambda;0)\psi_1(\lambda;1)$$
$$=\psi_1(\lambda;n)\psi_2(\lambda;n+1)-\psi_2(\lambda;n)\psi_1(\lambda;n+1). \tag{4.14}$$

Setting $\psi_1=\psi_+,\psi_2=\psi_-$ and choosing n large enough for the validity of (4.8), we obtain [using also (4.9)]

$$\psi_-(\theta;0)\psi_+(\theta;1)-\psi_+(\theta;0)\psi_-(\theta;1)=2i\sin\theta.$$

From (4.12) and (4.11) we have

$$e^{-v(1)/2}=A(\theta)\psi_+(\theta;1)+B(\theta)\psi_-(\theta;1), \tag{4.15}$$

which, combined with (4.13) rewritten in the form

$$0=A(\theta)\psi_+(\theta;0)+B(\theta)\psi_-(\theta;0)$$

and with (4.15), yields

$$A(\theta)=e^{-v(1)/2}[\psi_-(\theta;0)/2i\sin\theta] \tag{4.16}$$

and

$$B(\theta)=e^{-v(1)/2}[\psi_+(\theta;0)/2i\sin\theta]. \tag{4.17}$$

Finally,

$$A(\theta)B(\theta)=e^{-v(1)}[\psi_-(\theta;0)\psi_+(\theta,0)/4\sin^2\theta], \tag{4.18}$$

or, equivalently,

$$A(\theta)B(\theta)=e^{-v(1)}[P(e^{-i\theta})P(e^{i\theta})/4\sin^2\theta]. \tag{4.19}$$

There remains now to connect the spectral density with $A(\theta)B(\theta)=A(\theta)A^*(\theta)=|A(\theta)|^2$.

This is done most quickly by using Eq. (3.4) and setting $s_0=s$. Summing over s_0 from 1 to N and dividing by N, we get

$$\frac{1}{N}\sum_{s_0=1}^{N}E\left\{\exp\left(-\sum_{1}^{r}v(s_k)\right);s_0>0,\dots,s_{r-1}>0\,|\,s_r=s_0\right\}$$
$$=\int\lambda^r\frac{1}{N}\sum_{s_0=1}^{N}e^{-v(s_0)}\phi^2(\lambda;s_0)d\rho(\lambda). \tag{4.20}$$

If we let $N\to\infty$, then

$$\lim_{N\to\infty}\frac{1}{N}\sum_{s_0=1}^{N}e^{-v(s_0)}\phi^2(\lambda;s_0)=0$$

for every bound state, while

$$\lim_{N\to\infty}\frac{1}{N}\sum_{s_0=1}^{N}\exp(-v(s_0))\phi^2(\lambda;s_0)=2|A(\theta)|^2$$
$$=2|A(\cos^{-1}\lambda)|^2$$

for all scattering states. If we now look at the left-hand side of (4.20), we note that for $s_0>n_0+r$ the random walk cannot reach the part of the s-axis where $v(s)\neq 0$, and therefore the limit as $N\to\infty$ is the same as if v were identically zero. In other words,

$$\lim_{N\to\infty}\frac{1}{N}\sum_{s_0=1}^{N}E\left\{\exp\left(-\sum_{1}^{r}v(s_k)\right);s_0>0,\dots,s_{r-1}>0\,|\,s_r=s_0\right\}$$
$$=\int\lambda^r\lim_{N\to\infty}\frac{1}{N}\sum_{s_0=1}^{N}\phi^2(\lambda;s_0)d\sigma(\lambda)$$
$$=\frac{1}{\pi}\int_{-1}^{1}\lambda^r\frac{d\lambda}{(1-\lambda^2)^{1/2}}.$$

Combining all these considerations, we obtain that for all integers r

$$2\int_{-1}^{1}\lambda^r|A(\cos^{-1}\lambda)|^2d\rho(\lambda)=\frac{1}{\pi}\int_{-1}^{1}\lambda^r\frac{d\lambda}{(1-\lambda^2)^{1/2}}, \tag{4.21}$$

and we have

$$d\rho(\lambda)=\frac{1}{2\pi}\frac{d\lambda}{|A(\cos^{-1}\lambda)|^2(1-\lambda^2)^{1/2}}. \tag{4.22}$$

Thus, $|A(\theta)|^2$ determines $\rho(\lambda)$ for $-1\le\lambda\le 1$, and hence the potential (or rather) $[v(n)+v(n+1)]/2$.

However, it is clear that $|A(\theta)|^2$ cannot be prescribed arbitrarily.

By (4.19),

$$|A(\theta)|^2=e^{-v(1)}P(e^{-i\theta})P(e^{i\theta})/4\sin^2\theta, \tag{4.23}$$

and $P(z)$ must be a polynomial of degree $2n_0$ and of the form $Q(z^2)$.

5. DETERMINATION OF $|A(\theta)|^2$ FROM THE PHASE SHIFTS

If we write

$$P(e^{i\theta})=|P(e^{i\theta})|e^{-i\delta(\theta)}, \tag{5.1}$$

then

$$P(e^{-i\theta})=|P(e^{-i\theta})|e^{-i\delta(-\theta)}.$$

Since $P(e^{i\theta})$ and $P(e^{-i\theta})$ are complex conjugates, it follows that

$$\delta(-\theta)=-\delta(\theta). \tag{5.2}$$

For large n, we know that

$$\phi(\theta;n)\sim\sin[n\theta+\delta(\theta)]. \tag{5.3}$$

Given $\delta(\theta)$ for $0\le\theta\le\pi$, we ask what can be said about $\rho(\lambda)$. It will be seen that δ determines the *number* of bound states. If in addition one is given the position of the bound states, then $|A(\theta)|^2$ is determined, and hence the continuous part of the spectral function [see (4.22)].

One then still needs the normalizing constants to know the spectral function completely and hence to determine the potential.

Let Δ_c denote the change in going around the unit circle. Since $P(z)$ is analytic for $|z| < 1$, we see that

$$\Delta_c \arg(1/P(z)) = -2\pi N, \tag{5.4}$$

where N is the number of zeros of P within the unit circle (and hence the number of bound states).[7]

Consider first the case of no bound states. Then $P(z)$ has the following properties:

(a) $P(z)$ is analytic and nonzero in $|z| < 1$.

(b) $P(0) = \exp\left(\sum_1^{n_0} v(k)\right)$. (5.5)

(c) On $|z| = 1$,

$$S \equiv e^{2i\delta} = \frac{P^*(z)}{P(z)} = \frac{P(1/z)}{P(z)}. \tag{5.6}$$

We note that the decomposition of S such that P has properties (a), (b), and (c) is unique. Indeed, suppose there were two such P's, which we denote by P_1 and P_2. Let

$$q(z) = P_1(z)/P_2(z), \quad |z| < 1,$$
and
$$q(z) = P_1(1/z)/P_2(1/z), \quad |z| > 1. \tag{5.7}$$

Since P_1, P_2 are analytic and nonzero for $|z| < 1$, we see that $q(z)$ is analytic in the whole plane cut by the unit circle. However, on the unit circle

$$P_1(1/z)/P_1(z) = P_2(1/z)/P_2(z),$$
or
$$P_1(z)/P_2(z) = P_1(1/z)/P_2(1/z). \tag{5.8}$$

Therefore, q is continuous across the cut. Thus, q is analytic everywhere. It approaches 1 as $z \to 0$, since $P_1(0) = P_2(0)$. By Liouville's theorem

$$q \equiv 1$$
and
$$P_1 = P_2 \tag{5.9}$$

Consider now the function $e^{\Gamma_0(z)}$, where

$$\Gamma_0(z) = -\frac{1}{2\pi i} \oint \frac{\ln S(z')dz'}{z'-z} = -\frac{1}{\pi} \oint \frac{\delta(z')dz'}{z'-z}. \tag{5.10}$$

In virtue of the absence of bound states [Eq. (5.4) with $N = 0$], $\exp(\Gamma_0(z))$ is analytic and nonzero within c. As $z \to 0$, we have

$$\Gamma_0(z) = -\frac{\mathcal{P}}{\pi} \oint \frac{\delta(z')dz'}{z'-z} - i\delta(z). \tag{5.11}$$

To see reality properties, let us change to the variable θ. Using the antisymmetry of δ, this becomes

$$\Gamma_0(\theta) = \frac{\mathcal{P}}{\pi} \int_0^\pi \frac{\sin\theta'\delta(\theta')d\theta'}{\cos\theta - \cos\theta'} - i\delta(\theta). \tag{5.12}$$

Therefore,

$$\Gamma_0^*(z) = \Gamma_0(1/z) = \frac{\mathcal{P}}{\pi} \int_0^\pi \frac{\sin\theta'\delta(\theta')d\theta'}{\cos\theta - \cos\theta'} + i\delta(\theta). \tag{5.13}$$

We also note that

$$\Gamma_0(z)|_{z=0} = -\frac{1}{\pi} \oint \frac{\delta(z')dz'}{z'} = -\frac{i}{\pi} \int_{-\pi}^{\pi} \delta(\theta')d\theta' = 0. \tag{5.14}$$

Hence, setting

$$P(z) = Ae^{\Gamma_0(z)}, \tag{5.15}$$

with A chosen so as to satisfy the normalization

$$\int d\rho(\lambda) = 1$$

[with $\rho(\lambda)$ defined by (4.22) and (4.23)], we see that P is determined uniquely and

$$A = \exp\left(\sum_1^{n_0} v_k\right).$$

Hence,

$$|A(\theta)|^2 = A^2 \exp\left(\frac{2}{\pi} \mathcal{P} \int_0^\pi \frac{\sin\theta'\delta(\theta')d\theta'}{\cos\theta - \cos\theta'}\right) \Big/ 4\sin^2\theta, \tag{5.16}$$

and

$$\rho(\lambda) = \begin{cases} 0, & \lambda < -1, \\ A^2 \dfrac{2}{\pi} \displaystyle\int_{-1}^{\lambda} (1-\mu^2)^{1/2} \exp\left(\frac{2}{\pi} \mathcal{P} \int_{-1}^{1} \frac{\delta(\mu')d\mu'}{\mu'-\mu}\right) d\mu, \\ 1, & \lambda > 1. \end{cases}$$
$$-1 < \lambda < 1, \tag{5.17}$$

When bound states are present at z_i $(i = 1, 2, \ldots, N)$, the following modifications are made. Now by the principle of the argument,

$$\Delta_c \arg S = 2(-2\pi)N. \tag{5.18}$$

Consider then

$$S' = S \prod_{i=1}^{N} \frac{(z - z_i)}{[(1/z) - z_i]}.$$

Here $\Delta_c S' = 0$ and S' has all the properties S had with no bound states. Hence it has the decomposition

$$S' = e^{\Gamma^*(z)}/e^{\Gamma(z)}$$

with

$$\Gamma(z) = -\frac{1}{\pi} \oint_c \frac{\delta'(z')dz'}{z'-z}, \tag{5.19}$$

where

$$\delta' = \delta + \tfrac{1}{2} \arg \prod_{i=1}^{N} \frac{(z - z_i)}{[(1/z) - z_i]}.$$

Then,

$$S = \frac{\Gamma^*(z)}{e^{\Gamma(z)}} \prod_{i=1}^{N} \frac{[(1/z) - z_i]}{(z - z_i)}, \quad z \in c. \tag{5.20}$$

A decomposition of S into a ratio $P(1/z)/P(z)$ with properties (a)–(c) (except that now P has zeros at and only at z_i in the unit circle) is then obtained by inspection. Namely,

$$P(z) = Ae^{\Gamma(z)} \prod_{i=1}^{N} [1 - (z/z_i)], \tag{5.21}$$

where A is again chosen so as to satisfy a normalization condition. (The uniqueness argument proceeds as before.)

Since we have seen that the discrete eigenvalues occur in equal and opposite pairs, we can express everything in terms of those eigenvalues (z_i or λ_i) which are positive. For the spectral function we then find

$$d\rho(\lambda)=\begin{cases}\sum_{i=1}^{N/2}\frac{1}{C_i}\,\delta(\lambda+\lambda_i)d\lambda, & \lambda<-1,\\ \frac{2}{\pi}(1-\lambda^2)^{1/2}A^2\exp\left(\frac{2}{\pi}\,\wp\int_{-1}^{1}\frac{\delta(\lambda')d\lambda'}{\lambda'-\lambda}\right) & \\ \quad\times\prod_{i=1}^{N/2}\left[1-\left(\frac{\lambda+i(1-\lambda^2)^{1/2}}{\lambda_i-(\lambda_i^2-1)^{1/2}}\right)^2\right]d\lambda, & -1<\lambda<1,\\ \sum_{i=1}^{N/2}\frac{1}{C_i}\,\delta(\lambda-\lambda_i)d\lambda, & \lambda>1,\end{cases}\tag{5.22}$$

and A is such that

$$\int d\rho(\lambda)=1.$$

6. SUMMARY

Let us now put together the pieces of our solution. We are given the discrete eigenvalues λ_i ($|\lambda_i|>1$), the normalization constants C_i such that $C_i=\sum_n\phi^2(\lambda_i,n)$, and $\delta(\lambda)$ for $-1\le\lambda\le1$. From the phase shift and the λ_i, we calculate $|A(\theta)|^2$ for $-1\le\lambda\le1$ as in Sec. 5. From this we obtain $d\rho(\lambda)$ [Eq. (3.17) or (5.22)]. We then take the comparison function $\mathring{\phi}(\lambda,n)=(\sin n\theta)/(\sin\theta)$ with spectral function

$$d\sigma(\lambda)=(2/\pi)(1-\lambda^2)^{1/2}d\lambda,\qquad -1\le\lambda\le1.\tag{6.1}$$

Using these, we construct $g(n,m)$ with Eq. (2.20). The generalized Gel'fand–Levitan equation [Eq. (2.26)] is then solved for $K(n,m)$. Equation (2.27) gives $K(n,n)$. The average of two successive values of the potential then follows from Eq. (2.29). Requiring that the $\lim_{n\to\infty}v(n)=0$ then yields all $v(n)$ uniquely.

It is instructive to see the limiting form of our equations as $\Delta\to0$. For this it is convenient to change normalization. Let us replace $\phi,\mathring{\phi}$ by ϕ',ϕ_0', where

$$\begin{aligned}\phi'(\lambda,n)&=\Delta\phi(\lambda,n),\\ \phi_0'(\lambda,n)&=\Delta\phi_0(\lambda,n),\end{aligned}\tag{6.2}$$

and require that

$$\int_{-\infty}^{\infty}\phi'(\lambda,n)\phi'(\lambda,m)d\rho'(\lambda)=\int_{-\infty}^{\infty}\phi_0'(\lambda,n)\phi_0'(\lambda,m)d\sigma'=\frac{\delta(n,m)}{\Delta}.\tag{6.3}$$

(Thus $\rho'=\rho/\Delta^3$, $\sigma'=\sigma/\Delta^3$) Then in the limit $\Delta\to0$, $n\Delta=x$ finite, we obtain

$$\mathring{\phi}(\lambda,n)\to\sin\sqrt{2E}x/\sqrt{2E}\tag{6.4}$$

$$\begin{aligned}d\sigma'&\to0,\qquad E<0,\\ &\to(2/\pi)\sqrt{2E}dE,\qquad 0<E<\infty.\end{aligned}\tag{6.5}$$

Omitting bound states for simplicity, we similarly obtain

$$\begin{aligned}d\rho'&\to0,\qquad E<0,\\ &\to(2/\pi)\sqrt{2E}\exp\left(-\frac{2}{\pi}\,\wp\int_0^\infty\frac{\delta(E')dE'}{E'-E}\right)dE.\end{aligned}\tag{6.6}$$

The Gel'fand–Levitan equation [Eq. (2.26)] becomes

$$0=q'(x,y)+\kappa'(x,y)+\int_0^x\kappa'(x,t)q'(t,y)dt,\qquad x>y,\tag{6.7}$$

with

$$q'(x,y)=\int_{-\infty}^{\infty}\phi_0'(E,x)\phi_0'(E,y)d[\rho'-\sigma'].\tag{6.8}$$

The equation for the coefficient of $\phi_0'(E,n)$ in the expansion of $\phi(E,n)$ [Eq. (2.27)] becomes for small Δ

$$\frac{1}{K'^2(n,n)}\cong1-\Delta\kappa'(x,x).\tag{6.9}$$

Then

$$\begin{aligned}q(x)&=\lim_{\Delta\to0}\frac{1}{\Delta^2}[\ln K(n+1,n+1)-K(n,n)]\\ &=\frac{1}{2}\frac{d}{dx}\kappa'(x,x)\end{aligned}\tag{6.10}$$

In terms of the solution $\kappa'(x,y)$ of Eq. (6.7), the expression for $\phi(E,x)$ is

$$\phi(E,x)=\frac{\sin\sqrt{2E}x}{\sqrt{2E}}+\int_0^x\kappa'(x,y)\frac{\sin\sqrt{2E}y}{\sqrt{2E}}dy.\tag{6.11}$$

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APPENDIX: SOME PROPERTIES OF SYMMETRICAL THREE-TERM RECURSION RELATIONS

Consider the three-term recursion relation

$$a(n+1)\psi(\lambda,n+1)+b(n)\psi(\lambda,n)+a(n-1)\psi(\lambda,n-1)=\lambda g(n)\psi(\lambda,n),\qquad 1\le n,\tag{A1}$$

where

(i) The $a(n),b(n),g(n)$ are real.

(ii) The limits of these as $n\to\infty$ exist and are approached sufficiently rapidly. (A sufficient but certainly not necessary condition is that they are all constant after some N.)

(iii) $g(n)>0$.

We obtain an eigenvalue problem when we ask for those λ for which a "regular" solution exists in the sense that

$$\psi(\lambda,0)=0,\qquad\psi(\lambda,1)=A\ne0,\tag{A2}$$

and $\psi(\lambda;n)$ is bounded. The results are very similar to those for second-order self-adjoint differential operators; namely:

(1) There is a continuous spectrum for

$$\beta<-2\alpha<\lambda<\beta+2\alpha,\tag{A3}$$

where

$$\beta=b(\infty)/g(\infty),\qquad\alpha=a(\infty)/g(\infty).\tag{A4}$$

If we write $\lambda=2\alpha\cos\theta+\beta$, then in $z=e^{i\theta}$ the continuous eigenvalues lie on the upper half of the unit circle.

(2) There are at most a finite number of real, simple, discrete eigenvalues λ_i which lie outside of or at an edge of the continuum. (In z these are real and on or within the unit circle.)

(3) If $b(n)\equiv0$, the discrete eigenvalues occur in pairs $\pm\lambda_i$. (This is also true in z.)

(4) The eigenfunctions form a complete orthogonal set in that

$$\sum_{n=1}^{\infty} \psi(\lambda,n)g(n)\psi(\lambda',n)$$
$$= \delta(\lambda-\lambda') \frac{[Aa(1)]^2}{a(\infty)\sin\theta} |\psi_+(\lambda,0)|^2, \quad \lambda,\lambda' \in \text{continuous spectrum},$$
$$= 0, \quad \lambda=\lambda_i, \lambda' \in \text{continuous spectrum},$$
$$= \delta_{ij} \frac{[a(1)A]^2}{a(\infty)} \frac{\psi_+(\lambda_i,0)\psi_-(\lambda_i,0)}{2i\sin\theta_i}, \quad \lambda_i,\lambda_j \text{ discrete} \tag{A5}$$

Here $\psi_\pm(\lambda,n)$ are solutions of Eq. (A1) subject to the condition

$$\lim_{n\to\infty} |\psi_\pm(\lambda,n) - e^{\pm in\theta}| = 0, \tag{A6}$$

$$\delta(n,m) = \frac{a(\infty)}{[a(1)A]^2}\left(\sum_i \frac{2i\sin\theta_i\psi(\lambda_i,n)\sqrt{g(n)}\psi(\lambda_i,m)\sqrt{g(m)}}{\psi_+(\lambda_i,0)\psi_-(\lambda_i,0)} + \frac{1}{\pi}\int_{\lambda\min}^{\lambda\max} d\lambda\, \frac{\sin\theta\psi(\lambda,n)\sqrt{g(n)}\,\psi(\lambda,m)\sqrt{g(m)}}{|\psi_+(\lambda,0)|^2}\right). \tag{A7}$$

Many of these results follow from the following identity. Let $\psi_1(\lambda,n), \psi_2(\lambda',n)$ be two solutions of Eq. (A1). Then by standard manipulations, we obtain

$$a(n+1)[\psi_2(\lambda',n)\psi_1(\lambda,n+1) - \psi_1(\lambda,n)\psi_2(\lambda',n+1)] + a(n)[\psi_2(\lambda',n)\psi_1(\lambda,n+1) - \psi_1(\lambda,n)\psi_2(\lambda',n-1)] = (\lambda-\lambda')\psi_2(\lambda',n)g(n)\psi_1(\lambda,n). \tag{A8}$$

Putting $\lambda=\lambda'$, we obtain the result that

$$W[\psi_1,\psi_2] = a(n+1)[\psi_1(\lambda,n+1)\psi_2(\lambda,n) - \psi_1(\lambda,n)\psi_2(\lambda,n+1)] \tag{A9}$$

is independent of n.

There are two immediate applications.

(1) Since $\psi_\pm(\lambda,n)$ are two linearly independent solutions, we can express ψ satisfying the conditions of Eq. (A2) as a linear combination of these. Thus

$$\psi(\lambda,n) = \frac{W[\psi,\psi_-]}{W[\psi_+,\psi_-]}\psi_+(\lambda,n) - \frac{W[\psi,\psi_+]}{W[\psi_+,\psi_-]}\psi_-(\lambda,n). \tag{A10}$$

Evaluating the Wronskians at $n=1$ and in the limit $n\to\infty$ yields

$$\psi(\lambda,n) = \frac{a(1)A}{a(\infty)2i\sin\theta}[\psi_-(\lambda,0)\psi_+(\lambda,n) - \psi_+(\lambda,0)\psi_-(\lambda,n)]. \tag{A11}$$

Similarly, given any two linearly independent solutions (ψ_1,ψ_2) of Eq. (A1), we can express the Green's function, i.e., the solution of

$$a(n+1)G(\lambda,n+1;m) + b(n)G(\lambda,n;m) + a(n)G(\lambda,n;m) + a(n)G(\lambda,n-1;m) - \lambda g(n)G(\lambda,n;m) = \delta(m,m), \tag{A12}$$

in the form

$$G(\lambda,n;m) = \frac{-\psi_1(\lambda,n)\psi_2(\lambda,m)}{W[\psi_1,\psi_2]}, \quad n<m;$$
$$= \frac{-\psi_1(\lambda,m)\psi_2(\lambda,n)}{W[\psi_1,\psi_2]}, \quad n\ge m. \tag{A13}$$

In the special case of translational invariance—when the coefficients are independent of n—we have an even simpler result. Thus, let $\phi^0(\lambda,n)$ be the solution of

$$a_0\phi^0(\lambda,n+1) + b_0\phi^0(\lambda,n) + a_0\phi^0(\lambda,n-1) = \lambda g_0\phi^0(\lambda,n),$$

with

$$\phi^0(\lambda,0)=0, \quad \phi^0(\lambda,1) = 1/a_0,$$

i.e.,

$$\phi^0(\lambda,n) = (\sin n\theta)/(a_0\sin\theta), \tag{A14}$$

where $2a_0\cos\theta + b^0 = \lambda g_0$. Then two Green's functions are

$$G^{(1)}(\lambda,n;m) = \begin{cases}\phi^0(\lambda,n-m), & m<n,\\ 0, & m\ge n,\end{cases} \tag{A15}$$

and

$$G^{(2)}(\lambda,n;m) = \begin{cases}0, & m\le n,\\ \phi^0(\lambda,m-n), & m>n.\end{cases} \tag{A16}$$

With these we can write integral equations for solutions of

$$a_0\psi(\lambda,n+1) + b(n)\psi(\lambda,n) + a_0\psi(\lambda,n-1) = g(n)\lambda\psi(\lambda,n). \tag{A17}$$

So if ψ is to satisfy Eqs. (A2),

$$\psi(\lambda,n) = a_0A\phi^0(\lambda,n) + \sum_{m=0}^{n-1}\phi^0(\lambda,n-m) \times\{\lambda[g(m)-g_0] + [b_0 - b(m)]\}\psi(\lambda,m) \tag{A18}$$

and

$$\psi_\pm(\lambda,n) = e^{\pm in\theta} + \sum_{m=n+1}^{\infty}\phi^0(\lambda,m-n) \times\{\lambda[g(m)-g_0] + [b_0-b(m)]\}\psi_\pm(\lambda,m). \tag{A19}$$

From Eq. (A11) it follows that if $0\le\theta\le\pi$ (λ in the continuum), there are solutions satisfying the equation plus initial conditions which are bounded at infinity. "Bound states"–i.e., summable solutions–occur when there is a z_i, $|z_i|\le 1$, such that $\psi_+(\lambda_i,0)=0$.

Choosing $g_0 = g(\infty)$, $b_0 = b(\infty)$ in Eqs. (A18), (A19), we readily see a number of properties which are actually more generally true. Thus for real θ, replacing by $-\theta$ leaves ψ unchanged, while ψ_+ and ψ_- are interchanged. Also, $\psi_+ = \psi_-^*$. With some modest convergence requirements, we also see that ψ_+ is analytic for $|z|<1$, while ψ is analytic except for a pole at $z=0$.

The analyticity of ψ_+ for $|z|<1$ then implies that there are only a finite number of zeros of $\psi_+(\lambda,0)$ and hence a finite number of bound states. Bound states in the continuum are forbidden since $\psi_+=0$ implies $\psi_- = \psi_+^* = 0$, and then we see from Eq. (A11) that ψ vanishes identically. There can be exceptions. Since $\sin\theta$ vanishes at the edge of the continuum, there can be bound states there.

Further properties result when we sum Eq. (A8) from $n=1$ to $n=N$. The identity now becomes

$$a(N+1)[\psi_2(\lambda',N)\psi_1(\lambda,N+1) - \psi_1(\lambda,N)\psi_2(\lambda',N+1)] + a(1)[\psi_2(\lambda',1)\psi_1(\lambda,0) - \psi_1(\lambda,1)\psi_2(\lambda',0)] = (\lambda-\lambda')\sum_1^N \psi_2(\lambda',n)g(n)\psi_1(\lambda,n). \tag{A20}$$

If we choose ψ_1 to be a bound state $[\psi(\lambda_i,n)]$ and ψ_2 as its complex conjugate, we have $\lambda' = \lambda_i^*$. In Eq. (A20) the terms proportional to $a(1)$ are identically zero while those proportional to $a(N+1)$ vanish as $N \to \infty$. Hence we have

$$2i\,\mathrm{Im}\lambda_i \sum_{n=1}^{\infty} |(\psi_i,n)|^2 g(n) = 0. \tag{A21}$$

Thus the eigenvalues are real.

Similarly, if in Eq. (A20) we put $\psi_1 = \psi(\lambda_i,n)$ and $\psi_2 = \psi_+(\lambda',n)$ (with λ' near λ_i), we can again pass to the limit $N \to \infty$ with the result

$$\sum_{n=1}^{\infty} \psi_+(\lambda_i,n)g(n)\psi_+(\lambda',n) = \frac{a(1)\psi_+(\lambda',0)\psi_+(\lambda_i,1)}{\lambda'-\lambda_i}, \tag{A22}$$

since $\psi_+(\lambda_i,0)=0$. Passing to the limit $\lambda' \to \lambda_i$, we find

$$\sum_{n=1}^{\infty} \psi_+^2(\lambda_i,n)g(n) = a(1)\psi_+(\lambda_i,1)\dot{\psi}_+(\lambda_i,0), \tag{A23}$$

where $\dot{\psi}_+(\lambda_i,0) = (d/d\lambda)\psi_+(\lambda,0)|_{\lambda=\lambda_i}$. Thus $\dot{\psi}_+(\lambda_i,0) \neq 0$, and therefore the eigenvalues are simple. Further, since for bound states $\psi_+ \sim \psi$, we have the normalization

$$\sum_{n=1}^{\infty} |\psi(\lambda_i,n)|^2 g(n) = \frac{[a(1)A]^2}{a(\infty)}\,\frac{\mathring{\psi}_+(\lambda_i,0)\psi_-(\lambda_i,0)}{2i\sin\theta_i}. \tag{A24}$$

Finally, choosing $\psi_1 = \psi(\lambda_i,n)$ and ψ_2 either a $\psi(\lambda_i,n)$ $(i \neq j)$ or a continuum function, we obtain

$$\sum_{n=1}^{\infty} \psi(\lambda_i,n)g(n)\psi(\lambda,n) = 0, \quad \lambda \neq \lambda_i. \tag{A25}$$

If in Eq. (A20) we use two continuum wavefunctions, then the terms in $a(1)$ are zero and for large N we can replace the ψ's by their asymptotic forms. We obtain

$$(\lambda-\lambda')\sum_{n=1}^{\infty}\psi(\lambda',n)g(n)\psi(\lambda,n) = \frac{[a(1)A]^2|\psi_+(\lambda,0)|\,|\psi_+(\lambda',0)|\{\,\}}{2a(\infty)\sin\theta\,\sin\theta'}, \tag{A26}$$

where

$$\begin{aligned}\{\,\} = {} & (\cos\theta-\cos\theta')\cos(N\theta'+\delta'-N\theta-\delta)\\ & -(\cos\theta-\cos\theta')\cos(n\theta'+\delta'+N\theta+\delta)\\ & +(\sin\theta-\sin\theta')\sin(N\theta'+\delta'+N\theta+\delta)\\ & +(\sin\theta+\sin\theta')\sin(N\theta+\delta-N\theta'-\delta').\end{aligned} \tag{A27}$$

[Here $-\delta = \arg\psi_+(\lambda,0)$.] If we now divide Eq. (A26) by $(\lambda-\lambda')$ and integrate over a small region $\Delta\lambda'$, we find in the limit $N \to \infty$ that we get zero unless the region includes λ. If it does, the result is independent of the size of $\Delta\lambda'$. Thus the sum is proportional to $\delta(\lambda-\lambda')$. Evaluating the integral then gives

$$\sum_{n=1}^{\infty}\psi(\lambda,n)g(n)\psi(\lambda',n) = \frac{(\lambda-\lambda')[a(1)A]^2|\psi_+(\lambda,0)|^2\delta(\lambda-\lambda')}{a(\infty)\sin\theta}. \tag{A28}$$

We merely sketch the proof of the completeness relation [Eq. (A7)]. Let $h(m)$ be an arbitrary square summable function. Form

$$I(n) = \frac{1}{2\pi i}\int_c d\lambda \sum_{m=1}^{\infty} G(\lambda,n;m)h(m), \tag{A29}$$

where c is the unit circle in the z plane and the Green's function in accord with Eq. (A13) is taken to be

$$G(\lambda,n;m) = \begin{cases} \dfrac{-\psi(\lambda,n)\psi_+(\lambda,m)}{a(1)A\psi_+(\lambda,0)}, & n<m,\\[2ex] \dfrac{-\psi_+(\lambda,n)\psi(\lambda,m)}{a(1)A\psi_+(\lambda,0)}, & n \geq m. \end{cases} \tag{A30}$$

$I(n)$ is then evaluated in two ways. First, using the known properties under the reflection $\theta \leftrightarrow -\theta$ it can be written as an integral over the continuous spectrum of a product of the continuum eigenfunctions. Second, introducing the variable z we can evaluate the integral by residues. The singularities of the integrand within the unit circle lie at the zeros of $\psi_+(\lambda,0)$ and a pole at $z=0$. The first kind of singularities give contributions proportional to the bound state wave functions. (The reason for the appearance of $\psi_+'(\lambda_i,0)$ becomes clear here.) There is a simple pole at $z=0$ which appears only in the term where $n=m$. To evaluate the residue, we need the behavior of ψ and ψ_+ for $z \sim 0$. For simplicity, let us consider the case where all coefficients reach their asymptotic values at some $n=N$. Then directly from the recursion relation we find that for sufficiently small $|z|$ we have

$$\psi(\lambda,n) \approx \frac{\alpha}{z}^{n-1}\frac{g(n-1)\cdots g(1)}{a(n)\cdots a(z)} \tag{A31a}$$

and

$$\psi_+(\lambda,n) \approx \alpha^{N-n}z^n\frac{g(n+1)\cdots g(N)}{a(n+1)\cdots a(N)}. \tag{A31b}$$

For the crucial quantity determining the residue at $z=0$, we have

$$\left.\frac{-\psi(\lambda,n)\psi_+(\lambda,n)}{\psi_+(\lambda,0)2iz}\right|_{z=0} = \frac{-a(1)A}{2i\alpha g(n)}. \tag{A32}$$

This residue is proportional to $h(n)$. Then, equating the formulas for $I(n)$, we have an expression for $h(n)$ in terms of sums and integrals over the eigenfunctions. Inserting $h(n) = \delta(n,m)$ then yields Eq. (A7).[8]

Finally, we note the simplification occurring if $b(n) \equiv 0$. The eigenvalue equation is

$$a(n+1)\psi(\lambda,n+1) + a(n)\psi(\delta,n-1) = \lambda g(n)\psi(\lambda,n). \tag{A33}$$

Suppose λ_i is an eigenvalue corresponding to eigenfunction $\psi(\lambda_i,n)$. Let

$$\psi' = (-1)^{n+1}\psi(\lambda_i,n). \tag{A34}$$

We readily check that this satisfies the boundary conditions and Eq. (A33) with $\lambda = -\lambda_i$. Thus, in this case eigenvalues occur in equal and opposite pairs. It is readily checked that this statement carries over to the corresponding z_i.

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[1] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).
[2] R. Jost and W. Kohn, Phys. Rev. **87**, 977 (1952).
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[4]One should remember this when one contemplates passage to the limit ($\Delta \to 0$), and replace $\phi(\lambda; n)$ by $\Delta\phi(\lambda n)$ in all pertinent formulas.

[5]For example, if $n_0=2$, one obtains
$P(z) = e^{\nu(1)}(e^{\nu(2)} - 1)\, z^4 + [e^{\nu(1)}(2e^{\nu(2)} - 1) - 1]\, z^2 + e^{\nu(1)+\nu(2)}$.

[6]The reader will recognize the familiar theorem on the constancy of the Wronskian in one of its discrete versions.

[7]The reader will recognize this as a discrete version of Levinson's theorem [N. Levinson, Phys. Rev. **75,** 1445 (1949)]. There are minor technical modifications when there are bound states at the edge of the continuum. Since this is so special, we choose not to consider this case.

[8]It may be noted that we have sketched here an alternative proof of a theorem of Favard [J. Favard, C.R. Acad. Sci. (Paris) 200, 2052 (1935)]. This is to the effect that given the appropriate three-term recursion relation one can construct a spectral function. In the main body of the text we have effectively shown the converse. Given the spectral function, we construct the three-term recursion relation.

Weak quantization

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The present study shows the significance of weak quantization within the electric field dependence of optical absorption. This phenomenon is responsible for effects which cannot be derived from application of ordinary perturbation theory. It may play an important role in biochemical processes which occur in electric fields. In this paper the problems of how to treat higher-order radiation effects and how to include excited states in a molecule are mentioned.

I. INTRODUCTION

In the last twenty years many semiempirical methods have been developed for calculating the wave function of middle-sized and large organic molecules; most of the usual MO methods differ from one another only in details. Experience has shown that with these methods the calculated energies of low-lying electronic levels can be brought into reasonable agreement with the corresponding experimental results. In general, calculations of intensities have shown such great differences between theoretical and experimental values that so far there is no practical method which guarantees reasonable results for both energies and intensities simultaneously. It appears impossible to predict the field dependence of properties of large organic molecules as long as the corresponding values of the states without the external field are not known with sufficient accuracy.

Thus, methods based upon perturbation theory are mostly of practical use only for solving problems of symmetry. In regard to the uncertainty in the results, the effort required in numerical computation of perturbation does not appear to be justified.

The perturbation which arises from the external field can also be introduced directly into the Hartree–Fock operator. Thus, the inaccuracy for weak electric fields is reduced to that of the approximation without the external field. The difference between the results of the perturbation treatment and the direct, selfconsistent method could be used as a measure for the adaptibility of the considered order of perturbation expansion.

However, both methods are ultimately limited to a field-strength range which depends on the treated molecule and decreases generally with increasing size of the molecule. This is caused by the so-called "weak quantization."

This phenomenon is often disregarded—for example, the uncritical application of second order perturbation expansion for external electric fields—but may play an important role in biochemical processes which occur in electric fields.

Therefore, it is useful to demonstrate the significance of weak quantization by fundamental considerations. This is shown by a typical case, e.g., the electric field dependence of optical absorption. For example, these considerations are useful for application to problems of solvatochromy for large organic molecules or for electric field problems in quantum biochemistry.

II. THE SEMICLASSICAL MODEL OF OPTICAL ABSORPTION

In order to see the effect of weak quantization one has to examine the usual treatment of optical absorption and to compare it with the treatment under the influence of weak quantization.

The semiclassical model describes the absorption processes quantitatively. The probability per unit of time dP_{ga}/dt is a measure of the intensity of the absorption band, where the molecule undergoes a transition from state $|g\rangle$ to state $|a\rangle$. The frequency of the absorbed photon is ω_{ag}, which satisfies Bohr's frequency condition. In addition, the energy density is $\rho(\omega_{ag})$, and the polarization direction is defined by the unit vector $\mathbf{e}_L$ in this direction. A time-dependent perturbation calculation yields after application of the hypervirial theorem in dipole approximation and in the first order of the perturbation parameter the well-known formula[1]:

$$\frac{dP_{ga}}{dt} = \frac{2\pi}{\hbar^2}(\mathbf{e}_L \cdot \boldsymbol{\mu}^*_{ga})(\mathbf{e}_L \cdot \boldsymbol{\mu}_{ga}) \cdot \rho(\omega_{ag}).$$

Here $\boldsymbol{\mu}_{ga}$ is the transition moment of the molecule, which describes the transition from state $|g\rangle$ to state $|a\rangle$ as the only molecule-specific factor in this calculation.

It is defined as

$$\mu_{ga} = \langle g|\mathbf{M}|a\rangle,$$

where $\mathbf{M}$ is the dipole moment operator.

The semiclassical model is valid, provided that condition (1) holds.

$$\frac{1}{\omega_{ag}} \ll \Delta\tau \ll \frac{1}{dP_{ga}/dt}. \tag{1}$$

This means that observation of optical absorption must be limited to time intervals $\Delta\tau$, which are much greater than the reciprocal of the frequency of the absorbed light, but on the other hand are so small that the probability of finding the molecule in the state $|g\rangle$ is not considerably changed during this time.

In time-dependent theory the properties of the molecule are specified by the Hamiltonian, which is to have a complete set of eigenstates $|b\rangle$, with

$$\mathrm{H}_0|b(t,t_0)\rangle = i\hbar\frac{d}{dt}|b(t,t_0)\rangle = E_b|b\rangle. \tag{2}$$

According to the semiclassical model, the molecule is in its ground state $|g(t,t_0)\rangle$ at a time t before application of the electric field at time t_F and before light incidence at time t_L with

$$t_0 \le t \le t_F < t_L. \tag{3}$$

Immediately after switching on the electric field at time t_F, this molecular state undergoes a change variable with time which is dependent on the switch-on process for the external field.

The following definition is given:

$\Delta\tau_A^b$ = the interval of time which the adiabatic approximation for state $|b\rangle$ describes adequately.

The following then is required for the ground state:

$$t_F + \Delta\tau_A^g < t_L.$$

The field is thus switched on a sufficiently long time before the light, in such a way that the ground state can be treated adiabatically.

Thus, the Hamiltonian of the system becomes

$$\mathrm{H} = \mathrm{H}_0 - \mathbf{F} \cdot \mathbf{M}$$

with $\mathbf{F}$ as the field strength.

According to a fundamental axiom of quantum theory, the ground state for t with

$$t_F < t < t_L$$

in the Schrödinger representation can be described by

$$|b(t,t_F)\rangle\rangle = \mathrm{U}(t,t_F)\,|b(t_F,t_0)\rangle\rangle \tag{4}$$

with $|b\rangle = |g\rangle$.

Here $\mathrm{U}(t,t_F)$ as a time evolution operator represents a unitary transformation. In the further discussion this will be assumed to be known.

In addition, the following definition is given:

$\Delta\tau_F^b$ = the time interval in which the state $|b\rangle$ decays because of its energy uncertainty ΔE_b.

In principle ΔE_b can be evaluated by (4).

Then $\Delta\tau_F^b$ is a consequence of the uncertainty relation

$$\Delta\tau_F^b = \hbar/\Delta E_b.$$

Further, treatment of optical absorption in the electric field will then be determined by the following criteria:

1. the values of $\Delta\tau_F^g, \Delta\tau_F^a$ compared with $\Delta\tau$,

2. the values of $\Delta\tau_A^g, \Delta\tau_A^a$ compared with $\Delta\tau$.

Provided (5) holds true then the following can be discussed according to stationary methods:

$$\min(\Delta\tau_F^g, \Delta\tau_F^a) \gg \Delta\tau. \tag{5}$$

If (6) holds the ground state decays during the time interval of absorption; the well-known formula for calculating the transition probability loses its validity:

$$\Delta\tau_F^g \approx \Delta\tau \tag{6}$$

This case can offer itself experimentally by large bond broadening and, under extreme conditions, by a continuous spectrum in a discrete spectrum range without the external field.

Before discussing this phenomenon, it is useful to examine the external field dependence in time-independent representation. Since the Hamiltonian in the Schrödinger representation is explicitly time-independent, one may expect that the external field can be treated as a time-independent perturbation.

In this case, two basically differerent boundary considerations about the absorption process in the external field are conceivable:

1. At time t with

$$t_0 \le t \le t_F$$

the molecule is in the ground state of the unperturbed Hamiltonian. Thus, under the influence of the external field the ground state undergoes a change which differs from that in cases without field. In contrast, all excited states of the molecule can continue to be assumed as eigenstates of the unperturbed Hamiltonian. This occurs, if

$$\Delta\tau_A^a \gg \Delta\tau,$$

since then, during absorption, the "sudden approximation" holds good for the excited state $|a\rangle$ as long as it is exposed to the electric field by light stimulation. In this limiting case, a physical distinction is thus made between molecular potential and perturbation potential. If the excited state $|a(t,t_L)\rangle\rangle$ of the molecule in the field is evaluated in terms of the eigenstates of the unperturbed Hamiltonian, and if the probability amplitudes

$$\langle b(t,t_0)\,|\,a(t,t_L)\rangle\rangle$$

are calculated by use of time-dependent perturbation theory, then it is found that for low-lying excited states these oscillate with frequencies which are comparable with, or larger than, the frequency ω_{ag} of the absorbed photon.

From this it may be concluded that low excited states satisfy the following condition:

$$\Delta\tau_A^a \lesssim \frac{1}{\omega_{ag}}.$$

Taking into account relation (1), one can see that the low-lying excited states have to be treated in the following way.

2. For considering optical absorption in an external field the molecule is treated as if it continuously changes its properties when there is a steady increase in field strength. No physical distinction is made between molecular potential and perturbation potential. Thus, all states of the molecule undergo a change under the influence of the external field. If it is assumed that the time-independent Schrödinger equation

$$\mathrm{H}\langle\mathbf{x}|b\rangle = E_b\langle\mathbf{x}|b\rangle$$

has normalizable eigenstates $|b\rangle$, then the validity of the usual formula for calculating the intensities can be further assumed.

The electric field dependence of optical absorption can be calculated by evaluation of the electric field dependence of the transition moment calculated with the states of the field-dependent Schrödinger equation.

III. WEAK QUANTIZATION

Friedrichs and Rejto[2] have shown that the Schrödinger equation with the Hamiltonian

$$\mathrm{H} = \mathrm{H}_0 - \mathbf{F} \cdot \mathbf{M}$$

has no solution for normalizable states; rather, the oper-

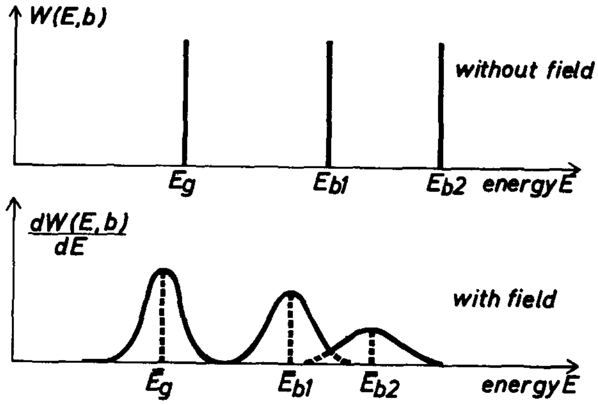

FIG. 1. Effect of weak quantization in energy representation.

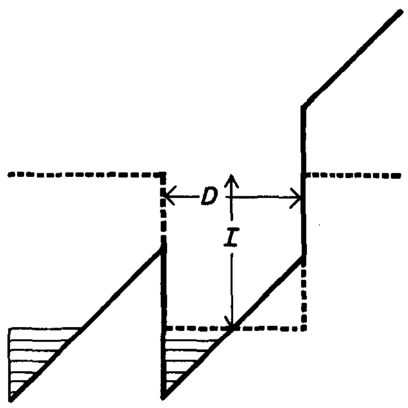

FIG. 2. Weak quantization as a consequence of tunnel effect.

ator for finite, arbitrarily small fields has a continuous spectrum with $-\infty < E < \infty$, exactly like the continuous unbound operator H.

This situation is denoted as "weak quantization," since in the energy representation for any given small field strength the probability $W(E, b)$ of finding an energy value E is concentrated around values $\overline{E}_b$ which in the case

$$\mathbf{F} = 0$$

change into the originally discrete spectrum without field. This is shown in Fig. 1, where the discrete spectrum without field alters into a continuous spectrum in an external electric field:

$$F_g = 2I/(e \cdot D). \tag{7}$$

In the position representation the energy of the wave function depends on the position. The hypervirial theorem is no longer applicable. The usual former relation for calculating the transition probability loses its validity. A state cannot be stationary in an external field, since the state must be normalizable. The molecular state becomes a "resonance" with an energy uncertainty of ΔE_b which depends on the state without the field and on the field strength.

Physically, weak quantization is closely related to "tunnel" effect, since after application of an arbitrarily weak external field, zones always appear in "outer regions" which energetically are more favorable than the original "potential well" necessary to bind the state. Thus, the tunnel effect yields a possibility of roughly determining the upper field strength, which no longer permits a stationary treatment of optical absorption because of the inapplicability of the time-independent Schrödinger equation.

Let D be the dimension of the molecule in the direction of the field, I the ionization energy of the molecule, and e the elementary charge. Then, a simple examination of a one-dimensional square potential well shows that the upper limit F_g of field strength which no longer permits stationary treatment of optical absorption as a result of field ionization is given by (7), as shown in Fig. 2.

Field ionization occurs at last if the potential $e \cdot \mathbf{F} \cdot (D/2)$ at the edge of the square well is equal to the potential barrier I. This leads to (7) for the upper limit of F.

These are fields which can affect large organic molecules in solvents. The electronic state in an external electric field can be considered as a linear combination of a bound state and a free wavepacket.

The probability amplitude for the free wavepacket in participating in the state increases generally with increasing transmission coefficient of the potential in the presence of the external field.

The mean value of momentum of these free states does not become zero. For this reason, the weak quantization gives rise to semiconductivity, which, for instance, plays a role in the quantum biochemistry of proteins in connection with problems of carcinogenesis. The free states can mostly be treated classically. But what about the bound states?

IV. STATIONARY APPROXIMATION METHODS

Taking into account weak quantization, an approximation method must be given which permits a stationary and adiabatic treatment of the field dependence of optical absorption.

Friedrichs[3] has written that the usual perturbation theory "is misleading in first order, and fails when it is pushed to second order." On the other hand, Kato[4] and Titschmarsh[5] have shown that usable results for the energy can be obtained in an "approximative way" if the calculation is limited to Hilbert space. An examination of the errors of the matrix elements of other operators than the Hamiltonian has yet to be made.

For field strength which are much smaller than the estimated upper limit F_g it would seem to be useful to postulate the existence of a stationary state $|\overline{b}_i\rangle$ which can represent the actual state in reasonable agreement. State $|\overline{b}_i\rangle$ must satisfy the following conditions:

1. Since it should be stationary, it must be normalizable. Furthermore, it is required that all the various $|\overline{b}_i\rangle$, $i = 1, 2, \cdots$ be orthonormal:

$$\langle \overline{b}_i | \overline{b}_j \rangle = \delta_{ij}.$$

2. For $F = 0$ the states $|\overline{b}_i\rangle$ must change into states $|b_i\rangle$ according to the Schrödinger equation without the external field:

$$\lim_{F \to 0} |\overline{b}_i\rangle = |b_i\rangle.$$

3. For weak fields state $|\overline{b}_i\rangle$ must have the energy $\overline{E}_{b_i}$ around which $W(E, b_i)$ concentrates:

$$\langle \overline{b}_i | H_0 - \mathbf{F} \cdot \mathbf{M} | \overline{b}_i \rangle = \overline{E}_{b_i}.$$

One way to satisfy these conditions is to obtain the $|\overline{b}_i\rangle$

by a unitary—or antiunitary—transformation

$$U(\mathbf{F})$$

from the corresponding states $|b_i\rangle$ which are solutions of the Schrödinger equation without the field:

$$\lim_{F\to 0} U(\mathbf{F}) = 1$$

Furthermore, the requirements can best be realized by using the Ritz variation principle in Hilbert space. In this procedure, the singularity of the kernel of the Hamiltonian for $F \to 0$ is neglected.

One physical consequence is the averaging of the energy over the whole region of the wavefunction.

The usual treatment of the problem by ordinary perturbation theory is equivalent to this point of view if the variation of the zero order wavefunction is limited to Hilbert space.

The Rayleigh–Schrödinger perturbation expansion yields in first order the well-known result

$$|b_i^{(1)}\rangle = \sum_{j\neq i} \frac{\langle b_j|\mathbf{M}\cdot \mathbf{e}_F|b_i\rangle}{E_{b_j} - E_{b_i}} |b_j\rangle$$

for the change of the wave function $|b_i\rangle$ in the external field, where the $|b_j\rangle$ are eigenfunctions of the unperturbated Hamiltonian. $\mathbf{e}_F$ is the unit vector in field direction.

This relation can also be obtained if the secular matrix with the elements

$$\langle b_j|\mathrm{H}|b_k\rangle$$

is diagonalized and all nondiagonal elements with $k \neq i$ are neglected. Thus it can be assumed that the limitation to the first order of the perturbation calculation will yield reasonable results if

1. $F\dfrac{|\langle b_j|\mathbf{M}\cdot \mathbf{e}_F|b_i\rangle|}{|E_{b_j} - E_{b_i}|} \ll 1 \quad$ for $j \neq i$
2. elements $\langle b_j|\mathbf{M}\cdot \mathbf{e}_F|b_k\rangle$ for $k \neq i$ do not become larger than those under consideration.

From the first condition a critical field strength can be calculated, which will likewise be of the same order as the upper limit F_g.

From this it can be concluded that if the perturbation calculation according to the first order does not yield reasonable results, the application of the second order perturbation terms will not necessarily lead to an improvement. It may be that selective summation methods are preferable. In any case, it is useful to analyze the elements

$$\langle b_j|\mathbf{M}\cdot \mathbf{e}_F|b_k\rangle$$

before choosing the special method of perturbation theory and to take into account the possible importance of free states.

In order to show the difficulties which are connected with the limitation to Hilbert space, a simple example will be treated. A particle in a one-dimensional potential is taken in an external field F. The ground state without the field is to be described by the wavefunction

$$\varphi_g(x).$$

Then the change in the wavefunction in first order perturbation expansion can be obtained from the differential equation of the Rayleigh–Schrödinger perturbation theory:

$$(\mathrm{H}_0 - E_g)\cdot \varphi_g^{(1)}(x) = \mathbb{X}\cdot \varphi_g(x) - \mu_{gg}\cdot \varphi_g(x).$$

With

$$\varphi_g^{(1)}(x) = G(x)\cdot \varphi_g(x)$$

the following is obtained:

$$G(x) = \int_0^x dz \cdot \varphi_g^{-2}(z)\cdot \int_0^z du(u - \mu_{gg})\varphi_g^2(u) + C_1 \int_0^x \varphi_g^{-2}(z)dz,$$

where μ_{gg} represents the dipole moment of the nonperturbed ground state. For illustration, it is sufficient to consider the particular solutions of the following examples:

1. $\varphi_g^2(x) = \text{const.} \to G(x) \sim x^3,$
2. $\varphi_g^2(x) = a\cdot x^\alpha, \alpha \neq -2 \to G(x) \sim (1/(\alpha+2))x^3,$
3. $\varphi_g^2(x) = a\cdot e^{-Ax^2} \to G(x) \sim (1/A)x,$
4. $\varphi_g^2(x) = \delta(0) \to G(x) = 0$

The first example is applicable for bound states only if φ_g is limited to a finite spatial region by a suitable "cutoff procedure." In the second case, the state φ_g is bound for $\alpha < -2$. However, the states remain square integrable after application of the electric field only for $\alpha < -8$. In the third and fourth case the states remain bound.

Here it can be seen that the stronger the particle is localized before perturbation, the weaker are the changes caused by the electric field in the "outer regions" of the unperturbed wavefunction.

An examination of the matrix elements

$$\langle b|\mathbf{M}\cdot \mathbf{e}_F|p\rangle$$

between an unperturbed state $|b\rangle$ and a free state $|p\rangle$ with

$$\mathrm{P}|p\rangle = p|p\rangle,$$

where P is the momentum operator, yields the interpretable result

$$\langle b|\mathbf{M}\cdot \mathbf{e}_F|p\rangle \sim (\nabla_p \mathbf{e}_F\langle b|p\rangle)_p.$$

The following qualitative conclusions can be drawn from the characteristics of the Fourier transformation:

1. The smaller the region in which the electrons can be localized before perturbation, the weaker is the participation of free states in the perturbed state. The upper field strength F_g will then be proportionately higher.

2. The stronger the spatial structure of the unperturbed wavefunction, the stronger is the structure of the participation to free states in the perturbed state, arranged according to the momentum.

These qualitative considerations connect electron density and field effect. In general, in the ground state the weakest change can be expected from an external electric field.

For completeness the generalized Hellmann–Feynman theorem[6] will have to be considered for taking into account field effects in optical absorption.

The first equation is the following relation, which is valid according to the use of the Ritz variation principle in determining the states $|\bar{b}_j\rangle$:

$$\bar{E}_{b_j}\delta_{ij} = \langle \bar{b}_j | \mathrm{H}_0 - \mathbf{F} \cdot \mathbf{M} | \bar{b}_i \rangle.$$

This relation is differentiated by $\mathbf{F} = \mathbf{F} \cdot \mathbf{e}_F$.

Here the following condition is to be satisfied:

$$\left| \frac{d\bar{b}_k}{dF} \mathfrak{H} \epsilon \right\rangle$$

The variation in states $|\bar{b}_j\rangle$ may be constructed only with the states of the Hilbert space $\mathfrak{H}$.

If a diagonal element is differentiated, the following equation is obtained:

$$\frac{d\bar{E}b_i}{dF} = -\langle \bar{b}_i | \mathbf{M} \cdot \mathbf{e}_F | \bar{b}_i \rangle$$

The differentiation of a nondiagonal with $|\bar{b}_i\rangle = |\bar{g}\rangle$ and $|\bar{b}_j\rangle = |\bar{a}\rangle$ yields the relation

$$\left\langle \bar{g} \left| \frac{d\bar{a}}{dF} \right.\right\rangle = \frac{1}{\bar{E}_g - \bar{E}_a} \langle \bar{g} | \mathbf{M} \cdot \mathbf{e}_F | \bar{a} \rangle.$$

Renewed differentiation finally yields

$$\frac{d}{dF} \langle \bar{g} | \mathbf{M} \cdot \mathbf{e}_F | \bar{a} \rangle = \frac{1}{\bar{E}_g - \bar{E}_a} \langle g | \mathbf{M} \cdot \mathbf{e}_F | a \rangle \cdot (\langle a | \mathbf{M} \cdot \mathbf{e}_F | a \rangle - \langle g | \mathbf{M} \cdot \mathbf{e}_F | g \rangle) + (\bar{E}_g - \bar{E}_a) \left(\frac{d}{dF} \left\langle \bar{g} \right\rangle \frac{d\bar{a}}{dF} \right).$$

This formula describes the change in the intensity responsible for a transition moment parallel to the electric field in case there is no marked line broadening as a result of weak quantization.

The first term on the right side reflects the direct coupling of states $|g\rangle$ and $|a\rangle$. It may predominate in isolated bands, and can be measured directly. The second term is responsible for the coupling of the states $|g\rangle$ and $|a\rangle$ with adjacent bands. This can be seen by comparison with the corresponding expression for perturbation calculation in first order. It is to be expected that the second term will be important when the band $|g\rangle \rightarrow |a\rangle$ is closely adjacent to an intensive band $|g\rangle \rightarrow |c\rangle$ with the same polarization direction, which also has a large transition moment

$$\langle c | \mathbf{M} \cdot \mathbf{e}_F | a \rangle.$$

It is possible to develop an analogous expression for the change of the transition moment directed perpendicular to the external field. The term which reflects the direct coupling of states $|g\rangle$ and $|a\rangle$ contains, instead of the dipole moment difference in field direction, the corresponding difference perpendicular to the field direction.

It may be useful to conclude that the term which does not reflect the direct coupling of the states $|g\rangle$ and $|a\rangle$ in any case includes the change of transition velocity and the energy differences of both states. It seems plausible that this term depends strongly on the participation of free states.

V. SUMMARY

The present study shows the significance of weak quantization within the electric field dependence of optical absorption. This phenomenon is responsible for effects which cannot be derived from application of ordinary perturbation theory. In this context the problems of how to treat higher-order radiation effects and how to include exited states in a molecule are mentioned.

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On the supplementary series of $SO_0(p,1)$

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We construct multiplier representations of the unitary irreducible supplementary series of $SO_0(p,1)$ on the sphere S^{p-1} with the aid of a certain bilinear functional. The matrix elements of these representations are shown to be the analytic continuation of the matrix elements of the principal series. The decomposition of such representations with respect to the noncompact subgroup $SO_0(p-1,1)$ is then performed by the analytic continuation of the "overlap" functions. Furthermore, the expansion of the relevant bilinear functional on the hyperboloid H^{p-1} is performed, and the connection is made with the previous decomposition.

1. INTRODUCTION

The study of the unitary irreducible representations of the special orthogonal groups has been an area of active research for many years now. There are many applications in physics as well as in the theory of special functions.[1] In the present article we deal with the connected component of the Lorentz-type orthogonal groups $SO_0(p, 1)$, and with a series of representations which have been called alternatively the supplementary, complementary, or exceptional series.

Our approach is a generalization of the classic work of Bargmann[2] by considering multiplier representation on the $(p-1)$-dimensional sphere[1] S^{p-1}. In Sec. 1 we construct representations of $SO_0(p, 1)$ as multiplier representations on S^{p-1}. In Sec. 2 we discuss harmonic analysis on the spheres S^{p-1} and then show that the matrix elements for the most degenerate supplementary series of $SO_0(p, 1)$ can be obtained by the analytic continuation of those from the principal series.[3] Then we consider the reduction of $SO_0(p, 1)$ according to the noncompact subgroup $SO(p-1, 1)$ for the supplementary series by the analytic continuation of the "overlap functions" obtained previously.[4] Finally, we consider some expansions on the two-sheeted hyperboloid H^{p-1} related to this reduction. All of the calculations are done explicitly only for the most degenerate representations.

For the general representations, one must construct vector-valued functions for which the vector space varies from point to point on S^{p-1}, that is one is dealing with vector bundles over S^{p-1}. If the vector space chosen is the vector space for an irreducible representation of $SO(p-1)$, then our problem is equivalent to doing harmonic analysis on[5] $SO(p)$ instead of S^{p-1}. In this case the necessary calculations are much more difficult, and so we consider only scalar-valued functions; however, we believe that our results are indicative of the general problem. We mention that in the classification of the unitary irreducible representations[6] of $SO_0(p, 1)$ our representations are designated by Schwarz as $D^{p-2/2}(\sigma_p)$ for p even and $D^{p-1/2}(\sigma_p)$ for p odd.

2. MULTIPLIER REPRESENTATIONS

The theory of multiplier representations developed by Bargmann,[2] Gel'fand and Naimark[7] has been elaborated into the very elegant theory of induced representations by Mackey.[8] We do not wish here to concern ourselves with induced representations as we are mainly interested in the supplementary series, which are obtained by analytic continuation of induced representations. We mention only that the principal series of $SO_0(p, 1)$ obtained as multiplier representations[1,3,5] can be viewed as induced representations.

Consider a representation of a group G by the transformation

$$T^\sigma(g)f(Z) = \mu^\sigma(g,g^{-1}Z)f(g^{-1}Z), \tag{2.1}$$

where the functions of f are say well-behaved vector-valued functions over a manifold $\mathfrak{M}$, $Z \in \mathfrak{M}$, over which the group action (in our case transitive) is defined. The function $\mu(g, Z)$ is called a multiplier and (2.1) is a multiplier representation. To insure that the operators $T(g)$ form a representation, $\mu^\sigma(g, Z)$ must satisfy the multiplier condition

$$\mu^\sigma(g_1g_2, Z) = \mu^\sigma(g_1, Z)\mu^\sigma(g_2,g_1Z) \tag{2.2}$$

and

$$\mu^\sigma(e, Z) = 1.$$

Furthermore, if we wish to describe unitary representations, we must introduce a suitable inner product

$$(f_1,f_2) = \int d\Omega(Z)d\Omega(Z')K(Z, Z')(f_1(Z),f_2(Z'))_V, \tag{2.3}$$

where $(f_1(Z),f_2(Z))_V$ refers to the inner product in a vector space V and $K(Z, Z')$ must be a suitably chosen symmetric kernel to assure the correct properties of an inner product. $\Omega(Z)$ is a measure on $\mathfrak{M}$. Then the demand for unitarity,

$$(T(g)f_1, T(g_2)f_2) = (f_1,f_2), \tag{2.4}$$

yields the constraint

$$\bar{\mu}^\sigma(g, Z)\mu^\sigma(g, Z')K(gZ, gZ')\left(\frac{d\Omega(gZ)}{d\Omega(Z)}\right)\left(\frac{d\Omega(gZ')}{d\Omega(Z')}\right) = K(Z, Z'), \tag{2.5}$$

where $[d\Omega(gZ)/d\Omega(Z)]$ is the Radon–Nikodym derivative defined by[9] $\Omega(gZ) = \int d\Omega(Z)[d\Omega(gZ)/d\Omega(Z)]$. Consider as a special case the kernel

$$K(Z, Z') = \delta(Z, Z'), \tag{2.6}$$

where

$$f(Z) = \int \delta(Z, Z')f(Z')d\Omega(Z'), \tag{2.7}$$

i.e., the delta function on $\mathfrak{M}$. Now by the transformation property (2.1), we must have

$$\delta(gZ, gZ')\left(\frac{d\Omega(gZ')}{d\Omega(Z')}\right) = \delta(Z, Z').$$

Then Eq. (2.5) reduces to

$$\left(\frac{d\Omega(gZ)}{d\Omega(Z)}\right) = |\mu^\sigma(g,g^{-1}Z)|^2, \tag{2.8}$$

and the Hilbert space would be $\mathcal{L}^2(\mathfrak{M})$.

We now wish to specialize to the case at hand, that is, $G = SO_0(p,1)$ and $\mathfrak{M} = S^{p-1}$, the $(p-1)$-dimensional sphere. We mention that S^{p-1} is isomorphic to a homogeneous space of $SO_0(p,1)$ obtained in the following way: Consider the Iwasawa decomposition[10] of $SO_0(p,1)$.

$$SO_0(p,1) = KAN.$$

where $K = SO(p), A$ is a one-parameter group generated by one of the boosts, and N is a $(p-1)$-dimensional Abelian group, and the subgroup MAN, where M is the centralizer of A in K and the normalizer of N in K. Actually $M = SO(p-1)$. Then

$$SO_0(p,1)/SO(p-1)AN \simeq SO(p)/SO(p-1) \simeq S^{p-1}.$$

With this choice for G and M, the representation (2.1) with the inner product (2.3) and kernel (2.6) yields the principal series of $SO_0(p,1)$.

We now give a few facts concerning S^{p-1}:

(i) The group of rigid transformations on S^{p-1} is $SO(p)$, and so with an arbitrary choice of phase we set

$$\mu(h,z) = 1, \quad h \in SO(p);$$

then (2.1) gives the quasiregular representation of $SO(p)$ on S^{p-1}.

(ii) The action of g on S^{p-1} for $g \in SO_0(p,1)$ is

$$g: z \to gz \equiv (g^\alpha{}_\beta z^\beta + g^\alpha{}_0)/(g^0{}_\beta z^\beta + g^0{}_0), \tag{2.9}$$

where $\alpha, \beta = 1, \ldots, p$, and the metric for $SO_0(p,1)$ is taken as

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(iii) The measure $d\Omega(z) = d^{p-1}z/|z^p|$ is invariant under the $SO(p)$ rotations, and quasiinvariant[9] under $SO_0(p,1)$. Furthermore,

$$\left(\frac{d\Omega(gz)}{d\Omega(z)}\right) = \left(\frac{d\Omega(z)}{d\Omega(gz)}\right)^{-1} = (g^0{}_\beta z^\beta + g^0{}_0)^{-p+1} \tag{2.10}$$

It then follows that, for $h \in SO(p)$, Eq. (2.5) yields

$$K(hz,hz') = K(z,z'), \quad h \in SO(p). \tag{2.11}$$

so that $K(z,z')$ must be of the form $K(z \cdot z')$. In accordance with the representations of the principal series[1,3,5,11]

$$\mu^\sigma(g,g^{-1}z) = (g^{-10}{}_\beta z^\beta + g^{10}{}_0)^\sigma. \tag{2.12}$$

Such representations are irreducible when σ is not an integer; when σ is a positive (negative) integer, there is an invariant subspace consisting of certain polynomials (factor space with respect to the polynomials), respectively.[1]

Putting Eqs. (2.10) and (2.12) into (2.5) yields the functional equation

$$(g^0{}_\beta z^\beta + g^0{}_0)^{-\bar\sigma-p+1}(g^0{}_\beta z'^\beta + g^0{}_0)^{-\sigma-p+1}K(gz,gz') = K(z,z'). \tag{2.13}$$

We make the ansatz: A solution to (2.13) is of the form

$$K(z,z') = C(1-z\cdot z')^\lambda = 2^{-\lambda}C(z-z')^{2\lambda}. \tag{2.14}$$

In fact, since the action is transitive (2.14) constitutes the most general solution. Considered as a generalized function[12] $K(z,z')$ given by (2.14) is analytic in λ except for simple poles at

$$\lambda = -[(p-1)/2] - k, \quad k = 0, 1, \cdots.$$

We thus concern ourselves with two cases:

(1) $\lambda \neq -[(p-1)/2] - k$, the regular case. Then (2.13) can be satisfied only if $\lambda = -\sigma - p + 1 = -\bar\sigma - p + 1$: hence σ is real.

(2) $\lambda = -[(p-1)/2] - k$, the singular case.

For now we are only interested in the case $k = 0$. Then we find (see Appendix A)

$$\operatorname{Res}(1-z\cdot z')^\lambda\Big|_{\lambda=-(p-1)/2} = \frac{(2\pi)^{(p-1)/2}}{\Gamma((p-1)/2)}\delta^{\mathrm{sph}}(z,z'), \tag{2.15}$$

and Eq. (2.13) is only satisfied if

$$\sigma + \bar\sigma = -(p-1)$$

or

$$\sigma = -[(p-1)/2] + i\rho, \quad \rho \text{ real}.$$

3. HARMONIC ANALYSIS ON S^{p-1}

Let $\mathfrak{D}$ denote the space of infinitely differentiable scalar-valued functions on S^{p-1}. The completion of $\mathfrak{D}$ with respect to the norm induced by the inner product

$$(f_1,f_2) = \int_{S^{p-1}} d\Omega(z)\overline{f_1}(z)f_2(z) \tag{3.1}$$

yields the Hilbert space $\mathcal{L}^2(S^{p-1})$. A complete orthonormal basis in $\mathcal{L}^2(S^{p-1})$ is given by the homogeneous harmonic polynomials[13]

$$Y_N(\theta_{p-1},\ldots,\theta) = N_p \prod_{j=2}^{p=2} C^{n_j+j/2}_{n_{j+1}-n_j}(\cos\theta_{j+1})\sin^{n_j}\theta_{j+1}e^{-in_1\theta_1}, \tag{3.2}$$

where the subscript N denotes $(n_{p-1},\ldots,n_1)$, N_p is given by

$$N_p = \frac{1}{\sqrt{2\pi}}\prod_{j=1}^{p-2}\Gamma(n_j + j/2)2^{n_j+(j-1)/2} \times\left(\frac{(n_{j+1}+j/2)\Gamma(n_{j+1}-n_j+1)}{\pi\Gamma(n_{j+1}+n_j+j)}\right)^{1/2}, \tag{3.3}$$

and the spherical coordinates for S^{p-1} have been used:

$$\begin{aligned} z^1 &= \sin\theta_{p-1}\cdots\sin\theta_1 \quad 0 \le \theta_1 < 2\pi, \\ z^2 &= \sin\theta_{p-1}\cdots\sin\theta_2\cos\theta_1, \\ &\qquad 0 \le \theta_i < \pi,\ i = 2,\ldots,p-1, \\ &\ \ \vdots \\ z^{p-1} &= \sin\theta_{p-1}\cos\theta_{p-2}, \\ z^p &= \cos\theta_{p-1}. \end{aligned} \tag{3.4}$$

Since we wish to describe the supplementary series arising from an inner product of the form (2.3), we are interested in the generalized function (2.14). It is regular for $\sigma < -(p-1)/2$, and for $-(p-1)/2 < \sigma$ can be given meaning in terms of its regularization.[12] In Appendix A the following expansion will be derived:

$$(1 - z \cdot z')^{-\sigma-p+1} = \frac{\pi^{(p-1)/2}\,\Gamma(-[(p-1)/2]-\sigma)}{2^{\sigma}\Gamma(\sigma+p-1)} \times \sum_N \frac{\Gamma(n+\sigma+p-1)}{\Gamma(n-\sigma)} Y_N(z)\overline{Y}_N(z'). \quad (3.5)$$

Again it is emphasized that this expansion has meaning as a generalized function even for $\sigma > -(p-1)/2$. The sum $\sum_N$ means the summation of n_j over the range $n_{p-1} = 0, 1, \ldots, n_i = 0, \ldots, n_{i+1}$ for $i = 2, \ldots, p-2$, and $n_1 = -n_2, \ldots, n_2$. We will use $n = n_{p-1}$ and $l = n_{p-2}$. Then the inner product (2.3) for scalar-valued functions can be written as

$$(f_1, f_2)_\sigma \equiv C \int \frac{d\Omega(z)d\Omega(z')}{(1 - z \cdot z')^{\sigma+p-1}} \overline{f}_1(z) f_2(z') \quad (3.6a)$$

$$= \sum_N \lambda_n(\sigma)(f_1, Y_N)(Y_N, f_2), \quad (3.6b)$$

where C is fixed by normalizing the kernel

$$C = \frac{2^{\sigma}\Gamma(-\sigma)}{\Gamma(-\sigma-(p-1)/2)\,\pi^{(p-1)/2}} \quad (3.7)$$

and

$$\lambda_n(\sigma) = (\sigma + p - 1)_n / (-\sigma)_n, \quad (3.8)$$

where $a_n \equiv \Gamma(a+n)/\Gamma(a)$ is Pochhammer's symbol. We find some useful properties of the function $\lambda_n(\sigma)$: It has the asymptotic behavior

$$\lambda_n(\sigma) \overset{n\to\infty}{\sim} n^{2\sigma+p-1}, \quad (3.9)$$

and it is positive definite when

$$\Gamma(\sigma + p - 1 + n)/\Gamma(n - \sigma) > 0. \quad (3.10)$$

In fact, (3.10) can be valid only if

$$-(p-1) < \sigma < 0. \quad (3.11)$$

Thus for σ in the range $-(p-1) < \sigma \leq -(p-1)/2$ we have a positive definite bilinear form with

$$\|f\|_\sigma^2 \equiv (f, f)_\sigma = \sum_N \lambda_n(\sigma)\,|(Y_N, f)|^2 \leq \sum_N |(Y_N, f)|^2 = \|f\|^2 < \infty. \quad (3.12)$$

Many of the properties of positive definite bilinear forms are best described by introducing a bounded Hermitian operator.[14] In fact, such an operator is used to show the equivalence between representations with σ replaced by $-\sigma - p + 1$. It is known[14,15] that with every positive definite bilinear form $(f_1, f_2)_\sigma$ one can associate a bounded Hermitian operator A^σ such that

$$(f_1, f_2)_\sigma = (f_1, A^\sigma f_2), \quad -(p-1) < \sigma < -(p-1)/2,$$

or

$$(Af)(z) = C \int d\Omega(z) \frac{f(z')}{(1 - z \cdot z')^{\sigma+p-1}}. \quad (3.13)$$

Putting $f(z) = Y_N(z)$ and using (3.5), we find

$$A^\sigma Y_N(z) = \lambda_n(\sigma) Y_N(z). \quad (3.14)$$

Thus the generalized spherical harmonics are eigenfunctions of A^σ with eigenvalues $\lambda_n(\sigma)$. But from (3.9)

$$\lim_{n\to\infty} \lambda_n(\sigma) \to 0 \quad \text{for } \sigma < -(p-1)/2$$

and such a condition characterizes a *compact*[16] operator.[15]

Theorem (Riesz): A bounded linear operator is compact if and only if it maps every weakly converging sequence into a strongly converging sequence.

Hence, there exist sequences of $\mathcal{L}^2(S^{p-1})$ functions which converge (strong) with respect to the σ-norm but do not converge (strong) in $\mathcal{L}^2(S^{p-1})$, and so $\mathcal{L}(S^{p-1})$ is not closed with respect to the σ-norm. The closure, however, yields a Hilbert space which we denote by $\mathcal{H}_\sigma$.

An orthonormal basis in $\mathcal{H}_\sigma$ can be easily constructed from Eq. (3.6b). Defining

$$e_N(z) \equiv [1/\eta_n(\sigma)] Y_N(z), \quad \eta_n(\sigma) = \eta_n^{-1}(-\sigma - p + 1) \equiv [\lambda_n(\sigma)]^{1/2}, \quad (3.15)$$

we obtain the orthonormality relation

$$(e_{N'}, e_N)_\sigma = \delta(N, N') \equiv \delta_{n_1 n_1'} \cdots \delta_{n_{p-1} n_{p-1}'} \quad (3.16)$$

and the completeness relation

$$(f_1, f_2)_\sigma = \sum_N (f_1, e_N)_\sigma (e_N, f_2)_\sigma. \quad (3.17)$$

In fact, these relations hold also for the principal series, i.e., $\sigma = -[(p-1)/2] + i\rho$ since then

$$\lambda_n(-[(p-1)/2] + i\rho) = \frac{([(p-1)/2] + i\rho)_n}{([(p-1)/2] - i\rho)_n},$$

which is nothing more than a phase factor and the e_N form a complete orthornormal basis in $\mathcal{L}^2(S^{p-1})$ for $\sigma = -[(p-1)/2] + i\rho$.

Before closing this section, we notice the analytic structure of the basis functions e_N as a function of σ. There are branch points at $\sigma = 0, 1, \ldots, n-1$ and $\sigma = -p+1, -p, \ldots, -n-p+2$. The branch cuts are chosen according to Fig. 1(a).

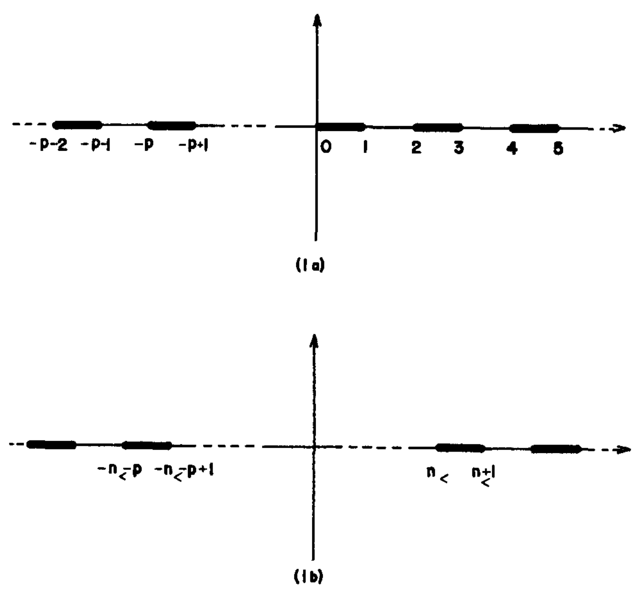


FIG. 1. (a) branch cuts of $e_N(\sigma)$ in complex σ plane. (b) branch cuts of $V^{\sigma}_{N',N}(g)$ in complex σ plane. See text for ranges.

4. THE REPRESENTATION FUNCTIONS

The representation functions or matrix elements for $SO_0(p, 1)$ have been discussed previously,[3,5] and for the most degenerate representation of the principal series an explicit expression[3] was given for matrix elements of a member of the double coset $SO(p)\backslash SO(p, 1)/SO(p)$. We shall denote the matrix elements as

$$(Y_{N'}, T^\sigma(g)Y_N) \equiv T^\sigma_{N',N}(g) \tag{4.1a}$$

and with respect to the basis e_N

$$(e_{N'}, T^\sigma(g)e_N) \equiv V^\sigma_{N',N}(g). \tag{4.1b}$$

Clearly, for the principal series

$$V^\sigma_{N',N}(g) = \frac{\eta_{n'}(\sigma)}{\eta_n(\sigma)} T^\sigma_{N',N}(g) \tag{4.2}$$

since $\eta_n(\bar\sigma) = \eta_n^{-1}(\sigma)$. Since $T^\sigma_{N',N}$ is an entire function of σ, the analytic structure of $V^\sigma_{N',N}(g)$ in σ is determined solely by $\eta_{n'}(\sigma)/\eta_n(\sigma)$ and we find that $V^\sigma_{N',N}(g)$ is an analytic function of σ in the cut plane, where the cuts are taken as shown in Fig. 1b. The branch points of $V^\sigma_{N',N}(g)$ occur at $\sigma = n_<, \ldots, n_> - 1$ and $\sigma = -n_< - p + 1, \ldots, -n_> - p + 2$ where $n_>(n_<)$ means the greater (lesser) of n' or n, respectively. Hence, we can analytically continue $V^\sigma_{N',N}(g)$ to the range $-(p-1) < \sigma < 0$, and by applying Eq. (3.6b) to $(e_{N'}, T^\sigma(g)e_N)_\sigma$, where $-(p-1) < \sigma < 0$, we arrive at

Theorem 1: The multiplier representation $(-p+1 < \sigma < 0)$ given by (2.1) with the prescribed action (2.9) and (2.12) for functions in $\mathcal{L}^2(S^{p-1})$ yields a unitary irreducible representation of $SO_0(p, 1)$ in $\mathcal{H}_\sigma$ which is equivalent to the analytic continuation of the principal series to the range $-p + 1 < \sigma < 0$.

As mentioned previously, the equivalence of the representations[14] under $\sigma \to -\sigma - p + 1$ is determined by the operator A^σ. First, consider the representation adjoint to $T^\sigma(g)$. This representation operates in $\mathfrak{D}'$, the space of antilinear functionals on $\mathfrak{D}$. By restricting this representation to $\mathfrak{D}$ and manipulating the multiplier (2.12) we obtain

$$(T^{-\bar\sigma-p+1}(g)f_1, f_2) = (f_1, T^\sigma(g^{-1})f_2). \tag{4.3}$$

Then, in the case of the supplementary series in the range $-(p-1) < \sigma < -(p-1)/2$, we can write

$$(T^\sigma(g^{-1})f_1, f_2)_\sigma = (f_1, (A^\sigma)^{-1}T^{-\sigma-p+1}(g)A^\sigma f_2)_\sigma. \tag{4.4}$$

It is noted by Eq. (3.14) that indeed A^σ is well defined and possesses an inverse for all σ except $\sigma = -p + 1 - k, + k$, where k is a nonnegative integer. Combining Eq. (4.4) with the unitarity condition (2.4), one finds

$$(f_1, T^\sigma(g)f_2)_\sigma = (f_1, (A^\sigma)^{-1}T^{-\sigma-p+1}(g)A^\sigma f_2)_\sigma. \tag{4.5}$$

Since this holds for all $f \in \mathcal{H}_\sigma$, we obtain

$$A^\sigma T^\sigma(g) = T^{-\sigma-p+1}(g)A^\sigma. \tag{4.6}$$

We note that for $-(p-1) < \sigma < -(p-1)/2$ the operator A^σ is one-to-one and compact and $(A^\sigma)^{-1}$ is unbounded, and since $\lambda_n^{-1}(\sigma) = \lambda_n(-\sigma - p + 1)$, $(A^\sigma)^{-1} = A^{-\sigma-p+1}$ which is compact for $-(p-1)/2 < \sigma_p < 0$. By taking Eq. (4.6) between basis states in $\mathcal{H}_\sigma$ we find

$$\lambda_{n'}(\sigma)V^\sigma_{N'N}(g) = \lambda_n(\sigma)V^{-\sigma-p+1}_{N'N}(g). \tag{4.7}$$

It suffices to discuss only the interval $-(p+1) < \sigma < -(p-1)/2$ where the generalized function (3.6) is regular. The operator $A^{-\sigma-p+1}$ corresponds to the generalized function $(1 - z\cdot z')^\sigma$.

Note Added in Proof: The statement of Theorem 1 deserves a comment. It was not stated explicitly in the theorem but is made explicit in the calculation as well as in the conclusion that the analytic continuation of the representations refers to analytic continuation in the weak sense, i.e., in terms of the matrix elements and not in terms of analytic continuation of operators. Also, I would like to add the following reference where the matrix elements of the supplementary series of the Lorentz group ($SO(3, 1)$) were calculated: S. Ström, Ark. Fys. **38**, 373 (1968).

5. THE DECOMPOSITION $SO_0(p, 1) \supset SO_0(p-1, 1)$

Previously this reduction has been obtained for the most degenerate representations of the principal series.[4,17] In terms of the V functions defined in Sec. 4, the reduction formula reads

$$V^\sigma_{N'N}(h) = \frac{\eta_{n'}(\sigma)}{\eta_n(\sigma)} \sum_{\tau=1}^{2} \int_0^\infty d\nu \frac{\eta_l(\nu)}{\eta_{l'}(\nu)} \overline{K^\sigma_{l'}(\nu, \tau, n')} \times V^{-[(p-2)/2]+i\nu}_{N'N}(h) K^\sigma_l(\nu, \tau, n), \quad h \in SO(p-1, 1), \tag{5.1}$$

where the "overlap" functions are given explicitly by (B2), and it should be understood that the N's in the V function of the integrand are of one lower dimension, i.e., $(n_{p-2}, \ldots, n_0)$.

For convenience we rewrite (5.1) with the aid of the symmetry relation (B3) as

$$V^{\sigma_p}_{N'N}(h) = \frac{-i\eta_{n'}(\sigma_p)}{\eta_n(\sigma_p)} \frac{[1 + (-1)^{n-l+n'-l'}]}{2} \int_c d\sigma_{p-1} \frac{\eta_n(\sigma_{p-1})}{\eta_{n'}(\sigma_{p-1})} \times K^{-\sigma_p-p+1}_{l'}(\sigma_{p-1}, 1, n') V^{\sigma_{p-1}}_{N'N}(h) K^{\sigma_p}_l(\sigma_{p-1}, n), \tag{5.2}$$

where the contour c runs from $-[(p-2)/2] - i\infty$ to $-[(p-2)/2] + i\infty$. Notice the selection rule for these totally symmetric representations owing to the factor $1 + (-1)^{n-l+n'-l'}$. Now both sides of Eq. (5.2) are analytic functions of σ_p and hence can be analytically continued to the supplementary series.[18] Upon doing so, some of the poles of the K functions may cause us to deform the integration contour. If this occurs, such poles give rise to a Regge-like contribution to (5.2). The analytic structure of the functions V and η have been given previously; they have no singularities for σ_p in the supplementary series. Also, the analytic structure of the K functions was given in Ref. 4; however, we repeat it here for convenience. The functions $K^{\sigma_p}_l(\sigma_{p-1}, +, n)$ have moving poles at $n - l$ even,

$$\sigma_{p-1} = -\sigma_p + 2k - (p-2) \\ = \sigma_p - 2k,$$

and at $n - l$ odd,

$$\sigma_{p-1} = -\sigma_p + 2k + 1 - (p-2) \\ = \sigma_p - (2k+1). \tag{5.3}$$

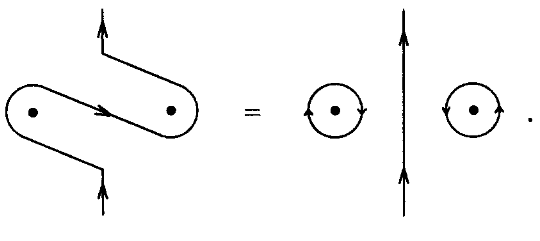
The moving poles of the integrand are thus shown in Fig. 2 along with the integration contour. There are other fixed singularities in the complex σ_{p-1} plane, but they do not interfere with either the migration of the moving poles or the path of integration. Then upon continuation of σ_p to the range $-(p-1) < \sigma_p < -(p-1)/2$, we find only the poles of $\overline{K_l^{-\sigma_p - p+1}}(\sigma_{p-1}, +, n)$ will cross the integration path. Denoting σ_{p-1}^k as these poles, the contour must be deformed when

$$\sigma_{p-1}^k \equiv \sigma_p + k + 1 = -(p-2)/2$$

or when

$$\sigma_p = -k - p/2. \tag{5.4}$$

The deformed contour can then be replaced by the original contour plus the pole contributions according to



(5.5)

Notice the poles cross the integration path in pairs due to the symmetry of the K function under $\sigma_{p-1} \to -\sigma_{p-1} - p + 2$. The results of the contribution from pole terms for various ranges of the supplementary series is summarized in Table I. Calculating the pole contributions by Cauchy's formula and inserting into Eq. (5.2),

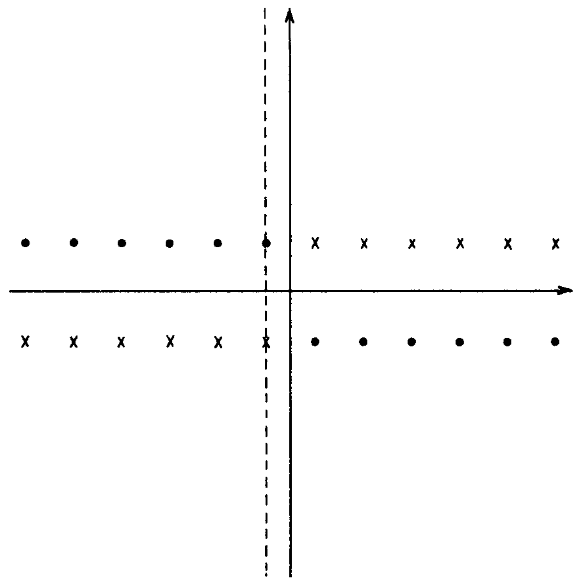


FIG. 2. The solid vertical line indicates the integration contour, the dotted vertical line is the principal series of $SO_0(p, 1)$, and the solid horizontal line is the supplementary series •... poles of $K_l^{\sigma_p}(\sigma_{p-1}, 1, n)$, ×... poles of $\overline{K_l^{\sigma_p}(\sigma_{p-1}, 1, n)}$

TABLE I.

Range of σ_p		Contributing poles
$-p/2 \le \sigma_p < -(p-1)/2$	$-(p-1)/2 < \sigma_p \le (p-2)/2$	none
$-p/2 - 1 \le \sigma_p < -p/2$	$-(p-1)/2 < \sigma_p \le -(p-4)/2$	0
$-p/2 - 2 \le \sigma_p < -p/2 - 1$	$-(p-4)/2 < \sigma_p \le -(p-6)/2$	0, 1
⋮	⋮	⋮
$-p/2 - k \le \sigma_p < -p/2 - k + 1$	$-(p-2k)/2 < \sigma_p \le -(p-2-2k)/2$	$0, 1, \ldots, k-1$
⋮	⋮	⋮
$-(p-1) < \sigma_p < -(p-1) + \begin{cases} \frac{1}{2} \ldots\ldots p \text{ odd} \ldots\ldots -\frac{1}{2} \\ 1 \ldots\ldots p \text{ even} \ldots\ldots -1 \end{cases} < \sigma_p < 0$		$0, 1, \ldots, \{(p-3)/2\}$

we obtain

$$V^{\sigma_p}_{n'N', nN}(h) = -i \frac{\eta_{n'}(\sigma_p)}{\eta_n(\sigma_p)} \frac{[1 + (-1)^{n-l+n'-l}]}{2} \int d\sigma_{p-1} \frac{\eta_l(\sigma_{p-1})}{\eta_{l'}(\sigma_{p-1})} V^{\sigma_{p-1}}_{N'N}(h) K_{l'}^{-\sigma_p - p+1}(\sigma_{p-1}, 1, n') K_l^{\sigma_p}(\sigma_{p-1}, 1, n)$$
$$+ 2\pi \frac{\eta_{n'}(\sigma_p)}{\eta_n(\sigma_p)} [1 + (-1)^{n-l+n'-l'}] \sum_{k=0}^{\{\sigma_p - p/2\}'} \frac{\eta_l(\sigma_p + k + 1)}{\eta_{l'}(\sigma_p + k + 1)} W_{n'l'}^{-\sigma_p - p+1, k} K_l^{\sigma_p}(\sigma_p + k + 1, n) V^{\sigma_p + k + 1}_{N'N}(h), \tag{5.6}$$

where $\{\alpha\}'$ means the smallest integer strictly less than α. The residue functions $W_{nl}^{\sigma, k}$ have been calculated in Appendix B. We mention that at the point $\sigma_p = -(p-1)/2 - k$ the kth pole does not contribute due to the vanishing of the normalization constant $N_{\sigma_p + k+1}$. This is indicated in the table.

Notice also that the residue functions (B6) vanish when $n - l$ and k are of opposite parity, which simply reflects the fact that the K functions have no poles then as can be seen from (5.3). This leads to the question of the multiplicities occurring in the decomposition. For the principal series of $SO_0(p, 1)$, there are two copies of each principal series of $SO_0(p-1, 1)$ occurring in the reduction.[4,17] This can be understood in several ways. Upon mapping S^{p-1} on to H^{p-1} [two-sheeted $(p-1)$-dimensional hyperboloid] we have two quasiregular representations of $SO_0(p-1, 1)$. Another way to understand this is to consider separately functions which are either even or odd under $\theta_{p-1} \to \theta_{p-1} - \pi$. Under $SO_0(p-1, 1)$ transformations this parity is preserved; hence, there are two copies of the quasiregular representation. The Hilbert space splits as the direct sum $\mathcal{H} = \mathcal{H}^{(+)} \oplus \mathcal{H}^{(-)}$. However, when we continue to the supplementary series the additional pole terms contribute either to the even functions or to the odd functions but not both; hence, these representations appear with multiplicity one. The new Hilbert space $\mathcal{H}_\sigma$ again splits according to $\mathcal{H}_\sigma = \mathcal{H}_\sigma^{(+)} \oplus \mathcal{H}_\sigma^{(-)}$, but now both $\mathcal{H}_\sigma^{(+)}$ and $\mathcal{H}_\sigma^{(-)}$ can have discrete contributions depending on the situation. For example, considering σ_p to be close enough to $-(p-1)$ to maximize the pole contributions, we find for $SO_0(3, 1)$ and $SO_0(4, 1)$ only the $k = 0$ term contributes and only in the space $\mathcal{H}_\sigma^{(+)}$ (see also Sec. 6 as well as Ref. 18), whereas for $SO_0(5, 1)$ and $SO_0(6, 1)$ the $k = 0$ term contributes to $\mathcal{H}_\sigma^{(+)}$ and the $k = 1$ term to $\mathcal{H}_\sigma^{(-)}$ and so on for the higher groups with the (even–odd) poles contributing to $\mathcal{H}_\sigma^{(\pm)}$, respectively. We summarize our results as follows:

Theorem 2: The supplementary series of representations of $SO_0(p,1)$ with $-(p-1) < \sigma_p < -(p-1)/2$ as described in Theorem 1 decompose into a direct integral of representations of the most degenerate principal series of $SO_0(p-1,1)$ with multiplicity two plus the direct sum of n-singleton representations of the supplementary series of $SO_0(p-1,1)$ with $\sigma_{p-1} = \sigma_p + n$ whenever σ_p is as indicated by Table I with $n = 1, \ldots, k+1, \ldots \{(p-3)/2\}$. These latter representations occur with multiplicity one.

6. HARMONIC ANALYSIS ON THE HYPERBOLOID H^{p-1}

In his investigation of the decomposition of the supplementary series of the Lorentz group [i.e., $SO_0(3,1) \supset SO_0(2,1)$], Mukunda[18] used a bilinear form on the two-sheeted hyperboloid and expanded the kernel in terms of harmonic functions. In this section we present an analogous discussion for the more general case of the groups $SO_0(p,1)$ and hyperboloids H^{p-1}. Of course the difficulties of harmonic analysis on noncompact manifolds such as H^{p-1} are well known; however, due to the pioneering work of Gel'fand and his collaborators,[14] such difficulties have been overcome. Our purpose then is to write down a Plancherel–Parseval formula for the hyperboloid H^{p-1} analogous to Eqs. (3.6b) and (3.17) for the sphere S^{p-1}.

We begin by considering the unitary map of S^{p-1} onto H^{p-1}. The $(p-1)$-dimensional two-sheeted hyperboloid H^{p-1} is given in spherical coordinates by

$$\begin{aligned}
\eta^0 &= \pm \cosh a, \\
\eta^1 &= \sinh a \sin\theta_{p-2} \cdots \sin\theta_1, \quad 0 \le \theta_1 < 2\pi, \\
\eta^2 &= \sinh a \sin\theta_{p-2} \cdots \cos\theta_1, \quad 0 \le \theta_i < \pi, i = 2, \ldots, p-2 \\
&\vdots \\
\eta^{p-1} &= \sinh a \cos\theta_{p-2}, \quad 0 \le a < \infty,
\end{aligned} \tag{6.1}$$

where $\pm$ refers to the (upper–lower) sheet of H^{p-1}.

The mapping of S^{p-1} onto H^{p-1} is given by

$$\eta^0 = 1/z^p, \quad \eta^i = z^i/z^p, \quad i = 2, \ldots, p-1$$

or

$$\begin{aligned}
\cos\theta_{p-1} &= \frac{1}{\cosh a}, \quad 0 \le \theta_{p-1} \le \pi/2, \ 0 \le a < \infty, \\
\cos\theta_{p-1} &= -\frac{1}{\cosh a}, \quad \pi/2 < \theta_{p-1} \le \pi, \ \infty > a \ge 0, \\
\sin\theta_{p-1} &= \tanh a, \quad 0 \le \theta_{p-1} < \pi, \ 0 \le a < \infty.
\end{aligned} \tag{6.2}$$

The functions on S^{p-1} are mapped as follows:

$$\begin{aligned}
f(z) &\to \cosh a^{-\sigma} f_1(\eta), \quad 0 \le \theta_{p-1} \le \pi/2, \\
f(z) &\to \cosh a^{-\sigma} f_2(\eta), \quad \pi/2 < \theta_{p-1} < \pi,
\end{aligned} \tag{6.3}$$

where the 1 or 2 denotes the upper or lower sheet, respectively. Following Mukunda, we define functions $f_\pm(\eta)$ which are even or odd under $\theta_{p-1} \to \pi - \theta_{p-1}$, $f_\pm \equiv (f_1 \pm f_2)/2$. Under (6.2) the measure $d\Omega(z)$ becomes

$$d\Omega(z) \to d\Omega(\eta)(1/\cosh a)^{p-1}, \tag{6.4}$$

where $d\Omega(\eta) = d^{p-1}\eta/|\eta_0|$. Combining Eqs. (6.2) and (6.4) with (3.6a), we obtain

$$(f,g)_\sigma = C \int d\Omega(\eta) d\Omega(\eta') [\bar{f}_+(\eta) g_+(\eta') K_+(\eta \cdot \eta') + \bar{f}_-(\eta) g_-(\eta') K_-(\eta \cdot \eta')] \tag{6.5}$$

where

$$\begin{aligned}
K_\pm(x) &= [(x-1)^{-\sigma-p+1} \pm (x+1)^{-\sigma-p+1}]/2, \\
x &= \cosh a \cosh a' - \sinh a \sinh a' \cos\beta, \\
\cos\beta &= \cos\theta_{p-2} \cos\theta'_{p-2} + \cdots \\
&\quad + \sin\theta_{p-2} \sin\theta'_{p-2} \cdots \sin\theta_1 \sin\theta'_1.
\end{aligned}$$

The expansion of $K_\pm(x)$ in a harmonic series can be performed by using the expansion formulas obtained by Vilenkin[2] using Gel'fand's method of horospheres.[14] The details are given in Appendix A. The result is

$$\begin{aligned}
K_\pm(x) &= \frac{\Gamma(-\sigma-(p-1)/2)\pi^{(p-3)/2}}{2^\sigma \Gamma(\sigma+p-1)} \\
&\quad \times \sum_N \int_0^\infty d\nu\, \Gamma(\sigma + \tfrac{1}{2}p + i\nu) \Gamma(\sigma + \tfrac{1}{2}p - i\nu) \\
&\quad \times \{\cosh\pi\nu \mp \sin\pi[\sigma + (p-1)/2)]\} \phi_{\nu,N}(\eta) \bar{\phi}_{\nu,N}(\eta')
\end{aligned} \tag{6.6}$$

for $-p/2 < \sigma < -(p-1)/2$, where the $\phi_{\nu,N}(\eta)$ have been given previously[4]

$$\begin{aligned}
\phi_{\nu,N}(\eta) &= N_\nu (\sinh a)^{-(p-3)/2} P^{-l-(p-3)/2}_{-(1/2)+i\nu} (\cosh a) \\
&\quad \times Y_N(\theta_{p-2}, \ldots, \theta_1)
\end{aligned}$$

$$N_\nu = [|\Gamma(i\nu + l + (p-2)/2)|^2 (\nu \sinh\pi\nu)/\pi]^{1/2}. \tag{6.7}$$

The inner product (6.5) then becomes

$$\begin{aligned}
(f,g)_\sigma &= \sum_N \int d\nu\, \lambda_\nu^+(\sigma)(f_+, \phi_{\nu,N})(\phi_{\nu,N}, g_+) \\
&\quad + \sum_N \int d\nu\, \lambda_\nu^-(\sigma)(f_-, \phi_{\nu,N})(\phi_{\nu,N}, g_-)
\end{aligned} \tag{6.8}$$

for $-p/2 < \sigma < -(p-1)/2$, where

$$\lambda_\nu^\pm(\sigma) = \frac{\Gamma(-\sigma)}{\pi\Gamma(\sigma+p-1)} \Gamma\left(\sigma + \frac{p}{2} + i\nu\right) \Gamma\left(\sigma + \frac{p}{2} - i\nu\right) \times \left[\cosh\pi\nu \mp \sin\pi\left(\sigma + \frac{p-1}{2}\right)\right].$$

It follows immediately that for $-(p-1) < \sigma < -(p-1)/2$, $\lambda_\nu^\pm(\sigma) > 0$, using Stirling's formula, we see that

$$\lambda_\nu^\pm(\sigma) \xrightarrow{\nu\to\infty} \nu^{2\sigma+p-1} \to 0 \tag{6.9}$$

for $\sigma < -(p-1)/2$; hence (6.8) converges and $\mathcal{L}^2(H)$ is dense in $\mathcal{H}_\sigma^\pm$. Now Eqs. (6.6) and (6.8) are defined only for σ in the range $-p/2 < \sigma < -(p-1)/2$. To define the kernel (6.6) for $\sigma < -p/2$, we must analytically continue the integrand of (6.6) in σ. Again when doing so we must deform the contour since the Γ functions exhibit poles when $i\nu = \mp(\sigma + \frac{1}{2}p + k)$. These poles will collide with the contour[19] when $\sigma = -\frac{1}{2}p - k$. Actually owing to the factor $\cosh\pi\nu \mp \sin\pi[\sigma + (p-1)/2]$ half of the poles are quenched. The even poles (k even) appear in $\lambda_\nu^+(\sigma)$ and the odd poles in $\lambda_\nu^-(\sigma)$. Hence, we get for σ, in the entire range $-(p-1) < \sigma < -(p-1)/2$,

$$\begin{aligned}
(f,g)_\sigma &= \sum_N \int_0^\infty d\nu\, \lambda_\nu^+(\sigma)(f_+, \phi_{\nu,N})(\phi_{\nu,N}, g_+) \\
&\quad + 2\Gamma(-\sigma) \sum_{k \text{ even}}^{\{-\sigma_p - p/2\}'_e} \frac{(-k-\frac{1}{2}p-\sigma) \sum_N (\sigma+p-1)_{k-l} \Gamma(-\sigma-k-1+l)(f_+, \psi_{\sigma+k+1,N})(\psi_{\sigma+k+1,N}, g_+)}{k!\,\Gamma(-2\sigma-p+1-k)}
\end{aligned}$$

$$+\sum_N \int_0^\infty d\nu\, \lambda_\nu^-(\sigma)(f_-,\phi_{\nu,N})(\phi_{\nu,N},g_-)$$
$$+\, 2\Gamma(-\sigma) \sum_{k\ \mathrm{odd}}^{\{-\sigma_p - p/2\}'_o} \frac{(-k-\frac{1}{2}p-\sigma)\sum_N (\sigma+p-1)_{k-l}\Gamma(-\sigma-k-1+l)(f_-,\psi_{\sigma+k+1,N})(\psi_{\sigma+k+1,N},g_-)}{k!\,\Gamma(-2\sigma-p+1-k)} \tag{6.10}$$

where $\{\alpha\}'_e, \{\alpha\}'_o$ denote greatest even (odd) integer strictly less than α respectively, and

$$\psi_{\sigma+k,N}(\eta) = (\sinh a)^{-(p-3)/2}\, P^{-[l+(p-3)/2]}_{\sigma+k+(p-1)/2}(\cosh a) \times Y_N(\theta_{p-2},\ldots,\theta_1)$$

It can be readily verified that (6.10) is a positive definite bilinear form. The question of the orthogonality of the functions $\psi_{\sigma+k,N}$ for different k and orthogonality between $\psi_{\sigma+k,N}$ and $\phi_{\nu,N}$ is somewhat difficult since $\psi_{\sigma+k,N}$ no longer exhibits the usual oscillatory behavior. The expression (6.10) converges even though the functions $\psi_{\sigma+k,N}(\eta)$ are more singular at $\cosh a \to \infty$ than $\phi_{\nu,N}(\eta)$. This is so since $\cosh a^\sigma\, \psi_{\sigma+k,N}$ converges in $\mathcal{L}^2(H^{p-1})$, and from (6.3) so does $\cosh a^{-\sigma} f_\pm$. As a result except for the points $\sigma = -\frac{1}{2}p - k$, $\mathcal{L}^2(H^{p-1})$ is dense in both $\mathcal{H}^\pm_\sigma$. At the points $\sigma = \frac{1}{2}p - k$

$$\lambda_\nu^\pm(\sigma) \xrightarrow{\nu\to 0} \nu^{-2};$$

hence, $\mathcal{L}^2(H^{p-1})$ is not dense in $\mathcal{H}^\pm_{-(p/2)-k}$. For a more thorough-going discussion of the Hilbert space structure the reader is referred to Mukunda.[18]

We remark that the integrands in (6.10) can be rewritten in terms of the σ-norms analogous to (3.17) by introducing

$$e^\pm_{\nu,N} \equiv [\lambda^\pm_\nu(\sigma)]^{-1/2}\phi_{\nu,N}. \tag{6.11}$$

These functions then form an orthonormal subset in $\mathcal{H}^\pm_\sigma$, but are not complete when $\sigma < -p/2$ owing to the contribution from the discrete terms in (6.10) [for $-(p+1)/2 \le \sigma < -p/2$, $e^-_{\nu,N}$ is complete in $\mathcal{H}^-_\sigma$]. Also the $e^\pm_{\nu,N}$ are a complete orthonormal basis for the principal series $\{\sigma = -[(p-1)/2] + i\rho\}$ since then $\lambda^\pm_\nu(\sigma)$ reduces to a phase factor.

The connection between the approach in this section and the approach in Sec. 5 can be made by noticing the relationship between the two functions $\lambda_n(\sigma)$ and $\lambda^\pm_\nu(\sigma)$. By making use of the unitary transformation between the representations on the sphere and on the hyperboloid, one finds

$$\lambda^\tau_{\nu'}(\sigma)\delta_{\tau,\tau'}\delta(\nu'-\nu) = \sum_n \lambda_n(\sigma) K^\sigma_l(\nu',\tau',n)\overline{K^\sigma_l(\nu,\tau,n)}. \tag{6.12}$$

Using (6.12) and the completeness property[4]

$$\sum_\tau \int d\nu\, \overline{K^\sigma_l(\nu,\tau,n')} K^\sigma_l(\nu,\tau,n) = \delta_{n',n}, \tag{6.13}$$

one finds that the matrix elements $(e_{N'}, T^\sigma(h)e_N)_\sigma$ for $h \in SO_0(p-1,1)$ and σ in the supplementary series with $-p/2 \le \sigma < -(p-1)/2$ gives exactly that given by Eq. (5.1) when σ is analytically continued to the above mentioned range.

CONCLUSION

We have used the generalized function $(1 - z\cdot z')^\lambda$ on the $(p-1)$-dimensional sphere to discuss representations of $SO_0(p,1)$. In particular, the supplementary series arises naturally while the principal series corresponds to the singular point $\lambda = -(p-1)/2$. It remains to investigate the remaining singular points and their possible connection with integer point representations. All in all, this procedure gives a unified way of handling the most degenerate representations of $SO_0(p,1)$ and possibly the general representations. At this point it is worth mentioning that the general groups $SO_0(p,1)$ have recently become of interest in physics in connection with the dual resonance models[20] in a way closely related to the multiplier representations we have used.

It is seen that the matrix elements for the supplementary series are the analytic continuation of those from the principal series. This allows us to discuss the decomposition according to the noncompact subgroup $SO_0(p-1,1)$ by the method of analytic continuation and it is shown to be consistent with the representations on the hyperboloid H^{p-1}. While this decomposition has been discussed previously for $p = 3$, our results contain as a special case the decomposition of the matrix elements which has not been given.

The question of applying these methods to the general representations is of foremost interest. Here we are concerned with representations on the $SO(p)$ group manifold with the basis vectors given by the $SO(p)$ matrix elements labeled by the usual Gel'fand–Tsetlin scheme. Owing to the usual decomposition of $SO_0(p,1)$ and the splitting of the Haar measure $\Omega(SO(p)) = \Omega(S^{p-1})\,\Omega(SO(p-1))$, the multipliers can be written as only multipliers[5] on S^{p-1}. For this reason we believe our results are somewhat indicative of the general pattern, modulo the appearance of certain discrete representations. This is analogous to what is sometimes referred to as "complications due to spin." Nonetheless, the general problem is quite formidable. One must know the analytic structure of the general "overlap" functions which itself presupposes the decomposition of the regular representation of $SO_0(p-1,1)$. Moreover, the factorization of the residues is now not at all trivial as it is in the most degenerate case. It is hoped that definite answers can be given to these problems in the future.

APPENDIX A: EXPANSIONS ON SPHERES AND HYPERBOLOIDS

We derive the expression (3.5). Expand $(1-x)^{-\gamma}$ in a Fourier Gegenbauer series:

$$(1-x)^{-\gamma} = \sum_{n=0}^\infty a_n(\gamma) C_n^{(p-2)/2}(x), \tag{A1}$$

with

$$a_n(\gamma) = N_n^2 \int_{-1}^1 dx (1-x)^{-\gamma}(1-x^2)^{(p-3)/2} C_n^{(p-2)/2}(x). \tag{A2}$$

This integral can be performed for $\mathrm{Re}\gamma < (p-1)/2$ with the aid of formula 7.311.3 of Ref. 21, yielding

$$a_n(\gamma) = \frac{2^{p-2-\gamma}[n+(p-2)/2]\Gamma(p-2)/2))\Gamma((p-1)/2-\gamma)(\gamma)_n}{\pi^{1/2}\Gamma(n+p-1-\gamma)}. \tag{A3}$$

Although the integral can be performed only for $\mathrm{Re}\gamma < (p-1)/2$, Eq. (A3) yields for $a_n(\gamma)$ an analytic function in the complex γ plane except for simple poles at $\gamma = [(p-1)/2] + k$; hence, the series (A1) has meaning as a generalized function for all γ except at these poles. Setting $x = z \cdot z'$, $\gamma = \sigma + p - 1$ and using the addition theorem for generalized spherical harmonics[13]

$$C_n^{(p-2)/2}(z \cdot z') = \frac{2\pi^{(p-1)/2}}{[n + (p-2)/2]\Gamma((p-2)/2)} \sum_N Y_N(z)\bar{Y}_N(z'), \quad \text{(A4)}$$

we readily obtain expression (3.5). It should be understood that the sum on N means the sum over all n_j, except n_{p-1}, over the ranges mentioned in the text.

For an analogous expansion on the hyperboloid, H^{p-1}, we use the expressions obtained by Vilenkin[1] using the Gel'fand–Graev transform[14]:

$$p \text{ even: } f(\cosh\alpha) = \frac{(-1)^{(p-2)/2}}{2i \sinh^{(p-2)/2}\alpha} \int_c d\sigma_{p-1} \times \frac{\Gamma(\sigma_{p-1} + p - 2)}{\Gamma(\sigma_{p-1})} a(\sigma_{p-1}) P^{-(p-3)/2}_{\sigma_{p-1}+(p-3)/2}(\cosh\alpha); \quad \text{(A5a)}$$

$$p \text{ odd: } f(\cosh\alpha) = \frac{(-1)^{(p-3)/2}}{2i \sinh^{(p-2)/2}\alpha} \int_c d\sigma_{p-1} \times \frac{\Gamma(\sigma_{p-1} + p - 2)}{\Gamma(\sigma_{p-1})} \cot\pi\sigma_{p-1} a(\sigma_{p-1}) P^{-(p-3)/2}_{\sigma_{p-1}+(p-3)/2}(\cosh\alpha), \quad \text{(A5b)}$$

with the inversion formula

$$a(\sigma) = \int_1^\infty f(x)(x^2 - 1)^{(p-3)/4} P^{-(p-3)/2}_{\sigma+(p-3)/2}(x). \quad \text{(A6)}$$

The contour c runs from $-(p-2)/2 - i\infty$ to $-(p-2)/2 + i\infty$. We have two integrals to perform one with $f_1(x) = (x-1)^\lambda$, the other with $f_2(x) = (x+1)^\lambda$. In the first case (A6) can be performed using formula 7.134.2 of Ref. 21 yielding

$$a_1 = \frac{-2^{\lambda+(p-1)/2}\Gamma(\lambda + (p-1)/2)\Gamma(\lambda - p + 2 - \sigma_{p-1})\Gamma(\sigma_{p-1} - \lambda)}{\pi\Gamma(-\lambda)} \sin\pi[\sigma_{p-1} + (p-3)/2]. \quad \text{(A7)}$$

The second integral can be done with the aid of formula 7.135.3 of Ref. 21, giving after some algebraic manipulations,

$$a_2 = \frac{2^{\lambda+p-1}\Gamma(\lambda + (p-1)/2)\Gamma(\sigma_{p-1} - \lambda)\Gamma(-\lambda - p + 2 - \sigma_{p-1})}{\pi\Gamma(-\lambda)} \sin\pi[\lambda + (p-1)/2]. \quad \text{(A8)}$$

Combining (A7) and (A8) to form $a_\pm = a_1 \pm a_2$ and setting $\lambda = -\sigma - p + 1$, we have

$$a_\pm = \frac{-\Gamma(-\sigma - (p-1)/2)\Gamma(\sigma + \tfrac{1}{2}p - i\nu)}{2^{\sigma+(p-1)/2}\pi\Gamma(\sigma + p - 1)} \times \Gamma(\sigma + \tfrac{1}{2}p + i\nu)\{\cosh\pi\nu \mp \sin\pi[\sigma + (p-1)/2]\} \quad \text{(A9)}$$

with $\sigma_{p-1} = -[(p-2)/2] + i\nu$. Strictly speaking, the above integrals can be performed only with the restrictions $\sigma > -p/2, \sigma < -(p-1)/2$; however, (A9) describes a function which is analytic in σ except for poles at $k - (p-1)/2$ and $-k - (p/2) \pm i\nu$. Thus the integrals can be given meaning in terms of their analytic continuation. To write the expansions in terms of the "spherical" functions on the hyperboloid, we make use of the addition theorem for the Legendre functions derived by Vilenkin[1]:

$$\sinh\alpha^{-(p-3)/2} P^{-(p-3)/2}_{\sigma+(p-3)/2}(\cosh\alpha) = 2^{(p-5)/2}\Gamma\left(\frac{p-3}{2}\right)\Gamma(\sigma+1)\Gamma(-p+3-\sigma) \times \sum_{l=0}^\infty (p-3+2l)\frac{(\sinh a)^{-(p-3)/2}(\sinh a')^{-(p-3)/2}}{\Gamma(-\sigma-p+3-l)} \times P^{-[(p-3)/2]-l}_{\sigma+(p-3)/2}(\cosh a) \times P^{-[(p-3)/2]-l}_{\sigma+(p-3)/2}(\cosh a') C_l^{(p-2)/2}(\cos\beta) \quad \text{(A10)}$$

with $\cosh\alpha = \cosh a \cosh a' - \sinh a \sinh a' \cos\beta$. Doing some algebra and using (A4), we find that the left-hand side of (A10) becomes for even p

$$\frac{2^{(p-1)/2}\pi^{(p-2)/2}(-1)^{(p-2)/2}}{i\nu} \times \frac{\Gamma(\sigma_{p-1} + 1)}{\Gamma(\sigma_{p-1} + p - 2)} \sum_N \phi_{\nu,N}(\eta)\bar{\phi}_{\nu,N}(\eta')$$

and for odd p

$$\frac{2^{(p-1)/2}\pi^{(p-2)/2}(-1)^{(p-3)/2}}{\nu} \coth\pi\nu \frac{\Gamma(\sigma_{p-1} + 1)}{\Gamma(\sigma_{p-1} + p - 2)} \times \sum_N \phi_{\nu,N}(\eta)\bar{\phi}_{\nu,N}(\eta'). \quad \text{(A11)}$$

Remembering that $\sigma_{p-1} = -[(p-2)/2] + i\nu$, we change the contour integral in (A5) to an integral over ν from 0 to ∞ and make use of the relations

$$p \text{ odd: } \operatorname{Im}\frac{\Gamma(\sigma_{p-1} + p - 2)}{\Gamma(\sigma_{p-1})} = \nu \frac{\Gamma(\sigma_{p-1} + p - 2)}{\Gamma(\sigma_{p-1} + 1)},$$

$$p \text{ even: } \operatorname{Re}\frac{\Gamma(\sigma_{p-1} + p - 2)}{\Gamma(\sigma_{p-1})} = i\nu \frac{\Gamma(\sigma_{p-1} + p - 2)}{\Gamma(\sigma_{p-1} + 1)} \quad \text{(A12)}$$

to obtain the expansion formulas (A5) as

$$f(x) = -2^{p-1/2}\pi^{p-1/2} \sum_N \int_0^\infty d\nu\, a(\nu)\phi_{\nu,N}(\eta)\bar{\phi}_{\nu,N}(\eta'), \quad \text{(A13)}$$

where

$$x = \cosh a \cosh a' - \sinh a \sinh a' \cos\beta,$$

$$\cos\beta = \cos\theta_{p-2}\cos\theta'_{p-2} + \cdots + \sin\theta_{p-2}\sin\theta'_{p-2}\cdots\sin\theta_1\sin\theta'_1.$$

This together with the Fourier coefficients (A9) then yields the expansion for the kernel $K_\pm$ given by Eq. (6.6).

It was mentioned previously that both the generalized functions $(1 - z \cdot z')^\lambda$ and $(\eta \cdot \eta' - 1)^\lambda$ (here $\eta_0, \eta'_0 > 0$) are singular when $\lambda = [(p-1)/2] - k$ or $\sigma = -[(p-1)/2] + k$. Considering only the case $k = 0$ and using the completeness of the spherical harmonics in Eq. (3.5), one easily obtains Eq. (2.15). Similarly using (A7), (A13) and the completeness of the functions $\phi_{\nu,N}(\eta)$, we obtain

$$\operatorname{Res}(\eta\cdot\eta' - 1)^{\lambda}\Big|_{\lambda=-(p-1)/2} = \frac{(2\pi)^{(p-1)/2}}{\Gamma((p-1)/2)}\,\delta^{\mathrm{hyp}}(\eta,\eta'). \tag{A14}$$

Note $(\eta\cdot\eta' + 1)^{\lambda}$ is regular.

APPENDIX B: THE RESIDUE FUNCTIONS

The residue functions are defined by

$$W_n^{-\sigma_p-p+1,k} = \lim_{\sigma_{p-1}\to-\sigma_p-k-p+1} (\sigma_{p-1} + \sigma_p + p - 1 + k) \times K_l^{-\sigma_p-p+1}(\sigma_{p-1}, 1, n), \tag{B1}$$

where the K functions were obtained in Ref. 4:

$$K_l^{-\sigma_p-p+1}(\sigma_{p-1}, 1, n) = \frac{\sqrt{\pi}N_{\sigma_{p-1}}N_n}{2^{l+(p-2)/2}\Gamma(l + (p-2)/2)} \sum_{j=0}^{\{(n-l)/2\}} \frac{(-1)^j}{j!} \frac{\Gamma(n + [(p-2)/2] - j)}{\Gamma([(n-l+1)/2] - j)} \times \frac{\Gamma([(n-l-\sigma_{p-1}+\sigma_p+1)/2]-j)\Gamma([(n-l+\sigma_{p-1}+\sigma_p+p-1)/2]-j)}{\Gamma([(n-l+2)/2]-j)\Gamma([(n+\sigma_p+p-1)/2]-j)\Gamma([(n+\sigma_p+p)/2]-j)} \tag{B2}$$

where the K function on the lower sheet is related by

$$K^{\sigma}(\nu, 2, n) = (-1)^{n-l}K^{\sigma}(\nu, 1, n). \tag{B3}$$

The relevant poles occur in $\Gamma([(n - l + \sigma_{p-1} + \sigma_p + p - 1)/2] - j)$. The residues of these poles can be found by analyzing the cases $n - l$ even and odd separately and using

$$\Gamma(z + i) = (-1)^i\Gamma(1 - z)\Gamma(z)/\Gamma(1 - z - i), \quad i \text{ integer.} \tag{B4}$$

We find

$$\operatorname{Res}\Gamma\left(\frac{\sigma_{p-1} + \sigma_p + p - 1 - n - l}{2} - j\right)\Big|_{\sigma_{p-1}=-\sigma_p-k-p+1} = \frac{(-1)^k[1 + (-1)^{n-l-k}](-1)^{(n-l+k)/2-j}}{\Gamma([(-n-l-k)/2] + j + 1)}. \tag{B5}$$

Inserting (B5) into (B1) and inverting some Γ functions we obtain explicitly

$$W_{nl}^{-\sigma-p+1,k} = \frac{(-1)^{(n-l-k)/2}[1 + (-1)^{n-l+k}]\sqrt{\pi}N_{\sigma_p+k+1}N_n\Gamma(n + [(p-2)/2] - j)\Gamma([(n-l+p+k)/2] + \sigma_p)}{2^{l+(p-2)/2}\Gamma(l+(p-2)/2)\Gamma(n-l+1)/2)\Gamma((n-l+2)/2)\Gamma((n+\sigma_p+p-1)/2)\Gamma((n+\sigma_p+p)/2)\Gamma(1-(n-l-k)/2)} \times {}_4F_3\left[\begin{matrix}-(n-l-1)/2, -(n-l)/2, -(\sigma_p-p-3+n)/2, -(\sigma_p+p-2+n)/2 \\ -n-(p-4)/2, -\sigma_p-(n-l+k+p+2)/2, -(n-l-k)/2+1\end{matrix}; 1\right]. \tag{B6}$$

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The explicit determination of the linear boson transformation coefficients

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The problem of determining the wavefunction is solved for the boson Bogoliubov transformation. The method of series expansion is applied to derive the general expression for the coefficients which connect the new Fock states of an arbitrary number of quasiparticles with the states before the transformation.

1. INTRODUCTION

The usefulness of the method of Bogoliubov transformations has manifested itself particularly in the theoretical treatments of superfluidity[1] and superconductivity.[2] In such a transformation the new boson annihilation operator $b_{\mathbf{k}}$ and creation operator $b_{\mathbf{k}}^\dagger$ of momentum $\mathbf{k}(\neq 0)$, satisfying the commutation relations, i.e.,

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'} \quad \text{and} \quad [b_{\mathbf{k}}, b_{\mathbf{k}'}] = [b_{\mathbf{k}}^\dagger, b_{\mathbf{k}'}^\dagger] = 0, \tag{1.1}$$

are related to the boson annihilation operator $a_{\mathbf{k}}$ and creation operator $a_{\mathbf{k}}^\dagger$ by

$$\begin{aligned} b_{\mathbf{k}} &= u_{\mathbf{k}} a_{\mathbf{k}} + v_{\mathbf{k}} a_{-\mathbf{k}}^\dagger = e^T a_{\mathbf{k}} e^{-T} \\ b_{\mathbf{k}}^\dagger &= u_{\mathbf{k}} a_{\mathbf{k}}^\dagger + v_{\mathbf{k}} a_{-\mathbf{k}} = e^T a_{\mathbf{k}}^\dagger e^{-T} \end{aligned} \tag{1.2}$$

with

$$T = -x_{\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger - a_{\mathbf{k}} a_{-\mathbf{k}}) = -T^\dagger. \tag{1.3}$$

Then the unitarity condition

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1 \tag{1.4}$$

holds for the real parameters

$$u_{\mathbf{k}} = u_{-\mathbf{k}} \equiv \cosh x_{\mathbf{k}} \quad \text{and} \quad v_{\mathbf{k}} = v_{-\mathbf{k}} \equiv \sinh x_{\mathbf{k}}. \tag{1.5}$$

The normalized Fock-state vector of $b_{\mathbf{k}}$ is expanded in terms of the states of $a_{\mathbf{k}}$ as follows:

$$|r,s\rangle_b = e^T |r,s\rangle_a = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} |p,q\rangle_a G_{pq;rs}(x_{\mathbf{k}}) \tag{1.6}$$

with

$$G_{pq;rs}(x_{\mathbf{k}}) = {}_a\langle p,q| e^T |r,s\rangle_a, \tag{1.7}$$

$$|r,s\rangle_a = \frac{1}{\sqrt{r!\,s!}}(a_{\mathbf{k}}^\dagger)^r (a_{-\mathbf{k}}^\dagger)^s |0\rangle_a$$

and (1.8)

$$|r,s\rangle_b = \frac{1}{\sqrt{r!\,s!}}(b_{\mathbf{k}}^\dagger)^r (b_{-\mathbf{k}}^\dagger)^s |0\rangle_b.$$

The vacuum $|0\rangle_a$ and $|0\rangle_b$ are respectively defined by

$$a_{\mathbf{k}}|0\rangle_a = 0 \quad \text{and} \quad b_{\mathbf{k}}|0\rangle_b = 0. \tag{1.9}$$

For the fermion case the expansion coefficient analogous to (1.7) is well known.[3]

There is also interest in the linear transformation for the boson with zero momentum.[4] In such a case, suppressing the momentum suffix, we have, instead of (1.2),

$$\begin{aligned} b &= ua + va^\dagger = e^S a e^{-S}, \\ b^\dagger &= ua^\dagger + va = e^S a^\dagger e^{-S}, \end{aligned} \tag{1.10}$$

with

$$S = -\tfrac{1}{2}x(a^\dagger a^\dagger - aa) = -S^\dagger. \tag{1.11}$$

Then the real parameters u and v are given by

$$u = \cosh x \quad \text{and} \quad v = \sinh x. \tag{1.12}$$

The normalized Fock-state vector of the quasiparticles is expanded as follows:

$$|l\rangle_b = e^S|l\rangle_a = \sum_{k=0}^{\infty} |k\rangle_a G_{kl}(x), \tag{1.13}$$

with

$$G_{kl}(x) = {}_a\langle k|e^S|l\rangle_a, \tag{1.14}$$

$$|k\rangle_a = (1/\sqrt{k!})(a^\dagger)^k|0\rangle_a \quad \text{and} \quad |k\rangle_b = (1/\sqrt{k!})(b^\dagger)^k|0\rangle_b. \tag{1.15}$$

The vacuum states are defined similarly to (1.9).

The purpose of the present paper is to derive the exact expression for the expansion coefficients defined by (1.7) and (1.14). In Sec. 2 the coefficient given by (1.14) is expanded into the infinite series in terms of the one-dimensional harmonic oscillator wavefunctions. In Sec. 3 further reduction of the series is carried out by frequent use of the properties of hypergeometric function, and its compact form is derived. In Sec. 4 it is shown that the coefficient defined by (1.7) is expressed in terms of the coefficients (1.14).

2. EXPANSION OF COEFFICIENT FOR ZERO MOMENTUM BOSON

To reexpress the quantity defined by (1.14) in analytic form, we replace the operators $a^\dagger$, a and the ket vacuum $|0\rangle_a$ by a scalar variable ξ, the differential operator $d/d\xi$, and unity, respectively. Then, due to the commutation relation $[d/d\xi, \xi] = 1$, the correct expectation value is obtained by putting $\xi = 0$, after all the differentiations are performed, i.e.,

$$\begin{aligned} G_{kl}(x) &= \frac{1}{\sqrt{k!\,l!}}\, {}_a\langle 0| a^k \exp\left(-\frac{x}{2}(a^\dagger a^\dagger - aa)\right)(a^\dagger)^l|0\rangle_a \\ &= \frac{1}{\sqrt{k!\,l!}} \frac{d^k}{d\xi^k}\left[\exp\left(-\frac{x}{2}\left(\xi^2 - \frac{d^2}{d\xi^2}\right)\right)\xi^l\right]_{\xi=0}. \end{aligned} \tag{2.1}$$

The power of ξ can be expanded in terms of the orthonormal set of harmonic oscillator wavefunctions $u_n(\xi) = N_n \exp(-\xi^2/2)H_n(\xi)$ satisfying

$$(\xi^2 - d^2/d\xi^2)u_n(\xi) = (2n+1)u_n(\xi), \tag{2.2}$$

where $N_n = (\pi^{1/2}2^n n!)^{-1/2}$ and $H_n(\xi)$ is the Hermite polynomial of nth order. Making use of the defining properties of the Hermite polynomial,[5] we obtain

$$\xi^l = \sum_{m=0}^{\infty} I_{lm} N_m u_m(\xi) \tag{2.3}$$

with

$$I_{lm} = \int_{-\infty}^{\infty} d\xi\, \xi^l H_m(\xi) \exp(-\tfrac{1}{2}\xi^2) = \pi^{1/2} l!\, m! \sum_{n=0}^{\min(l,m)}{}' \frac{2^{(l+n+1)/2}}{2^{l-n} n! [\frac{1}{2}(l-n)]! [\frac{1}{2}(m-n)]!}, \tag{2.4}$$

where the primed summation extends only over the values of n which make both $l - n$ and $m - n$ even integers.

The following formulas,

$$\frac{d^p}{d\xi^p} H_n(\xi) = 2^p \frac{m!}{(m-p)!} H_{n-p}(\xi), \tag{2.5}$$

$$H_{2q}(0) = (-1)^q \frac{(2q)!}{q!}, \quad \text{and} \quad H_{2q+1}(0) = 0, \tag{2.6}$$

are applied to give the relation

$$\frac{d^k}{d\xi^k}[H_m(\xi) \exp(-\tfrac{1}{2}\xi^2)]_{\xi=0} = (-1)^{(3k+m)/2} \sum_{p=0}^{\min(k,m)}{}' 2^{(3p-k)/2} \frac{k!\, m!}{p! [\frac{1}{2}(m-p)]! [\frac{1}{2}(k-p)]!}. \tag{2.7}$$

Making use of (2.3), (2.4) together with (2.7) in (2.1), we obtain

$$\begin{aligned} G_{kl}(x) &= \left(\frac{l!}{k!}\right)^{1/2} \sum_{m=0}^{\infty} \sum_{n=0}^{\min(l,m)} \frac{(2^{3n-l-2m} e^{-x(2m+1)})^{1/2}}{n! [\frac{1}{2}(l-n)]! [\frac{1}{2}(m-n)]!} \times \frac{d^k}{d\xi^k}[H_m(\xi) e^{-\xi^2/2}]_{\xi=0} \\ &= [(-1)^{3k} k!\, l!\, 2^{-(k+l-1)} e^{-x}]^{1/2} \sum_{m=0}^{\infty} \frac{(-1)^{m/2} m!}{2^m e^{mx}} \times \sum_{n=0}^{\min(l,m)}{}' \frac{2^{3n/2}}{n! [\frac{1}{2}(l-n)]! [\frac{1}{2}(m-n)]!} \\ &\quad \times \sum_{p=0}^{\min(k,m)}{}' \frac{2^{3p/2}}{p! [\frac{1}{2}(k-p)]! [\frac{1}{2}(m-p)]!}. \end{aligned} \tag{2.8}$$

Putting $q = (m-n)/2$, and changing the double summation $\sum_{m=0}^{\infty} \sum_{n=0}^{\min(l,m)}{}'$ into $\sum_{n=0}^{l}{}' \sum_{q=0}^{\infty}{}'$, and further $\sum_{q=0}^{\infty}{}' \sum_{p=0}^{\min(k,2q+n)}{}'$ into $\sum_{p=0}^{k}{}' \sum_{q=0}^{\infty}$, we can rewrite (2.8) as follows,

$$G_{kl}(x) = \left[\frac{(-1)^{3k} k!\, l!}{2^{k+l-1} e^x}\right]^{1/2} \sum_{n=0}^{l}{}' \frac{(-2)^{n/2} e^{-nx}}{n! [\frac{1}{2}(l-n)]!} \times \sum_{p=0}^{k}{}' \frac{2^{3p/2}}{p! [\frac{1}{2}(k-p)]!} \sum_{q=0}^{\infty} (-2e^x)^{-2q} \frac{(2q+n)!}{q! [q + \frac{1}{2}(n-p)]!}. \tag{2.9}$$

Further manipulations are required to reduce the infinite series in (2.9) to compact form. If we introduce the hypergeometric function[6] defined by

$$F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} \sum_{\lambda=0}^{\infty} \frac{\Gamma(\alpha+\lambda)\Gamma(\beta+\lambda)}{\Gamma(\gamma+\lambda)} \frac{z^\lambda}{\lambda!} \quad \text{for } |z| < 1, \tag{2.10}$$

and use the formula

$$\Gamma(2\nu) = (2^{2\nu}/2\pi^{1/2}) \Gamma(\nu) \Gamma(\nu + \tfrac{1}{2}), \tag{2.11}$$

we have for the summation in (2.9)

$$\sum_{q=0}^{\infty} (-2e^x)^{-2q} \frac{(2q+n)!}{q! [q + \frac{1}{2}(n-p)]!} = \frac{2^n}{\pi^{1/2}} \frac{\Gamma(\frac{1}{2}(n+1)) \Gamma(\frac{1}{2}n + 1)}{\Gamma(\frac{1}{2}(n-p)+1)} \times F(\tfrac{1}{2}(n+1), \tfrac{1}{2}n + 1, \tfrac{1}{2}(n-p) + 1; z). \tag{2.12}$$

To guarantee that the variable $z = -\exp(-2x)$ is within the convergence domain, we temporarily assume $x > 0$. However, we will find this restriction can be discarded in the final result.

According to the formula[7]

$$\begin{aligned} \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\gamma)} F(\alpha, \beta, \gamma; z) &= \frac{\Gamma(\alpha)\Gamma(\beta - \alpha)}{\Gamma(\gamma - \alpha)} (1-z)^{-\alpha} \times F\left(\alpha, \gamma - \beta, \alpha - \beta + 1; \frac{1}{1-z}\right) \\ &\quad + \frac{\Gamma(\beta)\Gamma(\alpha - \beta)}{\Gamma(\gamma - \beta)} (1-z)^{-\beta} F\left(\beta, \gamma - \alpha, \beta - \alpha + 1; \frac{1}{1-z}\right), \end{aligned} \tag{2.13}$$

for $|1 - z| > 1$ and $z \neq$ positive real number, (2.12) is rewritten in the alternative form

$$\begin{aligned} \sum_{q=0}^{\infty} (-2e^x)^{-2q} \frac{(2q+n)!}{q! [q + \frac{1}{2}(n-p)]!} &= \frac{2^n}{\pi^{1/2}} \left[\frac{\Gamma(\frac{1}{2}(n+1))\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}(1-p))} \times (1-z)^{-(n+1)/2} F\left(\frac{n+1}{2}, -\frac{p}{2}, \frac{1}{2}; \frac{1}{1-z}\right) \right. \\ &\quad \left. + \frac{\Gamma(\frac{1}{2}n+1)\Gamma(-\frac{1}{2})}{\Gamma(-\frac{1}{2}p)} (1-z)^{-\frac{n}{2}-1} \times F\left(\frac{n}{2}+1, \frac{1-p}{2}, \frac{3}{2}; \frac{1}{1-z}\right)\right] \\ &= \frac{2^n}{\pi^{1/2}} \left[\frac{\Gamma\left(\frac{n+1}{2}\right) \Gamma \frac{p+1}{2} \cos(\frac{1}{2}\pi p)}{(1-z)^{(n+1)/2}} \times F\left(-\frac{p}{2}, \frac{n+1}{2}, \frac{1}{2}; \frac{1}{1-z}\right) \right. \\ &\quad \left. - 2 \frac{\Gamma(\frac{1}{2}n+1)\Gamma(\frac{1}{2}p+1) \cos[\frac{1}{2}\pi(p+1)]}{(1-z)^{(n/2)+1}} \times F\left(\frac{1-p}{2}, \frac{n}{2}+1, \frac{3}{2}; \frac{1}{1-z}\right)\right]. \end{aligned} \tag{2.14}$$

In the above the last expression is obtained by using the formulas

$$\Gamma(\nu + \tfrac{1}{2}) \Gamma(\tfrac{1}{2} - \nu) = \pi / \cos \pi\nu \quad \text{and} \quad \Gamma(\nu)\Gamma(1-\nu) = \pi / \sin \pi\nu, \tag{2.15}$$

together with $\Gamma(1/2) = \pi^{1/2}$ and $\Gamma(-\frac{1}{2}) = -2\pi^{1/2}$.

Thus the double summation appearing in (2.9) is expressed as

$$\sum_{p=0}^{k}{}' \frac{2^{3p/2}}{p! [\frac{1}{2}(k-p)]!} \sum_{q=0}^{\infty} (-2e^x)^{-2q} \frac{(2q+n)!}{q! [q + \frac{1}{2}(n-p)]!} = \frac{2^n}{\pi^{1/2}} \frac{\Gamma(\frac{1}{2}(n+1))}{(\frac{1}{2}k)! (1-z)^{(n+1)/2}} \sum_{r=0}^{\infty}{}' \frac{(-2)^r (\frac{1}{2}k)!}{r! (\frac{1}{2}k - r)!}$$

$$\times F\left(-r,\frac{n+1}{2},\frac{1}{2};\frac{1}{1-z}\right)$$
$$+\frac{2^{n+3/2}}{\pi^{1/2}}\frac{\Gamma(\frac{1}{2}n+1)}{[\frac{1}{2}(k-1)]!(1-z)^{n/2+1}}\sum_{r=0}^{\infty}{}'$$
$$\times\frac{(-2)^r[\frac{1}{2}(k-1)]!}{r![\frac{1}{2}(k-1)-r]!}F\left(-r,\frac{n}{2}+1,\frac{3}{2};\frac{1}{1-z}\right), \quad (2.16)$$

only if we note that the replacement of the upper limit for the sum with respect to p does not affect the result because of the occurrence of the factorial of the negative integer in the denominator of the lhs.

Taking into account the fact that, in the primed summation, there also occur the factorials $(\frac{1}{2}k-r)!$ and $[\frac{1}{2}(k-1)-r]!$ in the denominators of rhs of (2.16), we separate two cases as follows:

$$(2.16)=\begin{cases}\dfrac{2^n}{\pi^{1/2}}\dfrac{\Gamma(\frac{1}{2}(n+1))}{(1-z)^{(n+1)/2}(\frac{1}{2}k)!}\displaystyle\sum_{r=0}^{\infty}(-2)^r\binom{\frac{1}{2}k}{r}F\left(-r,\frac{n+1}{2},\frac{1}{2};\frac{1}{1-z}\right), & \text{if } k \text{ even,}\\[2ex] \dfrac{2^{n+3/2}}{\pi^{1/2}}\dfrac{\Gamma(\frac{1}{2}n+1)}{(1-z)^{(n/2)+1}[\frac{1}{2}(k-1)]!}\displaystyle\sum_{r=0}^{\infty}(-2)^r\binom{\frac{1}{2}k-1}{r}F\left(-r,\frac{n}{2}+1,\frac{3}{2};\frac{1}{1-z}\right), & \text{if } k \text{ odd.}\end{cases} \quad (2.17)$$

It is obvious that if k is even (odd) and l odd (even), the coefficient vanishes by its definition (2.9).

To carry out the summation in (2.17), we make use of the formula

$$\sum_{\mu=0}^{\infty}\binom{\lambda}{\mu}s^{\mu}F(-\mu,\beta,\gamma;z)=(1+s)^{\lambda}F(-\lambda,\beta,\gamma;sz/(1+s)) \quad (2.18)$$

with $s=-2$. Thus, with (2.9) and (2.16), we immediately reach the following results:

$$G_{kl}(x)=\begin{cases}\dfrac{1}{(\frac{1}{2}k)!(\frac{1}{2}l)!}\left(\dfrac{k!l!}{2^{k+l}\cosh x}\right)^{1/2}\displaystyle\sum_{s=0}^{l/2}\binom{\frac{1}{2}l}{s}\left(\dfrac{-2e^{-2x}}{1+e^{-2x}}\right)^{s}F\left(s+\frac{1}{2},-\frac{k}{2},\frac{1}{2};\frac{2}{1+e^{-2x}}\right), & \text{if } k \text{ and } l \text{ even,}\\[2ex] \dfrac{1}{[\frac{1}{2}(k-1)]![\frac{1}{2}(l-1)]!}\left(\dfrac{k!l!}{2^{k+l-2}\cosh^3 x}\right)^{1/2}\displaystyle\sum_{s=0}^{(l-1)/2}\binom{\frac{1}{2}(l-1)}{s}\left(\dfrac{-2e^{-2x}}{1+e^{-2x}}\right)^{s}F\left(s+\frac{3}{2},-\frac{k-1}{2},\frac{3}{2};\frac{2}{1+e^{-2x}}\right), & \text{if } k \text{ and } l \text{ odd,}\\[2ex] 0, \quad \text{otherwise}\end{cases} \quad (2.19)$$

for $x>0$. However, we must be careful in dealing with the series for the hypergeometric function with the fourth argument greater than unity for $x>0$. This problem is solved in the next section.

3. DETERMINATION OF COEFFICIENT FOR ZERO MOMENTUM BOSON

The following analytic continuation formula[8] is appropriate for defining the concrete functional dependence of the hypergeometric function with the fourth argument greater than unity:

$$F(\alpha,\beta,\gamma;z)=\frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}z^{-\alpha}$$
$$\times F(\alpha,\alpha+1-\gamma,\alpha+\beta+1-\gamma;1-z^{-1})$$
$$+\frac{\Gamma(\gamma)\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\Gamma(\beta)}z^{\alpha-\gamma}(1-z)^{\gamma-\alpha-\beta}$$
$$\times F(\gamma-\alpha,1-\alpha,\gamma+1-\alpha-\beta;1-z^{-1}), \quad (3.1)$$

where it is assumed that $|\arg z|<\pi$ and that $1-\gamma$, $\beta-\alpha$, and $\gamma-\alpha-\beta$ are in general not integers. It is observed that, only if an infinitesimal quantity ϵ is added to the second arguments of the hypergeometric functions appearing in (2.19), are all the conditions presented below (3.1) satisfied. Applying (3.1), we have, if k is even,

$$F\left(s+\frac{1}{2},-\frac{k}{2}+\epsilon,\frac{1}{2};\frac{2}{1+e^{-2x}}\right)$$
$$=\frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2}k-s-\epsilon)}{\Gamma(-s)\Gamma(\frac{1}{2}(k+1)-\epsilon)}\left(\frac{1+e^{-2x}}{2}\right)^{s+1/2}$$
$$\times F\left(s+\frac{1}{2},s+1,s-\frac{k}{2}+1+\epsilon;\frac{1-e^{-2x}}{2}\right)$$
$$+\frac{\Gamma(\frac{1}{2})\Gamma(s-\frac{1}{2}k+\epsilon)}{\Gamma(s+\frac{1}{2})\Gamma(-\frac{1}{2}k+\epsilon)}\left(\frac{1+e^{-2x}}{2}\right)^{-s}\left(-\frac{1-e^{-2x}}{1+e^{-2x}}\right)^{k/2-s-\epsilon}$$
$$\times F\left(-s,\frac{1}{2}-s,\frac{k}{2}-s+1-\epsilon;\frac{1-e^{-2x}}{2}\right), \quad (3.2)$$

where the first term vanishes because of the divergence of the gamma function $\Gamma(-s)$ in the denominator and the fact that the hypergeometric function is well defined in terms of the convergent series. Thus, if k is even,

$$F\left(s+\frac{1}{2},-\frac{k}{2}+\epsilon,\frac{1}{2};\frac{2}{1+e^{-2x}}\right)$$
$$=\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(s+\frac{1}{2}\right)}\frac{(s-1-\frac{1}{2}k+\epsilon)(s-2-\frac{1}{2}k+\epsilon)\cdots(-\frac{1}{2}k+\epsilon)\Gamma(-\frac{1}{2}k+\epsilon)}{\Gamma(-\frac{1}{2}k+\epsilon)}\left(\frac{1+e^{-2x}}{2}\right)^{-s}\left(-\frac{1-e^{-2x}}{1+e^{-2x}}\right)^{k/2-s-\epsilon}$$
$$\times\sum_{\mu=0}^{\infty}\left(\frac{1-e^{-2x}}{2}\right)^{\mu}\frac{(-s)(-s+1)\cdots(-s+\mu-1)\cdot(\frac{1}{2}-s)(\frac{1}{2}-s+1)\cdots(\frac{1}{2}-s+\mu-1)}{\mu!(\frac{1}{2}k-s+1-\epsilon)(\frac{1}{2}k-s+2-\epsilon)\cdots(\frac{1}{2}k-s+\mu-\epsilon)}$$

$$\to \pi^{1/2}(\tfrac{1}{2}k)!\,s!\left(\frac{-2}{1+e^{-2x}}\right)^{s}\left(-\frac{1-e^{-2x}}{1+e^{-2x}}\right)^{k/2-s}\sum_{\lambda=\max(0,s-k/2)}^{s}\frac{[\frac{1}{2}(1-e^{-2x})]^{\lambda}}{\lambda!(\lambda+\frac{1}{2}k-s)!(s-\lambda)!(s-\frac{1}{2}-\lambda)!}, \tag{3.3}$$

as $\epsilon \to 0$. Similarly, if k is odd

$$F\left(s+\frac{3}{2},-\frac{k-1}{2}+\epsilon,\frac{3}{2};\frac{2}{1+e^{-2x}}\right)$$
$$\to \frac{\pi^{1/2}}{2}\left(\frac{k-1}{2}\right)!\,s!\left(\frac{-2}{1+e^{-2x}}\right)^{s}\left(-\frac{1-e^{-2x}}{1+e^{-2x}}\right)^{(k-1)/2-s}\sum_{\lambda=\max(0,s-(k-1)/2)}^{s}\frac{[\frac{1}{2}(1-e^{-2x})]^{\lambda}}{\lambda![\lambda+\frac{1}{2}(k+1)-s]!(s-\lambda)!(s+\frac{1}{2}-\lambda)!}, \tag{3.4}$$

as $\epsilon \to 0$. By adopting the expressions given by (3.3) and (3.4), the functional dependence of (2.19) is manifested at a glance in the following forms:

$$G_{kl}(x)=\begin{cases}\left(\dfrac{k!\,l!}{2^{k+l}\cosh x}\right)^{1/2}(-\tanh x)^{k/2}\displaystyle\sum_{\mu=0}^{l/2}\frac{(-\cosh x\,\sinh x/4)^{-\mu}}{(\frac{1}{2}l-\mu)!}\sum_{\nu=\max(0,\mu-k/2)}^{\mu}\frac{[\frac{1}{8}(1-e^{-2x})]^{\nu}}{\nu!(\nu+\frac{1}{2}k-\mu)!(2\mu-2\nu)!}, & \text{if } k \text{ and } l \text{ even},\\[2ex] \left(\dfrac{k!\,l!}{2^{k+l-2}\cosh^{3}x}\right)^{1/2}(-\tanh x)^{(k-1)/2}\displaystyle\sum_{\mu=0}^{(l-1)/2}\frac{(-\cosh x\,\sinh x/4)^{-\mu}}{(\frac{1}{2}(l-1)-\mu)!}\sum_{\nu=\max(0,\mu-(k-1)/2)}^{\mu}\frac{[\frac{1}{8}(1-e^{-2x})]^{\nu}}{\nu!(\nu+\frac{1}{2}(k-1)-\mu)!(2\mu+1-2\nu)!}, & \text{if } k \text{ and } l \text{ odd},\\[2ex] 0, \quad \text{otherwise.}\end{cases} \tag{3.5}$$

For the purpose of recovering the apparent symmetry between k and l we put $\lambda=\nu-\mu$, change the double summation $\sum_{\mu=0}^{l/2}\sum_{\nu=\max(0,\mu-k/2)}^{\mu}\left(\sum_{\mu=0}^{l/2}\sum_{\nu=\max(0,\mu-(k-1)/2)}^{\mu}\right)$ into $\sum_{\lambda=0}^{\min(k/2,l/2)}\sum_{\nu=0}^{l/2-\lambda}\left(\sum_{\lambda=0}^{\min((k-1)/2,(l-1)/2)}\sum_{\nu=0}^{(l-1)/2-\lambda}\right)$, and have

$$G_{kl}(x)=\begin{cases}\left(\dfrac{k!\,l!}{2^{k+l}\cosh x}\right)^{1/2}(-\tanh x)^{k/2}\displaystyle\sum_{\lambda=0}^{\min(k/2,l/2)}\frac{(-\sinh x\,\cosh x/4)^{-\lambda}}{(2\lambda)!(\frac{1}{2}k-\lambda)!(\frac{1}{2}l-\lambda)!}\left[\sum_{\nu=0}^{l/2-\lambda}\binom{\frac{1}{2}l-\lambda}{\nu}(-e^{x}\cosh x)^{-\nu}\right], & \text{for } k, l \text{ even},\\[2ex] \left(\dfrac{k!\,l!}{2^{k+l-2}\cosh^{3}x}\right)^{1/2}(-\tanh x)^{(k-1)/2}\displaystyle\sum_{\lambda=0}^{\min((k-1)/2,(l-1)/2)}\frac{(-\sinh x\,\cosh x/4)^{-\lambda}}{(2\lambda+1)![\frac{1}{2}(k-1)-\lambda]![\frac{1}{2}(l-1)-\lambda]!}\\ \quad\times\left[\displaystyle\sum_{\nu=0}^{(l-1)/2-\lambda}\binom{\frac{1}{2}(l-1)-\lambda}{\nu}(-e^{x}\cosh x)^{-\nu}\right], & \text{for } k, l \text{ odd}.\end{cases} \tag{3.6}$$

Since the sums in the square brackets in (3.6) are nothing but binomial expansions, we finally complete the compact expression of the functional dependence for the coefficient $G_{kl}(x)$ as follows:

$$G_{kl}(x)=\begin{cases}(-1)^{k/2}\left(\dfrac{k!\,l!}{2^{k+l}\cosh x}\right)^{1/2}(\tanh x)^{(k+l)/2}\displaystyle\sum_{\lambda=0}^{\min(k/2,l/2)}\frac{(-4/\sinh^{2}x)^{\lambda}}{(2\lambda)!(\frac{1}{2}k-\lambda)!(\frac{1}{2}l-\lambda)!}, & \text{for } k, l \text{ even},\\[2ex] (-1)^{(k-1)/2}\left(\dfrac{k!\,l!}{2^{k+l-2}\cosh^{3}x}\right)^{1/2}(\tanh x)^{(k+l)/2-1}\displaystyle\sum_{\lambda=0}^{\min((k-1)/2,(l-1)/2)}\frac{(-4/\sinh^{2}x)^{\lambda}}{(2\lambda+1)![\frac{1}{2}(k-1)-\lambda]![\frac{1}{2}(l-1)-\lambda]!}, & \text{for } k, l \text{ odd},\\[2ex] 0, \quad \text{otherwise.}\end{cases} \tag{3.7}$$

As the direct results from (3.7) we obtain

$$G_{kl}(-x)=\begin{cases}(-1)^{(k+l)/2}G_{kl}(x), & \text{for } k, l \text{ even},\\ (-1)^{(k+l)/2-1}G_{kl}(x), & \text{for } k, l \text{ odd},\end{cases} \tag{3.8}$$

and

$$G_{lk}(x)=\begin{cases}(-1)^{(k+l)/2}G_{kl}(x), & \text{for } k, l \text{ even},\\ (-1)^{(k+l)/2-1}G_{kl}(x), & \text{for } k, l \text{ odd}.\end{cases} \tag{3.9}$$

A simple relation follows from (3.8) and (3.9), i.e.,

$$G_{kl}(-x)=G_{lk}(x) \tag{3.10}$$

which can be directly proved from the definition of the coefficient in (2.1). This fact shows the correctness of (3.8) derived by assuming that our expressions in (3.7) hold for any value of x. Therefore, (3.7) gives correctly the desired expressions for $G_{kl}(x)$ defined for any real number x in (2.1). As special cases, (3.7) provides

$$G_{00}(x)=\cosh^{-1/2}x \text{ and } G_{11}(x)=\cosh^{-3/2}x \tag{3.11}$$

as given by Eq. (20) in Ref. 4.

It is straightforwardly proved that $G_{kl}(x)$ satisfies the following orthonormality condition:

$$\sum_{k=0}^{\infty}G_{kl}(x)G_{kl'}(x)=\delta_{ll'}. \tag{3.12}$$

4. DETERMINATION OF BOGOLIUBOV TRANSFORMATION COEFFICIENT

In calculating the expectation value defined by (1.7), it is profitable to replace the operators $a_{\mathbf{k}}^{\dagger}$, $a_{-\mathbf{k}}^{\dagger}$, and $a_{\mathbf{k}}$, $a_{-\mathbf{k}}$, and the ket vacuum $|0\rangle_a$ by two independent scalar variables α, β, differential operators $\partial/\partial\alpha$, $\partial/\partial\beta$, and unity, respectively. Similarly to (2.1) we set

$$G_{pq;rs}(x_{\mathbf{k}}) = \frac{1}{\sqrt{p!q!}} \frac{\partial^q}{\partial\alpha^p} \frac{\partial^q}{\partial\beta^q} \left[\exp\left(-x_{\mathbf{k}}\left(\alpha\beta - \frac{\partial^2}{\partial\alpha\partial\beta}\right)\right) \frac{\alpha^r\beta^s}{\sqrt{r!s!}}\right]_{\substack{\alpha=0\\ \beta=0}}. \quad (4.1)$$

If we introduce new variables ξ and η by

$$\xi = (\alpha + \beta)/\sqrt{2} \quad \text{and} \quad \eta = (\alpha - \beta)/i\sqrt{2}, \quad (4.2)$$

so that $\frac{\partial}{\partial\alpha} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial\xi} - i\frac{\partial}{\partial\eta}\right)$ and $\frac{\partial}{\partial\beta} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial\xi} + i\frac{\partial}{\partial\eta}\right)$, we have

$$\begin{aligned} G_{pq;rs}(x_{\mathbf{k}}) &= (2^{p+q+r+s}p!q!r!s!)^{-1/2} \left[\left(\frac{\partial}{\partial\xi} - i\frac{\partial}{\partial\eta}\right)^p \left(\frac{\partial}{\partial\xi} + i\frac{\partial}{\partial\eta}\right)^q \right. \\ &\quad \times \exp\left\{-\frac{x_{\mathbf{k}}}{2}\left(\xi^2 - \frac{\partial^2}{\partial\xi^2}\right) - \frac{x_{\mathbf{k}}}{2}\left(\eta^2 - \frac{\partial^2}{\partial\eta^2}\right)\right\} \\ &\quad \left. \times (\xi + i\eta)^r(\xi - i\eta)^s \right]_{\substack{\xi=0\\ \eta=0}} \\ &= (2^{p+q+r+s}p!q!r!s!)^{-1/2} \\ &\quad \times \sum_{\mu=0}^{p}\sum_{\nu=0}^{q}\sum_{\rho=0}^{r}\sum_{\sigma=0}^{s} \binom{p}{\mu}\binom{q}{\nu}\binom{r}{\rho}\binom{s}{\sigma} (-i)^{\mu+\sigma} i^{\nu+\rho} \\ &\quad \times \left[\frac{d^{p+q-\mu-\nu}}{d\xi^{p+q-\mu-\nu}} \left\{\exp\left(-\frac{x_{\mathbf{k}}}{2}\left(\xi^2 - \frac{d^2}{d\xi^2}\right)\right) \xi^{r+s-\rho-\sigma}\right\}\right]_{\xi=0} \\ &\quad \times \left[\frac{d^{\mu+\nu}}{d\eta^{\mu+\nu}} \left\{\exp\left(-\frac{x_{\mathbf{k}}}{2}\left(\eta^2 - \frac{d^2}{d\eta^2}\right)\right) \eta^{\rho+\sigma}\right\}\right]_{\eta=0}. \end{aligned} \quad (4.3)$$

Since the two square brackets in (4.3) correspond essentially to the quantities given by (2.1), we can rewrite (4.3) as follows:

$$\begin{aligned} G_{pq;rs}(x_{\mathbf{k}}) &= (2^{p+q+r+s}p!q!r!s!)^{-1/2} \sum_{\mu=0}^{p}\sum_{\nu=0}^{q}\sum_{\rho=0}^{r}\sum_{\sigma=0}^{s} \binom{p}{\mu}\binom{q}{\nu}\binom{r}{\rho}\binom{s}{\sigma} \\ &\quad \times [(-1)^{\mu+\sigma-\nu-\rho}(p+q-\mu-\nu)!(r+s-\rho-\sigma)! \\ &\quad \times (\mu+\nu)!(\rho+\sigma)!]^{1/2} G_{p+q-\mu-\nu,r+s-\rho-\sigma}(x_{\mathbf{k}}) G_{\mu+\nu,\rho+\sigma}(x_{\mathbf{k}}). \end{aligned} \quad (4.4)$$

The contributions to the sum come only from the terms in which both $\mu + \nu$ and $\rho + \sigma$ are even or odd, and both $p + q - \mu - \nu$ and $r + s - \rho - \sigma$ even or odd. Consequently $G_{pq;rs}(x_{\mathbf{k}})$ vanishes, if $p + q$ is odd (even) and $r + s$ even (odd). On the other hand, the conservation of momentum adds another restriction, $p - q = r - s$. It is straightforward to show by using (3.10) that

$$G_{rs;pq}(-x_{\mathbf{k}}) = G_{pq;rs}(x_{\mathbf{k}}), \quad (4.5)$$

which is also expected from the definition given by (1.7) or (4.1).

In conclusion the problem of determining the transformation coefficient explicitly is solved with the final expressions given by (3.7) and (4.5).

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Generating functional for covariant time-ordered products of currents

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Assuming that a functional of the form $F(A) = T\exp(iB(A))$ generates covariant time-ordered products of currents, general properties under Lorentz transformations are derived for the expansion coefficients of the functional $B(A)$. The functional $B(A)$ is explicitly constructed for the case of simple commutations relations between currents. The Feynman conjecture is discussed.

1. INTRODUCTION

It is well known that the usual time-ordered product (TP) of currents is not covariant under the general Lorentz transformation. The noncovariance is caused by the presence of Schwinger terms (ST) in the commutators of some currents.

The problem of covariant time-ordered products (CTP) was studied by Brown[1] in the framework of canonical theory and gauge principles. There, the approach is essentially functional, but the existence of the Hamiltonian and of a time evolution operator is assumed. In the present work the functional is treated only formally. It is generally needed to shorten expressions, to keep symmetrization, etc., with no effort made to give the functionals a strict mathematical meaning. The same problem was treated from the algebraic point of view by Dashen and Lee.[2] Our general form coincides with the low-ordered CTP given in Ref. 2. In this paper we shall assume that formally the CTP of currents can be given by the functional $F(A) = T[\exp(iB(A))]$, where T stands for the chronological time-ordering operator.

The CTP of n currents $T^*(J^{\mu_1}_{a_1}(x_1)\cdots J^{\mu_n}_{a_n}(x_n))$ is given by the formal functional derivative of order n, i.e.,

$$T^*(J^{\mu_1}_{a_1}(x_1)\cdots J^{\mu_n}_{a_n}(x_n)) = (i)^{-n}\partial_{A^{a_1}_{\mu_1}(x_1)}\cdots\partial_{A^{a_n}_{\mu_n}(x_n)}F(A)\Big|_{A=0} \tag{1.1}$$

We shall derive general transformation properties for the functional $B(A)$, which are necessary and sufficient for the functional $F(A)$ to be Lorentz covariant. The explicit form of $B(A)$ is given when the commutation relations among the currents involve at most first order derivatives of the δ function in ST. The Feynman conjecture is studied in this case.

2. DEFINITIONS

We denote by $G(A)$ a general functional which has a formal Volterra expansion:

$$F(A) = \sum_{n=0}^{\infty}\frac{1}{n!}\int\cdots\int F^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1\cdots x_n)\times A^{a_1}_{\mu_1}(x_1)\cdots A^{a_n}_{\mu_n}(x_n)dx_1\cdots dx_n. \tag{2.1}$$

μ_i stands for the Lorentz index, a_i for the symmetry index, x is the coordinate in Minkowski space. The coefficients $F^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1\cdots x_n)$ are operator-valued distributions. To give a mathematical meaning to the above expression, one should choose the functions $A^a_\mu(x)$ from a set of test functions and demand the convergence of (2-1) in the weak sense. Note that only the symmetric part of $F^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1\cdots x_n)$ contributes, and is given by

$$S_n F^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n} = \partial_{A^{a}_{\mu_1}(x_1)}\cdots\partial_{A^{a_1}_{\mu_n}(x_1)}F(A)\Big|_{A=0} \equiv D^{\mu_1}_{a_1}(x_i)\cdots D^{\mu_n}_{a_n}(x_n)F(A)\Big|_{A=0}, \tag{2.2}$$

where S_n stands for the symmetrizer of order n on the set of indices $(1\cdots n)$. We can therefore limit ourselves to symmetric coefficients. Often formal notations such as

$$F(A) = \sum(1/n!)F_nA^n,$$
$$D^{\mu_1}_{a_1}(x_i)\cdots D^{\mu_n}_{a_n}(x_n)F(A) = D^nF(A) \tag{2.3}$$

will be used.

It is known that the usual TP of currents is generated by the functional

$$F(A) = T\{\exp[i\textstyle\int dxJ^\mu_a(x)A^a_\mu(x)]\} \tag{2.4}$$

($\int dx$ stands for four-dimensional integration).

The above functional also satisfies the following conditions:

1. Unitarity, i.e., $F(A)F^\dagger(A) = F^\dagger(A)F(A) = 1$, $F^\dagger(A) = T^\dagger\{\exp[-i\int J^\mu_a(x)A^a_\mu(x)dx]\}$, $T^\dagger$ is the antichronological ordering operator.
2. Causality, i.e., $D^\mu_a(x)(F^\dagger(A)D^\nu_b(y)F(A)) = 0$ for $x \gtrsim y$, i.e., $x_0 > y_0$ and $(y-x)^2 < 0$.

The above form of $F(A)$ is also obtained from Assumptions 1 and 2 except for some "quasilocal" terms, which may be generated by a functional $B(A)$.[3,4] Therefore we take the $F(A)$ to be of the form[5]

$$F(A) = T\exp[iB(A)].$$

For the functional $B(A)$ we require that

$$B(A) = B^\dagger(A), \tag{2.5}$$

$$[B(A), B(\tilde{A})] = 0 \quad \text{for supp}\,A \sim \text{supp}\tilde{A}, \tag{2.6}$$

where $\text{supp}A = \{x; A^\mu_a(x) \neq 0\}$; $\theta \sim \omega$ means that the sets θ, ω are spacelike separated, i.e.,

$$x \in \theta;\ y \in \omega \to (x-y)^2 < 0$$

and that $B(A)$ generates quasilocal fields,[4] i.e.,

$$D^{\mu_1}_{a_1}(x)\cdots D^{\mu_n}_{a_n}(x_n)B(A)|_{A=0} = B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1\cdots x_n) \neq 0$$

for $x_1 = x_2 = \cdots = x_n$ only,

$$D^\mu_a(x)B(A)|_{A=0} = J^\mu_a(x). \tag{2.7}$$

Let L denote the set of all covariant functionals, i.e., $G(A) \in L \to U(\Lambda)G(A)U(\Lambda^{-1}) = G(\Lambda A)$, $\Lambda A^\mu = \Lambda^{\mu\nu}$

$A_\nu(\Lambda^{-1}x)$, where Λ is a 4×4 matrix representing a Lorentz transformation in Minkowski space.

We require

$$F(A) \in L. \tag{2.8}$$

Condition (2.5) assures unitarity and (2.6) gives causality. In general, $B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1\cdots x_n)$ will be of the form

$$\sum_{i=1}^{k} S_n P_i(\partial^{\mu_1}\cdots\partial^{\mu_n}) b^{\mu_1\cdots\mu_n}_{i,a_1\cdots a_n}(x_1)\delta(x_1-x_2)\cdots\delta(x_1-x_n),$$

where $P(\cdots\partial\cdots)$ is a polynomial of derivatives, and $b^{\mu_1\cdots\mu_n}_{i,a_1\cdots a_n}(x)$ is a local field.

In the case where the polynomial is a constant, the functional $B(A)$ is

$$B(A) = \sum_{n=0}^{\infty}\frac{1}{n!}\int B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x)A^{a_1}_{\mu_1}(x)\cdots A^{a_n}_{\mu_n}(x)dx. \tag{2.9}$$

The functional $B(A,t) = \sum\int B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(\mathbf{x},t)A^{a_1}_{\mu_1}(\mathbf{x},t)\cdots A^{a_n}_{\mu_n}(\mathbf{x},t)d^3x$ corresponds to the interaction Hamiltonian in the canonical formulation[1] and represents a power expansion in an external field $A^a_\mu(x)$ coupled to the current $J^\mu_a(x)$.

We shall call the set $\{k_i\}$ a partition of order n if $\forall i$, $1 \le i \le n$, $k_i \ge 0$, and $\sum_{i=1}^n k_i\cdot i = n$, and define the following functions:

$$C(\{k\}_n) = 1/\prod_{i=1}^{n} k_i!,$$
$$T(\{k\}_n) = T\left\{\prod_{j=1}^{n}\left[\left(\frac{iD^jB(A)}{j!}\right)\Big|_{A=0}\right]^{k_j}\right\}. \tag{2.10}$$

3. TRANSFORMATION PROPERTIES

In this section we examine some results of Assumption (2.8). As $F(A) = \sum(1/n!)F_nA^n$ and $F(A)\in L \Longleftrightarrow F_nA^n \in L$, we can write for the generators of the infinitesimal Lorentz transformations $M^{\mu\nu}$ the commutation relation

$$[M^{\mu\nu}, F_n\cdot A^n] = \sum_{j=1}^{n}\int\cdots\int F^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1\cdots x_n) \times A^{a_1}_{\mu_1}(x_1)\cdots\tilde{A}^{a_j}_{\mu_j}(x_j)\cdots A^{a_n}_{\mu_n}(x_n)dx_1\cdots dx_n,$$

where

$$\tilde{A}^a_\lambda(x) = i(x^\mu\partial^\nu - x^\nu\partial^\mu)A^a_\lambda(x) - i(g^\mu_\lambda g^{\nu\theta} - g^\nu_\lambda g^{\mu\theta})A^a_\theta(x), \tag{3.1}$$

while

$$[M^{\mu\nu}, J^\lambda_a(x)] = i(x^\mu\partial^\nu - x^\nu\partial^\mu)J^\lambda_a(x) + i[g^{\mu\lambda}J^\nu_a(x) - g^{\nu\lambda}J^\mu_a(x)]. \tag{3.1a}$$

The transformation (3.1)$\forall n$ is sufficient and necessary for $F(A)\in L$. The term $F_nA^n/n!$ can also be written as $(D^n/n!)F(A)|_{A=0}\cdot A^n$.

Let us now use the functional equality[3]

$$G(D)\cdot\exp[B(A)]\cdot Z(A) = \exp[B(A)]G(D+DB)Z(A), \tag{3.2}$$

where by $G(D)$ we denote the functional obtained from $G(A)$ by substituting in place of the function $A^a_\mu(x)$, the functional derivative $D^\mu_a(x)$. Taking $Z(A)=1$ and $G(A) = \int\cdots\int\delta(x_1-x_2)\cdots\delta(x_1-x_n)A^{a_1}_{\mu_1}(x)\cdots A^{a_n}_{\mu_n}(x_n)dx_1\cdots dx_n$, we get

$$F_nA^n = T[D+iDB(A)]^n|_{A=0}$$
$$= T\int\cdots\int\{[D^{\mu_1}_{a_1}(x_1) + D^{\mu_1}_{a_1}(x_1)iB(A)]\cdots \times [D^{\mu_n}_{a_n}(x_n) + D^{\mu_n}_{a_n}(x_n)iB(A)]\}|_{A=0},$$
$$A^{a_1}_{\mu_1}(x_1)\cdots A^{a_n}_{\mu_n}(x_n)dx_1\cdots dx_n. \tag{3.3}$$

The integration and summation over all variables with the functions $A^{a_j}_{\mu_j}(x_j)$, $j = 1\cdots n$ make the operator $D^\mu_a(x)$ similar to the ordinary derivative. This fact is used in Appendix A to prove

$$F_n\cdot A^n/n! = \sum_{\text{part }\alpha} C(\{k^\alpha\}_n)T(\{k^\alpha\}_n)\cdot A^n, \tag{3.4}$$

where $\{k^\alpha\}_n$ is a partition of order n, i.e., satisfying $\sum_{j=1}^n k^\alpha_j\cdot j = n$ and the sum $\sum_{\text{part}\,\alpha}$ runs through all distinct partitions of order n.

Using (3.4), we also prove in Appendix A that $F(A)\in L \Longleftrightarrow$

1. $$[M^{kl}, iD^nB(A)|_{A=0}]\cdot\frac{A^n}{n!} = \sum_{j=1}^{n} iD^nB(A)|_{A=0}\cdot\frac{A^{n-1}\cdot\tilde{A}_j}{n!}$$
$$\equiv \sum_{j=1}^{n}\int\cdots\int D^{\mu_1}_{a_1}(x_1)\cdots D^{\mu_n}_{a_n}(x_n)B(A)|_{A=0} \cdot\tilde{A}^{a_1}_{\mu_1}(x_1)\cdots A^{a_j}_{\mu_j}(x_j)\cdots A^{a_n}_{\mu_n}(x_n)dx_1\cdots dx_n$$

for $1\le k,l\le 3$ and $\tilde{A}^a_\mu(x)$ as in (3.1).

2. $$[M^{or}, iD^nB(A)|_{A=0}]\cdot\frac{A^n}{n!} = \sum_{j=1}^{n} iD^nB(A)|_{A=0}\cdot\frac{A^{n-1}\tilde{A}_j}{n!} + (-i)\sum_{k=1}^{[n/2]} d^n(k)\left[\frac{iD^kB(A)}{k!}\Big|_{A=0}, i\frac{D^{n-k}B(A)}{(n-k)!}\Big|_{A=0}\right]\delta(x^0-y^0)(x^r-y^r)\cdot A^n, \tag{3.5}$$

where $d^n(k) = \begin{cases}\frac{1}{2}; & k = n/2\\ 1; & \text{otherwise}\end{cases}$,

$$x\in\operatorname{supp}D^kB(A)|_{A=0},\quad y\in\operatorname{supp}D^{n-k}B(A)|_{A=0}.$$

The transformation properties stated in (3.5) are the generalization of the equations given in Ref. 2 for $n = 2, 3, 4$. Here no assumption has yet been made about the nature of the commutation relations in (3.5). The only conclusion that can be drawn is that the commutators are again quasilocal fields. This follows from Assumption (2.6), which guarantees that all the coefficients B_n are relatively local. For the case when $B(A)$ is given by (2.9), the explicit results can be found in Appendix B.

In the next chapter we shall see that a functional $B(A)$ satisfying (3.5) can be built explicitly for some models of current commutation relations.

4. AN EXPLICIT FUNCTIONAL

It is evident from (3.5) that the Lorentz covariance is connected with the equal time commutation relations among the quasilocal fields. Let us therefore study a model for which the commutation relations between the currents are known.

Let us assume that

$$[J^\mu_a(x), J^\nu_b(y)]\,\delta(x^0y^0) = k^{\mu\nu}_{ab}(x)\,\delta^4(x-y) + \text{ST}, \tag{4.1}$$

where $k^{\mu\nu}_{ab}(x)$ is a sum of local fields, and the ST involves first-order derivatives of the δ function. In general, ST will therefore be of the form

$$\mathrm{ST} = \sum_{j=1}^{3} S_{ab}^{\mu\nu,j}(y)\partial_j^x \delta^4(x-y) = \sum_{j=1}^{3} \partial_j^x [S_{ab}^{\mu\nu,j}(x)\delta^4(x-y)]. \quad (4.2)$$

We assume also that the commutation relation between the divergence $\partial_\mu J_a^\mu(x)$ and the currents is of the above type. We shall see that in the case of the Gell-Mann[6] algebra (with some other mild assumptions) all the assumptions stated above are satisfied.

Define a functional

$$\overline{B}(A) = \iint G(A,y) J_a^\mu(x) A_\mu^a(x) G^{-1}(A,y)\, dx dy,$$

where $G(A,y) = \exp[i \int dx J_b^0(x,y^0)(\mathbf{x}-\mathbf{y})\cdot \mathbf{A}^b(\mathbf{x},y^0)]$. (4.3)

As the currents are Hermitian and the fields $A_\mu^a(x)$ real, we have the following properties:

a. $G^\dagger(A,y) = G(A,y)$,
b. $\overline{B}^\dagger(A) = \overline{B}(A)$,
c. $[\overline{B}(A), \overline{B}(\tilde{A})] = 0$ for $\operatorname{supp} A \sim \operatorname{supp} \tilde{A}$,
d. $D^n \overline{B}(A)|_{A=0}$ is a quasilocal field,
e. $D_a(x)\overline{B}(A)|_{A=0} = J_a^\mu(x)$.

Therefore the functional $B(A)$ defined by the coefficients

$$B_{n,a_1\cdots a_n}^{\mu_1\cdots\mu_n}(x_1\cdots x_n) = (1/n) S_n \overline{B}_{n,a_1\cdots a_n}^{\mu_1\cdots\mu_n}(x_1\cdots x_n) \quad (4.4)$$

will satisfy the conditions (2.5)–(2.7) and the functional $F(A)$ defined by

$$F(A) = T\exp[iB(A)] \quad (4.5)$$

will also satisfy condition (2.8).

Using the expansion $e^A B e^{-A} = B + \sum_{n=1}^\infty (1/n!)[A\cdots[A,B]\cdots]$, we find

$$B_n A^n = \int\cdots\int [\mathbf{R}_{a_2}(x_2,x_1)\cdots[\mathbf{R}_{a_{n-1}}(x_{n-1},x_1), J_{a_1}^{\mu_1}(x_1)]\cdots]\cdot \mathbf{A}^{a_2}(x_2)\cdots \mathbf{A}^{a_{n-1}}(x_{n-1}) A_1^{a_1}(x_1) dx_1\cdots dx_n,$$

$$\mathbf{R}_a(x,y) = iJ_a^0(x)(\mathbf{x}-\mathbf{y})\delta(x^0-y^0).$$

The proof of covariance under spatial rotations is straightforward for the entire functional $F(A)$ and corresponds merely to exchange of the variables of integrations. For boosts we prove the infinitesimal version of covariance (3.5).

For the $n=1$ coefficient, $\int B_a^\mu(x)A_\mu^a(x)dx = \int J_a^\mu(x) A_\mu^a(x)dx$ and (3.5) is obtained from (3.1) and from partial integration [suppose $A_j^a(x)$ to be of compact support]. We present here the proof for $n=2$ to emphasize the importance of the assumptions made for the commutation relations. The last step of an inductive proof is given in Appendix C. For $n=2$, we have

$$B_2\cdot A^2 = \iint [J^0(x)(\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x)\delta(x^0-y^0), J^\mu(y)A_\mu(y)] \times dxdy.$$

Therefore,

$$[M^{or}, B_2\cdot A^2] = [M^{or}, \iint dxdy [J^0(x) \times (\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x)\delta(x^0-y^0) J^\mu(y)A_\mu(y)]$$
$$= \iint dx d^3y\, i(x^0\partial^r - x^r\partial^0)[J^0(x)(\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x), J^\mu(\mathbf{y},x^0)A_\mu(\mathbf{y},x^0)]$$
$$+ \iint dxd^3y\, i[J^r(x)(\mathbf{x}-\mathbf{y})\mathbf{A}(x), J^\mu(\mathbf{y},x^0)A_\mu(\mathbf{y},x^0)]$$
$$+ \iint dxd^3y [J^0(x)(\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x), i(x^0\partial_y^0 - y^r\partial^0)J^\mu(\mathbf{y},x^0)A_\mu(\mathbf{y},x^0)]$$
$$+ \iint dxd^3y [J^0(x)(\mathbf{x}-\mathbf{y})\cdot A(x), \times i(g^{0\mu}J^r(\mathbf{y},x^0) - g^{r\mu}J^0(\mathbf{y},x^0)A_\mu(\mathbf{y},x^0)], \quad (4.6)$$

where we used the Jacobi identity (3.1a) and ignore the summation over symmetry index, which is not essential here. Performing integration by parts, we rewrite Eq. (4.6) in the form

$$[M^{or}, B_2A^2] = \iint dxd^3y\, i(y^r - x^r)[\partial^0 J^0(x), \times J^\mu(\mathbf{y},x^0)](\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x)A_\mu(\mathbf{y},x^0)$$
$$+ \iint dxd^3y\, i[J^\mu(x)(\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x), J^\mu(\mathbf{y},x^0)A_\mu(\mathbf{y},x^0)]$$
$$+ \iint dxd^3y [J^0(x), J^\mu(\mathbf{y},x^0)]\, iy^\mu(\mathbf{x}-\mathbf{y})\cdot\partial^0\mathbf{A}(x)A_\mu(\mathbf{y},x^0)$$
$$+ \iint dxd^3y [J^0(x), J^\mu(\mathbf{y},x^0)] \times (-i)x^0(\mathbf{x}-\mathbf{y})\cdot\partial^\mu\mathbf{A}(x)A_\mu(\mathbf{y},x^0)$$
$$+ \iint dxd^3y [J^0(x), J(y,x^0)](\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x)\tilde{A}_\mu(y,x^0), \quad (4.7)$$

[$\tilde{A}_\mu(y,x^0)$ as in Eq. (3.1)].

We have assumed that at most, one spatial derivative of the δ function appears in the commutation relations involved.

Therefore,

a. $\int dx(x^r - y^r)[J^0(x), J^\mu(\mathbf{y},x^0)](\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x) = 0.$
b. Using $\partial^0 J^0(x) = \partial_\mu J^\mu(x) - \partial_l J^l(x)$, we rewrite the first term in the rhs of Eq. (4.7) in the form (after partial integrations):

$$\iint dxd^3y(-i)[J^r(x), J^\mu(y,x^0)](\mathbf{x}-\mathbf{y})\cdot\mathbf{A}(x)A^\mu(\mathbf{y},x^0)$$
$$+ \iint dxd^3y\, i[\mathbf{J}(x)\cdot\mathbf{A}(x), J^\mu(\mathbf{y},x^0)A_\mu(\mathbf{y},x^0)](x^r - y^r).$$

We subtract and add the expression

$$\iint dxd^3y\, i[J^0(x)A_0(x), J^\mu(\mathbf{y},x^0)A_\mu(\mathbf{y},x^0)](x^r - y^r)$$

and recollect various terms to obtain finally

$$[M^{or}, iD^2B(A)|_{A=0}]\cdot\tfrac{1}{2}A^2 = \sum_{j=1}^{2} iD^2B(A)|_{A=0}\tfrac{1}{2}A\tilde{A}_j$$
$$+ -\tfrac{1}{2}i\iint dxdy[iJ^\lambda(x)A_\lambda(x), iJ^\mu(y)A_\mu(y)]\delta(x^0-y^0)(x^r-y^r). \quad (4.8)$$

The result (4.8) is exactly the same as in (3.5) for $n=2$.

Having established the Lorentz covariance, let us write for comparison the covariant time order product for $n=2$. Using definitions (1.1) and (4.2), we get

$$T^*(J_a^0(x)J_b^0(y)) = T(J_a^0(x)J_b^0(y)),$$
$$T^*(J_a^0(x)J_b^k(y)) = T^*(J_a^k(x)J_b^0(y))$$
$$= T(J_a^0(x)J_b^k(y)) - \tfrac{1}{2}S_{ab}^{oo;k}(y)\delta(x-y),$$
$$T^*(J_a^l(x)J_b^k(y)) = T(J_a^l(x)J_b^k(y))$$
$$- \tfrac{1}{2}(S_{ab}^{ok;l}(y) + S_{ba}^{ol;k})\delta(x-y). \quad (4.9)$$

We note the appearance of the ST $S_{ab}^{oo;k}(y)$, which does not appear in the Gell-Mann type of algebra. It is simple to show, using Jacobi identity for the commutator $[M^{or}, [J_a^0(x), J_b^0(y)]]\delta(x^0-y^0)$ that

$$[M^{or}, S_{ab}^{oo,k}(x)] = i[S_{ba}^{ok;r}(x) - S_{ab}^{or;k}(x)] + i(x^0\partial^r - x^r\partial^0)S_{ba}^{oo;k}(x). \quad (4.10)$$

From (4.10) it is evident that for $S_{ba}^{oo;l}(x) = 0$, $1 \le l \le 3$, we have the symmetry $S_{ba}^{ok;r}(x) = S_{ab}^{or;k}(x)$, and (4.12) is the same as (2.9) and (2.10) in Ref. 2. The above symmetry property is reflected [for the case $S_{ab}^{oo;k}(x) = 0$] also in higher order terms of $B(A)$.[7] In the Gell-Mann algebra for $SU3 \times SU3$, one assumes that the local commutators of the time components of the currents, at equal times, do not contain ST. If one also assumes that the commutators $[J_a^0(x), \partial_\lambda J_b^\lambda(y)]\,\delta(x^0 - y^0)$, $[\partial_\mu J_a^\mu(x), \partial_\lambda J^\lambda(y)]\,\delta(x^0 - y^0)$ do not have ST, it follows that

a. $[J_a^\mu(x), J_b^\nu(y)]\,\delta(x^0 - y^0)$, $[J_a^\mu(x), \partial_\lambda J_b^\lambda(y)]\,\delta(x^0 - y^0)$ contain at most one derivative of δ function in ST;
b. All commutators obtained by successive commutation of the currents $J_a^\mu(x)$ with ST have the above-mentioned property.[7,8]

We conclude therefore that for currents satisfying the Gell-Mann algebra there exists a functional $F(A)$ [which can be taken from (4.5)] which generates CTP for the currents.

5. THE FEYNMAN CONJECTURE

The Feynman conjecture expressed in terms of CTP reads simply

$$\partial_{\mu_1} T^*(J_{a_1}^{\mu_1}(x_1)\cdots J_{a_n}^{\mu_n}(x_n)) = T^*(\partial_\mu J_{a_1}^\mu(x_1) J_{a_2}^{\mu_2}(x_2)\cdots J_{a_n}^{\mu_n}(x))$$
$$+ i \sum_{j=2}^{n} C_{a_1 a_j b} T^*(J_{a_2}^{\mu_1}\cdots J_b^{\mu_j}(x_j)\cdots J_{a_n}^{\mu_n}(x_n))\,\delta(x - x_j), \tag{5.1}$$

where C_{aa_jb} and the structure constants.

In the case of nonconserved currents, the new field $\partial_\mu J_a^\mu(x)$ is introduced. Assume first, therefore, that the currents are conserved.

Let us express (5.1) in terms of $(F_n \cdot A^n)/n!$, $n \ge 1$,

$$(-i)^n \partial_\mu D_a^\mu(x) F_n \cdot A^n (1/n!)$$
$$= iC_{abc}(-i)^{n-1} A_\mu^b(x) D_c^\mu(x) F_{n-1}\cdot A^{n-1}[1/(n-1)!]. \tag{5.2}$$

Remembering that $\partial_\mu J_a^\mu(x) = \partial_\mu D_a^\mu(x) F_1 \cdot A = 0$, we can sum up formally and obtain

$$\partial_\mu D_a^\mu(x) F(A) = (-) C_{abc} A_\mu^b(x) D_c^\mu(x) F(A). \tag{5.3}$$

Equation (5.3) is therefore equivalent to the Feynman conjecture for conserved currents.

Assume now that $F(A)$ is invariant under the gauge transformation

$$\delta A_\mu^a(x) = \partial_\mu \delta\lambda^a(x) - C_{abc} A_\mu^b(x)\,\delta\lambda^c(x). \tag{5.4}$$

Then

$$\delta F(A) = T\{i\delta B(A)\exp(iB(A))\}$$
$$= T\{i\textstyle\int \delta A_\mu^a(x) D_a^\mu(x) B(A)\exp[iB(A)]\,dx\}$$
$$= \textstyle\int T\{(iD_a^\mu(x)B(A))\exp[iB(A)]\}\,\delta A_\mu^a(x)\,dx$$
$$= \textstyle\int [-\partial_\mu(D_a^\mu(x)F(A)) - C_{abc}A_\mu^b(x) D_a^\mu(x) F(A)]\,\delta\lambda^a(x)\,dx,$$

$$\partial_\mu D_a^\mu(x) F(A) = -C_{abc} A_\mu^b(x) D_a^\mu(x) F(A).$$

We conclude therefore that the Feynman conjecture is equivalent for conserved current to the invariance of the generating function $F(A)$ under the gauge transformation (5.4).

We now write Eq. (5.3) in terms of the coefficients B_n using (3.4),

$$\frac{1}{n!}\partial_\mu D_a^\mu(x) T_n \cdot A^n$$
$$= \partial_\mu \sum_\alpha C(\{k^\alpha\}_n)\left\{\sum_{j=1}^{n} T\left[\prod_{l\ne j}\left(\frac{iB_l}{l!}\right)^l \frac{k_j\cdot j}{j!}\right.\right.$$
$$\left.\left.\times\, iD_a^\mu(x) D^{j-1}B(A)|_{A=0}\right]\cdot A^{n-1}\right\}$$
$$= \frac{-1}{n!} C_{abc} A_\mu^b(x) D_c^\mu(x) T_n \cdot A^n$$
$$= iC_{abc} A_\mu^b(x) \sum_\alpha C(\{k^\alpha\}_{n-1})\sum_{j=1}^{n-1}$$
$$\times\, T\left[\prod_{l\ne j}\left(\frac{iB_l}{l!}\right)^{k_l} \frac{k_j\cdot j}{j!}\, iD_c^\mu(x) D^{j-1}B(A)|_{A=0}\right]\cdot A^{n-2} \tag{5.5}$$

(with obvious notations).

In the case of $S_{ab}^{oo;k}(x) = 0$, it follows that $B_{n,a_1\cdots a_n}^{\mu_1\cdots\mu_n}(x_1\cdots x_n) \ne 0$ only for $\mu_j \ne 0$, $1 \le j \le n$, $n > 1$.[7] Therefore in (5.5) only three-dimensional divergences of the B_n appeared and commutators of the currents $J_a^0(x)$ with different B_n arise. Using the methods of Appendix A, it can be shown that (5.3) is satisfied. The non-Schwinger terms on the rhs of Eq. (5.3) are equal to the different terms on the lhs of Eq. (5.3) and the divergences are canceled against Schwinger terms. The cancellation would not take place in the case of a Schwinger term in the commutator $[J_a^0(x), J_b^0(y)]\,\delta(x^0 - y^0)$.

Coming back to the case of nonconserved currents, let us define a new "current" and a new function:

$$0 \le \lambda \le 4,\quad K_a^\lambda(x) = \begin{cases} J_a^\lambda(x);\ 0 \le \lambda \le 3 \\ \partial_\mu J^\mu(x);\ \lambda = 4 \end{cases},$$
$$E_\lambda^a(x) = \begin{cases} A_\lambda^a(x);\ 0 \le \lambda \le 3 \\ \phi(x);\ \lambda = 4 \end{cases}. \tag{5.6}$$

The "new" metric

$$g^{\mu\lambda} = \begin{cases} g^{\mu\lambda}, & 0 \le \mu,\lambda \le 3 \\ 0, & 0 \le \mu,(\lambda) \le 3, \lambda,(\mu) = 4 \\ -1, & \mu = \lambda = 4 \end{cases}.$$

The transformation of the "current" $K_a^\lambda(x)$ under infinitesimal Lorentz transformation reads as

$$0 \le \mu,\nu \le 3,\ [M^{\mu\nu}, K_a^\lambda(x)] = i(x^\mu\partial^\nu - x^0\partial^\mu) K_a^\lambda(x)$$
$$+ i[\tilde g^{\mu\lambda} K_a^\nu(x) - \tilde g^{\mu\lambda} K_a^\mu(x)]. \tag{5.7}$$

Let $D_a^\lambda(x)$ denote the functional derivative $\partial E_a^\lambda(x)$. It then follows that the functional

$$F(E) = T\{\exp[iB(E)]\} \tag{5.8}$$

will generate CTP for the currents and their divergences if and only if Eqs. (3.1) and (3.5) are satisfied, making the obvious substitutions $J \to K$, $A \to E$. To express the Feynman conjecture let us also define formally $\partial_4 = -1$; then (5.1) becomes

$$\partial_\lambda T^*(K_a^\lambda(x) K_{a_1}^{\lambda_1}(x_1)\cdots K_{a_n}^{\lambda_n}(x_n))$$
$$= i\sum_{j=1}^{n} C_{aa_jb} T^*(K_{a_1}^{\lambda_1}(x_1)\cdots K_{a_j}^{\lambda_j}(x_j)\cdots K_{a_n}^{\lambda_n}(x_n))\,\delta(x - x_j). \tag{5.9}$$

As before, the Feynman conjecture is equivalent to the invariance of the functional $F(E)$ under the general gauge transformation

$$\delta E_\theta^a(x) = (-)^{\delta_{\theta 4}} \partial_\theta \delta\lambda^a(x) - C_{abc} E_\theta^b(x) \delta\lambda^c(x) \quad (5.10)$$

and is also expressed in terms of the coefficient as in (3.5) with the necessary modifications.

We are able therefore to express, in terms of functionals, the necessary and sufficient conditions for $F(E)$ to generate CTP for currents and their divergences, and to satisfy the Feynman conjecture.

It follows (Appendix D) that in the case when no ST are present in the commutators $[K_a^0(x)K_b^0(y)]\delta(x^0 - y^0)$, $[K_a^4(x), K^4(y)]\delta(x^0 - y^0)$, $[K_a^0(x), K_b^4(y)]\delta(x^0 - y^0)$, the functional $F(E) = \exp iB(E)$ [where $B(E)$ is given by (4.3) and (4.4), making the substitutions $J \to K$, $A \to E$] will generate CTP as above.

Finally, let us note that if one looks on $B(A)$ as a Hamiltonian expressing the coupling of currents to an external field $A_\mu^a(x)$, among which some combinations express the electromagnetic field $[A_\mu^e(x) = A_\mu^3(x) + (1/\sqrt{3})A_\mu^8(x)$ in $SU3$ case], one would like to have invariance under gauge transformations of the second kind $\delta A_\mu^e(x) = \partial_\mu \delta\lambda(x) + A_\mu^e(x)$.

From this point of view, the currents are $J_a^\mu(x) = D_a^\mu(x)B(A)(A \neq 0)$ and they depend on the electromagnetic field. In particular, the commutation relations depend explicitly on the electromagnetic fields. For example, to first order in e,[9]

$$[J^0(x), J_5^0(y)] = (2ie/8\pi^2)\tilde{F}^{oj}(x)\partial_j\delta(x-y),$$

$$\tilde{F}^{oj}(x) = \epsilon^{oj\mu\nu}(\partial_\mu A_\nu^e - \partial_\nu A_\mu^e).$$

In this case the Feynman conjecture is not equivalent to the invariance under gauge transformations of the second kind, and it is impossible to satisfy both of them.[10]

APPENDIX A

We start with Eq. (5.3),

$$\begin{aligned}(1/n!)F_n \cdot A^n &= T[(D + DB)^n](1/n!) \\ &= (1/n!)\int \cdots \int T\{[D_{a_1}^{\mu_1}(x_1) + D_{a_1}^{\mu_1}(x_1)B(A)]|_{A=0} \cdots \\ &\quad \times [D_{a_n}^{\mu_n}(x_n) + D_{a_n}^{\mu_n}(x_n)B(A)]|_{A=0}\} \\ &\quad \times A_{\mu_1}^{a_1}(x_1) \cdots A_{\mu_n}^{a_n}(x_n)dx_1 \cdots dx_n. \end{aligned} \quad (A1)$$

We absorb here the factor i in the function B and prove (3.4) by induction. For $n = 1$, it is trivial. Assume (3.4) for all k, $k \leqslant n-1$ then

$$\begin{aligned}(1/n!)F_n \cdot A^n \\ = T\{[D + DB(A)]\cdot[D + DB(A)]^{n-1}\}|_{A=0} A \cdot A^{n-1}. \end{aligned} \quad (A2)$$

First it is clear that each term in $F_n \cdot A^n \cdot (1/n!)$ can be specified by some partition $\{k^\alpha\}_n$ and all partitions appear in Eq. (3.5). (This also follows from the proof indicated). Each configuration given by the partition $\{k^\alpha\}_n$, i.e., $T(\{k^\alpha\}_n)$ can be obtained from the configuration of order $(n-1)$, $T(\{k^\alpha\}_{n-1})$ by multiplication with $DB(A)|_{A=0}$ or by applying the functional derivative D [see (A2)]. Therefore let $\{k^\alpha\}_n$ be a partition of order n. Define

$$\{k^\alpha\}_{n-1}^1 = \begin{Bmatrix} k_i^\alpha; & i \neq 1 \\ k_1^\alpha - 1; & i = 1 \end{Bmatrix}, \quad k_1^\alpha \neq 0,$$

$$\{k^\alpha\}_{n-1}^j = \begin{Bmatrix} k_i^\alpha; & i \neq j, i \neq j-1 \\ k_j^\alpha - 1; & i = j \\ k_{j-1}^\alpha + 1; & i = j-1 \end{Bmatrix}, \quad k_j^\alpha \neq 0, j = 2 \cdots n.$$

The configuration given by the partition $\{k^\alpha\}_n$ is thus obtained by multiplying with DB the configuration given by $T(\{k^\alpha\}_{n-1}^1)$ and by applying the functional derivative on the expression D^jB appearing in the configuration $T(\{k^\alpha\}_{n-1}^j)$. Note that $\{k^\alpha\}_{n-1}^j$ defined above are really partitions of order $n-1$, i.e., $\sum_{i=1}^{n-1} k_i^{\alpha,j} \cdot i = n-1$. We note that by applying the functional derivative D we apply it to the expression

$$(D^jB)^{k_{j-1}^\alpha + 1}$$

and therefore a coefficient $(k_{j-1}^\alpha + 1)$ appears.

It remains to count the numerical coefficients. Let $k_j^\alpha \neq 0$, $j = 1 \cdots n$. Then the numerical coefficients (X) are by induction,

$$\begin{aligned} X &= \frac{1}{n} \frac{C(\{k^\alpha\}_{n-1}^1)}{\prod_{l=1}^{n-1} (l!)^{k_l^{\alpha,1}}} + \sum_{j=2}^n \frac{C(\{k^\alpha\}_{n-1}^j)\cdot(k_{j-1}^\alpha + 1)}{\prod_{l\neq j,j-1} (l!)^{k_l^{\alpha,j}}((j-1)!)^{k_{j-1}^\alpha+1}\cdot(j!)^{k_j^\alpha - 1}} \\ &= \frac{1}{n} \frac{k_1^\alpha}{\prod_{l=1}^n [(l!)^{k_l^\alpha}\cdot k_l^\alpha!]} + \sum_{j=2}^n \frac{k_j^\alpha \cdot j!\cdot(k_{j-1}^\alpha + 1)}{\prod_{l=1}^n [(l!)^{k_l^\alpha} k_l^\alpha!]\cdot(j-1)!(k_{j-1}^\alpha + 1)}. \end{aligned} \quad (A3)$$

The right-hand side of (A3) is valid without the restriction $k_j^\alpha \neq 0$, therefore,

$$X = \frac{1}{\pi[(l!)^{k_l^\alpha}\cdot k_l!]} \cdot \frac{\sum_{j=1}^n k_j^\alpha \cdot j}{n} = \frac{C(\{k^\alpha\}_n)}{\prod_{l=1}^n [(l!)^{k_l^\alpha}]} \quad (A3')$$

and (3.4) is proved.

Equation (3.5) is also proved by induction. Let us show that (3.5) is necessary for $F(A) \in L$. (The converse is proved along the same lines.) Assume $F(A) = F_n \cdot A^n \cdot 1/n!$ satisfies Eq. (3.1), i.e., $\sum_\alpha C(\{k^\alpha\}_n) T(\{k^\alpha\}_n)$ satisfies the same equation. Let (3.5) be true for all k, $k \leqslant n-1$, when the functions A have compact support (to ensure integration by parts if needed) and may be multiplied also by θ functions. We need only prove (3.5) for boosts; for rotations the proof is straightforward. Let us consider for demonstration one term in the sum (3.4) and look at the commutator

$$[M^{or}, C(\{k^\alpha\}_n) T(\{k^\alpha\}_n)]\cdot(A^n/n!). \quad (A4)$$

To apply the induction assumption, we take those partitions for which $k_n^\alpha = 0$. Because of θ functions appearing due to time ordering, the result of the commutation will contain, in addition to the sum of terms following from (3.5), extra commutation relations of the form

$$\begin{aligned} & i[D^lB(A)|_{A=0}, D^dB(A)|_{A=0}](x^r - y^r)\delta(x^0 - y^0), \quad \text{if} \\ & k_l^\alpha \cdot k_j^\alpha \neq 0, \quad x \in \operatorname{supp} D^lB(A)|_{A=0}, \\ & y \in \operatorname{supp} D^dB(A)|_{A=0}. \end{aligned} \quad (A5)$$

We show that the extra commutators cancel the commutators arising from (3.5) for all $\{k^\alpha\}_n$ if the partitions have more than two elements. For each extra commutator from the partition $\{k^\alpha\}_n$ coming from the cummutator $D^l B$, we associate a commutator coming from $[M^{\sigma r}, D^{l+j}B(A)|_{A=0}]$ [see Eq. (3.5) ($l+j<n$)], and from the term

$$(-i)/(n-l)!\,\{D^lB(A)|_{A=0}(1/l!),$$

$$D^{n-l}B(A)|_{A=0}](x^r-y^r)\,\delta(x^0-y^0)$$

(assume $l \leqslant j$) (this mapping is one to one).

As before, because of the k_p^α power of (D^pB) in $T(\{k^\alpha\}_n)$, we shall have numerical coefficients $k_l^\alpha \cdot k_j^\alpha$ for $l \neq j$ and $\binom{k_l^\alpha}{2}$ for $l=j$.

Let us define

(a). $$\{b^\alpha\}_n = \begin{Bmatrix} k_t^\alpha;\ t\neq l,\ t\neq j,\ t\neq l+j \\ k_{l+j}^\alpha+1;\ t=l+j \\ k_l^\alpha-1;\ t=l \\ k_{j-1}^\alpha-1;\ t=j \end{Bmatrix}, \quad l\neq j,$$

(b) $$\{b^\alpha\}_n = \begin{Bmatrix} k_t^\alpha;\ t\neq l,\ t\neq 2l \\ k_{2l}^\alpha+1;\ t=2l \\ k_l^\alpha-2;\ t=l \end{Bmatrix}, \quad l=j.$$

Because of the opposite sign of the commutators of (3.5) and (2.5), we need only count the numerical coefficients:

$$\text{(a)}\quad \frac{k_l^\alpha\cdot k_j^\alpha}{\prod_{t=1}^n[(t!)^{k_t^\alpha}k_t^\alpha!]} = \frac{k_l^\alpha\cdot k_j^\alpha\binom{l+j}{j}\cdot(k_{l+j}^\alpha+1)}{\prod_{t\neq l,j,l+j}[k_t^\alpha!(t!)^{k_t^\alpha}](l!)^{k_l^\alpha-1}(k_l^\alpha-1)!\,(l!)^{k_j^\alpha-1}(k_j^\alpha-1)!}\cdot$$

$$\frac{1}{((l+j)!)^{k_{l+j}^\alpha+1}(k_{l+j}^\alpha+1)!} = (k_{l+j}^\alpha+1)\binom{l+j}{2}\frac{1}{\prod_{t=1}^n[(t!)^{b_t^\alpha}\cdot b_t^\alpha!]}$$

$$\text{(b)}.\quad \binom{k_l^\alpha}{2}\cdot\frac{1}{\prod_{t=1}^n[(t!)^{k_t}k_t^\alpha!]}\ \frac{k_l^\alpha\cdot k_{l-1}^\alpha\cdot(k_{2l}^\alpha+1)\cdot(2l)!}{2\cdot(k_{2l}^\alpha+1)!\,((2l)!)^{k_{2l}^\alpha+1}\cdot l!\cdot l!(l!)^{k_l^\alpha-2}\cdot(k_l^\alpha-2)!\,(k_l^\alpha-1)k_l^\alpha\prod_{t\neq l,2l}[(t!)^{k_t^\alpha}k_t^\alpha!]}$$

$$= (k_{2l}^\alpha+1)\binom{2l}{2}\cdot\frac{1}{2}\ \frac{1}{\prod_{t=1}^n[(t!)^{b_t^\alpha}\cdot b_t^\alpha!]}. \tag{A6}$$

The right-hand side of Eqs. (A6) are exactly the numerical coefficients coming from (3.5) by induction. The terms of the form $\sum_j D^pB\cdot(A^{p-1}\cdot A_j/p!)$, $p<n$ will be canceled because we have assumed $F(A)\in L$ and we shall remain with the commutator $[M^{\sigma r}, D^nB]A^n/n!$ and the "extra" commutators coming from partitions which are of the form $\{k_l^\alpha, k_j^\alpha\}$ or $\{k_l^\alpha\}$ if $2l=n$, and as in (A6), we count the numerical coefficients and obtain after rearrangement, Eq. (3.5).

APPENDIX B

$B(A)$ is given by

$$B(A)=\sum_{n=0}^{\infty}\int B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x)A^{a_1}_{\mu_1}(x)\cdots A^{a_n}_{\mu_n}(x)\,dx. \tag{B1}$$

In order to apply (3.5), we rewrite the coefficients in the form

$$B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1)\,\delta(x_1-x_2)\,\delta(x_1-x_3)\cdots\delta(x_1-x_n) = B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1\cdots x_n).$$

We differentiate (3.5) functionally. As mentioned in (2.2) only symmetric parts contribute, and we obtain

$$[M^{\sigma r}, iB^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1)]\,\delta(x_1-x_2)\cdots\delta(x_1-x_n)$$

$$= n!\,S_n\Bigg(\sum_{j=1}^{(n/2)} d^n(j)\,[B^{\mu_1\cdots\mu_j}_{j,a_1\cdots a_y}(x_1)\,\delta(x_1-x_2)\cdots\delta(x_1-x_j),$$

$$B^{\mu_j\cdots\mu_n}_{n-j,a_{j+1}\cdots a_n}(x_{j+1})\,\delta(x_{j+1}-x_{j+2})\cdots\delta(x_{j+1}-x_n)]$$

$$\times\,\delta(x_1^0-x_{j+1}^0)(x_1^r-x_{j+1}^r)\Bigg)$$

$$+ S_n\{[i(x_1^0\partial_1^r - x_1^r\partial_1^0)B^{\mu_1\cdots\mu_n}_{n,a_1\cdots a_n}(x_1)]\,\delta(x_1-x_2)\cdots\delta(x_1-x_n)\}$$

$$+ S_n\Bigg(i\sum_{j=1}^{n}(g^{0\mu_j}B^{\mu_1\cdots r\cdots\mu_n}_{n,a_1\cdots a_j\cdots a_n}(x_1) - g^{r\mu_j}B^{\mu_1\cdots 0\cdots\mu_n}_{n,a_1\cdots a_j\cdots a_n}(x_1))$$

$$\times\,\delta(x_1-x_2)\cdots\delta(x_1-x_n)\Bigg). \tag{B2}$$

The symmetrizer in S_n acts on the set of indices $\{1\cdots n\}$. Equation (B2) is a generalization of Eq. (2.23) in Ref. 1. Indeed we recover (2.23) from (B2) when $B^{\mu_1\mu_2}_{2,a_1a_2}=0$ for $\mu_1(\mu_2)=0$ and is symmetric in the indices (1. 2).

APPENDIX C

From (4.5) it follows that (the i factor has been absorbed)

$$\frac{1}{n!}B_n\cdot A^n = \frac{1}{n}\int\left[J_a^0(x), B_{n-1}\cdot A^{n-1}\frac{1}{(n-1)!}\right]$$

$$\times\,\delta(x^0-y^0)(x^l-y^l)A_l^a(x)\,dx,\qquad y\in \operatorname{supp}B_{n-1}. \tag{C1}$$

Following the proof of (4.5) for $n=2$ and using induction, it is easy to obtain

$$\left[M^{\sigma r}, \frac{1}{n!}B_n\cdot A^n\right] = \frac{-i}{n}\int\left[J_a^\mu(x), \frac{1}{(n-1)!}B_{n-1}\cdot A^{n-1}\right]$$

$$\times\,(x^r-y^r)\,\delta(x^0-y^0)A_\mu^a(x)\,dx$$

$$-\frac{i}{n}\sum_{k=1}^{(n-1/2)} d^{n-1}(k)\int\Bigg[J_a^0(x), \left[\frac{1}{k!}B_k, \frac{1}{(n-k-1)!}B_{n-k-1}\right]$$

$$\times\,(y_k^r-z_k^r)\,\delta(y_k^0-z_k^0)\Bigg](x^l-y_k^l)\,\delta(x^0-y_k^0)$$

$$\times\,A^{n-1}\cdot A_\mu^a(x)\,dx + \sum_{j=1}^{n}\frac{1}{n!}B_n\cdot A^{n-1}\cdot\tilde{A}_j,$$

$$y_k\in\operatorname{supp}B_k,\qquad z_k\in\operatorname{supp}B_{n-k-1}. \tag{C2}$$

Using (C1), the fact that B is given in this case by an expression of the form (B1) and the Jacobi identity, we collect the numerical coefficients of similar expressions and get (3.5). [One should be careful in obtaining the k'th term of (3.5) for $n=2k$ or $n=2k+1$).]

APPENDIX D

Using the results obtained in Ref. 9, we need only prove that the commutators (the symmetry index neglected)

$$[K^l(x), K^4(y)]\delta(x^0 - y^0), \quad [K^4(x), B_n]\delta(x^0 - y^0),$$
$$y \in \operatorname{supp} B_n, \text{ do not contain ST.} \qquad \text{(D1)}$$

We have assumed that[11]

$$[K^0(x), K^4(y)]\delta(x^0 - y^0), \quad [J^0(x), \partial_\mu^y J^\mu(y)]\delta(x^0 - y^0)$$

do not have ST; therefore,

$$(x^l - y^l)[K^0(x), K^4(y)]\delta(x^0 - y^0) = 0, \quad l = 1, 2, 3.$$

Using the Jacobi identity, we get

$$\begin{aligned}
&[M^{or}, (x^l - y^l)[K^0(x), K^4(y)]\delta(x^0 - y^0)] \\
&\quad = (x^l - y^l)\{[i(x^0\partial^r - x^r\partial^0)K^0(x), K^4(y)]\delta(x^0 - y^0) \\
&\qquad + [K^r(x), K^4(y)]\}\delta(x^0 - y^0) \\
&\qquad + (x^l - y^l)i[K^0(x), (y^0\partial_y^r - y^r\partial_y^0)K^4(y)]\delta(x^0 - y^0) \\
&\quad = -i(x^l - y^l)\{[\partial^0 J^0(x), K^4(y)] - [K^r(x), K^4(y)]\}\delta(x^0 - y^0) \\
&\quad = -i(x^l - y^l)(x^r - y^r)\{[K^4(x), K^4(y)] \\
&\qquad - [\partial_j J^j(x), K^4(y)]\}\delta(x^0 - y^0) \\
&\qquad + i(x^l - y^l)[K^r(x), K^4(y)]\delta(x^0 - y^0) \\
&\quad = -i(x^r - y^r)[K^l(x), K^4(y)]\delta(x^0 - y^0) = 0.
\end{aligned}$$

Therefore, $[K^l(x), K^4(y)]\delta(x^0 - y^0)$ does not contain ST. The same is proved along similar lines using induction for the second commutator in (D1).[12]

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Identity satisfied by the d-type coefficients of $SU(n)$

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Using a very simple approach, we obtain *one* identity for each $SU(n)$, satisfied by its d-type coefficients.

I. INTRODUCTION

Though much is known about the properties of the Gell-Mann d and f type coefficients [1-3] that hold *for every* $SU(n)$, an identity, specific to a particular unitary unimodular group has been given only for $SU(3)$ by Macfarlane *et al.*[3] To obtain this identity, they have utlized the characteristic equation satisfied by the matrix $A = \sum_{i=1}^{8} a_i \lambda_i$. Their lengthy method can be laboriously used to go on to $SU(4), SU(5), \ldots$, but a general formulation is very hard to obtain. Also one does not acquire any insight into these *special* identities. In this work, using a very simple reasoning, we are able to write down these identities—one for each $SU(n)$—immediately. The identities we obtain have a neat and compact equivalent form. This is described in Secs. II and III. In Sec. IV, we list results for $SU(3)$ to $SU(6)$ derived by our method.

II. PARTICULAR IDENTITIES

We use the following ranges for the various types of indices.

index type	range
α	1 to n
i	1 to $n^2 - 1$
a	0 to $n^2 - 1$

The matrices λ_i of the n-dimensional representation of the $SU(n)$ group together with the matrix $\lambda_0 = (2/n)^{1/2} I_{n\times n}$ satisfy the usual multiplication rule[4]

$$\lambda_a \lambda_b = (d_{abc} + i f_{abc})\lambda_c \tag{1}$$

in terms of the completely antisymmetric structure constants f_{abc} and the completely symmetric coefficients d_{abc}.

Now for $SU(n)$,

$$\epsilon_{\alpha_1\alpha_2\cdots\alpha_{n+1}} \epsilon_{\beta_1\beta_2\cdots\beta_{n+1}} (\lambda_{a_1})_{\alpha_1\beta_1} \cdots (\lambda_{a_{n+1}})_{\alpha_{n+1}\beta_{n+1}} = 0 \tag{2}$$

as follows from the fact that *each* of the λ-matrices in Eq. (2) is n-dimensional (this is consistent with the notation described before, since the range of the indices $\alpha_1\beta_1\cdots$ is from 1 to n and n is the number of rows or columns of the λ matrices), while both the symbols $\epsilon_{\alpha_1\alpha_2\cdots\alpha_{n+1}}$, $\epsilon_{\beta_1\beta_2\cdots\beta_{n+1}}$, which contain antisymmetry in $(n+1)$ indices must be identically zero. Equation (2) is essentially the identity we are after expressed in a very compact form.

In order to express this equation as an identity amongst the d-coefficients, we have now to replace the product of the two ϵ_s' by a sum of products of δ functions, which when contracted against the matrix elements $(\lambda_a)_{\alpha\beta}$ will result in linear combinations of products of traces of these matrices. These traces can then be developed in terms of d-type coefficients. Before we carry this out in detail (Sec. III), we add a few remarks relevant to Eq. (2).

(i) This special identity for $SU(n)$ also holds for $SU(m)$ where $m < n$. This result, however, is uninteresting, since it is deducible from known identities for every $SU(n)$ together with an identity of our type for $SU(m)$.

(ii) Whenver anyone (or more) of the indices $a_1, a_2, \ldots, a_{n+1}$ takes (take) the value zero, since $(\lambda_0)_{\alpha\beta} = (2/n)^{1/2}\delta_{\alpha\beta}$, we shall have at least one contraction on the two ϵ symbols. When we express the product of ϵ'_s with one contraction as sums of products of δ-functions, we obtain zero identically. Thus in Eq. (2) we may replace an a-type index by an i-type one. This we shall henceforth do and replace Eq. (2) by

$$K_{i_1\cdots i_{n+1}} = \epsilon_{\alpha_1\alpha_2\cdots\alpha_{n+1}} \epsilon_{\beta_1\beta_2\cdots\beta_{n+1}} (\lambda_{i_1})_{\alpha_1\beta_1} \cdots (\lambda_{i_{n+1}})_{\alpha_{n+1}\beta_{n+1}} = 0. \tag{3}$$

(iii) The lhs $K_{i_1 i_2\cdots i_{n+1}}$ of Eq. (3) is evidently completely symmetrical in the indices $i_1, i_2, \ldots, i_{n+1}$. This remark will be useful later.

III. IDENTITY EXPRESSED IN TERMS OF THE d-TYPE COEFFICIENTS

In this section we try to express the tensor K in terms of the d-type coefficients of $SU(n)$. We expand the product of the two ϵ_s' in terms of sums of products of the δ functions and simplify to arrive at

$$K_{i_1 i_2\cdots i_N} = \sum \frac{(-1)^{N-N_2-\cdots-N_N}}{N_2!N_3!\cdots N_N! 2^{N_2}\cdot 3^{N_3}\cdots N^{N_N}} \times S[\mathrm{Tr}(\lambda_{i_1}\lambda_{i_2})\,\mathrm{Tr}(\lambda_{i_3}\lambda_{i_4})\cdots \mathrm{Tr}(\lambda_{i_{2N_2-1}}\lambda_{i_{2N_2}}) \times \mathrm{Tr}(\lambda_{i_{2N_2+1}}\lambda_{i_{2N_2+2}}\lambda_{i_{2N_2+3}})\cdots], \tag{4}$$

where

$$N = n + 1 \tag{5}$$

and the summation is over all partitions of N

$$N = 2\cdot N_2 + 3\cdot N_3 + \cdots + N\cdot N_N \tag{6}$$

into parts > 1[5] and S indicates that we have to symmetrize in the indices $i_1, i_2, \ldots, i_N$ and divide by $N!$. The structure of the quantity within the square brackets in Eq. (4) follows that of the partition in Eq. (6). Evidently on account of the complete symmetry of the tensor K, we may assume that the various traces occurring in Eq. (4) are also completely symmetrized.

We finally show how one can express the traces $S\,\mathrm{Tr}(\lambda_{i_1 i_2}\ldots\lambda_{i_r})$ as products of the d-type coefficients.

The procedure will become evident from the following four equations[6]

$$S\,\mathrm{Tr}(\lambda_a\lambda_b) = 2\delta_{ab}, \tag{7}$$

$$S\,\mathrm{Tr}(\lambda_a\lambda_b\lambda_c) = 2d_{abc}, \tag{8}$$

$$S\,\mathrm{Tr}(\lambda_{a_1 a_2}\cdots\lambda_{a_{2r}}) = S[d_{a_1a_2b_1}d_{a_3a_4b_1}\cdots d_{a_{2r-1}a_{2r}b_r} \times S\,\mathrm{Tr}(\lambda_{b_1}\lambda_{b_2}\ldots\lambda_{b_r})], \tag{9}$$

$$S\,\mathrm{Tr}(\lambda_{a_1}\lambda_{a_2}\ldots\lambda_{a_{2r+1}})^{(6)} = S[d_{a_1a_2b_1}d_{a_3a_4b_2}\cdots d_{a_{2r-1}a_{2r}b_r} \times S\,\mathrm{Tr}(\lambda_{b_1}\lambda_{b_2}\cdots\lambda_{b_r}\lambda_{a_{2r+1}})]. \tag{10}$$

By repeated use of Eqs. (9) and (10) we can reduce the symmetrical trace of any number of λ matrices to that of two or three matrices when we will apply Eq. (7) or (8) as the case may be. Substitution of expressions obtained from Eqs. (7)–(10) in Eq. (4) will finally lead to the identity we are after. Note that all these steps are straightforward, each term in the identity comes from a known source term in Eq. (4) (each source term corresponds to a given partition of $N = n + 1$), and has a well-defined coefficient as long as the symbol S is used. This coefficient will be the coefficient in Eq. (4) multiplied by $2^{N_2+N_3+\cdots+N_N}$ arising from the traces. Note also that in an actual computation, the symmetrization in Eqs. (9) and (10) may be dropped. One writes just one product of the d-type coefficients and performs symmetrization in all the N-indices after substituting the answers in Eq. (4). Also while performing symmetrization of Eq. (4), we may generally need quite fewer than $N!$ terms for various source terms.

IV. SPECIFIC CASES

After illustrating explicitly the calculation for $SU(3)$, we shall quote the results for $SU(4)$ to $SU(6)$.

(i) $SU(3)$:

$$K_{i_1i_2i_3i_4} = \epsilon_{\alpha_1\alpha_2\alpha_3\alpha_4}\epsilon_{\beta_1\beta_2\beta_3\beta_4}(\lambda_{i_1})_{\alpha_1\beta_1}(\lambda_{i_2})_{\alpha_2\beta_2} \times (\lambda_{i_3})_{\alpha_3\beta_3}(\lambda_{i_4})_{\alpha_4\beta_4}$$

$$= -6S\,\mathrm{Tr}(\lambda_{i_1i_2i_3i_4}) + 3S[\mathrm{Tr}(\lambda_{i_1i_2})\,\mathrm{Tr}(\lambda_{i_3i_4})]$$

$$= -12S(d_{i_1i_2a}d_{i_3i_4a}) + 12S(\delta_{i_1i_2}\delta_{i_3i_4}) = 0, \tag{11}$$

which can be written as

$$d_{i_1i_2a}d_{i_3i_4a} + d_{i_1i_3a}d_{i_2i_4a} + d_{i_1i_4a}d_{i_2i_3a} - (\delta_{i_1i_2}\delta_{i_3i_4} + \delta_{i_1i_3}\delta_{i_2i_4} + \delta_{i_1i_4}\delta_{i_2i_3}) = 0. \tag{12}$$

This is the same result as obtained previously by Macfarlane *et al. in our notation.*[3]

(ii) $SU(4)$:

$$3S(d_{i_1i_2a_1}d_{i_3i_4a_2}d_{i_5a_1a_2})_{15} - 5S(\delta_{i_1i_2}d_{i_3i_4i_5})_{10} = 0,$$

where 15 and 10 below the closing square brackets indicate that in order to perform symmetrization, *this many terms will have to be written down and the answer divided by this number*. Note that the numbers 15 and 10 are much smaller than 5!.

(iii) $SU(5)$:

$$6S(d_{i_1i_2a_1}d_{i_3i_4a_2}d_{i_5i_6a_3}d_{a_1a_2a_3})_{15} - 9S(\delta_{i_1i_2}d_{i_3i_4a}d_{i_5i_6a})_{45} - 4S(d_{i_1i_2i_3}d_{i_4i_5i_6})_{10} + 3S(\delta_{i_1i_2}\delta_{i_3i_4}\delta_{i_5i_6})_{15} = 0.$$

(iv) $SU(6)$:

$$30S(d_{i_1i_2a_1}d_{i_3i_4a_2}d_{i_5i_6a_3}d_{i_7a_1b}d_{a_2a_3b})_{105} - 42S(\delta_{i_1i_2}d_{i_3i_4a_1}d_{i_5i_6a_2}d_{i_7a_1a_2})_{315} - 35S(d_{i_1i_2a}d_{i_3i_4a}d_{i_5i_6i_7})_{105} + 35S(\delta_{i_1i_2}\delta_{i_3i_4}d_{i_5i_6i_7})_{105} = 0.$$

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[6]There are many different ways of expressing these symmetrized traces. Ours is the simplest and involves no f-type coefficients.

On the relationship between bifurcation points of the Kirkwood-Salsburg equation and phase transitions

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In this paper we explore the Vlasov conjecture on the relationship between bifurcation points and phase transitions. Because of the availability of the exact results of Ruelle, we focus our attention on the Kirkwood–Salsburg hierarchy, and recognizing that the first equation in this hierarchy is of the form of a Lichtenstein–Lyapunov nonlinear operator equation, we use a fundamental theorem of Krasnosel'skii to determine, under a suitable closure, bifurcation points for the same system considered by Ruelle. A special example is treated—that of a one-dimensional system of hard rods—and our main conclusion follows from the results of this study: namely, that "in this one-dimensional system" the bifurcation point does not seem to be related to the onset of a phase transition.

1. INTRODUCTION

The class of problems with which we shall be concerned in this paper deals with an approach to the study of phase transitions initiated by Kirkwood[1] and Vlasov[2] a generation ago. These authors suggested that changes in the behavior of solutions to certain of the nonlinear integral equations comprising the BBGKY hierarchy might be associated with the onset of a phase transition. In order to implement this suggestion, both authors derived instability criteria, Kirkwood using Fourier-transform methods and Vlasov using bifurcation theory, and, subject to the uncertainty involved in truncating the hierarchy (that is, use of superposition approximation), it was believed that the incidence of a phase transition could be identified with the point at which a well-defined solution exhibited an abrupt change in behavior. A problem of interpretation arises almost at once, however, in that it is very difficult to establish a one-to-one correspondence between the two criteria, although some progress has been made in simple cases.[3] Indeed, given the difference in approach of the two authors, there is no *a priori* reason to expect that the points of instability predicted by the Kirkwood theory are necessarily the same as the bifurcation points of the Vlasov theory. Of more consequence, however, is the observation that it has never been proved conclusively that these criteria represent either a necessary or a sufficient condition for the onset of a phase transition, a difficulty which is compounded by the fact that recent studies have shown that there can exist isolated branches of solutions to nonlinear problems which cannot be identified using standard analytical techniques.[4] The point of the latter remark is that, conceivably, a phase transition, viewed as a problem in nonlinear analysis, might be characterized by a switch from one branch of solutions to another, completely isolated branch, rather than by changes of the kind suggested by Kirkwood or Vlasov.

Recently, several authors[5] have re-examined the possibilities of the Kirkwood–Vlasov approach, bringing to the problem a variety of new analytical techniques complemented by a knowledge of recent results in the theory of classical fluids and phase transitions. While many of the results obtained by these authors are indeed suggestive, it must be pointed out that, for example, the exact relationship between bifurcation points on the one hand and phase transitions on the other has never been demonstrated. It is this task which is the objective of the present paper, and it is carried out in the following way. We recall that Ruelle, in his study of the Kirkwood–Salsburg hierarchy of linear integral equations, was able to obtain a bound which guaranteed the existence of a single phase for all values of the activity less than the one specified by the bound. At the same time, Groeneveld,[6] Penrose,[7] and Lebowitz[7] had obtained both upper and lower bounds on the radius of convergence of the virial expansion for certain potentials, and when this work was correlated with that of Ruelle,[8] it was found that the Ruelle bound corresponded to the lower bound on the radius of convergence. With these exact results at our disposal, we analyze here the first equation in the KS hierarchy, and note that this equation can be written formally as a Lichtenstein–Lyapunov operator equation. We obtain the linear operator equation whose eigenvalues determine the behavior of the nonlinear one, and then, after introducing a closure, we study the possibility of bifurcation for the same systems considered by Ruelle. As a concrete example, we determine explicitly the relationship between bifurcation points and bounds on the radius of convergence for a one-dimensional system of hard rods, a system for which detailed results are available. Our conclusions on validity of the Vlasov assumption follow from these studies, and are presented in the final section of this paper.

2. FORMULATION

We consider a classical, grand canonical ensemble of monatomic molecules in a volume V with activity z and pair intermolecular potential ϕ. For this system, the first equation in the Kirkwood–Salsburg hierarchy is

$$\rho(\underline{r}) = z\left(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_V K(\underline{r};(\underline{y})_n)\rho(\underline{y})_n d\underline{y}_1 d\underline{y}_2 \cdots d\underline{y}_n\right), \tag{2.1}$$

where

$$(\underline{y})_n = (\underline{y}_1, \underline{y}_2, \cdots, \underline{y}_n),$$

$$K(\underline{r};(\underline{y})_n) = \prod_{i=1}^{n} [\exp(-\beta\phi(|\underline{r} - \underline{y}_i|)) - 1] = \prod_{i=1}^{n} f(|\underline{r} - \underline{y}_i|). \tag{2.2}$$

Here, $\rho(\underline{y})_n$ is the n-body distribution function, and $f(|\underline{r} - \underline{y}_i|)$ is the Mayer f-function. (In this equation, and in what follows, we use the notation suggested by Ruelle in his book.[8]) By introducing the n-body correlation functions $g(\underline{y})_n$, where

$$g(\underline{y})_n = \rho(\underline{y})_n / \rho(\underline{y}_1)\rho(\underline{y}_2)\cdots\rho(\underline{y}_n), \tag{2.3}$$

Eq. (2.1) can be written as

$$\rho(\underline{r}) = z\left[1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_V K'(\underline{r}; (\underline{y})_n)\rho(\underline{y}_1)\rho(\underline{y}_2) \times \cdots \rho(\underline{y}_n) d\underline{y}_1 d\underline{y}_2 \cdots d\underline{y}_n\right], \quad (2.4)$$

where

$$K'(\underline{r}; (\underline{y})_n) = K(\underline{r}; (\underline{y})_n) g(\underline{y})_n. \quad (2.5)$$

We notice here that $K'(\underline{r}; (\underline{y})_n)$ is symmetric with respect to $(\underline{y})_n$. Now, Eq. (2.4) is an inhomogeneous nonlinear integral equation which can be transformed to a homogeneous equation by defining a new function $\rho'(\underline{r}) = \rho(\underline{r}) - \alpha$ for suitable choice(s) of constant α. By inserting $\rho(\underline{r}) = \rho'(\underline{r}) + \alpha$ into Eq. (2.4) and taking into account that $K'(\underline{r}; (\underline{y})_n)$ is symmetric with respect to $(\underline{y})_n$, we obtain, after grouping terms of each order of ρ',

$$\begin{aligned}\rho'(\underline{r}) + \alpha &= z\left(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \alpha^n \int_V K'(\underline{r}; (\underline{y})_n) d\underline{y}_1 \cdots d\underline{y}_n\right) \\ &+ z \sum_{n=1}^{\infty} \frac{n}{n!} \alpha^{n-1} \int_V K'(\underline{r}; (\underline{y})_n)\rho'(\underline{y}_1) d\underline{y}_1 \cdots d\underline{y}_n \\ &+ z \sum_{n=2}^{\infty} \frac{C_n^2}{n!} \alpha^{n-2} \int_V K'(\underline{r}; (\underline{y})_n)\rho'(\underline{y}_1)\rho'(\underline{y}_2) d\underline{y}_1 \cdots d\underline{y}_n \\ &+ \cdots, \end{aligned} \quad (2.6)$$

where $C_n^m = n!/[m!(n-m)!]$. Therefore, Eq. (2.6) can be written as follows:

$$\begin{aligned}\rho'(\underline{r}) + \alpha &= z\left(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \alpha^n \int_V K'(\underline{r}; (\underline{y})_n) d\underline{y}_1 \cdots d\underline{y}_n\right) \\ &+ z \sum_{n=1}^{\infty} \int_V K''(\underline{r}; (\underline{y})_n)\rho'(\underline{y}_1) \cdots \rho'(\underline{y}_n) d\underline{y}_1 \cdots d\underline{y}_n, \end{aligned} \quad (2.7)$$

where

$$K''(\underline{r}; (\underline{y})_n) = \sum_{m=n}^{\infty} \frac{C_m^n}{m!} \alpha^{m-n} \int_V K'(\underline{r}; (\underline{y})_m) d\underline{y}_{n+1} \cdots d\underline{y}_m. \quad (2.8)$$

By choosing α such that

$$\alpha = z\left[1 + \sum_{n=1}^{\infty} \frac{1}{n!} \alpha^n \int_V K'(\underline{r}; (\underline{y})_n) d\underline{y}_1 \cdots d\underline{y}_n\right], \quad (2.9)$$

we obtain the following homogeneous equation:

$$\rho'(\underline{r}) = z \sum_{n=1}^{\infty} \int_V K''(\underline{r}; (\underline{y})_n)\rho'(\underline{y}_n) d\underline{y}_1 \cdots d\underline{y}_n. \quad (2.10)$$

We now observe that this equation is similar in structure to the standard integral power series equation. An integral power term of order n relative to the function f is defined as

$$L(f) = \int K(s, y_1, y_2, \ldots, y_m) f^{\alpha_0}(s) f^{\alpha_1}(y_1) \times \cdots f^{\alpha_m}(y_m) dy_1 \cdots dy_m \quad (2.11)$$

if $\alpha_0 + \alpha_1 + \cdots + \alpha_m = n$, where $\alpha_0, \alpha_1, \ldots, \alpha_m$ are nonnegative numbers, and an integral power series is a summation from $n = 1$ to infinity of terms of the type (2.11). Returning, then, to the representation (2.10), we note that the right-hand side is an integral power series relative to the function ρ'. In operator notation, Eq. (2.10) can be written as

$$\rho'(\underline{r}) = z\mathrm{A}\rho'(\underline{r}), \quad (2.12)$$

where the operator A is defined as:

$$\mathrm{A}\rho'(\underline{r}) = \sum_{n=1}^{\infty} \int_V K''(\underline{r}; (\underline{y})_n)\rho'(\underline{y}_1) \cdots \rho'(\underline{y}_n) d\underline{y}_1 \cdots d\underline{y}_n. \quad (2.13)$$

This operator A, in the theory of nonlinear operator equations, is referred to as the Lichtenstein–Lyapunov integral power series operator. It is perhaps worth mentioning here that the integral power series equation, being an integral equation itself, is quite different from the usual power series expansion of a function in terms of some independent variable, e.g., the Mayer power series expansion of pressure p in powers of fugacity z.

Before one can make use of the various theorems on qualitative properties of the solutions of the operator equation (2.12), derived by Krasnosel'skii[9,10] and Vainberg,[11] it is necessary to establish first the conditions under which the operator A is completely continuous in function space.

Let C be the space of continuous functions on V, where V is a closed bounded set in a finite-dimensional space. We define the norm in C as

$$\|f\| = \sup_{x \in V} [|f(x)|]. \quad (2.14)$$

For simplicity we also introduce the notation

$$\int |e^{-\beta\phi(r)} - 1| dr = c(\beta) \quad (2.15)$$

and

$$\int (e^{-\beta\phi(r)} - 1) dr = c'(\beta). \quad (2.16)$$

By assuming that $c'(\beta) < \infty$ and $\sup_{y_i \in V} g(\underline{y})_n \leqslant d < \infty$, we have

$$\begin{aligned}|K''(\underline{r}; (\underline{y})_n)| &\leqslant \sum_{m=n} \frac{1}{n!(m-n)!} |\alpha|^{m-n} \times \int_V |K(\underline{r}; (\underline{y})_m)| \, |g(\underline{y})_m| d\underline{y}_{n+1} \cdots d\underline{y}_m \\ &\leqslant \sum_{m=n}^{\infty} \frac{1}{n!(m-n)!} d|\alpha|^{m-n} \int_V |K(\underline{r}; (\underline{y})_m)| d\underline{y}_{n+1} \cdots d\underline{y}_m \\ &= \sum_{m=n}^{\infty} \frac{1}{n!(m-n)!} d|\alpha|^{m-n} |K(\underline{r}; (\underline{y})_n)| \times \prod_{i=n+1}^{m} \int_V |K(\underline{r}; \underline{y}_i)| d\underline{y}_i \\ &= \frac{1}{n!} d|K(\underline{r}; (\underline{y})_n)| \sum_{m=n}^{\infty} [1/(m-n)!] |\alpha|^{m-n} c(\beta)^{m-n} \\ &= \frac{1}{n!} d|K(\underline{r}; (\underline{y})_n)| \exp[c(\beta)|\alpha|]. \end{aligned} \quad (2.17)$$

Thus,

$$\begin{aligned}\|\mathrm{A}\rho\| &\leqslant \sum_{n=1}^{\infty} \|\rho\|^n \int_V |K''(\underline{r}; (\underline{y})_n)| d\underline{y}_1 \cdots d\underline{y}_n \\ &\leqslant \sum_{n=1}^{\infty} \frac{\|\rho\|^n}{n!} d \exp[c(\beta)|\alpha|] \int_V |K(\underline{r}; (\underline{y})_n)| d\underline{y}_1 \cdots d\underline{y}_n \\ &= \sum_{n=1}^{\infty} \frac{\|\rho\|^n}{n!} d \exp[c(\beta)|\alpha|][c(\beta)]^n \\ &= d \exp[c(\beta)|\alpha|] \exp[c(\beta)\|\rho\|]. \end{aligned}$$

This shows that $\|\mathrm{A}\rho\|$ is bounded for bounded ρ provided that $c(\beta)$, d, and $\alpha < \infty$.

For equicontinuity, let us look at $\|A\rho(\underline{r}) - A\rho(\underline{r}')\|$:

$$\|A\rho(\underline{r}) - A\rho(\underline{r}')\| = \| \sum_{n=1}^{\infty} \int_V [K''(\underline{r};(\underline{y})_n) - K''(\underline{r};(\underline{y})_n)]$$

$$\times \rho(\underline{y}_1)\rho(\underline{y}_2)\cdots\rho(\underline{y}_n)d\underline{y}_1\cdots d\underline{y}_n\|$$

$$\leqslant \sum_{n=1}^{\infty} \|\rho\|^n \int_V |K''(\underline{r};(\underline{y})_n) - K''(\underline{r}';(\underline{y})_n)| d\underline{y}_1\cdots d\underline{y}_n$$

$$\leqslant \sum_{n=1}^{\infty} \|\rho\|^n \sum_{m=n}^{\infty} \frac{|\alpha|^{m-n}}{n!(m-n)!} \int_V |K(\underline{r};(\underline{y})_m) - K(\underline{r}';(\underline{y})_m)|$$

$$\times |g(\underline{y})_m| d\underline{y}_1\cdots d\underline{y}_m$$

$$\leqslant \sum_{n=1}^{\infty} \|\rho\|^n \sum_{m=n}^{\infty} \frac{d|\alpha|^{m-n}}{n!(m-n)!}$$

$$\times \int_V |K(\underline{r};(\underline{y})_m) - K(\underline{r}';(\underline{y})_m)| d\underline{y}_1\cdots d\underline{y}_m.$$

We now suppose that the pair potential $\phi(r)$ is continuous in intermolecular distance r. Then $K(\underline{r};\underline{y}_1) = f(|\underline{r} - \underline{y}_1|)$ is continuous as a function of $|\underline{r} - \underline{y}_1|$, and $K(\underline{r};(\underline{y})_n)$ is continuous as a function of $|\underline{r} - \underline{y}_1|, |\underline{r} - \underline{y}_2|, \ldots, |\underline{r} - \underline{y}_n|$. For a finite volume V in three-dimensional Euclidian space, $K(\underline{r};(\underline{y})_n)$ is therefore uniformly continuous in $V^n \subset \mathbb{R}^{3n}$. By taking into account the triangle inequality

$$|\underline{r} - \underline{r}'| \geqslant \Big| |\underline{r} - \underline{y}_1| - |\underline{r}' - \underline{y}_1| \Big|,$$

we conclude that for given $\epsilon' > 0$, there exists a $\delta > 0$ such that the condition $|\underline{r} - \underline{r}'| < \delta$ implies that

$$|K(\underline{r};(\underline{y})_m) - K(\underline{r}';(\underline{y})_m)| < \epsilon'.$$

Thus,

$$\|A\rho(\underline{r}) - A\rho(\underline{r}')\| \leqslant \sum_{n=1}^{\infty} \frac{1}{n!} d\|\rho\|^n$$

$$\times \sum_{m=n}^{\infty} \frac{1}{(m-n)!} |\alpha|^{m-n} \epsilon' (\text{mes} V)^m$$

$$= \sum_{n=1}^{\infty} \epsilon' d \|\rho\|^n (\text{mes} V)^n \frac{1}{n!} \sum_{m=n}^{\infty} \frac{1}{(m-n)!} (|\alpha| \text{mes} V)^{m-n}$$

$$= \sum_{n=1}^{\infty} \epsilon' d \|\rho\|^n (\text{mes} V)^n (1/n!) \exp(|\alpha| \text{mes} V)$$

$$= \epsilon' d \exp(\|\rho\| \text{mes} V) \exp(|\alpha| \text{mes} V)$$

$$= \epsilon' d \exp[\text{mes} V(\|\rho\| + |\alpha|)].$$

Therefore, for given $\epsilon > 0$, there exists a $\delta > 0$ such that the condition $|\underline{r} - \underline{r}'| < \delta$ implies that $\|A\rho(\underline{r}) - A\rho(\underline{r}')\| < \epsilon$ if we choose ϵ' to be such that

$$\epsilon' = \epsilon/d \exp[\text{mes} V(\gamma + |\alpha|)],$$

where $\gamma = \sup[\|\rho\|]$. Our conclusion that $A\rho$ is equicontinuous follows from the Ascoli–Arzela theorem. Hence, A is completely continuous on a bonded subset of C provided that $c(\beta)$, $\max[g(y)_n]$, and $|\alpha| < \infty$ and $\phi(r)$ is continous.

3. BIFURCATION THEORY

An examination of the homogeneous integral equation for $\rho'(\underline{r})$ reveals that $\rho'(\underline{r}) \equiv 0$ is a solution of Eq. (2.10); this solution shall be referred to as the trivial solution, and it corresponds to the choice $\rho(\underline{r}) \equiv \alpha$. In accordance with the notation of Krasnosel'skii, one identifies the trivial solution with the null vector θ, so that the operator equation (2.10) is written:

$$zA\theta = \theta.$$

For small values of the parameter z, it is straightforward to show that the null solution is unique. It is interesting to see if one can go beyond this result, however, and ask whether, for increasing values of the parameter z, starting at some value, say z_0, a nonzero solution of Eq. (2.10) makes its appearance in the neighborhood of θ. One says that z_0 is a bifurcation point of Eq. (2.10) if for every $\epsilon > 0$, $\delta > 0$ there exists an eigenfunction ρ of the operator A such that the norm $\|\rho\| < \delta$, and the eigenfunction ρ corresponds to a characteristic number z such that $|z - z_0| < \epsilon$.

If we now adopt the point of view taken by Vlasov, then the emergence of a new solution (or solutions) $\rho'(\underline{r})$ at the bifurcation point z_0 may, in some sense, be associated with the limit of stability of the phase described by $\rho'(\underline{r}) \equiv 0$. Given this interpretation and the availability of quite general theorems on bifurcation of nonlinear operator equations, it is our intention to study the possible bifurcation of Eq. (2.10), and to compare the results with the rigorous results obtained by Ruelle[12] on the one hand, and Groeneveld[6] and Lebowitz and Penrose[7] on the other. To carry out this program, we use the following fundamental theorem of Krasnosel'skii:

Theorem 2.1 (Ref. 9, p. 196): Let A be a completely continuous operator having a Fréchet derivative B at the point θ, and satisfying the condition

$$A\theta = \theta.$$

Then each characteristic value z_0 of odd multiplicity of the linear operator B is a bifurcation point of the operator A, and to this bifurcation point there corresponds a continuous branch of eigenvectors of the operator A.

Krasnosel'skii shows that for the Lichtenstein–Lyapunov operator A, the Fréchet derivative B at the origin of the space C is the linear integral operator (in our notation):

$$B\rho'(\underline{r}) = \int_V K''(\underline{r};\underline{y}_1)\rho'(\underline{y}_1)d\underline{y}_1. \tag{3.1}$$

Hence, according to the above theorem, the bifurcation points of the nonlinear operator A are determined by the eigenvalues of odd multiplicity of the linear operator equation

$$zB\rho = \rho. \tag{3.2}$$

That is, we have obtained the equation from which the bifurcation points of the first KS integral equation can be calculated, at least in principle.

An examination of the structure of the kernel in Eq. (3.1) for the case $n = 1$,

$$K''(\underline{r};\underline{y}_1) = \sum_{m=1}^{\infty} \frac{1}{(m-1)!} \alpha^{m-1} \int_V K'(\underline{r};(\underline{y})_m) d\underline{y}_2\cdots d\underline{y}_m$$

$$= \sum_{m=1}^{\infty} \frac{1}{(m-1)!} \alpha^{m-1} \int_V K(\underline{r};(\underline{y})_m) g(\underline{y})_m d\underline{y}_2\cdots d\underline{y}_m, \tag{3.3}$$

reveals the essential role played by the $g(y)_n$, the n-body correlation functions. This is, of course, the point in the analysis where n-body effects enter explicitly, and we note that the exact bifurcation point can be determined rigorously only when the whole hierarchy of KS integral equations is solved. In other words, the exact determination of the bifurcation point is linked to the n-body problem. This difficulty, so fundamental in its implications, not only arises in the present analysis, but is common to all studies of the Kirkwood–Vlasov type which focus attention on *one* equation of the BBGKY hierarchy. Such an equation is always coupled to an infinite hierarchy of nonlinear integral equations, regardless of the representation considered, with the consequence that before progress can be made, some approximation must be introduced to truncate the hierarchy. The point of view adopted in Refs. 1, 2, 3, 5 is that, although one cannot obtain *exact* results on the behavior of the hierarchy without solving the n-body problem, nonetheless one might be able to obtain an essentially correct description of this behavior by a fortunate choice of closure. Since it is our objective in this paper to determine the relationship between results obtained using bifurcation theory and exact results, we now introduce a closure, suggested by the structure of the kernel K'' in Eq. (3.3). In particular, we note that the kernel K'', as expressed in Eq. (3.3), is a summation of integral terms, with the kernel of each term a product function of $K(\underline{r};(\underline{y})_n)$ and $g(\underline{y})_n$. Furthermore, it is to be noted that $K(\underline{r};(\underline{y})_n)$ is the product of n Mayer f-functions, and, as illustrated in Fig. 1, this function tends to peak very sharply as the number n increases and goes to zero very quickly (to ~2 in reduced units) as the intermolecular distance increases. On the other hand, for short intermolecular distances $g(y)_n$ is nearly zero, particularly as n increases. These considerations on the composite behavior of $K(\underline{r};(\underline{y})_n)$ and $g(\underline{y})_n$, augmented by the observation that in a one-dimensional hard-rod system the product $K(\underline{r};(\underline{y})_n)g(\underline{y})_n$ is strictly zero for $n > 2$, suggest that the introduction of a closure which minimizes the importance of higher-order terms in Eq. (3.2) may not be serious. To explore this possibility, we recall that for a fluid phase (gas or liquid) the n-body correlation function approaches unity as the distance between particles becomes large. Therefore, as a first approximation on the $g(\underline{y})_n$ we set $g(\underline{y})_n \equiv 1$.

With this approximation, we have

$$\begin{aligned} K''(\underline{r};\underline{y}_1) &= \sum_{m=1}^{\infty} \frac{1}{(m-1)!}\,\alpha^{m-1} f(|\underline{r}-\underline{y}_1|) \\ &\quad\times \prod_{i=2}^{m} \int_V f(|\underline{r}-\underline{y}_i|)d\underline{y}_i \\ &= f(|\underline{r}-\underline{y}_1|)\sum_{m=1}^{\infty}\frac{1}{(m-1)!}\,\alpha^{m-1}c'(\beta)^{m-1} \\ &= f(|\underline{r}-\underline{y}_1|)\exp[c'(\beta)\alpha], \end{aligned} \tag{3.4}$$

and the linear equation (3.2) becomes

$$\rho'(\underline{r}) = z\int_V f(|\underline{r}-\underline{y}_1|)\exp[c'(\beta)\alpha]\rho'(\underline{y}_1)d\underline{y}_1. \tag{3.5}$$

Also, by Eq. (2.9) α is determined by

$$\begin{aligned} \alpha &= z\left(1+\sum_{n+1}^{\infty}\frac{1}{n!}\,\alpha^n\int_V K(\underline{r};(\underline{y})_n)d\underline{y}_1\cdots d\underline{y}_n\right) \\ &= z\left(1+\sum_{n=1}^{\infty}\frac{1}{n!}\,\alpha^n c'(\beta)^n\right) \\ &= z\exp[c'(\beta)\alpha]. \end{aligned} \tag{3.6}$$

To look for eigenvalues of Eq. (3.5), let $\rho'(\underline{r}) \equiv \rho'$, a constant. Then Eq. (3.5) reduces to

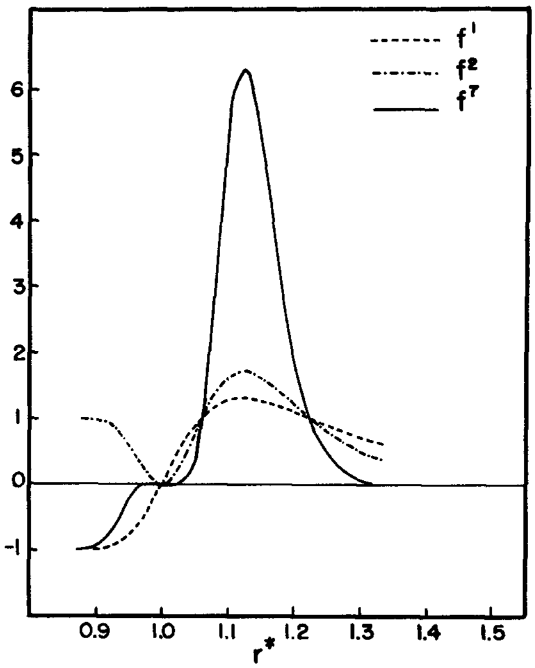

FIG. 1. Mayer f-function, f^2, and f^7 as functions of reduced intermolecular distance r^* for Lennard-Jones potential at reduced temperature $T^* = 1.2$.

$$\begin{aligned} 1 &= z\exp[c'(\beta)\alpha]\int_V f(|\underline{r}-\underline{y}_1|)d\underline{y}_1 \\ &= zc'(\beta)\exp[c'(\beta)\alpha]. \end{aligned} \tag{3.7}$$

By Eq. (3.6), Eq. (3.7) becomes

$$\alpha c'(\beta) = 1, \text{or } \alpha = 1/c'(\beta).$$

and from Eq. (3.6),

$$z = \alpha/\exp[c'(\beta)\alpha] = e^{-1}c'(\beta)^{-1}. \tag{3.8}$$

Hence we conclude that the linear operator equation (3.2) has a single eigenfunction $\rho'(\underline{r}) \equiv \rho'$, corresponding to a uniform density solution, and a simple eigenvalue given by Eq. (3.8). Given this information and the Krasnosel'skii theorem, we can identify Eq. (3.8) with the bifurcation point of the nonlinear operator equation (2.11).

The bifurcation point obtained can be compared with the result obtained by Ruelle in his rigorous analysis of the whole KS hierarchy.[12,8] Ruelle obtained the bound $|z| < e^{-2\beta B-1}c(\beta)^{-1}$ (henceforth, the activity corresponding to this bound will be called the Ruelle point), and showed that when $|z| < e^{-2\beta B-1}c(\beta)^{-1}$ the grand partition function has no zero;[8] therefore, according to Yang and Lee,[13] the system has no phase transition. It is important to note that the Ruelle point guarantees the existence of a single phase for values of $|z|$ less than $e^{-2\beta B-1}c(\beta)^{-1}$. In other words, a phase transition may occur only if $|z| \geqslant e^{-2\beta B-1}c(\beta)^{-1}$, at least, is satisfied.

We now show that the bifurcation point obtained above, Eq. (3.8), occurs at or beyond the Ruelle point. Returning to Eqs. (2.15), (2.16), we see that

$$c(\beta) \geqslant |c'(\beta)|.$$

Therefore, from the fact that $B \geqslant 0$, we have the relationship

$$e^{-2\beta B-1}c(\beta)^{-1} \leqslant e^{-1}c(\beta)^{-1} \leqslant |e^{-1}c'(\beta)^{-1}|.$$

This result suggests that for the particular closure $g(y)_n \equiv 1$, there does exist a simple relationship between the bifurcation point and the Ruelle point: In particular, the bifurcation point is always greater than or equal to the Ruelle point. For the case of purely repulsive potentials, this relationship is even simpler. Here we have that $B = 0$ and $c(\beta) = |c'(\beta)|$, and therefore the $|z|$ obtained from Eq. (3.8) is exactly the same as the Ruelle point. Moreover, for purely repulsive potentials $c'(\beta) < 0$, and therefore by Eq. (3.8) we have $z < 0$. This means that the bifurcation point cannot lie on the positive real axis for purely repulsive potentials. One might be tempted to conclude from this that there will be no phase transition for a system of molecules interacting via a purely repulsive potential, but it should be emphasized that the above result is a consequence of the analysis which followed from the assumption that $g(y)_n \equiv 1$. In fact, it will be shown in the next section that for a certain purely repulsive potential the bifurcation point can lie on the positive real axis but that this occurrence has nothing to do with a phase transition.

4. ONE-DIMENSIONAL SYSTEM OF HARD RODS

The relationship between bifurcation points and bounds on stability can be made more definite by considering a specific example, a system of one-dimensional hard rods of length a. Strictly speaking, this class of potentials is not accessible to our study, given the conditions on complete continuity of the operator A. However, one can proceed by identifying a continuous potential function which, in a suitably defined limit, yields the hard-rod potential; in particular, we consider the potentials

$$\phi(r) = \begin{cases} m^m, & 0 \leq r < a + 1/m - 1 \\ 1/(r - a + 1)^m, & r \geq a + 1/m - 1 \end{cases}$$

in the limit when $m \to \infty$. For this one-dimensional hard-rod system, $c'(\beta) = -2a$, and therefore by Eq. (3.8),

$$z = -1/2ea = -0.184a^{-1}.$$

We note in passing that in bifurcation theory one deals with z explicitly, rather than with the absolute value of z; so we conclude that the bifurcation point lies on the negative z axis. Furthermore, in agreement with the result obtained in the previous section relative to a system of molecules interacting via a purely repulsive potential, the absolute value of z obtained using bifurcation theory is the same as the bound obtained from the Ruelle analysis.

Our result for the hard-rod system can be compared to the one derived by Penrose in his analysis of the radius of convergence of the virial expansion; there the lower bound on the radius of convergence R was found to be $0.184a^{-1}$, whereas the upper bound for R was found to be $0.368a^{-1}$. Furthermore, Penrose found that the function $p(z) = kT \sum b_l z^l$ was analytic on the positive real axis, but had a branch point at $z = -0.368a^{-1}$. Since the hard-rod system exhibits no phase transition, a result first obtained by Tonks,[14] Penrose concluded that the divergence in the fugacity expansion for real $z > R$ has no physical significance. In light of the above analysis, we conclude here, similarly, that the bifurcation point for this system has no physical significance as regards phase transitions.

A strong result that supports this conclusion can be obtained by noticing that for a hard-rod system $K(r;(y)_n)$ $g(y)_n) = 0$ for $n > 2$. Hence, the linear equation (3.2) becomes

$$\rho'(r) = z \int_V \Big(K(r; y_1) + \alpha \int_V K(r;(y)_2) g^{(2)}(|y_2 - y_1|) dy_2 \Big) \rho'(y_1) dy_1.$$

After setting $\rho'(r) \equiv \rho'$ and taking into account the fact that $K(r;(y)_2) g(y)_2 = 0$ except when $|r - y_1|, |r - y_2| < a$ and $|y_1 - y_2| > a$, one obtains

$$1 = z\Big(2 \int_0^a (-1) dy_1 + 2\alpha \int_0^a \int_a^{a+y_1} (-1)(-1) g^{(2)}(y_{12}) dy_1\Big),$$

$$z = 1 \Big/ \Big(-2a + 2\alpha \int_0^a \int_a^{a+y_1} g^{(2)}(y_{12}) dy_{12} dy_1\Big). \quad (4.1)$$

In the low density limit

$$g^{(2)}(y_{12}) = \begin{cases} 0, & y_{12} < a \\ 1, & y_{12} \geq a \end{cases},$$

and because of the geometry of hard-rod configurations, the value of $g(r)$ exceeds unity when r becomes greater than a. One would expect, therefore, that, for the second term in the denominator in Eq. (4.1),

$$2 \int_0^a \int_a^{a+y_1} g^{(2)}(y_{12}) dy_{12} dy_1 > 2 \int_0^a \int_a^{a+y_1} dy_{12} dy_1 = a^2.$$

This shows that for the hard-rod system, one might find a bifurcation point on the positive real axis. But, as mentioned earlier, the hard-rod system has no phase transition, and therefore it appears that the bifurcation point has nothing whatever to do with the signalling of a phase transition.

5. CONCLUSION

The principal objective of this paper was to investigate the relationship, if any, between bifurcation points and the signalling of a phase transition. In our analysis, we focused attention on the first equation in the Kirkwood–Salsburg hierarchy, an equation which was recognized to have the form of an integral power series equation. Such an integral series defines a nonlinear integral operator, usually referred to as the Lichtenstein–Lyapunov operator, and the possible bifurcation of the full nonlinear equation was investigated by determining the eigenvalues of an associated linear operator equation. In particular, by a fundamental theorem of Krasnosel'skii, the bifurcation points of the full nonlinear equation are just the eigenvalues of odd multiplicity of the associated linear equation.

In order to obtain well-defined estimates of the bifurcation point for specific systems, it was necessary to introduce a closure. Our choice of closure was motivated by the structure of the kernel K'' and, once introduced, led to a simple relationship between the absolute value of the bifurcation point and the Ruelle point, a relationship which, for the case of purely repulsive potentials, reduced to an identity. The bifurcation point itself, when related to the activity, was found to lie on the negative real axis. We then considered the specific case of a one-dimensional system of hard rods, for which exact bounds on the radius of convergence of the virial expansion had been determined by Penrose and Lebowitz,[8] and it led to the interesting result that the bifurcation point was related to the lower bound (rather than the upper bound as might have been expected) on the radius of convergence. Since, for this system, the bifurcation point could be located on the positive real axis, and since it is known explicitly that a one-dimensional system of hard rods does *not* exhibit a phase transition, the conclusion was reached that "for this one-dimensional system" the bifurcation point seemed to have nothing to do with the signalling of a phase transition. Indeed, the overall conclusion one reaches in the present study is that there may well exist a fundamental relationship between bifurcation points, on the one hand, and bounds on the radius of convergence, on the other. However, in light of the specific example treated in this paper, the bifurcation point seems to be related to a lower bound rather than an upper bound on the radius of convergence, which, together with the *location* of the bifurcation point, would seem to invalidate the basic assumption of Vlasov, namely, that there may exist a fundamental relationship between bifurcation points and phase transitions.

Finally, it should be emphasized that the above analysis has been carried through subject to the closure defined by setting $g(y)_n = 1$. Possibly, then, the above conclusions should be tempered by the statement that if one were to impose other closures, the bifurcation point might shift around on the real activity axis, perhaps even coinciding with an upper bound on the radius of convergence for certain systems. A less delicate way of phrasing this possibility would be to suggest that the use of our closure so mutilates the nonlinear equation under study that, quite possibly, the results obtained in this paper are misleading, if not incorrect. The seriousness of this objection can be neutralized, at least in part, by directing the reader's attention to a truly remarkable feature of the Krasnosel'skii theorem cited in Sec. 3. Essentially, this theorem states that the possible bifurcation of the full nonlinear integral operator is determined by an associated *linear* operator equation; for the specific case of the Lichtenstein–Lyapunov operator, the associated linear operator is, in fact, the leading term on the right-hand side of the full nonlinear operator equation. Now, whereas one might expect that the use of different closures would affect higher-order terms in the integral power series, perhaps in a dramatic way (although from our arguments in Sec. 3, we do not believe this to be the case), the effect of these changes on the *linear* term is expected to be small. That this is reasonable may be inferred from the following calculation. Suppose, instead of introducing a "horizontal" closure, one introduces a "vertical" one; that is, suppose one truncates terms beyond the first linear one in *every* equation of the Kirkwood–Salsburg hierarchy. It turns out that one can carry through an analysis on this truncated set of equations in exactly the same way that Ruelle analyzed the full KS hierarchy. The infinite volume limit can be constructed and a bound obtained which can then be compared directly with the exact one obtained by Ruelle. One finds the discrepancy between the two bounds to be $1/e$. Phrased differently, it seems that n-body effects are imbedded in the Kirkwood–Salsburg hierarchy in such a way that the difference between considering these effects explicitly, as Ruelle did, and bypassing their importance almost entirely, as was done in the above calculation, is a factor of $1/e$. While not conclusive, this observation, coupled with the fact that the structure of the kernel K'' itself suggested the closure adopted, lends support to our premise that the principal conclusions of this paper may not change in an essential way with a different choice of closure.

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Conformal group in a Poincaré basis. III. Degenerate series

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We construct systematically all the unitary irreducible representations of the group $SU(2,2)$ which are realized on the two manifolds Z and Z introduced in Paper I of this series; these include all the degenerate representations at present known apart from the exceptional or ladder series. This particular realization of the global theory displays the Poincaré subgroup in a simple form, and we examine the reduction products under this group. We find that the degenerate first series contain only spacelike momenta and a single spin fixed by the invariants of $SU(2,2)$; the degenerate second series on the other hand contain only spinless representations of $\mathbb{P}$, while the nature of the momenta which appear depends on the particular series concerned.

I. INTRODUCTION

In the third paper of this series[1] we study all those representations of $SU(2, 2)$ which are realized upon the manifolds Z or $\hat{Z}$ that were introduced previously. Since these are degenerate representations (that is, they are defined over manifolds of lower than maximum dimensionality), they do not in general belong to the principal series and hence will not enter into the generalized Plancherel measure.[2] Despite this, they are of considerable interest: both mathematically, because the well-known groups $SL(2,C)$ and $SL(2,R)$ have no degenerate series except the trivial representation, and physically, because all the applications of the representation theory of the conformal *group* (as opposed to its Lie algebra) have used degenerate series exclusively. We find that these manifolds carry all the degenerate representations that are at present known,[3] with the single exception of the ladder or exceptional series; fortunately this has been fairly well covered[4,5] in the literature—at least algebraically—and so its omission here is less serious.

Let us recall the nature of the phenomenon of degeneracy. Any representation of a group G is defined by operators on a space of functions over some homogeneous space of the group; and we know that all such spaces are of the form G/H, where H is a closed subgroup of G. Consider a sequence of such H_i which satisfies $H_i \subset H_j$ for $i < j$; and let H_0 be the subgroup consisting of the identity alone. Then $G/H_0 = G$, and upon G itself is defined the (reducible) regular representation. Proceding further, we know of the existence of H_1 such that G/H_1 is the carrier of the *principal series* of representations of G; we can extend the functions on G/H_1 to functions on G itself by simple invariance or homogeneity requirements, but they will not in general be Haar-square-integrable on G. Now consider $H_2 \supset H_1$; this defines a manifold of lower dimension than G/H_1, but which is still a perfectly possible carrier space for representations of G. Such representations are termed *degenerate*; if we insist upon regarding them as defined over G/H_1, we find that the dependence of the functions upon one or more variables is trivial, and so they are not square-integrable over that manifold.

A simple example of such degeneracy is the one-dimensional (unitary irreducible) representation of $G = GL(2,R)$ realized on the space G/G, and given by

$$r \to |\det r|^{i\rho}[\operatorname{sgn}(\det r)]^{\epsilon}, \quad r \in G.$$

Slightly more complicated examples are to be found in Ref. 6, Chap. III, which treats the sequence of increasingly degenerate series of $SL(n,C)$ specified by the sequence of subgroups $H_2 \subset H_3 \subset \cdots$.

In the present paper we are concerned with two distinct degenerate series of $\mathcal{G} \simeq SU(2,2)$. In paper I we introduced a subgroup Λ of $\mathcal{G}$ (which corresponds to what we have called H_2 here) which defined a manifold Y, and found that there were actually two distinct groups K and $\mathcal{K}$ which contained Λ and hence defined each a submanifold of Y which we called Z (zee) and Z (zeta) respectively, neither of which was a submanifold of the other. (Notice the interesting feature that the sequence of subgroups H_i has branched into two). In that paper we did not make use of these manifolds per se—they were defined merely as stepping-stones to Y—but they clearly satisfy the criteria for carrier spaces of degenerate representations, and we now investigate them in that light.

Because of the very much simpler structure of these representations when compared with those of the principal series, we are able to treat them systematically. It is clear from our previous remarks that degenerate representations do indeed exist with these manifolds as carrier spaces; we therefore have only to investigate the twin problems of unitarity and irreducibility. We do this by deriving systematically all possible Hermitian forms which are invariant under the postulated representation operators. Suppose that for a given set of parameters specifying the representation (i.e., Casimir operators) there exists only one such form: Then if it is positive-definite, it constitutes a scalar product, and the representation is unitary; the absence of an alternative form implies the absence of operators commuting with all the representation operators, and demonstrates its irreducibility. If we find two or more such forms, the representation is reducible, and we must display explicitly the invariant subspaces, but the argument is very similar.

There is, of course, no objection to this procedure for the principal series of representations—indeed Gel'fand uses this method in Ref. 7 to construct those of $SL(2,C)$ and $SL(2,R)$—but the manifold Y was of too great a complexity for us to use it with ease (recall that the principal discrete series d_0 is sixfold reducible!) and so in Papers I and II we used more specific theorems to obtain the representations. The advantage of the procedure here, when practicable, is that it ensures both irreducibility and completeness; but it does not, of course, mean that there do not exist other degenerate representations, defined over other carrier spaces. As we have remarked already, the exceptional series is not defined over either of the manifolds examined here.

Section II then starts by deriving all possible invariant bilinear forms on spaces over the four-dimensional manifold Z, which is essentially Minkowski space, by a method which is the exact analog of Gel'fand's treatment of $SL(2,R)$ in Ref. 7, Chap. VII; with a knowledge of these we can then write down all the unitary representations in the degenerate second series. Not surprisingly, they are all degenerate representations of the Poincaré group too; they are spinless. As an exception to the general rule that they do not appear in the principal series, two of the representations (which we call $d_2^{k\pm}$) turn out to be special cases of the discrete series $d_0^{\pm}$ ($K = k - 1, p = 0 = q$).

Section III treats the degenerate first series in a similar way, although the analysis is less straightforward, deriving as before a continuous series, a complementary, and (this time) two discrete. We find that when restricted to the Poincaré group, only spacelike momenta occur, while the spin is fixed by the Casimir operators of $SU(2,2)$. Section VI summarizes our results and compares them with those of other workers—in particular with the analysis of Yao.[3] We find some disagreement. Finally, two appendices treat incidental material which is made use of in the body of the paper.

We retain most of the notation and conventions of Papers I and II; in particular, the subgroups and matrices in Paper I, Sec. 2, and their complexifications (needed for a study of the reducibility of the discrete series) from Paper II, Sec. 2. There is one slight change: Lest the similarity of the type used to denote Z (zee) and Z (zeta) give rise to confusion, we have added a caret to Z (zeta) defined by (I. 9) or (15), and in this paper denote this manifold by $\hat{Z}$. We have introduced a new notation and nomenclature for the various degenerate series which is an obvious extension of the systematic notation of Graev for the principal series of $U(p,q)$, and is intended to be clearer and more specific than the current tendency to call every series the "most degenerate" and ignore the branched structure of the sequence of subgroups H_i.

II. SECOND DEGENERATE SERIES

The degenerate second series of representations are defined on the space H_z of functions over the manifold Z of (I. 8). The transformation law under $g \in \mathcal{G}$ has been given in (I. 13):

$$T_g : f(z) = |\Delta|^{s-2}(\operatorname{sgn}\Delta)^{\epsilon} f(z'), \qquad zg = kz', \tag{1}$$

where k is a member of the block-diagonal subgroup K of (I. 8). Our task is to find all values of s and ϵ which admit a positive-definite invariant Hermitian form—i.e., a scalar product. We approach this systematically by deriving all possible bilinear functionals on the subspace $H_z^0 \subset H_z$ of functions of compact support: the extension to H_z itself then follows as in Ref. 7, Chap. III, Sec. 4. 4.

A. Invariant bilinear functionals

Suppose then that we have a bilinear form $B(f,g)$ which is invariant under all $g \in \mathcal{G}$. As we pointed out in II, it is convenient to choose a set $\{g_i\}$ of elements of $\mathcal{G}$ and examine the invariance under each g_i separately; such a set was given in II, Sec. 2, and we shall make use of it here. We shall suppose that f transforms under the representation $(s_1\epsilon_1)$ and g under $(s_2\epsilon_2)$.

Consider first the requirement of invariance under the translation group Z. Gel'fand's results[7] tell us at once that this implies that

$$B(f,g) = [B_0, \omega], \tag{2}$$

where

$$\omega(z) = \int f(z')g(z + z')d\mu(z') = f * g(z)$$

and B_0 is some generalized function on H_z^0. Now examine the dilatation operator. We find

$$T_d : f(z) = |d|^{2s_1-4} f(zd^{-2})$$

so that

$$B(f,g) = |d|^{8-2s_1-2s_2} B[f(d^2z), g(d^2z)]$$

and

$$[B_0, \omega(z)] = d^{-s_1-s_2}[B_0, \omega(dz)]: \tag{3}$$

That is, B_0 is a homogeneous generalized function in z of degree $-(s_1 + s_2) - 4$. We now look at an arbitrary element $a \in SL(2,C) \subset \mathcal{G}$ and find

$$[B_0, \omega(z)] = [B_0, \omega(z')]; \tag{4}$$

and therefore B_0 is constructed entirely out of quantities which are invariant under $SL(2,C)$. Since only one such exists, we know that B_0 is a homogeneous generalized function of $(a\bar{a} + bc)$ [i.e., $x_\mu x^\mu$] of degree $-\frac{1}{2}(s_1 + s_2) - 2$. Its parity is not yet determined.

Finally we consider the element $J \in \mathcal{G}$ of (II. 3), in order to find the remaining restrictions upon B_0. It is easy to show that the transformations under J are

$$\left.\begin{aligned} a' &= -a\Delta^{-1} \\ b' &= -c\Delta^{-1} \\ c' &= -b\Delta^{-1} \end{aligned}\right\} \quad \Delta = -a\bar{a} - bc \tag{5}$$

so that

$$[|a_1 - a_2|^2 + (b_1 - b_2)(c_1 - c_2)]' = [\ \ ]\Delta_1^{-1}\Delta_2^{-1}. \tag{6}$$

There are two possibilities we must consider, according to whether or not $\frac{1}{2}(s_1 + s_2)$ is a nonnegative integer; let us start with the nonsingular case, when it is not. Then the homogeneous generalised function B_0 is defined uniquely[8] up to parity:

$$\int f(z_1)[|a_1 - a_2|^2 + (b_1 - b_2)(c_1 - c_2)]^{-[(s_1+s_2)/2]-2} \times (\operatorname{sgn}[\ \ ])^{\nu} g(z_2)d\mu(z_1)d\mu(z_2). \tag{7}$$

This is already invariant under the similitude group. Examining the behavior under $J \in \mathcal{G}$ with the aid of (5) and (6), we find that it is conformal-invariant too, provided

$$s_1 = s_2, \qquad \epsilon_1 = \nu = \epsilon_2. \tag{8}$$

We are left with the singular case to consider, when $(s_1 + s_2)$ is an even integer. There are then three linearly independent generalized functions associated with the quadratic form $(a\bar{a} + bc)^{-n-2}$ (see, for instance, Ref. 8, Chap. III, Sec. 2. 2), and we must examine them all for invariance. The calculations are tedious and largely routine, paralleling Gel'fand's treatment[7] of $SL(2,R)$, and we do not give them here but instead just state the results. We find that invariant functionals exist when

$$s_1 + s_2 = 0, \qquad \epsilon_1 = \epsilon_2$$

and when

$$s_1 - s_2 = 0, \qquad \epsilon_1 = \epsilon_2. \tag{9}$$

In the first case just one functional exists (unless both s vanish), and can be written

$$B(f,g) = \int f(z)g(z)d\mu(z). \tag{10}$$

In the second, which includes the special case of $s_1 = 0 = s_2$, all three functionals are invariant if the parity of s is ϵ; of these, one is concentrated on the entire eight-dimensional space $\{z_1, z_2\}$, one upon the surface $|a_1 - a_2|^2 + (b_1 - b_2)(c_1 - c_2) = 0$, and one at $z_1 = z_2$. We shall not need the former two; the last is given by

$$B(f,g) = \int f(z)(\partial_a\partial_{\bar{a}} + \partial_b\partial_c)^s g(z)d\mu(z). \tag{11}$$

If the parity of s differs from ϵ, only this one functional is invariant.[9] To summarize: If $s_1 = s_2$ is not an integer, there exists the unique bilinear form (7), usually to be understood in the sense of its regularization; if $s_1 = -s_2 \neq 0$, there is the form (10); and if $s_1 = s_2$ is an integer, there are three linearly independent bilinear forms of which the simplest is (11). If $s_1 \neq \pm s_2$, no such forms can exist.

B. Unitary representations

We now ask that the representation (1) be unitary; that is, we must find all positive-definite Hermitian functionals on H_z. We have just found all bilinear functionals, and hence we know all Hermitian ones, which are obtained by setting $s_2 = \bar{s}_1$, $\epsilon_1 = \epsilon_2$. Let us start with the first case of (9). This tells us that if

$$s = i\rho$$

where ρ is real, then just one invariant Hermitian functional exists, and is given by

$$(f,g) = B(\bar{f},g) = \int \overline{f(z)}g(z)d\mu(z). \tag{12}$$

This is manifestly positive-definite, and it therefore defines a scalar product. This makes (1) a unitary representation, which is also irreducible since no further invariant forms exist. We shall call it the second degenerate continuous series $d_2^{\rho\epsilon}$.

Now turn to (7). For hermiticity (9) implies that

$$s = \sigma,$$

where σ is real. Let us change our parametrization of z from $\{a,b,c\}$ to $\{x_\mu\}$ as defined in (I.15); then (7) becomes

$$B(\bar{f},g) = \int \overline{f(x)}\,|(x-x')^2|^{-\sigma-2}[\operatorname{sgn}(x-x')^2]^\epsilon \times g(x')d^4x d^4x'. \tag{13}$$

It can be shown that this is positive definite only for $\epsilon = 1 \pmod 2$ and σ in the open interval $(-1, 0)$; under these conditions (1) and (13) define a unitary irreducible representation of $\mathcal{G}$ which we call the second degenerate complementary series d_2^σ. We assert that $\sigma \in (0,1)$ defines a representation which is equivalent to this.

We are left with the two possibilities when $s_1 = s_2$ is an integer: $\epsilon_1 = \epsilon_2 = s \pmod 2$ and $\epsilon_1 = \epsilon_2 = s+1 \pmod 2$. Consider first the former. We know that there are just three invariant Hermitian functionals, and hence at most three irreducible components of this representation. To determine the irreducible subspace of H_z in this case (it is no longer sufficient to work with H_z^0) we must introduce the complexification Z_c of the manifold Z, as we did in II with the larger manifold Y. We can then make use of the results of II, Sec. 3A, to find three invariant domains of Z_c: the forward, backward, and spacelike tube domains T^+, T^-, and T^0. Therefore, we can decompose H_z into the sum of three subspaces $H_z^\pm$ and H_z^0, of functions which are boundary values of others analytic in T^+ or T^- and of functions which are not. When $\epsilon = s \pmod 2$ the transformations T_g are analytic in the variables z_c (see Paper II, Sec. 2) and hence this decomposition is invariant under all of $\mathcal{G}$; if the parity relation is not satisfied, then neither is the decomposition invariant and (11) is then not of definite sign.

We therefore obtain three second degenerate discrete series d_2^k. With the variables x_μ of (I.15) we have

$$T_g^k: f(x) = \Delta^{k-2}f(x'),$$
$$(f,g) = \int \overline{f(x)}[\partial_\mu\partial^\mu]^k g(x)d^4x. \tag{14}$$

The irreducible subspaces are defined above as boundary value spaces.

C. Reduction under $\mathbb{P}$

We now turn to the reducibility of these representations under the Poincaré group. First notice that they are all degenerate representations: They are defined over the manifold of space–time points alone, with no provision for spin. For timelike momenta, such representations are usually regarded as the spin-zero representations of the principal series; but for spacelike momenta they are often overlooked, as the little-group representation to which they correspond is the *trivial* representation of $SU(1,1) \sim O(2,1)$. In the context of degenerate (i.e., nonprincipal series) representations of the Poincaré group, however, they must be remembered.

We start with the continuous series $d_2^{\rho\epsilon}$ and the complementary d_2^σ. Since there are no analyticity constraints upon H_z in these two cases, we find that all momenta (timelike and spacelike) occur. For the discrete series d_2^k, however, the situation is more interesting. The analyticity criteria of Sec. 2.2 show that there are two timelike series (which we shall call $d_2^{k\pm}$) which contain timelike positive and negative mass momenta, respectively, and one spacelike series d_2^{k0}. We have in fact met $d_2^{k\pm}$ before: They are exactly the principal discrete series $d_0^\pm$ in the special case $p = 0 = q$ (that is, $m = 0, L = K + 2$); it is not difficult to show that the scalar product in that case degenerates into ours. The spacelike series d_2^{k0} too is not entirely new: It occurred in II but was discarded when we redefined the carrier spaces $\mathfrak{D}^i$ modulo the space $\mathcal{E}$ of polynomials in $\omega, \overline{\omega}$ (II, Secs. 3A and 4B). Notice incidentally that (14) is positive-definite on H_z^0 but negative-definite upon $H_z^\pm$ if k is odd.

Finally, we can summarize our results in the following theorem:

Theorem 5: When restricted to $\mathbb{P}$, each representation $d_2^{\rho\epsilon}$ or d_2^σ of the second degenerate continuous or complementary series of $\mathcal{G}$ contains a direct integral over all (timelike and spacelike momenta) spinless representations of $\mathbb{P}$. The representations d_2^{k+} and d_2^{k-} of the positive or negative discrete series contain all timelike momenta with positive or negative masses respectively, whereas d_2^{k0} contains only all spacelike momenta. Each representation occurs with unit multiplicity.

III. FIRST DEGENERATE SERIES

The degenerate first series are defined on the space H_ζ introduced in I, section 3.2, of C^∞ functions over the manifold $\hat{Z}$ of (I.9):

$$\hat{Z} \ni \zeta = \left(\begin{array}{c|cc|c} 1 & & & \\ \hline -\bar{\beta} & 1 & & \\ -\bar{\alpha} & & 1 & \\ \hline \epsilon & \alpha & \beta & 1 \end{array}\right), \tag{15}$$

$$\epsilon + \bar{\epsilon} + \alpha\bar{\beta} + \bar{\alpha}\beta = 0. \tag{16}$$

We shall sometimes satisfy this condition upon ϵ by writing $\epsilon = c - \bar{\alpha}\beta$, where c is pure imaginary. The transformation law is

$$\begin{aligned} T_g: f(\zeta) &= k_1^A \bar{k}_1^B f(\zeta') \\ &= |k_1|^{2B} k_1^{A-B} f(\zeta'), \\ \zeta g &= \mathcal{K}\zeta' \quad [\text{cf. (I. 13)}], \end{aligned} \tag{17}$$

and we shall proceed as in the last section to find all admissible values of the constants A and B. To do this, it is best to use a somewhat different set of elements of $\mathcal{G}$: we shall choose $\zeta \in \hat{Z}$, the dilation d, the operator $\phi \equiv \exp(\phi J_3)$, and the inversion $I = \exp(\pi J_2)$ of (II. 2), and the unimodular subgroup R corresponding to the matrix k_0 of (I. 22):

$$R = \left(\begin{array}{c|cc|c} 1 & & & \\ \hline & r_{11} & ir_{12} & \\ & ir_{21} & r_{22} & \\ \hline & & & 1 \end{array}\right), \quad r_{11}r_{22} + r_{12}r_{21} = 1. \tag{18}$$

It is simple to show that these are a sufficient set of elements of $\mathcal{G}$.

A. Invariant bilinear functionals-general case

Consider first the restraints imposed upon a bilinear functional $B(f,g)$ by invariance under ζ, assuming that f transforms under the representation (A_1B_1) and g under (A_2B_2). We find as before that such invariance implies that B is some generalized function acting upon the (generalized) convolution of f and g:

$$\begin{aligned} B(f,g) &= [B_0, \omega], \\ \omega(\zeta) &= \int f(\zeta')g(\zeta\zeta')d\mu(\zeta'). \end{aligned} \tag{19}$$

Notice that $\hat{Z}$ is not an Abelian group; hence this convolution cannot be written additively. The measure is given by (I. 12):

$$d\mu(\zeta) = D\alpha D\beta dc. \tag{20}$$

Invariance under $\phi = \exp(\phi J_3)$ is trivial; and examining d after the manner of the last section, we find that, for fixed β, B_0 is homogeneous in $|\alpha|$ and c together of degree $-\frac{1}{2}(A_1 + A_2 + B_1 + B_2)$. Turning to the group R, we obtain

$$\begin{aligned} \alpha \to \alpha' &= \alpha r_{11} + i\beta r_{21}, & c' &= c, \\ \beta \to \beta' &= \beta r_{22} + i\alpha r_{12}, & k_1 &= 1, \end{aligned} \tag{21}$$

so that B_0 must be unchanged by all such transformations. It therefore depends only upon the invariants of this group: that is, upon c itself and the combination $-2\mathrm{Re}\,\epsilon = \alpha\bar{\beta} + \bar{\alpha}\beta$. We can summarize our results by stating

B_0 is a homogeneous function of $|\epsilon|$ of degree $-\frac{1}{2}(A_1 + A_2 + B_1 + B_2)$.

There are as before two alternatives to consider, according to whether or not $s \equiv \frac{1}{2}(A_1 + A_2 + B_1 + B_2)$ is a positive integer; we start with the nonsingular alternative, when it is not. Then B_0 is arbitrary only up to a dependence upon the phase of ϵ: We have

$$[B_0, \omega] = \int |\epsilon|^{-s}\Phi(\arg\epsilon)\omega(\zeta)d\mu(\zeta), \tag{22}$$

where Φ is some (generalized) function to be determined. Invariance under $I \in a$ leads us to

$$\begin{aligned} B(f,g) &= B(T_I f, T_I g) \\ &= \int f(\alpha_1'\beta_1'\epsilon_1')\beta_1^{A_1 * B_1}|\bar{\beta}_1\beta_2\epsilon_{12}'|^{-s}\Phi[\arg(\bar{\beta}_1\beta_2\epsilon_{12}')] \\ &\quad \times \beta_2^{A_2 * B_2} g(\alpha_2'\beta_2'\epsilon_2')|\beta_1|^6 d\mu(\zeta_1)|\beta_2|^6 d\mu(\zeta_2), \end{aligned}$$

where we have set

$$\alpha' = -\epsilon/\beta, \quad \beta' = -1/\beta, \quad \epsilon' = \alpha/\beta,$$

and

$$\epsilon_{12} \equiv \epsilon(\zeta_2\zeta_1^{-1}) = \epsilon_2 - \epsilon_1 + \bar{\beta}_1(\alpha_2 - \alpha_1) + \bar{\alpha}_1(\beta_2 - \beta_1). \tag{23}$$

The notation $z^{A*B} \equiv z^A \bar{z}^B$ was introduced in II. For this equation to be satisfied, we must have

$$A_1 + B_1 = A_2 + B_2,$$

$$\Phi(\arg\epsilon_{12}' + \arg\beta_2 - \arg\beta_1)e^{i(A_1-B_1)\arg\beta_1}e^{i(A_2-B_2)\arg\beta_2} = \Phi(\arg\epsilon_{12}')$$

which tells us that $A_1 + A_2 = B_1 + B_2$ and

$$\Phi(\phi) = e^{i(A_1-B_1)\phi}. \tag{24}$$

Therefore, unless s is a positive integer, there exists an invariant bilinear functional only if

$$\begin{aligned} A_1 &= \sigma + \tfrac{1}{2}m - \tfrac{3}{2} = B_2, \\ B_1 &= \sigma - \tfrac{1}{2}m - \tfrac{3}{2} = A_2, \end{aligned} \tag{25}$$

where m is an integer and σ is arbitrary complex. (The factors of $\frac{3}{2}$ are inserted for convenience.) In this case it is given by

$$B(f,g) = \int f(\zeta_1)|\epsilon_{12}|^{-m-2\sigma-3}\epsilon_{12}^m g(\zeta_2)d\mu(\zeta_1)d\mu(\zeta_2)$$

(generally to be understood in the sense of its regularization). It is unique. If σ is real, we can therefore obtain a Hermitian functional

$$(f,g) = \int \bar{f} * g(\zeta)|\epsilon|^{-m-2\sigma-3}\epsilon^m d\mu(\zeta). \tag{26}$$

We show in Appendix A that if m is even and σ lies in the open interval $(-\frac{1}{2}, 0)$, this is positive-definite and hence defines a scalar product; the resulting unitary irreducible representation of $\mathcal{G}$ we shall call the first degenerate complementary series $d_1^{m\sigma}$. In Appendix B we show that the representation with parameters $(m, -\sigma)$ is equivalent.

B. Invariant bilinear functionals-singular case

We now turn to the singular alternative, in which $s = \frac{1}{2}(A_1 + A_2 + B_1 + B_2)$ is a positive integer. We have not been able to treat this case systematically because of the complexity of the non-Abelian manifold $\hat{Z}$, which makes it difficult to determine invariant regularizations of the integral (26) and even more difficult to investigate their positivity. There are, however, two series of representations that we already know to exist, a continuous series and a discrete, and we shall investigate these individually. We start with the first degenerate continuous series $d_1^{m\rho}$, specified by $2A = 2i\rho - m - 3$, $2B = 2i\rho + m - 3$:

$$T_g: f(\zeta) = |k_1|^{m+2i\rho-3} k_1^{-m} f(\zeta'). \tag{27}$$

This has the manifestly invariant, positive-definite inner product

$$(f,g) = \int \overline{f(\zeta)} g(\zeta) d\mu(\zeta). \tag{28}$$

C. Discrete series of representation

Consider the representation d_1^{AB} of $\mathcal{G}$ by

$$T_g^{AB}: f(\zeta) = k_1^A \bar{k}_1^B f(\zeta'), \tag{29}$$

where A and B are nonnegative integers. This is reducible: in particular, it contains an (irreducible) *finite-dimensional* representation over a space M of multinomials of total degree in $(\alpha, \beta, \epsilon)$ of A or less and $(\bar{\alpha}, \bar{\beta}, \bar{\epsilon})$ of B or less. [This can easily be verified by using the standard set of elements of $\mathcal{G}$.] The dimensionality d of this representation is

$$36(d+1) = (A+1)(A+2)(A+3)(B+1)(B+2)(B+3) \tag{30}$$

(we have given the trivial representation dimension zero). According to a theorem[10] of Harish-Chandra, then, there are a pair of *unitary* irreducible representations contained in (29) as well. We have not been able to find a particularly convenient inner product with these parameter values, however, and shall therefore study the equivalent representation of $\mathcal{G}$ in which A and B are *negative* integers. That there is indeed a true equivalence is shown in Appendix B.

First then consider the reducibility of the representation T^{-A-B}. As in the last section, we must complexify the manifold $\hat{Z}$; this is arranged in direct analogy with (II. 4), by replacing $(-\bar{\alpha})$ and $(-\bar{\beta})$ in the matrix ζ of (15) by γ and δ. The complexified matrix ζ_c then transforms with the complexified $\mathcal{K}_c$[cf. (II. 6), (II. 8)]:

$$\begin{aligned} T_g^{-A-B}: f(\zeta_c) &= k_1^{-A} k_{-1}^{-B} f(\zeta_c'), \\ \zeta_c g &= \mathcal{K}_c \zeta_c'; \end{aligned} \tag{31}$$

we have replaced $\bar{k}_1$ by k_{-1}^{-1} [for the notation see (I. 9)], which on the "real boundary" is no change at all. Then because A and B are integers, we find that the transformations preserve analyticity in the set of variables $\{\alpha, \beta, \gamma, \delta, \epsilon\}$: The argument exactly parallels that of II, Sec. 3. We find four invariant domains in this five-dimensional complex space, entirely analogously to (II. 18):

$$\Omega_1 \equiv \epsilon + \bar{\epsilon} + \bar{\alpha}\beta + \alpha\bar{\beta} \gtrless 0$$
$$U_1 \equiv \epsilon + \bar{\epsilon} - \delta(\alpha + \bar{\gamma}) - \bar{\delta}(\bar{\alpha} + \gamma) - \beta\gamma - \bar{\beta}\bar{\gamma} \gtrless 0;$$

of these four domains, however, only those two for which $\Omega_1 u_1 > 0$ possess boundary values onto $\gamma = -\bar{\alpha}, \delta = -\bar{\beta}$, and so we anticipate twofold reducibility. Unlike the situation in II, however, we have no "independent" variable in which to have analyticity [$\Omega_1 > 0$ cannot be a domain of holomorphy in all three variables α, β, and ϵ] and so are forced into more involved considerations.

We assert then that the space H_ζ is the union of two (intersecting) spaces H_ζ^+ and H_ζ^- which are defined as follows: H_ζ^+ contains all those functions $f(\alpha, \beta, c) \in H_\zeta$ which by some orientation-preserving[11] change of variables $\zeta \to \zeta'(\zeta)$ can be expressed as $f'(\alpha', \beta', c')$ where f' is analytic in c' in $\mathrm{Re}\, c' > 0$. H_ζ^- is defined to have analyticity in $\mathrm{Re}\, c' < 0$. Since the transformations (31) preserve analyticity in $\{\alpha, \beta, \gamma, \delta, \epsilon\}$—and hence in $c \equiv \epsilon - \beta\gamma$—it is almost obvious that these spaces are invariant; we omit a detailed proof since an indirect proof of the reducibility of this representation will be given shortly by displaying two scalar products. As a simple example of a function with the desired properties we cite

$$\begin{aligned} H_\zeta^- \ni f &= (\epsilon - \beta\gamma - 1)^{-N} \exp(\epsilon - \beta\gamma + \alpha\gamma + \beta\delta) \\ &= (c-1)^{-N} \exp(c - |\alpha|^2 - |\beta|^2) \end{aligned}$$

on the boundary.

The space H_ζ^+ is found by reversing the sign of c. The intersection of H_ζ^+ and H_ζ^- is a finite-dimensional space (which for certain parameter values is empty); let us introduce the notations

$$E = H_\zeta^+ \cap H_\zeta^-, \quad F^+ = H_\zeta^+/E, \quad F^- = H_\zeta^-/E. \tag{32}$$

Upon F^+, F^-, and E the representation (31) then acts irreducibly.

We now consider the scalar product. By the results of Sec. 3A there is a unique invariant Hermitian form for the space H_ζ^{-A-B}, given by

$$(f,g)_0 = \int \overline{f(\zeta_1)} \epsilon_{12}^{A-3} \bar{\epsilon}_{12}^{B-3} g(\zeta_2) d\mu(\zeta_1) d\mu(\zeta_2). \tag{33}$$

The integral converges in a classical sense for $(A+B) > 3$ (the asymptotics of H_ζ are satisfactory) and in the case of equality we replace this by the scalar product for the continuous series (28). Since we show in Appendix B that the representations (A, B) and $(-B-3, -A-3)$ are equivalent, we have covered all possibilities. In what follows we shall ignore the trivial case $A + B = 3$.

Now if A and $B \geqslant 3$ the integral is degenerate upon a subspace $D \subset H_\zeta$ of functions whose generalized moments vanish; if A or $B < 3$, more complicated arguments are needed, and the degeneracy subspace is H_ζ itself. The factor space H_ζ/D is finite-dimensional, and isomorphic to E; D itself is just the direct sum of F^+ and F^-. That E is empty for A or $B < 3$ implies the nonexistence of a finite-dimensional representation of $\mathcal{G}$ for these parameter values, which correspond to A or B of (29) (but not both) being negative.

Therefore the Hermitian form (33) vanishes identically upon the spaces of interest, and we must seek another. It is natural to try replacing the homogeneous function of ϵ_{12} in the integrand by an associated homogeneous function (see for example Gel'fand,[7] Chap. VII, Sec. 5.3): we consider the form

$$(f,g) = \int \overline{f(\zeta_1)} \epsilon_{12}^{A-3} \bar{\epsilon}_{12}^{B-3} \ln(\epsilon_{12}) g(\zeta_2) d\mu(\zeta_1) d\mu(\zeta_2).$$

It is simple to show that this is invariant upon D (but not upon H_ζ itself unless $A + B < 6$) and nondegenerate there. We can indeed now introduce two independent Hermitian forms which are separately invariant on D; to do so, we write (33) as

$$(f,g) = \int \bar{f} * g(\zeta) \epsilon^{A-3} (-\alpha\bar{\beta} - \bar{\alpha}\beta - \epsilon)^{B-3} \ln\epsilon \, d\epsilon D\alpha D\beta$$

where the ϵ integration is along the contour $\mathrm{Re}\epsilon =$

$-\operatorname{Re}\alpha\bar{\beta}$ and we run the logarithmic cut along the imaginary axis. Suppose $g \in F^+$; then if $\operatorname{Re}(\alpha\bar{\beta}) < 0$ we can close the contour of ϵ integration to the right and the integral vanishes. Similarly for $g \in F^-$ we can close it to the left if $\operatorname{Re}(\alpha\bar{\beta}) > 0$. We can therefore define the two conditionally invariant[12] Hermitian forms

$$(f,g)_\pm = \int_{\alpha\bar{\beta}+\bar{\alpha}\beta \gtrless 0} \bar{f} * g(\zeta)\epsilon^{A-3}\bar{\epsilon}^{B-3}\ln\epsilon d\mu(\zeta); \tag{34}$$

then $(f,g)_+$ vanishes upon F^- but is nonzero upon F^+, while $(f,g)_-$ is nondegenerate upon upon F^-. If $f \in F^+$ and $g \in F^-$ (or vice versa), the form vanishes. Notice that while both these functionals can be extended to the entire space H_ζ, they are not invariant there.

Since both these forms are Hermitian, we have only to show positivity in order to constitute them as scalar products for the series d_1^{-A-B} and complete the proof of the unitarity of the representations. We have not succeeded in finding a direct proof of this; however, we have shown that the scalar product (if it exists) is (34), unique up to multiplicative factors, and since Harish-Chandra's theorem assures us of the existence of a UIR (and hence of a scalar product), positivity of the normalized integral follows.[13] A direct proof would of course be more satisfactory.

Let us summarize our results on the series $d_1^{A,B}$ which is equivalent to $d_1^{-B-3,-A-3}$. When A and B are nonnegative, we are assured of unitarity by Harish-Chandra's theorem; and when $A + B = -3$, we can use the scalar product (28) of the continuous series, which is manifestly positive-definite. For other parameter values we cannot at present prove unitarity.

D. Reduction under $\mathbb{P}$

We now consider the reduction under the Poincaré group of these representations over the manifold $\hat{Z}$. For the second degenerate series it was immediately clear what was the situation, but here it is less so and we must examine the Casimir operators of $\mathbb{P}$.

First we consider the momentum dependence—that is, the way the functions $f \in H_\zeta$ transform under translations z_0. Consider for fixed β a translation in the direction

$$(x_0, \mathbf{x}) = (\tfrac{1}{2}(1 + \beta\bar{\beta}),\ -\operatorname{Re}\beta, \operatorname{Im}\beta, \tfrac{1}{2}(1 - \beta\bar{\beta}));$$

that is, a transformation by a matrix z_0 given by

$$(a,b,c) = (-b\bar{\beta}, b, b\beta\bar{\beta}).$$

For all the first degenerate series we obtain hence

$$T_{z_0}: f(\alpha,\beta,c) = f(\alpha,\beta,c)$$

so that the function is unaltered by this displacement—in other words, the momentum must be orthogonal to this direction. But this is parallel to a *lightlike* vector; no timelike vector can be orthogonal to this, and hence the momentum is purely spacelike for all representations on the spaces H_ζ. We can obtain this result another way by remarking that the basis functions $\mathfrak{D}^{p}_{A'A}(\zeta)$ of Appendix A are actually eigenfunctions of momentum; and a short calculation shows that $p_\mu p^\mu = -|A'|^2$.

We turn now to the spin content. To investigate this, we evaluate the fourth-order Casimir operator w^2 of $\mathbb{P}$ in terms of the generators of the group expressed as differential operators[14] on H_ζ. w is given by

$$w_\mu = -\tfrac{1}{2}\epsilon_{\mu\nu\rho\sigma}J^{\nu\rho}P^\sigma$$

and after a tedious but straightforward calculation we obtain the remarkable result

$$w_\mu w^\mu = k(k+1)P_\mu P^\mu,$$

where we have assumed that the representation is specified by (29) (where A and B are not necessarily integers), and set

$$k = 1 + \tfrac{1}{2}(A + B). \tag{35}$$

In other words, the representation T^{AB} contains only the single spin $s = k$ (the missing minus signs are caused by the anti-Hermitian nature of our generators). Inserting the values of A and B appropriate to the series concerned, we find that the continuous series (27) has spin $s = -\frac{1}{2} + i\rho$ and the complementary series (25) has spin $s = \sigma - \frac{1}{2}$; the parity of the representations of the little groups is that of m. The first of these is on the principal continuous series of $SU(1,1)$ or $O(2,1)$ and the second on the complementary series, and confirm our result that the momenta concerned are all spacelike.

There remains the discrete series (29), or more strictly the two separate parts of the series specified by $A + B = -3$ and $A, B \geqslant 0$. On the first part we find that the spin lies on the discrete series[15] of $SU(1,1)$, $s = -\frac{1}{2}$; on the second, that it lies on the discrete series but at a value of $s = 1$ or above. The problem is now to decide which discrete series $-k^+$ or k^- — and to investigate the effects of the reducibility of $d_1^{A,B}$.

First consider the former problem. Recall that for the principal series of $\mathcal{G}$ the parameter $\frac{1}{2}m = \frac{1}{2}(B - A)$ plays the role of an "allowed helicity"; a brief calculation now shows, however, that for A and B of the same sign the helicity $\frac{1}{2}m$ is incompatible with both the series k^+ and k^- of $SU(1,1)$. This paradox is resolved quite simply by observing that the actual helicity is given by a more complicated operator (if $p_1 = 0 = p_2$ it is just $\frac{1}{2}m - i\partial/\partial\theta$, where $\theta = \arg\beta$); the derivatives in this have a spectrum with an excluded center portion because of the requirement that (33) vanish on the space D, and because of this the helicity does indeed always lie in an allowed range. We find in fact that both the series k^+ and k^- occur in the reduction under the Poincaré group.[16]

Finally, we turn to the significance of the reducibility of the representation d_1^{AB}. This is linked to the invariance of the analyticity in c in some reference frame, and we know that analyticity in $\operatorname{Re}c > 0$ implies that $(p_0 + p_3) > 0$. Since this is itself not a Lorentz-invariant restriction for spacelike momenta, we need concern ourselves with it no further since it cannot restrict the representations of $\mathbb{P}$ which occur. We can now summarize our results:

Theorem 6: When restricted to $\mathbb{P}$, each representation of the first degenerate series of $\mathcal{G}$ contains all spacelike momenta. The first degenerate continuous series $d_1^{m\rho}$ contains the spin $s = -\frac{1}{2} + i\rho$ only; the complementary series $d_1^{m\sigma}$ only the spin $s = \sigma - \frac{1}{2}$. In either case the parity of the representation of the little group is that of m. The representations $d_1^{mk\pm}$ of the positive or negative discrete series contain the spin k only.

IV. COMMENTS AND COMPARISONS

In this section we summarize our results on the degenerate series and compare them with those of other workers. To relate our representations unambiguously to those of others we make use of the expressions (I.38) for the Casimir operators; with the representation (II.12),

$$T_g: f(y) = |\Delta|^{K-1}(\mathrm{sgn}\Delta)^\epsilon |\lambda|^{m-K+L-2}\lambda^{-m} f(y') \quad (36)$$

these are

$$C_2 = 5 - \tfrac{1}{4}m^2 - \tfrac{1}{2}(K^2 + L^2),$$
$$C_3 = \tfrac{1}{8}im(K^2 - L^2), \quad (37)$$
$$C_4 = \tfrac{1}{8}m^2(K^2 + L^2 - 2) - \tfrac{1}{2}(K^2 + L^2) + \tfrac{1}{16}(K^2 - L^2)^2 + 1$$

and the fourth-order operator is related to that of Yao[3] by (I.39). In the table at the end of this section we list the representations, their scalar products, and the allowed values of the parameters K, L, and m, together with the representations in Yao's list[3] to which they correspond and their reduction products under the Poincaré group. The Casimir operators can all be found by straightforward substitution in (37), and we do not give them explicitly.

We start by discussing the second degenerate series. The complementary series d_2^{σ} has been given by Yao alone, but the continuous series $d_2^{\rho\epsilon}$ by several authors,[3,17,18] although the presence of the parameter ϵ (which does not appear in representations of the Lie algebra) has been overlooked. Castell[17] has shown how this reduces under $\mathbb{P}$; Limić *et al.*[17] have realized the representation on spaces of functions over the hyperboloids $O(4,2)/O(4,1)$ and $O(4,2)/O(3,2)$ and the cone $O(4,2)/O(3,1) \times T^4$: these are, of course, all unitarily equivalent by virtue of the Gel'fand–Graev transform. All these results are in agreement with ours.

The discrete series have also been investigated. Rączka and Fischer[19] consider $U(2,2)$; hence their representation is actually d_2^{kn}, where n is an integer of the same parity as k [corresponding to our parameter $\epsilon = k(\mathrm{mod}\ 2)$], and is irreducible by virtue of the extra generator that that group has; the threefold reducibility is given in Refs. 18 and 20, where the authors treat the orthogonal group $SO(4,2)$. Yao's conclusion[3] that all these series are spacelike disagrees with ours; he also regards $k = 0$ as a separate class of representation (his class X) and implies that it is irreducible. Castell[17] has examined the special case $k = 0 = \epsilon$ and its reduction under $\mathbb{P}$, and his results agree with our own; the alternative situation $k = 0, \epsilon = 1$ belongs to the continuous series $d_2^{\rho\epsilon}$ and is irreducible.

We now turn to the degenerate first series, and as far as we are aware the only treatment of these is that of Yao.[3] For the continuous series $d_1^{m\rho}$ (his "principal series," case XIII) and the complementary series $d_1^{m\sigma}$ his results agree with ours; so too do his results on that part $d_1^{m\pm}$ of the discrete series characterized by $A + B = -3$ (his cases V, VI); although we obtain a UIR for all integer values of m whereas he requires it to be odd.

For the other part of the discrete series $d_1^{A,B}$ (his "discrete series $D^\pm$," cases III, IV) our results differ. Yao has obtained these series by citing the theorem[10] by Harish–Chandra that we employed in Sec. 3C, which to be applicable requires the existence of a finite-dimensional representation of $SU(2,2)$. Now we have shown explicitly that such a finite-dimensional representation exists when A and B are both either positive integers or negative and less than -3, while by substituting into (37) his values for the Casimir operators of these series we find that Yao's representations have one of the parameters A, B positive and the other negative. We have not been able to convince ourselves that a finite-dimensional representation does indeed exist with such parameter values, and so the Casimir operators that we give for this series do not agree with those of Yao. He finds like us that his series are spin-irreducible, but states that they are purely timelike. Since our series are defined over the manifold $\hat{Z}$, they are purely spacelike; the spin then belongs to the discrete series of $SU(1,1)$.

It is interesting to note that the degenerate first series we have given here contain between them every spacelike spin[15] except for $k = 0$ and $k = \frac{1}{2}$. Whether or not the discrete series d_1^{AB} and d_1^m are in fact separated by these points requires an investigation of the positivity of the scalar product (34) in the range where the integral converges but is not guaranteed positive by the Harish-Chandra theorem.

Finally, we notice that the exceptional or ladder series of representations[4,5] are not present above. This is because they are not defined over either of the manifolds Z or $\hat{Z}$; indeed they are not given by any formula of the type (36). To see this, we remark that the Casimir operators of that series are[3]

$$C_2 = -\tfrac{3}{4}(k^2 - 4), \quad C_3 = \tfrac{1}{8}ik(k^2 - 4), \quad C_4 = \tfrac{3}{16}k^2(k^2 - 4), \quad k \text{ an integer}; \quad (38)$$

there are many sets of values of K, L, and m which satisfy these relations, but none of them in addition can yield the dilation operator whose generator has been given by Castell[4] or Mack and Todorov.[5]

Table of results

$d_1^{m\rho}$ $\quad K = 1 \quad L = 2i\rho \quad m$

$(f,g) = \int \overline{f(\zeta)} g(\zeta) d\mu(\zeta)$

Yao case XIII, "principal series"
Spacelike. Spin $s = -\frac{1}{2} + i\rho$

$d_1^{m\sigma}$ $\quad K = 1 \quad L = 2\sigma \quad m$ even $\quad \sigma \in (-\frac{1}{2}, 0)$ or $(0, \frac{1}{2})$

$(f,g) = \int \overline{f(\zeta_1)} |\epsilon_{12}|^{-m-2\sigma-3} \epsilon_{12}^m g(\zeta_2) \times d\mu(\zeta_1) d\mu(\zeta_2)$

Yao case XIV, "complementary series"
Spacelike. Spin $s = \sigma - \frac{1}{2}$

$d_1^{AB\pm}$ $\quad K = 1 \quad L = 3 + A + B \quad m = A - B$
$A, B \geqslant 0$

Spacelike. Spin $s = 1 + \frac{1}{2}(A + B)$

$d_1^{-A-B\pm}$ $\quad K = 1 \quad L = 3 - A - B \quad m = A - B$
$A, B \geqslant 3$

$(f,g) = \int \bar{f} * g(\zeta) \epsilon^{A-3} \bar{\epsilon}^{B-3} \ln \epsilon \, d\mu(\zeta)$

Spacelike. Spin $s = -2 + \frac{1}{2}(A + B)$
Yao cases III, IV, "discrete series $D^\pm$".
But see above.

$d_1^{m\pm}$ $\quad K = 1 \quad L = 0 \quad m$

$(f,g) = \int \overline{f(\zeta)} g(\zeta) d\mu(\zeta)$

Spacelike. Spin $s = -\frac{1}{2}$ only.
Yao cases V, VI "most degenerate discrete series".

$d_2^{\rho\epsilon}$ $\quad K = i\rho - 1 \quad L = i\rho + 1 \quad m = 0$

$\rho \in (-\infty, 0)$ or $(0, \infty) \quad \epsilon = 0$

$\rho \in (-\infty, 0]$ or $[0, \infty) \quad \epsilon = 1$

$(f,g) = \int \overline{f(z)} g(z) d\mu(z)$

All momenta (time- and spacelike). Spinless. Yao case I, "most degenerate principal continuous series."

d_2^{σ} $\quad K = \sigma - 1 \quad L = \sigma + 1 \quad m = 0 \quad \epsilon = 1$

$\sigma \in (-1, 0)$ or $(0, 1)$

$$(f,g) = \int \overline{f(x)}\, |(x - x')^2|^{-\sigma-2} \operatorname{sgn}(x - x')^2 \times g(x') d^4x d^4x'$$

All momenta (time- and spacelike). Spinless. Yao case II, "most degenerate complementary continuous series."

$d_2^{K\pm}, d_2^{K_0}$ $\quad K = k - 1 \quad L = k + 1 \quad m = 0$

$\epsilon = k \pmod 2$

$(f,g) = \int \overline{f(x)}\, \Box^k g(x) d^4x$

$d_2^{K\pm}$ has timelike momenta;

$d_2^{K_0}$ has spacelike momenta. All spinless. Yao cases VII–IX, "most degenerate discrete series."

When $k = 0$ Yao case X, "most degenerate discrete representation."

APPENDIX A: POSITIVITY OF SCALAR PRODUCT IN $d_1^{m\sigma}$

We wish to find the conditions under which

$$I \equiv \int \overline{f(\zeta_1)}\, (\overline{\alpha}\beta - c)^{m/2-\sigma-3/2} (\alpha\overline{\beta} + c)^{-m/2-\sigma-3/2} \times f(\zeta\zeta_1) d\mu(\zeta) d\mu(\zeta_1) \tag{A1}$$

is of definite sign. To do so, we notice that this is an integral operator acting upon the generalized convolution $\overline{f} * f(\zeta)$, and so it is natural to pass to the Fourier transform over $\hat{Z}$.

We first remark that $\hat{Z}$ is a five-parameter non-Abelian group with only one Casimir operator, corresponding to the element c. Choosing a Fourier integral pseudobasis for the space of functions of α on which the representations of the principal series are defined, we find that the representation functions (matrix elements) of an arbitrary group element are

$$\mathfrak{D}^p_{A'A}(\zeta) = e^{pc + i\operatorname{Re}(A\overline{\alpha})} \delta^2(A' - A + 2ip\beta); \tag{A2}$$

here the real number p labels the UIR, and the complex A, A' the basis. If we define

$$\tilde{f}^p(A', A) \equiv \int f(\zeta) \overline{\mathfrak{D}^p_{A'A}(\zeta)} d\mu(\zeta), \tag{A3}$$

then we find the analog of the Plancherel theorem

$$\int \overline{f(\zeta)} g(\zeta) d\mu(\zeta) = \pi^{-3} \int \overline{\tilde{f}^p(A', A)}\, \tilde{g}^p(A', A) DADA' p^2 dp. \tag{A4}$$

All these results are easily verified by straightforward classical Fourier transforms; the details of the group theory are irrelevant. We can now approach the problem of positivity. It is easy to verify that if $\sigma < 0$, the asymptotic behavior of $f \in H_\zeta$ implies that f is μ-measurable; hence the Fourier transform (A3) exists. By the representation property of the $\mathfrak{D}$ functions and the Plancherel theorem then we find

$$I = \pi^{-3} \int p^2 dp DADA'\, \tilde{\mathfrak{M}}^p(A, A') \int \overline{\tilde{f}^p(A, A'')}\, \tilde{f}^p(A', A'') DA'', \tag{A5}$$

where

$$\begin{aligned}\tilde{\mathfrak{M}}^p(A, A') &= \mathfrak{F}\{(\overline{\alpha}\beta - c)^{m/2-\sigma-3/2}(\alpha\overline{\beta} + c)^{-m/2-\sigma-3/2}\}(p, A, A') \\ &= \int (\overline{\alpha}\beta - c)^{m/2-\sigma-3/2}(\alpha\overline{\beta} + c)^{-m/2-\sigma-3/2} e^{-pc - i\operatorname{Re}(A\overline{\alpha})} \\ &\quad \times D\alpha dc\, \delta^2(A' - A + 2ip\beta) D\beta.\end{aligned} \tag{A6}$$

Change to the variables $\omega = \alpha\overline{\beta} + c, \overline{\omega}, c$; then we can perform the ω integral in a distribution sense (Gel'fand,[8] Appendix B, Eq. B1.7.7) and the c integral gives a $\delta[p - \operatorname{Im}(A/\beta)]$. Let us write

$$A = A_0 e^{i\alpha}, \quad A' = A_0' e^{-i\alpha};$$

then the final result takes the form

$$\begin{aligned}\tilde{\mathfrak{M}} &= 2^{-2\sigma-1} i^{-|m|} \pi^2 \frac{\Gamma(|m/2| - \sigma - \frac{1}{2})}{\Gamma(|m/2| + \sigma + \frac{3}{2})} |p|^{2\sigma} (\operatorname{sgn} p)^m \\ &\quad \times |\sin\alpha|^{-2\sigma-1} [\operatorname{sgn}(\sin\alpha)]^m e^{-im\alpha} \\ &\quad \times |A_0|^{-1} \delta(|A_0| - |A_0'|).\end{aligned} \tag{A7}$$

We shall denote the constant part of this by $c(m, \sigma)$. The integral (A5) then becomes

$$\begin{aligned}&c(m, \sigma)\pi^{-3} \int |p|^{2\sigma+2} (\operatorname{sgn} p)^m dp \int DA''.\, |A_0| d|A_0|.\, d(\arg A_0) \\ &\quad \times \int_0^\pi \overline{\tilde{f}^p(A_0 e^{i\alpha}, A'')}\, \tilde{f}^p(A_0 e^{-i\alpha}, A'') \\ &\quad \times e^{-im\alpha} |\sin\alpha|^{-2\sigma-1} [\operatorname{sgn}(\sin\alpha)]^m d\alpha.\end{aligned} \tag{A8}$$

Clearly we can have positivity of the scalar product (that is, of the normalized integral) only if m is even. The p integral certainly converges for $-\frac{1}{2} < \sigma < 0$ and we shall show that in this interval the integrand is positive.

Consider then the α integral in (A8), with m an even integer. Let us set

$$\tilde{f}^p(A, A'') = \tilde{f}^p(|A|, \alpha = \arg A, A'') \equiv F(\alpha)$$

and concentrate upon the dependence on α for fixed p, A'', and $|A_0|$. The integrals over α and $(\arg A_0)$ become

$$\int_0^{2\pi} d\alpha' \int_0^\pi \overline{F(\alpha' + \alpha)}\, F(\alpha' - \alpha) e^{-im\alpha} (\sin\alpha)^{-2\sigma-1} d\alpha.$$

This is of the form of an integral operator acting on the convolution over the unit circle of $\overline{F}$ and F. Define

$$\tilde{F}_N = \int_0^{2\pi} F(\varphi) e^{iN\varphi} d\varphi;$$

then after a little manipulation we can use the Plancherel theorem to write the integral as

$$\begin{aligned}&\frac{1}{8\pi^2} \sum_N \overline{\tilde{F}}_{-N} \tilde{F}_{-N} \int_0^\pi e^{i\varphi(N - m/2)} (\sin\tfrac{1}{2}\varphi)^{-2\sigma-1} d\varphi \\ &\quad = \sum_N \frac{2^{2\sigma-1}\pi^{-1}(-1)^{N-m/2}\Gamma(-2\sigma)}{\Gamma(\frac{1}{2} - \sigma + \frac{1}{2}m - N)\Gamma(\frac{1}{2} - \sigma - \frac{1}{2}m + N)} |\tilde{F}_{-N}|^2\end{aligned} \tag{A9}$$

(we have used HTF 2.4.8).[21] Consider the constant factors here; if $N \geqslant m/2$, we can write them as

$$\frac{2^{2\sigma-1}\Gamma(-2\sigma)}{\pi[\Gamma(\frac{1}{2}-\sigma)]^2}\,\frac{(\frac{1}{2}+\sigma)(\frac{3}{2}+\sigma)\cdots(N-\frac{1}{2}m-\frac{1}{2}+\sigma)}{(\frac{1}{2}-\sigma)(\frac{3}{2}-\sigma)\cdots(N-\frac{1}{2}m-\frac{1}{2}-\sigma)}.$$

The denominator is always positive for $\sigma < 0$, and the numerator is positive too if $(\sigma + \frac{1}{2}) > 0$. Similar considerations apply if $N < m/2$. By combining (A8) and (A9) we have therefore proved that the scalar product (A1) is positive definite if m is even and $\sigma \in (-\frac{1}{2}, 0)$. For σ outside this range the integrals must be understood in the sense of their regularizations, and will not in general be positive.

APPENDIX B: EQUIVALENCE OF REPRESENTATIONS OF d_1

We asserted in section 3.3 that the representations (A,B) and $(-B-3,-A-3)$ of the first degenerate series were equivalent. To show this, we display an intertwining operator between them, which we shall denote V. Such an operator $V: H_\zeta(-B-3,-A-3) \to H_\zeta(A,B)$ is given in general by

$$V: f(\zeta) = \int f(\zeta_1)[\epsilon(\zeta_1\zeta^{-1})]^{B*A} d\mu(\zeta_1); \tag{B1}$$

it is trivial to verify that

$$T_g^{A,B}[Vf] = V[T_g^{-B-3,-A-3}f] \tag{B2}$$

by using the standard set of operators, and we need not show it here. This displays the equivalence of the representations (m,ρ) and $(m,-\rho)$ of the first continuous series, and also of (m,σ) and $(m,-\sigma)$ of the complementary. In both these cases the integrals converge in a classical sense.

If A and B are positive integers the situation is more complicated. It is clear that the factor space H_ζ/D of functions whose generalized moments do not vanish [see Eq. (33)ff.] is mapped onto the multinomial subspace $M \subset H_\zeta(A,B)$, while the subspaces F^+ and $F^- \subset H_\zeta(-B-3,-A-3)$ are annihilated. We introduce for them the operators

$$V_\pm f(\zeta) = \int f(\zeta_1)[\epsilon(\zeta_1\zeta^{-1})]^{B*A}\ln[\epsilon(\zeta_1\zeta^{-1})]\, d\mu(\zeta_1); \tag{B3}$$

on these spaces (but not on H_ζ itself) this is an intertwining operator in the sense (B2), and it is simple to check that it both preserves the analytic structure in c and is continuous. The set of equivalences is therefore proved.

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[9] To prove the invariance of (11), it is easier to use the element B of (II.3) rather than J; we then need the identity $[b^2(\partial_a\partial_{\bar{a}} + \partial_b\partial_c) - b\partial_c]^N b^{2-N} f = b^{2+N}(\partial_a\partial_{\bar{a}} + \partial_b\partial_c)^N f$, which is easily proved by induction.

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[11] That is, the Jacobian $d\mu(\zeta')/d\mu(\zeta)$ of the transformation must be positive.

[12] It is easy to show that the contribution to (33) from the singular part of the integrand actually vanishes.

[13] A similar argument can be adduced to argue the positivity of the scalar product (II.25) that we introduced for $d_0^{\,i}$.

[14] The generators are not the same as (I.31), nor can we obtain them by ignoring some of the terms there, as we can for the degenerate *second* series. A fresh derivation is necessary.

[15] The conventional specification of the discrete series adds one to our values of k.

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Hill's functions and the one-dimensional Schrödinger equation*

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Over a region of finite width in which the potential varies with respect to a single Cartesian coordinate, it is possible to transform the one-dimensional Schrödinger equation into Hill's equation. It is thus possible to express the connection of the wavefunction and its normal derivative across the region exactly, in terms of the Fourier expansion coefficients of the potential profile. As a consequence, the reflection and transmission amplitudes and the bound-state energies associated with such a region may be directly calculated without actually solving an equation in the interior of the region. These results are applied to the solution of several examples, including the problem of s-wave scattering by a central potential.

I. INTRODUCTION

Exact solutions of the one-dimensional Schrödinger equation in regions of varying potential may be obtained in terms of known functions only when the potential profile takes on one of a limited number of forms. The harmonic oscillator[1] is perhaps the best-known example; another is the periodic cosinusoidal potential considered by Morse,[2] who obtained solutions in terms of Mathieu functions.

If a solution in terms of familiar functions (generally speaking, solutions of the hypergeometric equation) cannot be obtained, alternate approaches have been useful. These include direct series solution of the differential equation, yielding results which are most often useful in the long-wavelength limit; and the WKB method,[3] which is appropriate in the short-wavelength limit.

In this paper we present an approach to this problem which is applicable when the potential variation occurs over a region of finite width and possesses a Fourier series expansion. The solutions obtained are formally exact and may be applied in any wavelength regime; this is particularly important when the scale of the inhomogeneity is comparable to the wavelength. The approach is based upon the fact that an almost arbitrary *periodic* potential may be dealt with by transforming the Schrödinger equation into Hill's equation[4]; we simply focus attention on a single half-period or full period of an equivalent even-periodic potential.

In the following sections of this paper, we first transform the Schrödinger equation in one dimension into the Hill equation and present the connection of the wavefunction and its normal derivative across the region of varying potential. This connection turns out to involve the Fourier coefficients of the potential profile in a relatively simple way and does not require the actual solution of the Hill equation. As a consequence, the wavefunction in the exterior regions may be determined exactly without solving the differential equation in the interior. We then illustrate the application of this formalism to the solution of several examples and present numerical data for some concrete cases.

II. FORMULATION OF THE PROBLEM

The one-dimensional Schrödinger equation is written

$$\frac{\hbar^2}{2m}\frac{d^2\hat{\psi}}{dx^2} + [E - V(x)]\hat{\psi} = 0, \tag{1}$$

where $\psi(x) = \hat{\psi}(x)\exp(-iEt/\hbar)$; $V(x)$ is presumed to vary on $0 \le x \le d$. On $0 \le x \le d$, introduce the following substitutions into (1):

$$\xi = \frac{\pi x}{2d}, \tag{2a}$$

$$u(\xi) = \hat{\psi}(x), \tag{2b}$$

$$\lambda + 2\sum_{n=1}^{\infty} g_n \cos 2n\xi = \left(\frac{2d}{\pi}\right)^2\left(\frac{2m}{\hbar^2}\right)[E - V(x)]. \tag{2c}$$

We find that $u(\xi)$ satisfies Hill's equation[5]

$$\frac{d^2u}{d\xi^2} + (\lambda + 2\sum_{n=1}^{\infty} g_n \cos 2n\xi)u = 0. \tag{3}$$

We term solutions of (3) "Hill's functions." Solutions of Hill's equation are readily obtained when the series of coefficients g_n is absolutely convergent; this is the only restriction placed on the function $V(x)$. Let the basic set of solutions be denoted $u_{1,2}(\xi)$, where

$$u_1(0) = u_2'(0) = 1, \tag{4a}$$

$$u_2(0) = u_1'(0) = 0 \tag{4b}$$

(primes denote differentiation with respect to the argument); then $\hat{\psi}(x)$ is given on $0 \le x \le d$ by a linear combination of these functions:

$$\hat{\psi}(x) = \left[u_{1,2}\left(\frac{\pi x}{2d}\right)\right]. \tag{5}$$

It is possible to solve Hill's equation and thereby obtain $\hat{\psi}(x)$ throughout the region $0 \le x \le d$. However, for many problems of interest, all that is required in addition to (4) is the set of values $u_{1,2}(\pi/2)$ and $u_{1,2}'(\pi/2)$, so that boundary conditions on $\hat{\psi}$ and $\hat{\psi}'$ at $x = 0$ and $x = d$ may be imposed. These values are known and are expressible directly in terms of the coefficients λ and g_n. We have[6,7]

$$u_1(\pi/2) = \cos(\pi\sqrt{\lambda}/2)C_1(\lambda), \tag{6a}$$

$$u_2(\pi/2) = (1/\sqrt{\lambda})\sin(\pi\sqrt{\lambda}/2)S_0(\lambda), \tag{6b}$$

$$u_1'(\pi/2) = -\sqrt{\lambda}\sin(\pi\sqrt{\lambda}/2)C_0(\lambda), \tag{6c}$$

$$u_2'(\pi/2) = \cos(\pi\sqrt{\lambda}/2)S_1(\lambda), \tag{6d}$$

in which C_0, C_1, S_0, and S_1 are the infinite determinants[8]

$$C_0(\lambda) = \left\| \delta_{n,m} + \frac{(g_{n-m} + g_{n+m})(1 + \operatorname{sgn} n \operatorname{sgn} m)}{\sqrt{\epsilon_n \epsilon_m}(\lambda - 4n^2)} \right\|_0^\infty \tag{7a}$$

$$C_1(\lambda) = \left\| \delta_{n,m} + \frac{(g_{n-m} + g_{n+m+1})}{\lambda - (2n+1)^2} \right\|_0^\infty \tag{7b}$$

$$S_0(\lambda) = \left\| \delta_{n,m} + \frac{(g_{n-m} - g_{n+m})}{\lambda - 4n^2} \right\|_1^\infty \tag{7c}$$

$$S_1(\lambda) = \left\| \delta_{n,m} + \frac{(g_{n-m} - g_{n+m+1})}{\lambda - (2n+1)^2} \right\|_0^\infty \tag{7d}$$

In (7), $\epsilon_n = 2$ if $n > 0$ and $\epsilon_0 = 1$; $\delta_{n,m} = 1$ if $n = m$ and $\delta_{n,m} = 0$ otherwise; sgn $n = 1$ if $n > 0$, and sgn $0 = 0$; $g_{-n} = g_n$ and $g_0 = 0$.

The poles of the infinite determinants which occur when λ is the square of an integer are exactly canceled by the zeros of the trigonometric functions which multiply them. Thus $u_{1,2}(\pi/2)$ and $u'_{1,2}(\pi/2)$ are analytic functions of λ; their zeros are those of the associated determinants.

The connection of the wavefunction and its normal derivative across the region of varying potential may now be expressed in terms of a connection matrix as follows:

$$\begin{bmatrix} \hat{\psi}(d) \\ \hat{\psi}'(d) \end{bmatrix} = \begin{bmatrix} u_1\left(\frac{\pi}{2}\right) & \frac{2d}{\pi} u_2\left(\frac{\pi}{2}\right) \\ \frac{\pi}{2d} u_1'\left(\frac{\pi}{2}\right) & u_2'\left(\frac{\pi}{2}\right) \end{bmatrix} \begin{bmatrix} \hat{\psi}(0) \\ \hat{\psi}'(0) \end{bmatrix}. \tag{8}$$

The matrix elements depend only on the coefficients λ and g_n via (6) and (7). In the symmetric case, where $V(x) = V(-x)$ in the region $-d \le x \le d$, the connection is readily shown to be given by

$$\begin{bmatrix} \hat{\psi}(-d) \\ \hat{\psi}'(-d) \end{bmatrix} = \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix} \begin{bmatrix} \hat{\psi}(d) \\ \hat{\psi}'(d) \end{bmatrix} \tag{9}$$

in which

$$\alpha_{11} = \alpha_{22} = u_1'(\pi/2)u_2(\pi/2) + u_1(\pi/2)u_2'(\pi/2), \tag{10a}$$

$$\alpha_{12} = -(4d/\pi)u_1(\pi/2)u_2(\pi/2), \tag{10b}$$

$$\alpha_{21} = -(\pi/d)u_1'(\pi/2)u_2'(\pi/2). \tag{10c}$$

We have used the fact that u_1 is an even and u_2 an odd function; again, the matrix elements depend only on the coefficients λ and g_n.

III. APPLICATIONS

The method given in the previous section is particularly well suited to the solution of problems that involve the matching of wavefunctions at the boundaries of a region without requiring knowledge of the wavefunction in the interior of the region. Reflection and transmission at a region of varying potential, scattering from a finite range central potential, as well as the associated eigenvalue problems for bound states are natural examples.

In this and the following sections, we present the formal solutions to these problems and consider some concrete examples.

Reflection and transmission by $V(x)$ on $0 \le x \le d$

Consider the potential

$$V = \begin{cases} V_1 & (x < 0) \\ V(x) & (0 \le x \le d) \\ V_2 & (x > d) \end{cases} \tag{11}$$

We expand $V(x)$ as in (2c) and define $k_i^2 = \frac{2m}{\hbar^2}(E - V_i)$, $i = 1, 2$. Then for $x < 0$, let

$$\hat{\psi}(x) = e^{ik_1x} + Re^{-ik_1x}; \tag{12}$$

and for $x > d$, let

$$\hat{\psi}(x) = Te^{ik_2(x-d)}. \tag{13}$$

R and T are respectively the reflection and transmission amplitudes to be determined. Evaluating $\hat{\psi}$ and $\hat{\psi}'$ at $x = 0$ and $x = d$, substituting these values into (8) and solving for R and T yields

$$R = \frac{1}{D}\{-u_1'(\pi/2) + i\kappa_2 u_1(\pi/2) - i\kappa_1[u_2'(\pi/2) - i\kappa_2 u_2(\pi/2)]\}, \tag{14a}$$

$$T = \frac{-2i\kappa_1}{D} \tag{14b}$$

with

$$D = u_1'(\pi/2) - i\kappa_2 u_1(\pi/2) - i\kappa_1[u_2'(\pi/2) - i\kappa_2 u_2(\pi/2)], \tag{14c}$$

in which $\kappa_i = 2k_i d/\pi$, $i = 1, 2$. $u_{1,2}(\pi/2)$ and $u'_{1,2}(\pi/2)$ are known, thus determining R and T for an essentially arbitrary potential profile. The energies of bound states, if any exist, are obtained from the roots of the equation $D = 0$.

Reflection and transmission by $V(x) = V(-x)$ on $-d \le x \le d$

Consider the potential

$$V = \begin{cases} V_2 & (|x| > d) \\ V(x) = V(-x) & (|x| \le d) \end{cases} \tag{15}$$

For $x < -d$, let

$$\hat{\psi}(x) = e^{ik_2(x+d)} + R_s e^{-ik_2(x+d)} \tag{16}$$

and for $x > d$, let

$$\hat{\psi}(x) = T_s e^{ik_2(x-d)}. \tag{17}$$

R_s and T_s are respectively the reflection and transmission amplitudes to be determined. Evaluating $\hat{\psi}$ and ψ' at $x = \pm d$, substituting in (9), and solving for R_s and T_s, we obtain

$$R_s = -\frac{1}{D_s}[u_1'(\pi/2)u_2(\pi/2) + \kappa_2^2 u_1(\pi/2)u_2(\pi/2)], \tag{18a}$$

$$T_s = \frac{-i\kappa_2}{D_s} \tag{18b}$$

with

$$D_s = [u_1'(\pi/2) - i\kappa_2 u_1(\pi/2)][u_2'(\pi/2) - i\kappa_2 u_2(\pi/2)]. \tag{18c}$$

Note that the roots of D_s, which determine the bound-state energies, separate into two groups because of the symmetry of the potential. Bound states for which $\hat{\psi}(-x) = \hat{\psi}(x)$ are characterized by

$$u_1'(\pi/2) = i\kappa_2 u_1(\pi/2) \tag{19}$$

and those for which $\hat{\psi}(-x) = -\hat{\psi}(x)$ by

$$u_2'(\pi/2) = i\kappa_2 u_2(\pi/2). \tag{20}$$

$u_{1,2}$ and $u_{1,2}'$ are real, so roots may exist only if $\kappa_2^2 < 0$.

S-Wave scattering by a central potential

Consider the central potential in spherical coordinates

$$V = \begin{cases} V(r) & (0 \le r \le r_0) \\ 0 & (r > r_0) \end{cases} \tag{21}$$

The scattering of the $l = 0$ partial wave (the s-wave) is treated in a manner analogous to that of reflection and transmission at a symmetric one-dimensional potential. It is easy to show that on $0 \le r \le r_0$, the wavefunction for $l = 0$ which is regular at $r = 0$ is given by

$$\hat{\psi}(r) = \frac{2r_0 A_0}{\pi r} u_2(\pi r/2r_0), \tag{22}$$

where r_0 takes the place of d in the previous calculations. A_0 is the form factor; $\hat{\psi}(0) = A_0$, to be determined.

In the region $r > r_0$, we have

$$\psi(r) = \frac{\sin k_0 r}{k_0 r} + B_0 \frac{e^{ik_0 r}}{ik_0 r}, \tag{23}$$

where $k_0^2 = 2mE/\hbar^2$ and B_0 is the scattering amplitude to be determined. Ensuring that $\hat{\psi}$ and $\hat{\psi}'$ are continuous at $r = r_0$ determines the values of A_0 and B_0. We obtain

$$A_0 = e^{-ik_0 r_0}\left[1\Big/\left(u_2'(\pi/2) - \frac{2ik_0 r_0}{\pi} u_2(\pi/2)\right)\right], \tag{24a}$$

$$B_0 = e^{-ik_0 r_0} i \sin(-k_0 r_0)\left[\left(u_2' \frac{\pi}{2} - \frac{2k_0 r_0}{\pi} \cot k_0 r_0 u_2 \frac{\pi}{2}\right)\Big/ \left(u_2' \frac{\pi}{2} - \frac{2ik_0 r_0}{\pi} u_2 \frac{\pi}{2}\right)\right]. \tag{24b}$$

The equation determining the energies of the bound states is simply

$$u_2'(\pi/2) = (2ik_0 r_0/\pi) u_2(\pi/2). \tag{25}$$

The scattering cross-section σ_0 is given by $(4\pi/k_0^2)|B_0|^2$. In the low-energy limit $k_0 r_0 \to 0$, we obtain for σ_0 and A_0

$$\lim_{k_0 r_0 \to 0} \sigma_0 = 4\pi r_0^2 \left[1 - \frac{(2/\pi) u_2(\pi/2)}{u_2'(\pi/2)}\right]^2, \tag{26a}$$

$$\lim_{k_0 r_0 \to 0} A_0 = 1/u_2'(\pi/2). \tag{26b}$$

For this limiting case, $\lambda = (8mr_0^2/\pi^2\hbar^2)V_a$, where V_a is the average potential in the region $r \le r_0$. We turn now to the consideration of some numerical examples.

IV. NUMERICAL EXAMPLES

In the examples considered in this section, the potentials are of the form

$$V(x) = \tfrac{1}{2}[V(d) + V(0)] - \tfrac{1}{2}[V(d) - V(0)]\cos(\pi x/d) + \Gamma \cos(2\pi x/d) - \Gamma \tag{27}$$

in which Γ is a parameter. The coefficients λ and g_n are given by

$$\lambda = (2d/\pi)^2 (2m/\hbar^2)\left[E - \tfrac{1}{2}V(d) - \tfrac{1}{2}V(0) + \Gamma\right], \tag{28a}$$

$$g_1 = \tfrac{1}{4}(2d/\pi)^2 (2m/\hbar^2)[V(d) - V(0)], \tag{28b}$$

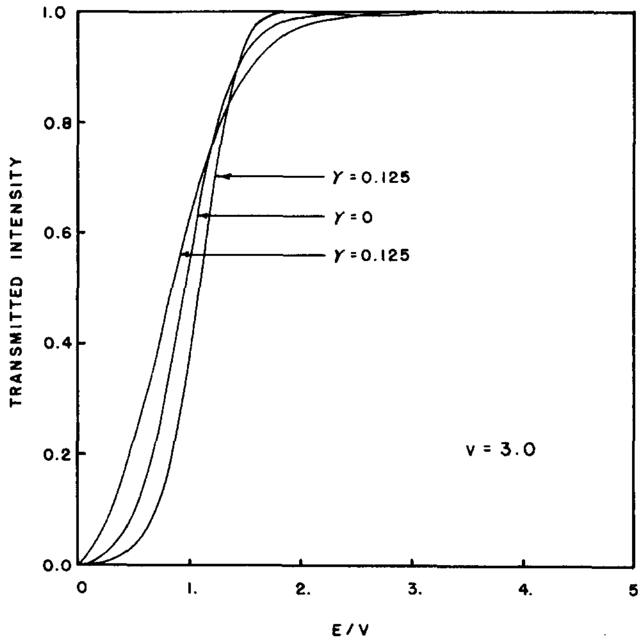

FIG. 1. Transmitted intensity vs E/V.

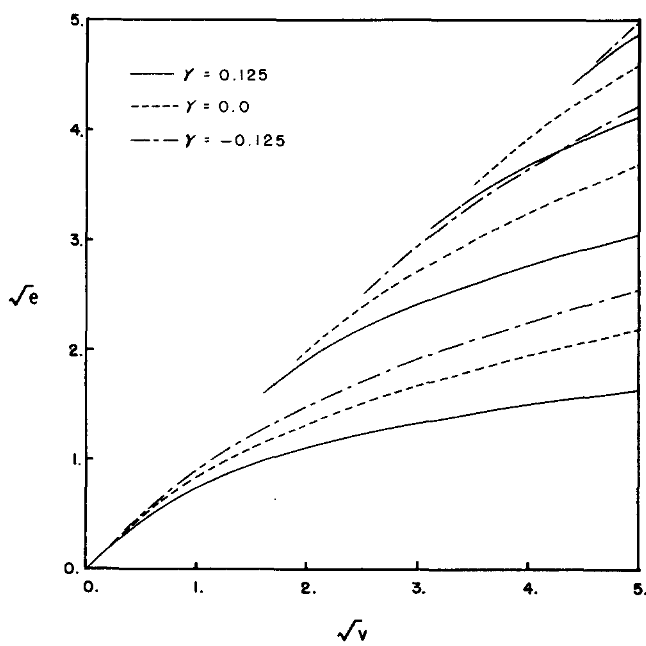

FIG. 2. Bound-state energies in a symmetric well.

$$g_2 = -(\Gamma/2)(2d/\pi)^2(2m/\hbar^2), \tag{28c}$$

$$g_n = 0, \quad (n > 2). \tag{28d}$$

We shall use the abbreviations $e \equiv (2d/\pi)^2(2mE/\hbar^2)$ and $v \equiv (2d/\pi)^2(2mV/\hbar^2)$ as appropriate in what follows.

Transmission through a symmetric barrier

The relative transmitted intensity τ_s of a beam incident from $x < -d$ on a region of symmetrically varying potential ($-d \leq x \leq d$) is obtained from Eq. (18b):

$$\tau_s = |T_s|^2 = \kappa_2^2/\{[u_1'(\pi/2)^2 + \kappa_2^2 u_1(\pi/2)^2][u_2'(\pi/2)^2 + \kappa_2^2 u_2(\pi/2)^2]\}. \tag{29}$$

We assume $V(0) = V_1 = V$ and $V(\pm d) = V_2 = 0$. Curves of τ_s as a function of E/V are given in Fig. 1 for $v = 3.0$ and $\gamma = \Gamma/V = -0.125$, 0.0, and 0.125. The three cases correspond respectively to (1) a barrier of height $v = 3.0$ with $V''(0) = 0$; (2) a barrier of height $v = 3.0$ of cosinusoidal shape; and (3) a barrier of height $v = 3.0$ with $V''(\pm d) = 0$.

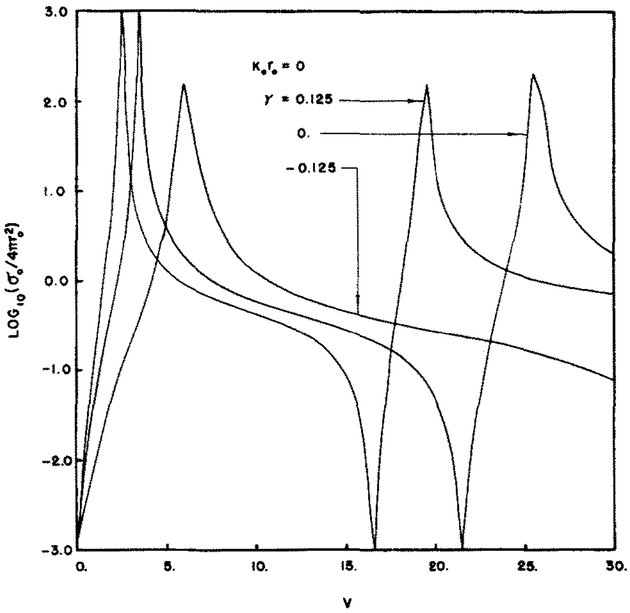

FIG. 3. Scattering cross-section vs. v; $k_0 r_0 \to 0$.

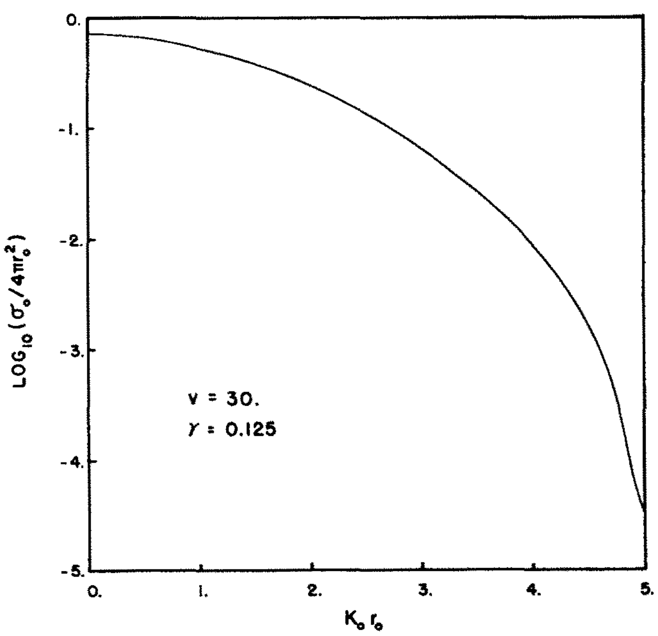

FIG. 4. Scattering cross-section vs. $k_0 r_0$; $v = 30$, $\gamma = 0.125$.

Bound states in a symmetric potential well

Let the parameters of a symmetric potential well extending over $|x| \leq d$ be chosen so that $V(\pm d) = V$ and $V(0) = 0$. The bound-state energies are obtained from (19). We have calculated $\sqrt{e}$ as a function of $\sqrt{v}$ for $\gamma = E/V = 0.125$, $\gamma = 0$, and $\gamma = -0.125$. The results are shown in Fig. 2. The case $\gamma = 0.125$ represents a well for which $V''(0) = 0$; while for $\gamma = 0.125$, $V''(\pm d) = 0$. It will be noted that the bound-state energies increase as γ is decreased. This is a consequence of the increase of average potential in the well with decreasing γ.

Scattering from a central potential

Consider a central potential for which $V(0) = -V$ and $V(r_0) = 0$. The scattering cross-section in the limit $k_0 r_0 \to 0$ is given in (26a). Curves of the normalized cross-section $\sigma_0/4\pi r_0^2$ in this limit are shown in Fig. 3 as functions of v for $\gamma = 0.125$, $\gamma = 0$, and $\gamma = -0.125$. The resonance peaks corresponding to the onset of new virtual energy levels are evident; their shift to larger values of V as γ is decreased is due to the increase in average potential in the region. Also apparent are the nulls associated with the passage of the phase shift δ_0 through 180°.

The normalized scattering cross-section $\sigma_0/4\pi r_0^2$ is shown as a function of $k_0 r_0$ for $v = 30$ and $\gamma = 0.125$ in Fig. 4. This set of parameters approximates a Woods–Saxon potential of depth 60 MeV and radius 5 f.

V. SUMMARY

We have proposed a method by which solutions of the one-dimensional Schrödinger equation may be obtained in terms of Hill's functions. The method is applicable to potentials which vary over a region of finite width, and may be applied if the series of Fourier expansion coefficients of the potential profile is absolutely convergent. If these conditions are met, Hill's equation may be solved throughout the region of varying potential.

The determination of the wavefunction in the exterior region can be carried out without solving the Hill equation. This is possible by virtue of the fact that the values of the Hill functions and their derivatives at the boundaries are expressible directly in terms of the Fourier coefficients of the potential profile. Thus reflection and transmission coefficients and bound-state energies are easily calculated for any profile which possesses a Fourier cosine expansion.

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Generation of stationary Einstein–Maxwell fields

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The Einstein–Maxwell field equations in the presence of one Killing vector are shown to possess covariance under an eight-parameter group of linear substitutions in the field variables. This internal symmetry group is isomorphic to $SU(2,1)$. Three of the degrees of freedom correspond to gage transformations, but the remaining ones allow us to generate a five-parameter family of solutions given a single solution.

1. INTRODUCTION

The Einstein–Maxwell equations which describe the coupling of the electromagnetic field with gravity have so far proven too complicated to yield solutions except in a few special cases. However, as several authors have pointed out, they possess a large amount of hidden symmetry. Given one solution, one may use certain transformations to generate other solutions (often more complicated ones). Ehlers[1] was the first to discover such a method. He gave a discrete transformation which mapped static vacuum solutions into stationary ones. Harrison[2] considered a subclass of stationary electromagnetic solutions, namely those for which the various gravitational and electromagnetic potentials were all functionally dependent. He gave several cases of continuous transformations connecting such solutions. Matzner and Misner[3] and also Ernst[4,5] studied the problem of stationary vacuum fields with axial symmetry. They produced field equations and effective Lagrangians which were manifestly covariant under rotations in an abstract $(2 + 1)$-dimensional Minkowski space. Geroch[6] showed that this $SO(2, 1) \approx SU(1, 1)$ symmetry was present for all stationary vacuum fields, with no further restrictions imposed, and that it directly implied the existence of Ehlers–Harrison transformations.

In this paper we will extend Geroch's results to include electromagnetism once more. We will study the symmetry of the Einstein–Maxwell equations in the presence of one timelike Killing vector. Using the formulation of the field equations given by Israel and Wilson,[7] we will show the equations possess an enlarged symmetry group isomorphic to $SU(2, 1)$. Some of the group transformations merely produce gage changes, while the remaining ones are transformations of the Ehlers–Harrison type. Making use of them enables us to generate a five-parameter family of stationary Einstein–Maxwell solutions from any one such solution.

2. FIELD EQUATIONS

The electromagnetic field may be conveniently described by means of the complex Maxwell tensor

$$\mathfrak{F}_{\mu\nu} \equiv F_{\mu\nu} + i^*F_{\mu\nu}, \tag{2.1}$$

where $F_{\mu\nu}$ is the usual Maxwell tensor and $^*F_{\mu\nu}$ is its dual. In a source-free region the entire set of Maxwell's equations is

$$\mathfrak{F}_{[\mu\nu;\sigma]} = 0.$$

This is the integrability condition for the existence of a complex vector potential $\mathfrak{A}_\mu$ such that

$$\mathfrak{F}_{\mu\nu} = \mathfrak{A}_{\nu,\mu} - \mathfrak{A}_{\mu,\nu}. \tag{2.2}$$

In fact $\mathfrak{A}_\mu$ provides a redundant description of the field, and one can show that knowledge of the fourth component $\mathfrak{A}_4 \equiv \Psi$ is entirely sufficient. The real and imaginary parts of Ψ turn out to be the usual electrostatic and magnetic scalar potentials.

If the space–time in which $\mathfrak{F}_{\mu\nu}$ resides is stationary, there must exist a coordinate system in which all physically measurable quantities are time-independent. In this case the line element may be written as

$$ds^2 = f(dt + w_j dx^j)^2 - f^{-1}h_{jk}dx^j dx^k, \quad j,k = 1, 2, 3, \tag{2.3}$$

where f, w_j, h_{jk} do not depend on t. By a suitable gage transformation one may make $\mathfrak{A}_\mu$ time independent also.

All field equations may be written as equations in a 3-space H with metric tensor h_{jk}. Let ∇ denote the covariant derivative in H. We define a twist vector[7]

$$\boldsymbol{\tau} \equiv f^2 \nabla \times \mathbf{w} + i(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*). \tag{2.4}$$

Using a portion of the Einstein equations,

$$G_{j4} = 8\pi T_{j4},$$

one can prove that[7]

$$\nabla \times \boldsymbol{\tau} = 0,$$

implying the existence of a scalar "twist potential" ψ, such that

$$\boldsymbol{\tau} = \nabla\psi. \tag{2.5}$$

In a manner analogous to the treatment above of electromagnetism, we define a complex scalar potential for gravitation

$$\mathcal{E} \equiv f - \Psi\Psi^* + i\psi, \tag{2.6}$$

the "Ernst potential." Once h_{jk} is given, $\mathcal{E}$ completely suffices to determine the metric and hence the gravitational field. However, note that the relation between $\mathcal{E}$ and ds^2 is a nonlocal one, since $\mathbf{w}$ and ψ are not locally related.

The Maxwell equations and the remaining Einstein equations may now be cast in terms of $\mathcal{E}, \Psi$. They yield[7]

$$f\nabla^2\mathcal{E} = (\nabla\mathcal{E} + 2\Psi^*\nabla\Psi)\cdot\nabla\mathcal{E}, \tag{2.7}$$

$$f\nabla^2\Psi = (\nabla\mathcal{E} + 2\Psi^*\nabla\Psi)\cdot\nabla\Psi, \tag{2.8}$$

as well as specifying the curvature tensor of H:

$$f^2R^{(3)}_{jk} = \tfrac{1}{2}\mathcal{E}_{,(j}\mathcal{E}^*_{,k)} + \Psi\mathcal{E}_{,(j}\Psi^*_{,k)} + \Psi^*\mathcal{E}^*_{,(j}\Psi_{,k)} - (\mathcal{E} + \mathcal{E}^*)\Psi_{,(j}\Psi^*_{,k)}. \tag{2.9}$$

The 3-metric h_{jk} may be any metric whatever for which this is the curvature tensor.

3. $SU(2, 1)$ SYMMETRY

The easiest way to make the symmetry in Eqs. (2.7)–(2.9) manifest is to replace $\mathcal{E}, \Psi$ by three complex scalar fields u, v, w:

$$\mathcal{E} = (u - w)/(u + w), \qquad \Psi = v/w. \tag{3.1}$$

Of course, there is redundancy in a description of this sort. In particular, we may choose w to obey any field equation we please, in order to obtain simple ones for u, v. Upon substituting Eq. (3.1) in Eqs. (2.7), (2.8), we find a possible choice to be

$$\begin{aligned}(uu^* + vv^* - ww^*)\nabla^2 u &= 2(u^*\nabla u + v^*\nabla v - w^*\nabla w)\cdot\nabla u,\\ (uu^* + vv^* - ww^*)\nabla^2 v &= 2(u^*\nabla u + v^*\nabla v - w^*\nabla w)\cdot\nabla v,\\ (uu^* + vv^* - ww^*)\nabla^2 w &= 2(u^*\nabla u + v^*\nabla v - w^*\nabla w)\cdot\nabla w.\end{aligned} \tag{3.2}$$

We now introduce an abstract complex 3-space M with an indefinite metric,

$$\eta_{\alpha\beta} = \mathrm{diag}(1, 1, -1).$$

We regard the fields u, v, w as components of a single vector field

$$y^{\alpha} = (u, v, w)$$

which takes values in this 3-space. That is, at each point of H the electromagnetic and gravitational fields determine a vector which lies in M.

Due to the fact that only the ratios of u, v, w enter into Eq. (3.1), their normalization is not significant, and it is actually only the *rays* in M we are concerned with rather than vectors.

Equation (3.2) may now be written compactly as

$$Y_{\beta}Y^{\beta}\nabla^2 Y^{\alpha} = 2Y_{\beta}{}^*\nabla Y^{\beta}\cdot\nabla Y^{\alpha}; \tag{3.3}$$

Equation (2.9) for the curvature of H becomes

$$R_{jk} = (Y_{\alpha}{}^* Y^{\alpha})^{-2} V_{\alpha(j}V^{\alpha}{}_{k)}{}^*, \tag{3.4}$$

where

$$V^{\alpha}{}_{j} \equiv Y_{\beta}{}^* Y_{\gamma,j}\epsilon^{\alpha\beta\gamma}. \tag{3.5}$$

Now consider what happens if we perform a constant unitary transformation in M. That is, we make a linear replacement

$$Y^{\alpha} \to Y'^{\alpha} = A^{\alpha}{}_{\beta}Y^{\beta} \tag{3.6}$$

such that

$$Y'_{\alpha}{}^* Y'^{\alpha} = Y_{\alpha}{}^* Y^{\alpha} \tag{3.7}$$

and $A^{\alpha}{}_{\beta}$ is not a function of position in H. According to Eqs. (3.4), (3.5), R_{jk} transforms as a scalar in M and hence retains a fixed value. We may assume that h_{jk} remains fixed also. Under these circumstances, the appearances of ∇ in Eq. (3.3) transform as a vector in M, and if Y^{α} satisfies the equation, so does Y'^{α}.

Thus if (Y^{α}, h_{jk}) *specify a stationary Einstein–Maxwell solution, so do* (Y^{α}, h_{jk}).

The group of all unitary transformations $A^{\alpha}{}_{\beta}$ in M is denoted by $U(2, 1)$. However, since we are only interested in the rays of this space rather than the vector, the addition of a common phase factor to the components of Y^{α} is immaterial. We may therefore restrict ourselves to the subgroup $SU(2, 1)$.

4. PARAMETRIZATION OF $SU(2, 1)$

It would be useful to have an explicit representation of the most general $SU(2, 1)$ matrix in terms of eight real parameters, e.g., "Euler angles." In $SU(2)$ or even $SU(3)$ this is relatively straightforward, due to Euler's theorem that any finite rotation is a rotation leaving some axis fixed. However, the presence of an indefinite metric requires us to consider a number of different cases. For example, in Minkowski space there are certain exceptional "null rotations" which must be handled separately. The easiest approach is to look at the eigenvalue problem for A. The usual result for unitary matrices is that the eigenvectors form a complete orthonormal set and that all eigenvalues have unit modulus. However, when null eigenvectors are possible, two exceptions arise to this rule. There is no restriction on the eigenvalue corresponding to a null eigenvector, and two null eigenvectors need not be orthogonal. For matrices in $SU(2, 1)$ we will have the following list of possibilities:

(A) two spacelike eigenvectors, one timelike eigenvector;

(B) one spacelike eigenvector, two distinct null eigenvectors;

(C) one spacelike, one (double) null eigenvector;

(D) one (triple) null eigenvector.

We will write the matrix in factored form, and need to consider the following five simple classes of $SU(2, 1)$ transformation:

$$\text{(I)}\quad \begin{aligned}(u + w) &\to (u + w),\\ v &\to V + a(u + w),\\ (u - w) &\to (u - w) - 2a^* v - aa^*(u + w),\end{aligned} \tag{4.1}$$

$$\text{(II)}\quad \begin{aligned}(u + w) &\to (u + w),\\ v &\to v,\\ (u - w) &\to (u - w) + i\alpha(u + w),\end{aligned} \tag{4.2}$$

$$\text{(III)}\quad \begin{aligned}(u + w) &\to b(u + w),\\ v &\to (b^*/b)v,\\ (u - w) &\to (1/b^*)(u - w),\end{aligned} \tag{4.3}$$

$$\text{(IV)}\quad \begin{aligned}(u + w) &\to (u + w) + i\beta(u - w),\\ v &\to v,\\ (u - w) &\to (u - w),\end{aligned} \tag{4.4}$$

$$\text{(V)}\quad \begin{aligned}(u + w) &\to (u + w) - 2c^* v - cc^*(u - w),\\ v &\to v + c(u - w),\\ (u - w) &\to (u - w)\end{aligned} \tag{4.5}$$

Here a, b, c are arbitrary complex parameters and α, β are arbitrary real parameters. Let I, II, etc. stand for arbitrary $SU(2, 1)$ matrices in the corresponding class. We will represent A by first rotating one of its eigenvectors to a standard position, performing further rotations which leave this vector fixed, then rotating back to the initial position.

In case (A) we make one of its spacelike eigenvectors coincide with v, writing it as

$$A = (\mathrm{I}\cdot\mathrm{V})\cdot(\mathrm{III}\cdot\mathrm{II}\cdot\mathrm{IV})\cdot(\mathrm{I}\cdot\mathrm{V})^{-1}. \tag{4.6}$$

In all of the cases (B), (C), (D), there exists at least one null eigenvector, and we bring it into coincidence with $(u - w)$. The form of A will then be

$$A = (\mathrm{I}\cdot\mathrm{II})\cdot(\mathrm{III}\cdot\mathrm{IV}\cdot\mathrm{V})\cdot(\mathrm{I}\cdot\mathrm{II})^{-1}. \tag{4.7}$$

Starting from a single solution all members of its symmetry class may be obtained by application of one or the other of Eqs. (4.6) and (4.7).

We will now look at the effect of these $SU(2,1)$ transformations on the physics. From Eqs. (2.6), (3.1) we have

$$f = (uu^* + vv^* - ww^*)/(u + w)(u^* + w^*). \tag{4.8}$$

$SU(2,1)$ matrices belonging to classes I and II have a particularly simple effect since they leave $(u + w)$ fixed and therefor f as well. Under I,

$$\Psi \to \Psi + a, \quad E \to E - 2a^*\Psi - aa^*, \quad f \to f, \quad \tau \to \tau, \tag{4.9}$$

Under II,

$$\Psi \to \Psi, \quad E \to E + i\alpha, \quad f \to f, \quad \tau \to \tau. \tag{4.10}$$

These two transformations leave both the electromagnetic field and the geometry unchanged, and correspond to electromagnetic and gravitational gage transformations.

Under a class III transformation,

$$E \to (bb^*)^{-1}E, \quad \Psi \to (b^*b^{-2})\Psi. \tag{4.11}$$

When b has absolute value unity the transformation is a "duality rotation," which changes electric fields into magnetic ones and vice versa, but does not affect the geometry. If instead we choose $bb^* \neq 1$, the effect of Eq. (4.11) may be shown to be

$$ds^2 \to (bb^*)^{-1}ds^2,$$

a uniform conformal transformation or rescaling. It is a well-known general result that such a transformation always leads to new solutions of the field equations either in the case of vacuum or when only mass-zero fields are present.[8]

Class IV maps static vacuum fields into stationary ones and is a transformation of the type discovered by Ehlers.[1] Class V transformations do not preserve vacuum and correspond to the ones found by Harrison.[2]

5. DISCUSSION

Given a stationary Einstein–Maxwell solution we proceed as follows. Determine f, w_i, h_{jk} from the metric. Calculate the potentials ψ, Ψ which obey Eqs. (2.2), (2.4), (2.5). The $SU(2,1)$ transformations given in Sec. 4 may all be re-expressed in terms of their action on $\mathcal{E}$, Ψ. (The potentials u, v, w are useful because they transform more simply than $\mathcal{E}$, Ψ, but in practice they are *never needed*.) The five-parameter family of solutions may be obtained in one step from Eqs. (4.6), (4.7), or it may be built up in gradually increasing generality through successive applications of Eqs. (4.1)–(4.5).

There is one important circumstance in which a smaller family will be obtained. If the range of the vector field Y^α happens to lie entirely in a proper subspace of M, there will be certain transformations of $SU(2,1)$ having no effect whatever. For example, if we start with a vacuum field, Y^α lies entirely in the subspace $v = 0$. The duality rotation in the case is clearly futile! As pointed out in Ref. 2, a Schwarzchild metric leads only to a four-parameter family, Brill–NUT space[9] with the conventional parameters (m, l, e, d).

In fact, most known stationary solutions are either vacuum themselves or occur in a family with a vacuum member. One might even wonder whether more general ones are possible. However, Harrison[10] has given Einstein–Maxwell solutions of sufficient generality to be used in generating five-parameter families of solutions.

It should be noted that certain other transformations are known[7] which may be used to produce new stationary solutions but which are not included in the present discussion. The methods used to generate the Kerr metric and the recent Tomimatsu-Sato metric[11] from static solutions remain unclear.

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Mixed basis matrix elements for the subgroup reductions of $SO(2,1)$

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By using the irreducible decomposition on the two-dimensional light cone, the mixed basis matrix elements for the three subgroup reductions of $SO(2,1)$ are calculated. These matrix elements are calculated for the principal series only and can be expressed in terms of well-known special functions. As a consequence of appearing in this context, some new properties of these special functions are given.

INTRODUCTION

An intensive study of the representation theory of $SU(1,1)$, the covering group of $SO(2,1)$, has been carried out in recent years[1-3]. The basic motivation for such a study stems from the crossed channel partial wave expansion of the scattering amplitude in which the group $SO(2,1)$ figures as the "little group" of the spacelike momentum transfer[3]. It is also of some mathematical interest to make such a study. In this paper we are concerned with different ways of realizing a unitary irreducible representation (UIR) of $SO(2,1)$ in terms of different subgroup bases and how these realizations are related. The representation theory of $SO(2,1)$ in the compact basis corresponding to the subgroup reduction $SO(2,1) \supset SO(2)$ has been thoroughly examined by Bargmann[4]. More recently the UIR's of $SO(2,1)$ in the noncompact basis corresponding to the group reduction $SO(2,1) \supset SO(1,1)$ have been studied. Mukunda[5-7] has explicitly performed this reduction for all possible UIR's of $SO(2,1)$ and calculated the corresponding matrix elements. Macfadyen[8] has given these matrix elements in terms of known special functions, namely, the generalized Legendre functions of the second kind[9]. The only remaining subgroup basis for $SO(2,1)$ is that corresponding to the group reduction $SO(2,1) \supset T_1$. This has been partially investigated by Vilenkin,[10] who has given the matrix elements in this basis for the principal series of $SO(2,1)$.

In this paper we will show how by using the irreducible decomposition of the space of square integrable functions defined on the cone we can calculate explicit expressions for the mixed basis matrix elements in the three subgroup bases of $SO(2,1)$[11]. This method only enables us to calculate matrix elements of the single valued principal series. The explicit expressions for the matrix elements which we obtain can be expressed in terms of well-known special functions. As a consequence of appearing in this context, we use standard techniques to derive some new properties of these functions.

The content of the paper is arranged as follows; In Sec. 1 we review the irreducible decomposition on the cone and give the expansions on the cone corresponding to the three subgroup reductions of $SO(2,1)$. In Sec. 2 we carry out the explicit calculation of the mixed basis matrix elements.

1. THE IRREDUCIBLE DECOMPOSITION ON THE CONE

The problem we are concerned with here is the decomposition into irreducible components of the representation

$$U(g)\,|\xi\rangle = |\xi g\rangle \tag{1.1}$$

of functions $|\xi\rangle$ defined on the two-dimensional cone

$$[\xi,\xi] = \xi_0^2 - \xi_1^2 - \xi_2^2 = 0$$

(the reason for the notation $|\xi\rangle$ will become clear subsequently). This problem is well known[12,13] to be equivalent to the decomposition of $|\xi\rangle$ into homogeneous components. This is achieved via the formulas

$$|\xi\rangle = \frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} |\xi;\sigma\rangle\, d\sigma, \tag{1.2}$$

$$|\xi;\sigma\rangle = \int_0^\infty |t\xi\rangle\, t^{-\sigma-1}\, dt. \tag{1.3}$$

[Comment: The notation we will use is essentially that of Vilenkin[10] with the exception that the generators of the pure Lorentz transformations along the i axis ($i = 1, 2$) are denoted by N_i and the generator of the rotation subgroup is M_3. The corresponding one-parameter subgroups are then $h_i(a) = e^{N_i a}$, $r_3(\phi) = e^{M_3\phi}$.] Group-theoretically, (1.2) is an expansion of $|\xi\rangle$ in terms of the irreducible representations

$$l = \delta - i\rho, \quad \epsilon = 0 \quad (-\infty < \rho < \infty) \tag{1.4}$$

of $SO(2,1)$. We recover the unitary case when $\delta = -\frac{1}{2}$. This corresponds to the single valued principal series of $SO(2,1)$. Each irreducible component as expected satisfies the homogeneity condition

$$|\xi a;\sigma\rangle = a^\sigma\,|\xi;\sigma\rangle, \quad a \text{ real}. \tag{1.5}$$

The expansion (1.2) is made explicit by choosing a coordinate system for ξ. The three expansions are now given for the coordinate systems corresponding to the three subgroup reductions of $SO(2,1)$. (i) The spherical or S system corresponding to the subgroup reduction $SO(2,1) \supset SO(2)$. Here ξ is parametrized according to

$$\xi = \omega_S(1, \cos\phi, \sin\phi), \quad 0 < \omega_S < \infty, 0 \le \phi < 2\pi. \tag{1.6}$$

From the homogeneity condition (1.6),

$$|\xi;\rho\rangle = \omega_S{}^{[-(1/2)+i\rho]}\,|\phi;\rho\rangle. \tag{1.7}$$

(Here we have introduced the notation $|\xi;\rho\rangle = |\xi; -\tfrac{1}{2} + i\rho\rangle$ etc.) By expanding $|\phi;\rho\rangle$ in a Fourier series according to

$$|\phi;\rho\rangle = \sum_{M=-\infty}^{\infty} |\rho;M\rangle\, e^{iM\phi} \tag{1.8}$$

the resulting S system expansion on the cone is

$$|\xi\rangle = \sum_{M=-\infty}^{\infty} \int_{\infty}^{\infty} d\rho\, |\rho;M\rangle\, \omega_S{}^{[-(1/2)+i\rho]} e^{iM\phi}. \tag{1.9}$$

(ii) The hyperbolic or H system corresponding to the subgroup reduction $SO(2,1) \supset SO(1,1)$. Here ξ is parametrized according to

$$\xi = \omega_{H\pm}(\cosh\beta_\pm, \pm 1, \sinh\beta_\pm), \quad 0 < \omega_{H\pm} < \infty, -\infty < \beta_\pm < \infty, \tag{1.10}$$

and we define $\eta = \operatorname{sgn}\xi_2$ in the H system. To write the expansion correctly, we split $|\xi\rangle$ into two parts according to

$$|\xi\rangle = |\xi\rangle_+ + |\xi\rangle_-, \qquad |\xi\rangle_\pm = |\xi\rangle\,\theta(\pm\xi_1). \tag{1.11}$$

Then from the homogeneity condition (1.6) we have

$$|\xi;\rho,\pm\rangle = \omega_{H\pm}{}^{[-(1/2)+i\rho]}|\beta_\pm;\rho\rangle \tag{1.12}$$

By expanding $|\beta_\pm;\rho\rangle$ by means of a Fourier transform according to

$$|\beta_\pm;\rho\rangle = \int_{-\infty}^{\infty} |\rho;\pm,\tau\rangle e^{i\tau\beta_\pm} d\tau, \tag{1.13}$$

the resulting H system expansion on the cone is

$$|\xi\rangle_\pm = \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\rho\, |\rho;\pm,\tau\rangle\, \omega_{H\pm}{}^{[-(1/2)+i\rho]} e^{i\tau\beta_\pm}. \tag{1.14}$$

(iii) The horospherical or HO system corresponding to the subgroup reduction $SO(2,1) \supset T_1$. Here T_1 is the subgroup generated by $M_3 - N_2$. ξ is parametrized according to

$$\xi = \omega_E((r^2+1),(r^2-1),2r), \quad 0 < \omega_E < \infty, \quad -\infty < r < \infty. \tag{1.15}$$

From the homogeneity condition (1.6) we have

$$|\xi;\rho\rangle = \omega_E{}^{[-(1/2)+i\rho]}|r,\rho\rangle. \tag{1.16}$$

By expanding $|r,\rho\rangle$ by means of a Fourier integral transform according to

$$|r,\rho\rangle = \int_{-\infty}^{\infty} ds\, |\rho,S\rangle e^{iSr}, \tag{1.17}$$

the resulting HO system expansion is

$$|\xi\rangle = \int_{-\infty}^{\infty} dS \int_{-\infty}^{\infty} d\rho\, |\rho,S\rangle\, \omega_E{}^{[-(1/2)+i\rho]} e^{iSr}. \tag{1.18}$$

2. CALCULATION OF THE MIXED BASIS MATRIX ELEMENTS

We give here those mixed basis matrix elements which are necessary in order to completely determine a matrix element of the form $\langle A|U(g)|B\rangle$, with g a general group element. Here $|A\rangle$ and $|B\rangle$ are basis vectors of different subgroup reductions of the same UIR of the principal series of $SO(2,1)$. The corresponding parametrization of the group element g is then of the form

$$g = g_A \delta g_B, \tag{2.1}$$

where g_A and g_B are the two one-parameter group elements generated by the diagonalized operators in the bases A and B.

For the calculation of the $S \leftrightarrow HO$ mixed basis matrix elements the parametrization of g is

$$g = r_3(\phi)h_1(a)p_1(r), \tag{2.2}$$

where $p_1(r) = e^{(M_3 - N_2)r}$. For the explicit calculation of the general mixed basis matrix element we rewrite (1.1) in the following form:

$$\int_{-\infty}^{\infty} U(g)|\rho,S\rangle\, \omega_E{}^{-(1/2)+i\rho} e^{iSr} dS = \sum_{M=-\infty}^{\infty} |\rho,M\rangle\, \overline{\omega}_S{}^{-(1/2)+i\rho} e^{iM\phi'} \tag{2.3}$$

with

$$\xi g = \overline{\omega}_S(1, \cos\phi', \sin\phi').$$

This then gives the integral representation of the general matrix element

$$\langle \rho,M|U(g)|\rho,S\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{\overline{\omega}_S}{\omega_E}\right)^{-(1/2)+i\rho} e^{iM\phi'} e^{-iSr} dr. \tag{2.4}$$

Because of the group parametrization (2.2) we need only calculate the matrix element of $g = h_1(a)$. We then have that

$$\overline{\omega}_S/\omega_E = e^{a}(r^2 + e^{-2a}), \qquad e^{i\phi'} = (r + ie^{-a})/(r - ie^{-a})$$

and the explicit expression for the mixed basis matrix element is then

$$\begin{aligned}\langle \rho,M|h_1(a)|\rho,S\rangle &= \frac{(-1)^M S^{-1/2}}{\Gamma(\frac12 - i\rho - M)}(2S)^{(1/2)-i\rho} W_{-M,i\rho}(2e^{-a}S), \quad S > 0,\\ &= \langle \rho,-M|h_1(a)|\rho,-S\rangle, \quad S < 0,\end{aligned} \tag{2.5}$$

where $W_{\mu\nu}(Z)$ is the Whittaker function as defined in Ref. 14. The standard techniques of the infinitesimal method now enable us to derive the raising and lowering operators in the index M of these functions. To do this, we use a fixed column of the mixed basis matrix element $\langle \rho,M|U(g)|\rho,S\rangle$ as an S system basis for the UIR $l = -\frac12 - i\rho$, $\epsilon = 0$ of $SO(2,1)$. In the parametrization (2.2) this basis vector has the form

$$\langle \rho,M|U(g)|\rho,S\rangle = e^{iM\phi}\langle \rho,M|h_1(a)|\rho,S\rangle e^{iSr}, \tag{2.6}$$

and the generators of $SO(2,1)$ are expressed as differential operators in the parameters a, ϕ, r according to

$$M_3 = \frac{\partial}{\partial\phi}, \qquad N_1 \pm iN_2 = e^{\pm i\phi}\left(\frac{\partial}{\partial a} \pm i\frac{\partial}{\partial\phi} \mp ie^{-a}\frac{\partial}{\partial r}\right). \tag{2.7}$$

Then from the formulas, for the action of the generators $N_1 \pm iN_2$, on an S system basis[9] f_M, viz.,

$$(N_1 \pm iN_2)f_M = (-\tfrac12 + i\rho \mp M)f_{M\pm1} \tag{2.8}$$

we have on separating out the ϕ and r dependence the well-known recurrence relations for the Whittaker functions,

$$-xW_{M,i\rho}(x) + (\tfrac12 x - M)W_{M,i\rho}(x) = W_{M+1,i\rho}(x), \tag{2.9}$$

$$xW'_{M,i\rho}(x) + (\tfrac12 x - M)W_{M,i\rho}(x) = (\tfrac12 + i\rho - M)(\tfrac12 - i\rho - M)W_{M-1,i\rho}(x). \tag{2.10}$$

These relations are, however, known to be true for the functions $W_{\mu\nu}(Z)$ quite generally (i.e., with μ, ν, Z complex). As a further illustration of our calculation we write the identity

$$\int_{-\infty}^{\infty} ds\,\langle \rho,M|h_1(a)|\rho,S\rangle\langle \rho,S|h_1(b)|\rho,N\rangle = \langle \rho,M|h_1(a+b)|\rho,N\rangle \tag{2.11}$$

explicitly and obtain the new identity

$$\int_0^\infty dS[\tilde{W}_{M,i\rho}(e^{-a}S)\tilde{W}_{N,-i\rho}(e^{b}S) + \tilde{W}_{-M,i\rho}(e^{-a}S)\tilde{W}_{-N,-i\rho}(e^{b}S)] = \tfrac{1}{2}(-1)^{M+N}P_{MN}^{-(1/2)+i\rho}(\cosh(a+b)) \quad (2.12)$$

where

$$\tilde{W}_{M,i\rho}(x) = W_{-M,i\rho}(x)/\Gamma(\tfrac{1}{2}-i\rho-M).$$

We note in particular that if $a=-b$, the right-hand side of this identity is $\frac{1}{2}\delta_{MN}$.

For the calculation of the $S\leftrightarrow H$ mixed basis matrix elements, the parametrization of g is

$$g = r_3(\phi)h_1(a)h_2(\beta) \quad (2.13)$$

(remember for our choice of H system coordinates on the cone we have diagonalized N_2). The explicit calculation is achieved by writing (1.1) in the form

$$\sum_{\pm}\int_{-\infty}^{\infty} d\tau\, U(g)|\rho;\pm,\tau\rangle\, \omega_{H\pm}^{-(1/2)+i\rho}e^{i\tau\beta\pm} = \sum_{M=-\infty}^{\infty}|\rho,M\rangle\,\overline{\omega}_S^{-(1/2)+i\rho}e^{im\phi'} \quad (2.14)$$

with $\overline{\omega}_S$ and ϕ' as in (2.3). The integral representation of the general matrix element is then

$$\langle\rho,M|U(g)|\rho;\pm,\tau\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{\overline{\omega}_S}{\omega_{H\pm}}\right)^{-(1/2)+i\rho} e^{iM\phi}e^{-i\tau\beta_\pm}d\beta_\pm. \quad (2.15)$$

Because of the parametrization (2.13) we need only calculate the matrix element of $g=h_1(a)$. We then have that

$$\frac{\overline{\omega}_S}{\omega_{H\pm}} = \cosh a\cosh\beta_\pm \pm \sinh a,$$

$$e^{i\phi'} = \frac{\sinh a\cosh\beta_\pm \pm \cosh a + i\sinh\beta_\pm}{\cosh a\cosh\beta_\pm \pm \sinh a},$$

and the explicit expression for the mixed basis matrix element is then

$$\langle\rho,M|h_1(a)|\rho;+,\tau\rangle = \frac{1}{\pi}e^{-\pi(iM+\tau)}\frac{\Gamma(\frac{1}{2}-i\rho-i\tau)}{\Gamma(\frac{1}{2}-i\rho-M)} \times Q_{i\tau,M}^{(1/2)+i\rho}(-i\sinh a), \quad (2.16)$$

where $Q_{\mu\nu}^{j}(Z)$ is the generalized Legendre function of the second kind as defined by Azimov[9]. The other matrix element is given by the relation

$$\langle\rho,M|h_1(a)|\rho;-,\tau\rangle = (-1)^{M+1}\langle\rho,M|h_1(-a)|\rho;+,-\tau\rangle. \quad (2.17)$$

Using the infinitesimal method we may, as we did with the Whittaker functions find the raising and lowering operators in the index M for the $Q_{\mu\nu}^{j}(Z)$ functions as they appear in (2.16). The S system basis vector is now, for the parametrization (2.13),

$$\langle\rho,M|U(g)|\rho;\pm,\tau\rangle = e^{iM\phi}\langle\rho,M|h_1(a)|\rho;\pm,\tau\rangle e^{i\tau\beta}, \quad (2.18)$$

and the generators $N_\pm = N_1 \pm iN_2$ have the form

$$N_\pm = e^{\pm i\phi}\left(\frac{\partial}{\partial a} \pm i\tanh a\frac{\partial}{\partial\phi} \pm \frac{i}{\cosh a}\frac{\partial}{2\beta}\right). \quad (2.19)$$

Using (2.8) and separating out the ϕ and β dependence, we get the new recurrence relations

$$\left(\frac{d}{da} - M\tanh a + \frac{\tau}{\cosh a}\right)Q_{i\tau,M}^{(1/2)+i\rho}(i\sinh a) = [(M+\tfrac{1}{2})^2+\rho^2]Q_{i\tau,M+1}^{(1/2)+i\rho}(i\sinh a), \quad (2.20)$$

$$\left(\frac{d}{da} + M\tanh a - \frac{\tau}{\cosh a}\right)Q_{i\tau,M}^{(1/2)+i\rho}(i\sinh a) = Q_{i\tau,M-1}^{(1/2)+i\rho}(i\sinh a). \quad (2.21)$$

The analogous identity to (2.12) for the $S\leftrightarrow H$ mixed basis matrix elements is

$$\frac{1}{\pi^2}\int_{-\infty}^{\infty} d\tau[\tilde{Q}_{\tau M}^{\rho}(i\sinh a)\tilde{Q}_{\tau M}^{-\rho}(-i\sinh b) + (-1)^{M+N} \times \tilde{Q}_{-\tau M}^{\rho}(i\sinh a)\tilde{Q}_{\tau N}^{-\rho}(-i\sinh b)] = P_{MN}^{(1/2)+i\rho}(\cosh(a+b)), \quad (2.22)$$

where

$$\tilde{Q}_{\tau M}^{\rho}(i\sinh a) = \frac{\Gamma(\frac{1}{2}-i\rho-i\tau)}{\Gamma(\frac{1}{2}-i\rho-M)}Q_{i\tau,M}^{(1/2)+i\rho}(-i\sinh a)$$

Again the interesting case of this identity is when $a=-b$.

There are two group parametrizations necessary for the calculation of the $HO\leftrightarrow H$ mixed basis matrix elements, viz.,

$$g = h_2(\beta)h_1(a)p_1(r), \qquad \eta = -, \quad (2.23a)$$

$$g = h_2(\beta)h_1(a)r_3(\pi)p_1(r), \qquad \eta = +. \quad (2.23b)$$

The explicit calculation is achieved by writing (1.1) in the form

$$\sum_{\pm}\int_{-\infty}^{\infty} d\tau\, U(g)|\rho;\pm,\tau\rangle\,\omega_{H\pm}^{-(1/2)+i\rho}e^{i\tau\beta_\pm} = \int_{-\infty}^{\infty} ds|\rho,S\rangle\,\omega_E^{-(1/2)+i\rho}e^{iSr'}, \quad (2.24)$$

with

$$\xi g = \overline{\omega}_E(r'^2+1, r'^2-1, 2r').$$

The integral representation of the general matrix element is then

$$\langle\rho,S|U(g)|\rho;\pm,\tau\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{\omega_E}{\omega_{H\pm}}\right)^{-(1/2)+i\rho}e^{iSr'}e^{-i\tau\beta_\pm}d\beta_\pm. \quad (2.25)$$

Because of the parametrizations (2.23a), (2.23b) we need only calculate the matrix element of $h_1(a)$ for $\eta=-$ and $h_1(a)r_3(\pi)$ for $\eta=+$. We then have that

$$(\overline{\omega}_S/\omega_{H\pm}) = e^{-a}\cosh\tfrac{1}{2}\beta_\pm,\; r' = e^{a}\tanh\tfrac{1}{2}\beta_\pm,$$

and the explicit expression for these matrix elements is

$$\langle\rho,S|h_1(a)|\rho;-\tau\rangle = \langle\rho,S|h_1(a)r_3(\pi)|\rho;+,\tau\rangle = 1/2\pi(\tfrac{1}{4}e^{-a})^{[-(1/2)+i\rho]}B(\tfrac{1}{2}-i\rho-i\tau,\tfrac{1}{2}-i\rho+i\tau)e^{-iSe^{a}} \times {}_1F_1(\tfrac{1}{2}-i\rho-i\tau, 1-2i\rho, 2iSe^{a}), \quad (2.26)$$

where

$$B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$$

and ${}_1F_1(b;c;z)$ is the confluent hypergeometric function[15].

We also give here the expression for the matrix element $\langle \rho, S | h_1(a) | \rho; +, \tau \rangle$, it is

$$\langle \rho, S | h_1(a) | \rho; +, \tau \rangle = \frac{1}{4\pi} (-\tfrac{1}{4} e^a S^2)^{-(1/2)+i\rho} \times [\Gamma(\tfrac{1}{2} - i\rho + i\tau) W_{-i\tau,-i\rho}(-2iSe^a) + \Gamma(\tfrac{1}{2} - i\rho - i\tau) W_{i\tau,-i\rho}(2iSe^a)]. \quad (2.27)$$

We also have directly from the integral representations the asymptotic equality

$$\langle \rho, M | h_1(a) | \rho; \pm, \tau \rangle = [\langle \rho, S | h_1(a) | \rho; \pm, \tau \rangle]_{S=M}, \quad (2.28)$$

which holds for large a. This is the direct analogy of a similar relation which is known to hold for the subgroup reductions of $SO(3,1)$[12].

CONCLUDING REMARKS

We have seen in this paper how the method on the cone can be used to directly calculate the mixed basis matrix elements for the principal series of $SO(2,1)$. The use of this method for calculating matrix elements is due to Verdiev[15] and has been extensively used for the subgroup reductions of $SO(3,1)$[12]. From our calculations we can immediately find the overlap functions by putting $a = 0$. These overlap functions can be used to factorize the overlap functions of the subgroup reductions of $SO(3,1)$. An example of this factorization is

$$\langle J, m | \pm, l, s \rangle = \langle J, m | \pm, l, m \rangle \langle m | s \rangle.$$

Here $|J, m\rangle$, $|\pm, l, m\rangle$, and $|\pm, l, s\rangle$ are basis vectors for the same UIR of $SO(3,1)$ corresponding to the group reductions $SO(3,1) \supset SO(3) \supset SO(2)$, $SO(3,1) \supset SO(2,1) \supset SO(2)$, and $SO(3,1) \supset SO(2,1) \supset T_1$, respectively. The Lorentz group labels have been suppressed in these vectors. The matrix $\langle m | s \rangle$ is then the S–HO overlap function which is given by (2.5) after putting $a = 0$.

[Note: We have assumed here that l is in the principal series $l = -\frac{1}{2} + i\rho$, $\epsilon = 0$ of $SO(2,1)$.] We intend in the near future to make a complete study of matrix elements in the subgroup reductions of $SO(2,1)$ for all possible UIR's.

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A linked cluster evaluation of contour integrals in statistical mechanics

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A linked cluster expansion is obtained for the logarithm of the partition function which constitutes an asymptotic expansion in $1/N$ for a normal system. The result is obtained by means of a new and rather general way of asymptotically evaluating a type of integral common in statistical mechanics.

1. INTRODUCTION

The statistical mechanics of many-particle systems is usually studied employing the grand canonical ensemble (GCE). This choice is dictated by its being, in most cases, the most convenient ensemble to use for quantum problems and the most appropriate one when using second quantization or, in general, quantum field theoretical methods. Since the principal interest in quantum statistical mechanics is in systems large enough so that the results are almost ensemble-independent, this choice of ensemble is usually satisfactory.[1]

On the other hand, as we have discussed in an earlier paper[2] (hereafter denoted I), there are circumstances under which it is either convenient or, in certain cases, necessary to use other ensembles with various constraints, such as fixed number of particles N (the petit-canonical ensemble), fixed N and constant pressure (the isobaric petit-canonical ensemble), fixed N and the energy either constant or constrained to a small variation $E_0 - \alpha \leq E \leq E_0 + \alpha, \alpha \ll E_0$ (the microcanonical ensemble).

In I we developed an asymptotic expansion in l/N, for the constant volume and constant pressure petit-canonical ensembles, more specifically an asymptotic expansion for the respective partition functions for the two ensembles. In the present paper a much more powerful method of handling the asymptotic evaluation of the contour integrals is developed. This is a rather general technique which has numerous possible applications. By this means we are able to obtain a linked cluster diagram expansion for the *logarithm* of the partition function $Z_N(V, T)$, i.e., for the thermodynamic potential which in this case is the Helmholtz free energy [multiplied by $-(kT)^{-1}$]. We are further able to exploit the form of the expansion to develop a perturbation expansion for the petit canonical ensemble. This result constitutes a more fundamental proof and a generalization, with some minor corrections, of the earlier work of Brout and Englert[3] and Horwitz, Englert, and Brout[4] for interacting fermions and of De Coen, Englert, and Brout[5] for bosons.[6]

This linked cluster evaluation of the contour integral is formulated in the present work for the special case of the constant-volume petit-canonical ensemble. The present formulation can be expected to be valid for a single phase region, not too close to a phase transition. Thus for quantum systems these conditions will, crudely speaking, correspond to the assumption of what is called a "normal" fermion or boson system. We may also speculate that a suitable resummation of the series may make the method applicable to cases having a phase transition.[6] We shall discuss some conditions of validity for the expansion, but since we are not yet able to rigorously define the conditions, the expansion remains, in fact, a formal expansion, subject to test of validity in each application.

In I we used a complex integral representation of the partition function; by selecting a contour tangent to the steepest descents path, we obtained a general expression for the asymptotic expansion for Z_N. The present formulation allows the contour to cross the real axis at an arbitrary point P if there is a sufficiently large region of analyticity containing both P and the saddle-point of the integral. We are then able to obtain a general expression for the asymptotic expansion for the $\log Z_N$.

A specific application of the above procedure leads to a perturbation expansion. If one chooses the point P to be the saddle point of the partition function Z_0, corresponding to some reference Hamiltonian $\hat{H}_0$, the linked cluster expansion obtained combines both a perturbation expansion and an asymptotic expansion in $1/N$. A comparison with the previous work mentioned above[3-5] shows agreement with their results to order N, for normal systems. For terms smaller than order N, there are corrections to earlier work coming from $1/N$ corrections to the unperturbed distribution and correlation functions. When setting up this asymptotic perturbation expansion, it is convenient for some applications to also regroup the ordinary linked cluster graphs as obtained from the grand canonical ensemble expansion. This regrouping is related to the operator diagram formulation of Brout and Englert[3] and the grand canonical ensemble methods of Balian, Bloch, and De Dominicis.[7] To order N this regrouping is quite straightforward, being closely related to Goldstone graphs for zero temperature perturbation theory; carrying out this regrouping to higher order in $1/N$ becomes increasingly complicated to describe as compared with the usual Wick's theory results obtained for the customary grand canonical ensemble formalism.

In a forthcoming paper we develop a linked cluster expansion for the microcanonical ensemble. This microcanonical formalism is currently being exploited for the study of critical phenomena.

2. THE LINKED CLUSTER EXPANSION

The partition function $Z_N(V, T)$ is the appropriate statistical mechanical function to describe all equilibrium properties of a system with a fixed number of particles N contained in a volume V in contact with a heat reservoir at temperature T:

$$Z_N(V, T) = \mathrm{Tr}^{(N)} \exp(-\beta\hat{H}) = \sum_s \exp[-\beta E_s(N, V)] = \exp[-\beta F(N, V, T)], \quad (1)$$

where $\hat{H}$ is the Hamiltonian for the system, $\beta^{-1} = kT$, k being the Boltzmann constant, and where $\mathrm{Tr}^{(N)}$ denotes the trace in any convenient representation spanning the Hilbert space of eigenfunctions of the N particle Hamiltonian, and s enumerates the eigenstates of $\hat{H}$.

Z_n has the well-known complex integral representation[8]

$$Z_N(V, T) = (1/2\pi i)\int_C (d\zeta/\zeta^{N+1})Q(\zeta, V, T), \quad (2)$$

where the contour C encloses the origin, but excludes any poles of $Q(\zeta, V, T)$ and

$$Q(\zeta, V, T) = \sum_{N'=0}^{\infty} \zeta^{N'} Z_{N'}(V, T). \tag{3}$$

This then readily becomes the unrestricted trace in a Fock space representation (denoted Tr) and particularly with $[\hat{N}, \hat{H}] = 0$, i.e., the number operator commuting with the Hamiltonian

$$Q(\zeta, V, T) = \mathrm{Tr}\, \exp(-\beta \hat{H} + \ln\zeta \hat{N}). \tag{4}$$

The quantity in (3) or (4) is seen to be the analytic continuation of the grand partition function for complex values of the fugacity $z = \exp\alpha$.

It is then convenient to transform Z_N to the form

$$Z_N(V, T) = (1/2\pi i) \int_C (d\zeta/\zeta) \exp[\phi(\zeta)] \tag{5}$$

with

$$\phi(\zeta, N, T) = \ln[Q(\zeta, V, T)] - N \ln\zeta \tag{6}$$

and then to introduce the variables

$$\ln\zeta = u + iv = y \tag{7}$$

whence

$$Z_N(V, T) = (1/2\pi i) \int_{C'} dy\, \exp[\phi(e^y, V, T)], \tag{8}$$

where C' is the mapping of the contour C on the (u, v) plane. Let us assume for simplicity a single phase region in which $Q(\zeta, V, T)$ is analytic and also has no zeros out to some radius $|\zeta|<|\zeta_1|$.[9] Then we choose a contour C to be a circle with radius ζ_0, $|\zeta_0|<|\zeta_1|$ or, in terms of the contour C' in the y-plane,

$$u = u_0 = \ln|\zeta_0|, \quad -\pi < v < \pi.$$

Then

$$Z_N(V, T) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dv\, \exp[\phi(e^{u_0+iv}, V, T)]. \tag{9}$$

Under the extreme conditions defined above, this expression would be exact. The usual procedure is then to choose u_0, by the saddle-point condition $\partial\phi/\partial\zeta\,[\zeta = e^{u_0}, V, T] = 0$, $u_0 = \alpha$ being β times the chemical potential, and take the steepest-descent path through $\zeta = e^{\alpha}$, which is normally along v. This we shall not do at present, but rather leave ζ_0 arbitrary.

Let us proceed to expand $\phi(e^{u_0+v}, V, T)$ in iv,

$$\phi(e^{u_0+iv}, V, T) = \sum_{r=0}^{\infty} [C'_r(u_0)(iv)^r(r!)^{-1}] - u_0 N - ivN, \tag{10}$$

where

$$C'_r(u_0) = \frac{\partial^r}{\partial y^r} \ln[Q(e^y, V, N)] = \frac{\partial^r}{\partial u_0^r} C'_0(u_0),$$
$$C'_0(u_0) = \ln[Q(e^{u_0}, V, N)] = \beta\pi(e^{u_0}, V, T), \tag{11}$$

and it is to be observed from the definition of $\ln Q$ that the C'_r are the rth-order cumulant averages of the number operator, evaluated at the fugacity $\exp(u_0)$. It is convenient to use, in place of the quantities C'_r, the quantities C_r, which are defined as follows $C_0 = C'_0 - Nu_0$, $C_1 = C'_1 - N$, and $C_r = C'_r$ for r greater than 1. The C_r are then the cumulant averages of $\hat{N} - N$, the fluctuation of the number operator from the value N. Then (9) can be written

$$Z_N(V, T) = (1/2\pi) \int_{-\pi}^{\pi} dv\, \exp[C_0 + C_1 iv - \tfrac{1}{2} C_2 v^2 + S(v)], \tag{12}$$

where

$$S(v) = \sum_{r=3}^{\infty} C_r(u_0)(iv)^r(r!)^{-1}. \tag{13}$$

This result (12) can now be represented in the following operator form where the limits of integration can be replaced by $\pm\infty$ up to terms asymptotically small, $O[\exp(-C_2)]$ cf. Appendix A):

$$Z_N(V, T) = (1/2\pi) e^{C_0} \exp[D(\partial/\partial C_1)] \int_{\infty}^{\infty} \frac{dv}{2\pi} \times \exp(ivC_1 - \tfrac{1}{2} C_2 v^2) \tag{14}$$

with

$$D\left(\frac{\partial}{\partial C_1}\right) = \sum_{r=3}^{\infty} C_r(u_0)(r!)^{-1} \frac{\partial^r}{\partial C_1} r. \tag{15}$$

On integrating, (14) becomes

$$Z_N(V, T) = (e^{C_0}/\sqrt{2\pi C_2}) e^D \exp(-\tfrac{1}{2} C_2^1/C_2) \tag{16}$$

and then

$$\ln[Z_N(V, T)] = C_0 + \ln\sqrt{2\pi C_2} + \ln(\exp D)\, [\exp(-\tfrac{1}{2} C_1^2/C_2)]. \tag{17}$$

Exploiting the algebraic structure of the exponential as a generator of a cumulant expansion with the differential operator $\exp D$ taking the place of an averaging, we find

$$\ln(\exp D)\, [\exp(-\tfrac{1}{2} C_1^2/C_2)] = \sum_{n=1}^{\infty} (-\tfrac{1}{2} C_2)^n \mu_n[C_1^2], \tag{18}$$

where the μ_n are defined in analogy with the usual cumulants:

$$\mu_2[C_1^2] = e^D C_1^4 - (e^D C_1^2)^2 = C_4 + 4C_3 C_1,$$
$$\mu_3[C_1^2] = e^D C_1^6 - 3(e^D C_1^2)(e^D C_1^4) + 2(e^D C_1^4)$$
$$\mu_4[C_1^3] = \ldots; \tag{19}$$

in general, then,

$$\mu_n[x^2] = \frac{\partial^n}{\partial\lambda^n} \ln(e^D e^{\lambda x^2}) \Big|_{x=0}. \tag{20}$$

This already represents a substantial simplification over the result in I. But one can make use of the analogy of the exponent $-\frac{1}{2} C_1^2/C_2$ with a two-particle diagonal potential for which $-1/C_2$ is the interaction, $\frac{1}{2}$ the symmetry factor, and the interaction is regarded as quadratic in C_1. The result of this purely algebraic connection between single-variate and multi-variate cumulants is that $\ln(\exp D)\, [\exp(-\frac{1}{2} C_1^2/C_2)]$ can be expanded in a linked cluster expansion in the quantities $\mu_n[C_1]$. Symbolically, we write

$$\ln(\exp D)\, [\exp(-\tfrac{1}{2} C_1^2/C_2)] = L\{\mu_n[C_1]\}. \tag{21}$$

We note[11] that $\mu_n[C_1] = C_n$.

One has the following prescription for the linked cluster expansion: Draw the usual unlabelled line graphs consisting of points (vertices) joined by lines (bonds). The contribution of each bond is $(-1/C_2)$, and that of a vertex with r bonds attached C_r. There is also a weight factor associated with each diagram corresponding to the order of the symmetry group of the diagram. These diagrams are essentially the same as those used for the Ising model by Horwitz and Callen[12] (HC). The proof there is essentially algebraic and goes through here as well. There is one trivial modification that while in HC the interaction was bilinear in unequal operators, here the operators are equal. This merely adds to the diagram scheme bonds which are connected at both ends to the same vertex.

There is one other difference: Since $S(v)$ begins with C_3, there are no diagrams with only two bonds attached to a vertex. Thus, for example,

(a)  has contribution $(3!)^{-1}C_3C_1^3(-C_2)^{-3}$,

(b) has contribution $(\frac{1}{2})^3C_3^2(-C_2)^{-3}$,

(c)  has contribution $(\frac{1}{2})^3C_5C_1(-C_2)^{-3}$,

(d)  has contribution $(\frac{1}{2})(1/3!)(-C_2)^{-3}C_3^2$.

Let us now consider the classification of the diagrams in order of N. For a normal expansion, all C_r are of order N. Thus, every bond carries a factor $1/N$, while every vertex carries a factor N. The net result is that only Cayley tree diagrams, i.e., diagrams which have no closed paths are of order N. Diagrams having a single closed path are of order N^0. Diagrams with two closures of order N^{-1}, etc.

The sum of all Cayley tree diagrams corresponds to the $C_0(u_0)$ being replaced by $C_0(u')$, u' being the saddle-point value of y in the integral (12). To verify this, we first note the obvious converse that had we chosen u_0 to be the saddle-point value, $C_1(u_0) = \langle\hat{N}\rangle - N = 0$; there would remain none of the graphs which are not multiply connected and hence none of the graphs of order N. In Appendix B we evaluate the sum of the Cayley tree diagrams and confirm the above statement. Cayley tree attachments to stars, diagrams with closed parts when summed replace the dependence on u_0 in the $C_r(u_0)$ in the closed parts by $C_r(u')$.

3. PERTURBATION THEORY

The linked cluster expansion developed in the last section for the Helmholtz free energy can readily be made into a linked cluster perturbation expansion for the petit-canonical ensemble. The central feature of the method of Sec. 2 was the freedom of choice of the point where the contour crosses the real axis. We shall now proceed to set up a perturbation expansion inside the integral for ϕ. The Hamiltonian for the system being first assumed separated in some convenient way into a single particle part H_0 and some interaction part λV:

$$\hat{H} = \hat{H}_0 + \lambda\hat{V}, \tag{22}$$

λ denoting a coupling constant characterizing the perturbation. Setting up a perturbation expansion for

$$\phi = \phi_0 + X, \tag{23}$$

where

$$\phi_0 = \ln \operatorname{Tr} [\exp(-\beta\hat{H}_0 + \hat{N}\ln\zeta)] - N\ln\zeta,$$

$$X = \ln\langle T \exp(-\int_0^\beta du\lambda\hat{V}(u))\rangle_0, \tag{24}$$

and $V(u) = [\exp(u\hat{H}_0)]\hat{V}[\exp(-u\hat{H}_0)]$, the (imaginary time) interaction representation of the operator V and

$$\langle A\rangle_0 = [\operatorname{Tr} A \exp(-\beta\hat{H}_0 + \ln\zeta N)]/\operatorname{Tr}\exp(-\beta\hat{H}_0 + N\ln\zeta). \tag{25}$$

If we now make the specific choice of ζ_0, that $\ln\zeta_0 = \alpha_0$, corresponding to the saddle-point value for the single particle Hamiltonian H_0,

$$\frac{\partial\phi}{\partial\ln\zeta}\Big|_{\zeta=\exp\alpha_0} = 0, \tag{26}$$

which just corresponds to choosing the chemical potential for the unperturbed system macroscopically to give $\langle\hat{N}\rangle_0 = N$, the zero denoting a density operator defined in terms of $\hat{H}_0$, as in (25).

Let us assume that the domain of analyticity of $\phi(\zeta)$ includes both the saddle point of ϕ (corresponding to $\hat{H}$) and the saddle point of $\hat{H}_0$ (corresponding to $\hat{H}_0$), in addition to which it extends out a sufficient distance from both saddle points to attain the asymptotic form described in Appendix A.

We can then carry through our previous expansion, but now have a new interpretation of the expansion, and a separation into two types of terms: one corresponding to finite N corrections to the partition function of the $\hat{H}_0$ and the other to contributions due to the interaction terms, order N and smaller.

Expanding the exponent ϕ, taking $\zeta = \exp(\alpha_0 + iv)$, we have

$$\phi_0(v) = f_0(\alpha_0) + \sum_{n=1}^{\infty} f(\alpha_0)\frac{(iv)^n}{n!},$$

$$X(v) = h_0(\alpha_0) + \sum_{n=1}^{\infty} h(\alpha_0)\frac{(iv)^n}{n!}, \tag{27}$$

where

$$f_n = M_n^{(0)}[\hat{N} - N], \tag{28}$$

while

$$h_n = M_n[\hat{N} - N] - M_n^{(0)}[\hat{N} - N], \tag{29}$$

i.e., the f_n are the cumulant averages of the mean fluctuation of the number operator evaluated with a density operator determined by $\hat{H}_0$, while the h_n represent the modification of the nth-order cumulant due to the interaction terms. The $h_n(\alpha_0)$ will be obtainable as an expansion in V by means of the usual Wick's theorem results derivable for the grand canonical ensemble, and hence will be representable as a sum of graphs in one of the various graphical expansions known for the grand canonical ensemble.[13]

We have as noted above chosen $f_1 = \langle\hat{N}\rangle - N = 0$. Asymptotically as before

$$Z_N(V,T) = e^{\phi_0 + X}\int_{-\infty}^{\infty}\frac{dv}{2\pi}\exp[-\tfrac{1}{2}v^2 f_2 + h_1 iv + T'(v)], \tag{30}$$

where

$$T'(v) = \sum_{n=3}^{\infty} f_n(\alpha_0)\frac{(iv)^n}{n!} + \sum_{n=2}^{\infty} h_n(\alpha_0)\frac{(iv)^n}{n!} \tag{31}$$

$$= \sum_{n=2}^{\infty}\frac{\psi_n(\alpha_0)(iv)^n}{n!} \tag{32}$$

with

$$\psi_2 = h_2, \quad \Psi_n = f_n + h_n, \quad n \ge 2. \tag{33}$$

Thus

$$\ln[Z_N(V,T)] = f_0 + h_0 - \tfrac{1}{2}\ln(2\pi f_2) + \ln\{\exp[D(\partial/\partial h)]\exp(-\tfrac{1}{2}h_1^2/f^2)\} \quad (34)$$

$$= f_0 + h_0 - \tfrac{1}{2}\ln(2\pi f_2) + L[f_n, h_n', \alpha_0], \quad (35)$$

where L is the sum linked graphs.

The linked cluster result is immediate as before. There are now, however, two modifications. First the separation graphically into f_n vertices and h_n hypervertices: One is to be indicated by a small dot and the latter by an open large dot. Secondly, the large dots contain vertices of order two, whereas our previous result began only with vertices of order 3.

The first two terms of (34) represent the Legendre transform of the grand potential to the Helmholtz free energy, but evaluated at the macroscopic chemical potential[14] corresponding to $\hat{H}_0$, i.e., α_0, rather than that corresponding to $\hat{H}$, denoted α. The effect of the terms in the expansion of order N will, by arguments like those at the one of Sec. 2, shift α_0 to α. A remark is in order about the partial summations in the coupling constant and in $1/n$ (see, for example, remarks in Ref. 3). The hypervertices h_n as well as h_0 are obtainable from the infinite sum of perturbation graphs in the grand canonical ensemble formalism, here evaluated, however, at α_0 rather than α. This is just the opposite extreme from the more common case where one is expanding the G.C.E. graphs term by term in the coupling constant in terms of the fully interacting chemical potential α. Both of these cases represent a separate resummation—in one case of the perturbation expansion and in the other of the chemical potential—in a mutually inconsistent fashion. There are a number of problems, even quite trivial ones, where this leads to serious difficulties; maintaining this consistency can be shown to be equivalent to conserving variational properties of F and preserving the Hugenholtz–Van Hove–Pines type relations.[15]

This type of consistency can, of course, also be maintained in the GCE formalism by evaluating α at each order of approximation, determining α by maintaining the derivative of the grand potential equal to zero at fixed N. The advantage of the present method is in having an explicit graphical representation to keep track of the consistency.

4. COMPARISONS WITH OTHER PERTURBATION EXPANSIONS

The perturbation expansion for the free energy developed in Sec. 3 as an asymptotic expansion in $1/N$ will now be examined in some more detail and an explicit comparison made with the constant volume petit-canonical ensemble perturbation expansion of Brout and Englert, *et al.*[3-5] The terms of order N (topologically Cayley tree diagrams) represent the Legendre transform of the grand potential in which the macroscopic chemical potential has been expanded out diagrammatically in terms of the interaction. It is convenient to speak of the perturbation terms as divided into two classes, GCE linked cluster diagrams corresponding to the hypervertices h_n (beginning with h_0) and the correlation-bonding of these disjoint linked parts to make up the graphs analyzed in the previous sections. The h_n hypervertices are, of course, just the nth derivative with respect to α_0 of the sum of the GCE linked graphs, which could be evaluated in any of the various GCE perturbation schemes. By choosing a specific formalism for the GCE expansion we shall make an explicit connection with the Brout and Englert expansion. We shall discuss in detail the Cayley tree terms, which for a "normal" fermion or boson system represents the order N terms. For that case (order N and normal fermion or bosons), our result is in agreement with the previous canonical ensemble perturbation results.[16]

Of the various forms of perturbation for the grand potential developed by Bloch, De Dominicis, and Balian,[17] a particular one[7] is most appropriate to make connection with the petit-canonical ensemble expansion of Brout and Englert. This expansion is obtained by a rearrangement of the terms of the usual formalism and can be obtained in both time dependent and time independent forms. Let us refer the reader for the detailed rules of the expansions to the original papers or the review of Bloch.[17] For our present purpose we need only to know certain characteristic properties of the rearranged expansion. The rules for the linked parts given below are identical with that of the Brout-Englert expansion except for being evaluated at α instead of α_0.

(1) The central point of difference from the usual linked cluster methods is the handling of terms having more than a single pair of equal indices. In principle, the approach could apply to multiple repetitions of pairs of operators with equal indices. In practice, only for graphs in which the repeated indices occur from momentum conservation (macroscopic limit), i.e., as self-energy insertions—leading to the necklase structure in the notation of Balian *et al.*[7]—are these effects of order N. We shall not consider except in passing the higher order terms in this rearrangement (but cf. Appendix C).

(2) The rearrangement of these repeated indices leads to a new definition for the linked diagrams, in which there are two modifications:

(i) a line with repeated indices and self-energy insertions is unidirectional, only descending or ascending lines for a given propagator, like in the Goldstone expansion.

(ii) Such state has only a single statistical factor $n(r) = \langle a^+(r)a(r)\rangle_0$ for descending lines and $n'(r) = \langle a(r)a^+(r)\rangle_0$ for descending lines, no matter how many self-energy insertions. This is indicated in the diagrams by drawing a dotted line for all lines connecting self-energies but one.

(iii) In addition to the single necklace, which will comprise, for us, the redefined linked GCE diagrams—the redefined hypervertex h_n'—there are a set of disjoint necklaces with a common index in all internal lines of the necklaces being dashed lines, and there is a common

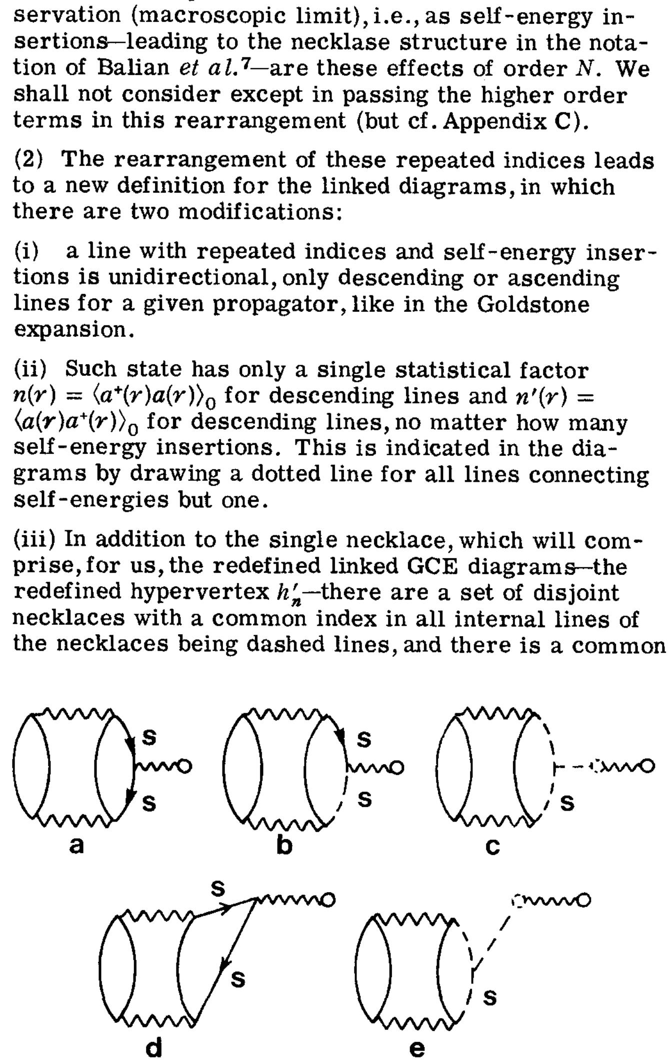


FIG. 1. A comparison of the graphs of the conventional GCE expansion and the modified one of Brout and Englert or Balian, Bloch, and De Dominicis.

statistical factor for n necklaces having a common index, which is just $m_n(s)$, the nth cumulant average of $n(s)$.

Thus if we consider the diagrams in Fig. 1, the graph of Fig. 1a is replaced in the above described formalism by the two graphs Figs. 1b and 1c comprising a redefined linked graph (1b) and two disjoint linked graphs linked by equal-index correlation bonds (1c). Correspondingly, the graph at Fig. 1d disappears as a linked graph and appears only as an equal-index correlation linked graph. We note further for reference purposes that all the dependence in the GCE perturbation on α is contained in the dependence in the functions $n(r), n'(r)$ and the equal index cumulants $m(1, 2 \ldots, N)$.

If we now rearrange our perturbation expansion within the h_0 and h_n hypervertices, in the manner described above, we obtain for each such hypervertex the following structure: the redefined hypervertices h_n', which we shall denote by open squares corresponding to the above redefined linked parts and equal index correlation bonding of these h_n' hypervertices. As far as we have described this expansion of the h_n', we have only the leading order contribution (in N), and the structure consists only of Cayley tree structures of equal index correlation bonding of the h_n' hypervertices.

Having done the above, we now have two types of vertices: the f_n vertices and the h_n' hypervertices, the latter being joined by two types of correlation bonds, the solid line and the dashed-line, equal-index, correlation bond. Since the equal-correlation bonds connect specific equal states of disjoint linked parts, and since it is otherwise convenient to separate a correlation link which acts several times on the same state, we shall introduce an infrastructure on our h' hypervertices: a window to a particular labeled line on the linked graph. Then, to lowest order we have (Fig. 2), denoting by L' the evaluation of the redefined linked graphs, then defining[18]

$$G(r) = \frac{\partial L'\{n(r)\}}{\partial n(r)}, \quad G(r, s) = \frac{\partial^2 L'}{\partial n(r) \partial n(s)}, \cdots. \tag{36}$$

The sum of the contributions of the two graphs of Fig. 2 then give

$$\tfrac{1}{2} \sum_{r,s} G(r)G(s)\big(m_2(r)\delta_{r,s} - m_2(r)m_2(s)/\textstyle\sum_t m_2(t)\big) \tag{37}$$

and we define $m_2(r, s)$ by

$$m_2(r, s) = m_2(r) - m_2(r)m_2(s)/\textstyle\sum_t m_2(t). \tag{38}$$

For the next order one distinguished two classes of graphs, those of Fig. 3a having only pairs of states connected by correlation, while those of Fig. 3b have correlations between three states. The contribution of the sum of graphs in Fig. 3a gives

$$\tfrac{1}{2} \sum_{r,s,t,u} G(r)G(s,t)G(u)m_2(r,s)m_2(t,u), \tag{39}$$

and the sum of the graphs of Fig. 3b gives

$$(1/3!) \sum_{r,s,t} G(r)G(s)G(t)m_3(r, s, t), \tag{40}$$

where

$$\begin{aligned} m_3(r, s, t) = {} & m_3(r)\delta_{r,s}\delta_{s,t} - [m_2(r)m_2(s)/\textstyle\sum m_2(t)]\delta_{s,t} \\ & - m_3(s)m_2(r)/\textstyle\sum m_2(t)\delta_{r,t} \\ & - m_3(t)m_2(s)\delta_{s,r}/\textstyle\sum m_2(t) \\ & + [\textstyle\sum m_2(t)]^{-2}[\textstyle\sum_{r,s,t} m_3(r)m_2(s)m_2(t) \\ & + m_3(s)m_2(r)m_2(t) \\ & + m_3(t)m_2(r)m_2(s)] \\ & - \textstyle\sum_u m_3(u)m_2(r)m_2(s)m_2(t)\Big/\Big(\textstyle\sum_u m_2(u)\Big)^3. \end{aligned}$$

Thus the resulting correlation bonding on combining the two classes of terms is just the multivariate cumulant: this result together with the identical structure of the linked parts leads us to conclude that our expansion is identical to order N with that of Brout and Englert.

In the present paper we will not go into the details of the higher order terms in this formalism. Carrying this procedure to higher orders leads to a much more complex set of rules for the structure of the hypervertices than the usual GCE perturbation expansions. In Appendix C we illustrate some of the higher order effects. In one example showing a typical type of term contributing a higher order contribution to $m_2(i, j)$ and in the second case indicating a type of $1/N$ diagram leading to treatment of equal indices not on a necklace in a linked diagram (hypervertex).

One might well raise the question why one should bother with the complications involved in this rearrangement of the GCE to higher order, since as far as the treatment of the $1/N$ terms goes, one can handle the matter more simply with the perturbation expansion. There are two motivations, one formal and one practical, though it may well be that it is generally desirable whenever such expansions in $1/N$ are of interest. The formal argument is that such an expansion represents the obvious generalization that one would expect to be of interest for a finite

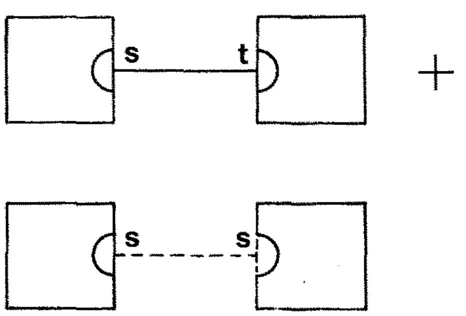


FIG. 2. The combination of the second-order correlation term of the modified GCE graphs and those in the expansion of the present work.

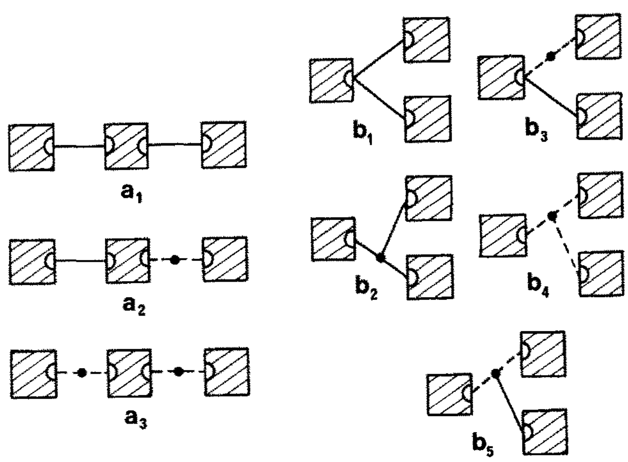


FIG. 3. Two classes of third-order correlation terms combining the modified GCE graphs and the graphs of the expansion in the present work.

system for which the functional expression of the free energy is given not only in terms of single-particle distribution functions, but in terms of the many-particle correlation functions, and our $m_n(1,2,\ldots,n)$ are just of this character. The practical reason of interest is our experience in working on a pairing approximation for interacting bosons, where, in order to reestablish the order-N character of the leading order terms of the linked cluster expansion, it was necessary to establish this functional dependence on the canonical ensemble correlation functions, the above $m_n(1,2\cdots)$.

APPENDIX A: ASYMPTOTIC PROPERTIES OF ln Z

The object of this appendix is to show more specifically the structure of the terms ignored in arriving at (12) or (14). In fact, much less restrictive conditions on the analytic properties of $\phi(\zeta)$ are necessary. It will be clear that if $\phi(\zeta)$ is a decreasing function of ζ along the contour chosen and has a domain of analyticity of radius $O(N^{-1/2-\eta}), \eta > 0$, that will suffice to give (12) as the asymptotic expansion, ignored terms being of order $\exp(-N^{\eta})$.

Let us then consider the dependence of the integral in Eq. (12) on its limits here to be denoted $\pm\theta_0$, transforming to the variable $t = \sqrt{C_2}/2\theta, t_0 = \sqrt{C_2}/2\theta_0$,

$$I(t_0) = \frac{e^{C_0}}{2\pi\sqrt{C_2/2}} \int_{-t_0}^{t_0} dt\, e^{-t^2+T(t)} \tag{A1}$$

where (cf. I)

$$T(t) = \sum_{\substack{n=1\\ n\neq 2}}^{\infty} \frac{D_n (it)^n}{n!}, \quad e^{T(t)} = \sum_{n=0} (it)^n \sum_{\substack{\{m_r\}\\ \sum r m_r = n}} \left(\frac{D_r}{r!}\right)^{m_r} \frac{1}{m_r!} \tag{A2}$$

and

$$D_n = (2/C_2)^{n/2} C_n. \tag{A3}$$

From (A1) and (A2), we find, noting that odd moments vanish, that even ones are given by

$$\int_{-t_0}^{t_0} dt\, t^{2n} e^{-t^2} = \int_0^{t_0} d\tau\, \tau^{n-1/2} e^{-\tau} = \gamma(n+\tfrac{1}{2}, t_0^2), \tag{A4}$$

where $\gamma(\chi)$ is the incomplete gamma function; this can be written as the difference of the complete gamma function and

$$\Gamma(\nu,\alpha) = \int_0^{\infty} d\tau\, t^{\nu-1} e^{-\tau}. \tag{A5}$$

Therefore,

$$I(t_0) = \frac{e^{C_0}}{2\pi\sqrt{C_2/2}} \sum_{n=0}^{\infty} (-1)^{2n} [\Gamma(n+\tfrac{1}{2}) - \Gamma(1+\tfrac{1}{2}, t_0^2)] \times \sum_{\substack{\{m_r\}\\ \sum_r r m_r = 2n}} \prod_{r=0}^{\infty} \left(\frac{D_r}{r!}\right)^{m_r} \frac{1}{m_r!}. \tag{A6}$$

We note that

$$\sum_{\substack{\{m_r\}\\ \sum r m_r = 2n}} \prod_r \left(\frac{D_r}{r!}\right)^{m_r} \frac{1}{m_r!} = \frac{D_1^{2n}}{(2n)!} + \frac{D_1^{2n-3}}{(2n-3)!}\frac{D_3}{3!} + \frac{D_1^{2n-3}}{(2n-3)!}\left(\frac{D_3}{3!}\right)^2 \frac{1}{2} + \cdots \tag{A7}$$

can be obtained from the generator

$$\left[\exp\left(\sum_{r=3}^{\infty} \frac{D_r}{r!} \frac{\partial^r}{\partial D_1^r}\right)\right] \left(D_1^{2n}\right). \tag{A8}$$

Hence

$$I(t_0) = \frac{e^{C_0}}{\sqrt{2C_2}} \sum_{n=0}^{\infty} (-1)^{2n} \frac{[\Gamma(n+\frac{1}{2}) - \Gamma(n+\frac{1}{2}, t_0^2)]}{\Gamma(\frac{1}{2})} \times \exp\left(\sum_{n=3}^{\infty} \frac{D_r}{r!} \frac{\partial^r}{\partial D_1^r} \left[\frac{D_1^2}{(2n)!}\right]\right). \tag{A9}$$

We note further that

$$\Gamma(n+\tfrac{1}{2})/\Gamma\tfrac{1}{2} = (2n)!/2^{2n} n! \tag{A10}$$

and asymptotically

$$\Gamma(n+\tfrac{1}{2}, t_0^2) = t_0^{2n} e^{-t_0^2} [G_n(t_0)], \tag{A11}$$

$$G_n(t_0) = \sum_{m=0}^{M} \frac{\Gamma(1-n-\frac{1}{2}+m)}{\Gamma(\frac{1}{2}-n)} [t_0^{-2m} + O(t_0^{-2M})], \tag{A12}$$

and if C_2 is of order N, as is the case for normal systems, then if $\theta_0 = O(N^{-1/2-\eta})$ for $\eta > 0$, $\exp(-t_0^2)(-N\eta)]$, and for a macroscopic system; these do not contribute to the asymptotic expansion.

Combining (A10) and (A12) with (A9), we obtain

$$I(t_0) = \frac{1}{\sqrt{2\pi C_2}} e^{-\beta F_0} \exp\sum_3 \frac{D_r}{r!} \times \frac{\partial}{\partial D_1^r} \left(e^{-D_1^2/2} - e^{-t_0^2} \sum_{n=0}^{\infty} \frac{D_1^{2n}}{(2n)!} t_0^{2n} G_n(t_0)\right) \tag{A13}$$

and, going back to variables θ_0, C_n,

$$I(\theta_0) - \frac{e^{C_0}}{\sqrt{2C_2}} e^{D} \left(e^{-C_1^2/C_2} - e^{-C_2\theta^2/2} \sum \frac{(C_1\theta_0)^{2n}}{(2n)!} G_n(\theta_0)\right) \tag{A14}$$

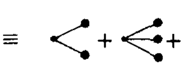
with

$$G_n(\theta_0) = \sum_{m=0} \frac{\Gamma(1-n-\frac{1}{2}+m)}{\Gamma(\frac{1}{2}-n)} \left(\frac{2}{C_2\theta_0}\right)^m + O\left[\left(\frac{C_2\theta_0^2}{2}\right)^{-m}\right]. \tag{A15}$$

Thus the results of (12) are verified asymptotically provided that $C_2\theta_0^2 = O(N^{\eta})$, i.e., $\theta_0 = O(N^{-1/2-\eta})$.

APPENDIX B: SUM OF CAYLEY TREE GRAPHS

(i) Summing insertions on a single vertx, we obtain the integral equation from the Cayley tree sum

• ≡  ··· , (B1)

thus on adding + —• — —• ,

$$\overline{C}_1 = C_1(u - \overline{C}_1/2) + \overline{C}_1 \tag{B2}$$

whence

$$C_1(u_0 - \overline{C}_1/C_2) = 0,$$

which has the solution

$$C_1(u_0') = 0, \quad u' = u_0 - \overline{C}_1/C_2 \tag{B3}$$

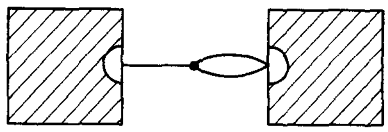


FIG. 4. A higher-order term in the evaluation of $m_2(r,t)$.

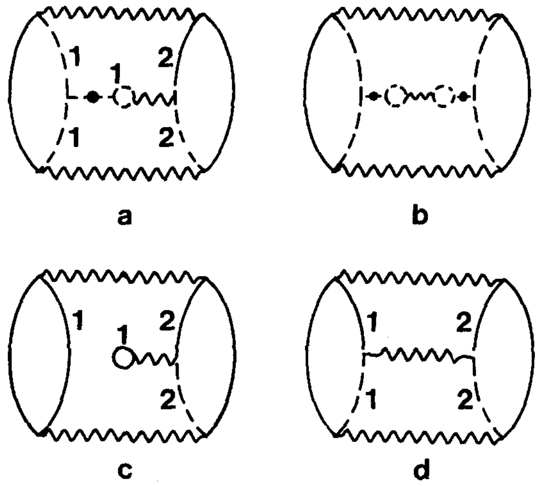


FIG. 5. An example of higher-order structure of the modified GCE graphs.

determining u_0', as the value for which

$$\langle\hat{N}\rangle = N \quad \text{and} \quad \overline{C}_1 = C_2(u_0 - u_0'). \tag{B4}$$

(ii) The addition of Cayley tree branches to any vertex produces the replacement at $\overline{C}_n$ by $C_n(u_0')$.

(iii) The sum of all Cayley tree graphs is given by

$$C_0(u_0') + \frac{C_1^2(u_0')}{C_2} - \frac{1}{2}\frac{C_1^2(u_0')}{C_2} - \frac{1}{2}\frac{C_1^2(u_0')}{C_2} = C_0(u_0');$$

The last term arises from the fact that the renormalization of a single vertex there is missing not only the single term •—•, but also the term •—•—• . The x vertices represent the same expression as the large dot but with the symmetry corresponding to the vertex distinguished.

Thus the net result is that the expansion no longer has Cayley tree graphs and that all vertices $C_r(u_0)$ are replaced by $C_r(u_0')$, $C_1(u_0') = 0$. The $\overline{C}_r$ play the role of dummy variables.

APPENDIX C: ILLUSTRATION OF SOME HIGHER ORDER CORRECTIONS, IN 1/N

Case 1: An example of a higher-order correction to $m_2(1,2)$. The contribution to $m_2(r,t)$ from Fig. 4 is

$$-m_2(r)\sum_s m_3(s)m_3(t)/(\sum m_2)^3. \tag{C1}$$

Case 2: A higher-order term in the rearranged GCE linked cluster expansion.

The term of Fig. 5a adds to the class bonds which close on the same hypervertex O—O an equal index correlation bond. The contribution of Fig. 5b is of the form of two disjoint graphs joined by a pair of equal index correlation bonds. Figure 5c indicates that self-energy type terms remain even when one has overlapping indices. Figure 5d represents an additional higher order modification of the bare hypervertex. Figures 5a-5d, of course, arise from the rearrangement.

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[1]Note that a variety of size dependent effects such as surface effects also appear in GCE, and these usually dominate over the differences between grand- and petit-canonical ensemble results except insofar as the thermodynamic constraints are involved, and these can be obtained to the same accuracy by Legendre transformation of the GCE results. Thus, for example, it is obvious that for the petit-canonical ensemble fluctuations in N are zero; while for the GCE they are not. On the other hand, a given thermodynamic function, such as compressibility, would be the same in the macroscopic limit in both ensembles.

[2]G. Horwitz, J. Math. Phys. **7**, 2261 (1966).

[3]R. Brout and F. Englert, Phys. Rev. **120**, 1519 (1960).

[4]G. Horwitz, F. Englert, and R. Brout, Phys. Rev. **130**, 409 (1963).

[5]De Coen, F. Englert, and R. Brout, Physica (Utr.) **30**, 1293 (1964).

[6]In a forthcoming paper we shall illustrate this in treating the pairing approximation for superfluid bosons as well as for superconductors, in which the advantage of this approach in setting up perturbation theory is manifest and an appropriate grouping of terms keeping self-energy and chemical potential corrections to the same order leads to a "well-defined" expansion, well-defined in the sense of restoring the order N character to the redefined linked cluster expansion.

[7]R. Balian, C. Bloch, and C. De Dominicis, Nucl. Phys. **25**, 529 (1961).

[8]See, for example, E. Schrödinger, *Statistical Thermodynamics* (Cambridge U.P., London, 1948).

[9]This is much more stringent a condition than is necessary. It would suffice to have a domain including a part of the positive real axis containing the saddle-point value, which being without poles or zeros is still large enough to attain asymptotic conditions for the expansion (cf. Appendix A). As mentioned to me by J. Lebowitz, the Lee and Yang[10] argument that a single phase region has no dense approach of zeros to the real axis does not guarantee that there cannot be isolated zeros approaching the real axis whose presence would break down the force of the above argument.

[10]C. N. Yang and T. D. Lee, Phys. Rev. **82**, 404 (1952); Phys. Rev. **87**, 410 (1952).

[11]Comparing with (20), $\mu_n[C_1] = (\partial^n/\partial\lambda^n)\ln e^D e^{\lambda C_1}$, but $\ln e^D e^{\lambda C_1} = \ln e^{(\lambda C_1 + \Sigma_3^\infty C_n\lambda^n/n!)} = \lambda C_1 + \Sigma_3^\infty(\lambda^n/n!)C_n$, $\mu_n[C_1] = C_n$.

[12]G. Horwitz and H. B. Callen, Phys. Rev. **114**, 1757 (1961).

[13]C. Bloch, in *Studies in Statistical Mechanics*, edited by J. De Boer and G. E. Uhlenbeck (North-Holland, Amsterdam, 1965), Vol. 3.

[14]We use the term macroscopic chemical potential corresponding to some Hamiltonian in the sense of the saddle-point value for the petit-canonical ensemble, which is identical with the grand-canonical chemical potential, but only equal to the canonical ensemble chemical potential in the macroscopic limit.

[15]L. Van Hove and N. M. Hugenholtz, Physica (Utr.) **29**, 363 (1958); N. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).

[16]In contrast to the Brout–Englert *et al.* approach, we have a graphical evaluation of the canonical ensemble multivariate cumulants the leading order evaluation being included in our Cayley tree correlation graphs. Thus, for example, $m_2(r,s) = \langle\hat{n}(s)\hat{n}(r)\rangle 0 - \langle\hat{n}(r)\rangle 0 \langle\hat{n}(s)\rangle 0$, which vanishes for the GCE and has the leading order contribution of order $1/N$ for the canonical ensemble $m_2(r,s) = m_2(r)\delta_{r,s} - m_2(r)m_2(s)/\Sigma_t m_2(t)$. Brout and Englert's evaluation of the $m_n(1,2,\ldots,n)$ is obtained by a method equivalent to saddle-point evaluation of the m_n and is correct only to the leading order in $1/N$ for normal systems. Furthermore, in more complicated cases, such as that of superfluid bosons, the procedure proves ambiguous.

[17]A summary of these methods can be found, for example, in the review of C. Bloch, in Ref. 13 and a general review of quantum statistical expansions, in *Quantum Field Theoretical Methods in Statistical Physics*, edited by A. A. Abrikosov, L. O. Gorkev, and I. Ye Dzaloshinskii (Pergamon, Oxford, 1965), 2nd ed.

[18]On summing the diagrams there is no difficulty with these quantities $G(r)$ and $G(r,s)$, etc. On linked diagrams the singular regions are

not reached and the net contribution of correlation diagrams at $T = 0$ is only dependent on $G(r)$ for r at the Fermi energy. However, a strict general handling of these quantities as a statistical Landau energy requires a regularization procedure since the functions become singular off the Fermi surface. De Dominicis and Balian have studied this matter in detail. See, for example, C. De Dominicis, CEA 1873 Saclay 1961 and R. Balian and C. De Dominicis, Ann. Phys. (N.Y.) **62,** 229 (1971).

Unstable particle scattering in the LSZ formalism

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The properties of the unstable particles are studied by investigating the Lee model and a modified form of it. We define the unstable particle to be the complex pole of the analytically continued Green's function on the unphysical Riemann sheet. The mass and lifetime of the unstable particles are determined. Different ways of calculating the renormalization constant are discussed. The Lehmann–Symanzik–Zimmermam (LSZ) formalism is extended to include the unstable particles. Decay and scattering amplitudes for the unstable particles are calculated. The formalism is exact and does not depend on the arbitrary separation of the total Hamiltonian. Comparison with results obtained by other methods is discussed.

I. INTRODUCTION

The main difficulty in dealing with the unstable particle problem is that the unstable particle has complex mass. For a Hermitian Hamiltonian, the eigenvalue has to be real. Therefore, it is impossible to find an eigenstate for the unstable particle. Without the concept of eigenstate, the usual definition of a particle can not be obtained. In order to overcome this difficulty, there have been various prescriptions[1-4] for constructing the "approximate" eigenstate for the unstable particles. Perturbation theory[4] is the one used in most applications. This approach depends crucially on the separation of the total Hamiltonian into the unperturbed part and the interaction part which is responsible for the decay. Viewing the fact that the majority of the particles in the physical world are actually unstable, it is desirable if we can have a formalism to describe the unstable particles without an arbitrary application of the Hamiltonian.

It is thus the purpose of this paper to illustrate the possibility of extending the LSZ formalism to include the unstable particles, both unstable elementary particles and unstable composite states. The formalism is exact and does not rely on an artificial separation of the total Hamiltonian. All the decay and scattering amplitudes of the unstable particles can be calculated.

We shall illustrate our extended LSZ formalism in two examples: (1) Unstable elementary V particle in a modified Lee model; (2) Unstable $(V\theta)$ composite state in the Lee model.

It is well known that there are three stable elementary particles in the Lee model,[5] namely V, N and θ particles. In addition, it was shown that a stable $(V\theta)$ composite state can occur for sufficiently large coupling constant g in the V-θ sector.[6] When the value of g is decreased less than some critical value g_B, this $(V\theta)$ composite state becomes unstable. This state serves as an excellent example for illustrating the LSZ formalism for unstable composite state.

An example of another type of the unstable particles, namely, the unstable elementary particle results from the addition of an extra repulsive four-point interaction between the N and θ particles to the regular Lee model. We can make the elementary V particle become unstable. This modified Lee model was suggested by R. B. Marr and Y. Shimamoto[7] and from now on we will refer to it as the Lee model II.

Due to the uncertainty principle,[8] the definition of an unstable particle is not unique. If we let m be the mass and Γ^{-1} be the lifetime (i.e., Γ is the width) of an unstable particle, then there will be an uncertainty in the definition of mass of the order $\Delta m \simeq \Gamma$. Furthermore, since the width Γ can be considered as a kind of mean square deviation from the average of a mass distribution, so there is also an uncertainty on Γ itself of the order $\Delta\Gamma \simeq \Gamma^2/m$. It is, therefore, clear that m and Γ can be defined to a good approximation only if Γ is very small, i.e., if the lifetime is very long.

Among different definitions which we will not go into detail here, the one we choose is to relate the unstable particle to be the complex pole of the analytically continued Green's function on the unphysical Riemann sheet. The real part of the pole is defined to be the "observed mass" of the unstable particle and imaginary part of the pole is related to the lifetime of the unstable particle. The determination of the renormalization constant will be discussed.

The outline of this paper is as follows. In Sec. II, the Lee model II is investigated for illustrating the properties of the unstable elementary V particle. The mass, lifetime, and the renormalization constant are determined. The asymptotic assumption and reduction formula for unstable particle are developed in Sec. III. The decay amplitude of the unstable V particle is calculated in Sec. IV. In Sec. V, the properties of the unstable $(V\theta)$ composite state in the Lee model is investigated. The extended LSZ formalism for the unstable composite state is illustrated in Sec. VI by calculating the decay amplitudes of the processes

$$(V\theta)_u \to V + \theta, \quad (V\theta)_u \to N + \theta + \theta,$$

and in Sec. VII by calculating the scattering amplitude for the process

$$(V\theta)_u + \theta \to (V\theta)_u + \theta.$$

Summary and conclusion follow in Sec. VIII.

II. THE LEE MODEL II; UNSTABLE ELEMENTARY V PARTICLE

The total renormalized Hamiltonian for the Lee model II can be written as

$$H = H_0 + H', \tag{1}$$

where

$$H_0 = Z' m_v' \psi_v^+ \psi_v + m_N \psi_N^+ \psi_N + \sum_k w_k a_k^+ a_k,$$

$$H' = g'\left(\psi_v^+\psi_N \sum_k \frac{u(w)}{(2w)^{1/2}}\, a_k + \psi_N^+ \sum_k \frac{u(w)}{(2w)^{1/2}}\, a_k \psi_v\right) + Z'\delta m_v' \psi_v^+\psi_v + G\psi_N^+\psi_N \sum_k \frac{u(w)}{(2w)^{1/2}}\, a_k^+ \sum_{k'} \frac{u(w')}{(2w')^{1/2}}\, a'_k,$$

$$w_k = (k^2 + \mu^2)^{1/2}, \tag{1'}$$

$G > 0$, is the coupling constant of the repulsive four-point interaction. The renormalization constant Z' and mass renormalization δm_v are to be determined. The renormalized coupling constant g' is defined to be $g'^2 = g_0^2 Z'$.

The two constant in the Lee Model[5], namely Q_1 and Q_2 defined as

$$Q_1 = Z'\psi_v^+\psi_v + \psi_N^+\psi_N, \qquad Q_2 = Z'\psi_v^+\psi_v + \sum_k a_k^+ a_k \tag{2}$$

are again the two constant in the Lee model II because

$$[Q_i, H] = 0, \qquad i = 1, 2. \tag{3}$$

The eigenvalues of the Q_i are denoted by q_i. Consequently, the Lee model II can also be decomposed into the isolated sectors.

We now consider the V-sector which is characterized by the four tau functions:

$$\tau^1(t) = \langle 0 \mid T(\psi_v(t)\psi_v^+(0)) \mid 0\rangle, \tag{4a}$$

$$\tau^2(t,w) = \langle 0 \mid T(\psi_N(t)a_k(t)\psi_v^+(0)) \mid 0\rangle \frac{(2w)^{1/2}}{u(w)}, \tag{4b}$$

$$\tau^3(t,w) = \langle 0 \mid T(\psi_v(t)\psi_N^+(0)a_k^+(0)) \mid 0\rangle \frac{(2w)^{1/2}}{u(w)}, \tag{4c}$$

$$\tau^4(t,w,w') = \frac{(4ww')^{1/2}}{u(w)u(w')} \langle 0 \mid T(\psi_N(t)a_k(t)\psi_N^+(0)a_k^+(0)) \mid 0\rangle. \tag{4d}$$

The Fourier transform of these tau functions can be shown to satisfy the following equations

$$(W - m_0)\hat\tau'(W) = \frac{1}{Z'} + \frac{g'}{Z'} \sum_k \frac{u^2(w)}{2w}\, \hat\tau^2(W,w), \tag{5a}$$

$$(W - m_N - w)\hat\tau^2(W,w) = g'\,\hat\tau^1(W) + G \sum_{k'} \frac{u^2(u')}{2w'}\, \hat\tau^2(W,w'), \tag{5b}$$

$$(W - m_N - w)\hat\tau^3(W,w) = g'\tau^1(W) + G \sum_{k'} \frac{u^2(w')}{2w'}\, \hat\tau^3(W,w'), \tag{5c}$$

and

$$(W - m_N - w)\hat\tau^4(W,w,w') = \frac{2w}{u^2(w)}\,\delta_{kk'} + g'\hat\tau^3(W,w') + G \sum_{k''} \frac{u^2(w'')}{2w''}\, \hat\tau^4(W,w'',w'). \tag{5d}$$

From Eqs. (5a) and (5b), $\tau'(W)$ can be solved to be

$$\hat\tau'(W) = \left(1 + \frac{G}{4\pi^2}\int_\mu^\infty \frac{dw\,u^2(w)(w^2-\mu^2)^{1/2}}{(m_N + w - W - i\epsilon)}\right)\Big/\left(Z'L(W + i\epsilon)\right)^{-1}, \tag{6}$$

where

$$L(W + i\epsilon) = [g_0^2 + G(W - m_0) \times [P_1(W) - P_2(W)], \tag{7a}$$

$$P_1(W) = \frac{1}{4\pi^2}\int_\mu^\infty \frac{dw\,u^2(w)(w^2-\mu^2)^{1/2}}{(m_N + w - W - i\epsilon)}, \tag{7b}$$

$$P_2(W) = \frac{m_0 - W}{g_0^2 + G(W - m_0)}, \tag{7c}$$

and

$$\tau^2(W,w) = \tau^3(W,w) = g'\hat\tau'(W)(W - m_N - w + i\epsilon)^{-1} \times \left(1 + \frac{G}{4\pi^2}\int_\mu^\infty \frac{dw'u^2(w')(u'^2-\mu^2)^{1/2}}{(m_N + w' - W - i\epsilon)}\right)^{-1}. \tag{8}$$

Similarly, $\hat\tau^4(W,w,w')$ can be solved to give

$$\hat\tau^4(W,w,w') = \frac{2w\delta_{kk'}}{u^2(w)(W - m_N - w)} + \frac{1}{(W - m_N - w')(W - m_N - w)} \times \left[G + g'^2\hat\tau'(W)\Big/\left(1 + \frac{G}{4\pi^2} \times \int_\mu^\infty dw_1 \frac{u^2(w_1)(w_1^2 - u^2)^{1/2}}{m_N + w_1 - W - i\epsilon}\right)\right] \times \left(1 + G\int_\mu^\infty \frac{dw''u(w'')(w''^2-\mu^2)^{1/2}}{4\pi^2(m_N + w'' - W - i\epsilon)}\right)^{-1}. \tag{9}$$

Now we investigate the analytic properties of the function $L(W + i\epsilon)$ defined in Eq. (7a). It is obvious that when $W < m_N + \mu$, $L(W + i\epsilon)$ is a real analytic function. There can be only one zero of $L(W)$ which corresponds to a physical stable V particle (c.f. Fig. 1). This zero reduces to that of the original Lee model in the limit of $G \to 0$. As $G \to \infty$, the zero moves toward the value of the bare mass m_0. For sufficiently large $(m_0 - m_N)$, $L(W)$ will no longer have any zero below the threshold $m_N + \mu$ (c.f. Fig. 2). In other words, by choosing the parameters properly, we will not have a stable V particle in the Lee model II.

In the physical region, i.e., $W > m_N + \mu$, we get from Eq. (7a) that

$$\operatorname{Im} L(W + i\epsilon) = [g_0^2 + G(W - m_0)]\,\frac{u^2(W - m_N)}{4\pi} \times [(W - m_N)^2 - \mu^2]^{1/2}, \tag{10}$$

which will not vanish for any value of W. Hence, $L(W)$ cannot vanish in the entire physical region.

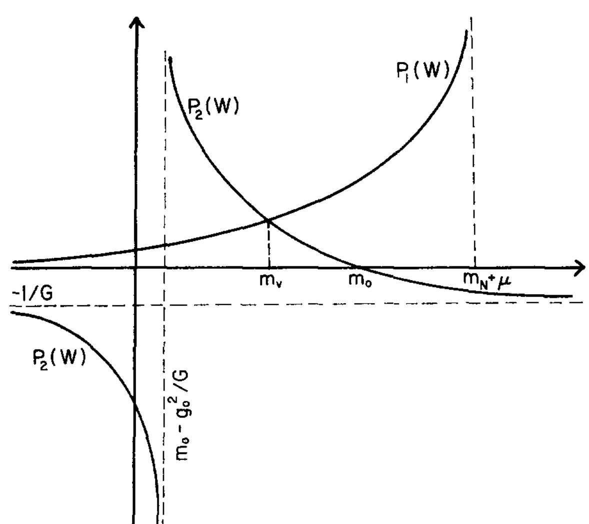

FIG. 1. Graphs for functions $P_1(W)$ and $P_2(W)$ with $m_0 < m_N + \mu$.

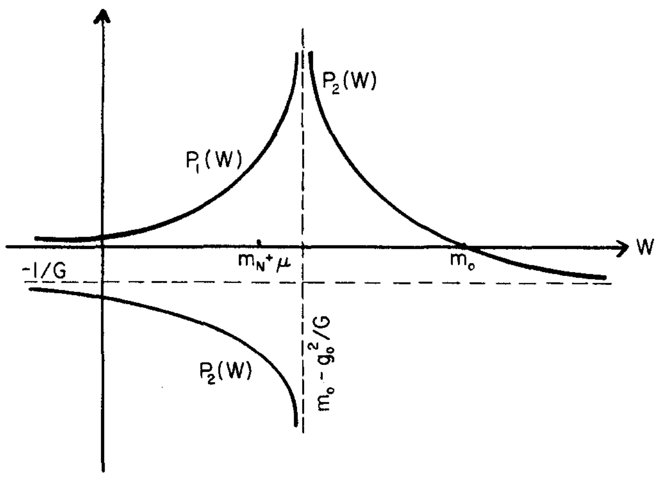

FIG. 2. Graphs for functions $P_1(W)$ and $P_2(W)$ with $m_0 > m_N + \mu$.

With the above analysis, we see that by properly choosing the parameters, $\hat{\tau}^1(W)$ will not have any pole in the entire physical sheet.

Let us analytically continue the Green's function $\hat{\tau}^1(W)$ in Eq. (6) onto the second Riemann sheet and define

$$L^{\text{II}}(Z) = L(Z) + 2i \operatorname{Im} L(Z). \tag{11}$$

We now define the unstable elementary V particle to be the complex pole of the Green's function $\hat{\tau}^1(W)$ on the second Riemann sheet. By Eq. (11) this means a complex zero of $L^{\text{II}}(z)$ at $z = M_v$:

$$L^{\text{II}}(M_v) = 0, \tag{12}$$

where

$$M_v \equiv m'_v - i\Gamma/2Z'. \tag{12'}$$

M_v will be referred to as the complex mass of the unstable elementary V particle. The real part m'_v is defined to be the "observed" mass and the imaginary part Γ is defined to be the width (inverse of the lifetime) of this unstable V particle.

m'_v and Γ can be solved exactly by substituting Eqs. (6), (10), and (11) into Eq. (12a). In the case that $\Gamma/Z' \ll m'_v - m_N$, the results of m'_v and Γ are

$$m'_v = m_0 - \left(\frac{g_0^2}{4\pi^2} P \int_\mu^\infty \frac{dw u^2(w)(w^2-\mu^2)^{1/2}}{(m_N + w - m'_v)} \Big/ - \frac{G\Gamma}{8\pi Z'}[(m'_v - m_N)^2 - \mu^2]^{1/2} u^2(m'_v - m_N)\right) \Big/ \left(1 + GP \int_\mu^\infty \frac{dw u^2(u)(w^2-\mu^2)^{1/2}}{(m_N + w - m'_v)}\right)^{-1} \tag{13}$$

and

$$\Gamma = \left(Z'[g_0^2 + G(m'_v - m_N)][(m'_v - m_N)^2 - \mu^2]^{1/2} u^2(m'_v - m_N)\right) \Big/ \left(1 + \frac{G}{4\pi^2} P \int_\mu^\infty \frac{dw u^2(w)(w^2-\mu^2)^{1/2}}{(m_N + w - m'_v)}\right)^{-1}, \tag{14}$$

where P denotes the principal value of the integral. The mass renormalization $\delta m'_v$ is

$$\delta m'_v \equiv m_0 - m'_v. \tag{15}$$

If the coupling constant G is very small, then to the first order in G, Eq. (14) becomes

$$\Gamma = \frac{g'^2}{2\pi}[(m'_v - m_N)^2 - \mu^2]^{1/2} u^2(m'_v - m_N) \times \left(1 - \frac{G}{2\pi^2} P \int_\mu^\infty \frac{dw u^2(w)(w^2-\mu^2)^{1/2}}{(m_N + w - m'_v)}\right). \tag{16}$$

The determination of the renormalization constant Z' for the unstable particle is ambiguous. Numerous prescriptions[9] have been given in the literature. In the stable case, the renormalization constant Z represents the probability of finding a bare V particle in the physical V particle state. There are two equivalent ways of determining Z

$$\operatorname*{Res}_{W=m_v} \hat{\tau}^1(W) = 1, \tag{17a}$$

$$\langle\langle N | j | V \rangle\rangle = \langle N | j_0 | V \rangle, \tag{17b}$$

where j is the renormalized current of the θ field

$$j = j_0 Z^{1/2} = g(\psi_N^+ \psi_v + \text{h.c.}). \tag{18}$$

Since we do not have an eigenstate for unstable particles, the renormalization constant can no longer be interpreted as the "probability". By analogy with the stable case, we list three ways of determining the renormalization constant Z' for the unstable V particle.[8]

(i) $$\operatorname*{Res}_{W=M_v} [\hat{\tau}^1(W)]^{\text{II}} = 1, \tag{19}$$

where

$$[\hat{\tau}^1(W)]^{\text{II}} = \hat{\tau}^1(W) + 2i \operatorname{Im} \hat{\tau}^1(W). \tag{20}$$

This would lead to a complex value for Z' which implies the fields ψ_v and ψ_v^* are not Hermitically conjugate.

(ii) $$\left| \operatorname*{Res}_{W=M_v} [\hat{\tau}^1(W)]^{\text{II}} \right| = 1. \tag{21}$$

Z' determined by this condition can be a real quantity.

(iii) $$\left| \operatorname*{Res}_{W=m'_v} \hat{\tau}^1(W) \right| = 1. \tag{22}$$

III. ASYMPTOTIC CONDITION AND REDUCTION FORMULA FOR UNSTABLE STATE

Let us now discuss the asymptotic condition for the unstable V particle in the Lee model II. The in and out states are defined at time $t \to \pm\infty$. Since an unstable particle will decay in a finite time, there can exist no in and out states associated with an unstable particle. We must modify our asymptotic assumption to allow for this property. The extension of the asymptotic condition to unstable particle can be constructed by a slight modification of the stable case. It was shown[10] in the stable case that the physics remains the same no matter whether we use the field $\psi_v(t)$ or $\psi_N(t) \int d^3k\, a_k(t)$ or linear combination of them as the interpolating field for the stable V particle. In other words, a physical particle can be described by various interpolating fields as long as they have the correct quantum numbers. Now in the Lee model II, the most general local field operator for the unstable V particle with quantum numbers $q_1 = 1$, $q_2 = 1$ can be written as

$$B_0^v(t) = A\psi_v(t) + C\psi_N(t) \int d^3k\, a_k(t), \tag{23}$$

where A and C are c-numbers.

We no longer associated the unstable V particle with the field $\psi_v(t)$, but together with the field $\psi_N(t) \int d^3k\, a_k(t)$ as we did in the stable case. By analogy to the stable case, we assume the following asymptotic condition for the unstable V particle:

$$\lim_{t\to\mp T} \langle\langle \beta \mid e^{-iM_v t} B_0^{v+}(t) \mid \alpha\rangle\rangle = (Z^{v*}_u)^{1/2} \langle\langle \beta \mid B^{v+}_{u_{\substack{\text{in}\\ \text{out}}}} \mid \alpha\rangle\rangle, \tag{24}$$

where

$$M_v = m_v' - i\Gamma/2Z'$$

is the complex mass of the unstable V particle determined by the position of pole on the complex plane. We relate the in and out fields that characterize the unstable V particle with the field operator $B_0^v(t)$ at time t becoming a very large value T. Notice that as $T \to \pm\infty$, $e^{-iM_vT} \to {0 \atop \infty}$; the in and out fields become meaningless. This is expected because we know that the unstable particles do not exist in the infinite past or future.

The other notations in the assumption (24) are standard: $\langle\langle\, \alpha \mid$ and $\langle\langle\, \beta \mid$ are arbitrary physical states, Z^v_u is the renormalization constant such that the renormalized field operator $B^v_u(t)$ is defined as

$$B^v_u(t) = B^v_0(t)/(Z^v_u)^{1/2}. \tag{25}$$

The value of Z^v_u will be determined later.

An unstable V particle is created by operating with the in-field operator B^{v+}_{in}.

The asymptotic conditions for the fields $\psi_N(t)$ and $a_k(t)$ are assumed to be[11]

$$\lim_{t\to\mp T} \langle\langle \beta \mid e^{-im_N t} \psi^+_N(t) \mid \alpha\rangle\rangle = \langle\langle \beta \mid \psi^+_{N_{\substack{\text{in}\\ \text{out}}}} \mid \alpha\rangle\rangle \tag{26}$$

and

$$\lim_{t\to\mp T} \sum_{k'} f(w',w)\, e^{-iw't} \langle\langle \beta \mid a^+_{k'}(t) \mid \alpha\rangle\rangle = \langle\langle \beta \mid a^+_{k_{\substack{\text{in}\\ \text{out}}}} \mid \alpha\rangle\rangle, \tag{27}$$

where $f(w',w)$ is a good function of w' centered about the point $w' = w$ satisfying the condition

$$\sum_{k''} f^*(w'',w) f(w'',w') = \begin{cases} 0 & \text{as} \quad k \neq k' \\ 1 & \phantom{\text{as}} \quad k = k'. \end{cases} \tag{27'}$$

We can extend T to $\pm\infty$ without causing any trouble because mass m_N and energy w are real quantities. However, for the convenience in deriving the reduction formulation, we will keep the conditions as written in Eq. (26) and (27).

Consider the matrix element

$$S_{\alpha\beta} \equiv \langle\langle \beta\,;\, m_{\text{out}} \mid \alpha\,;\, n_m \rangle\rangle, \tag{28}$$

where α, β, represent the N particle or the unstable V particle. m, n represent the number of the θ particles in the incoming and outgoing states, respectively.

With the LSZ asymptotic assumptions in Eqs. (24), (26) and (27), the reduction formula can be derived, in an analogous way to the stable case in the Lee model, to be[11]

$$S_{\alpha\beta} = \delta_{mn}\delta_{\alpha\beta} + \frac{1}{(n\,!\,m\,!)^{1/2}} \int_{-T}^{T}\!\!\int dt\, dt' \exp\Big[i\Big(m_\beta + \sum_{j=1}^{m} w_j\Big)t'\Big] \times \overrightarrow{\Big(i\frac{d}{dt'} - m_\beta - \sum_{j=1}^{m} w_j\Big)}\, \tau_{\alpha\beta}(t',t)\, \overleftarrow{\Big(i\frac{d}{dt} + m_\alpha + \sum_{i=1}^{n} w_i\Big)}$$

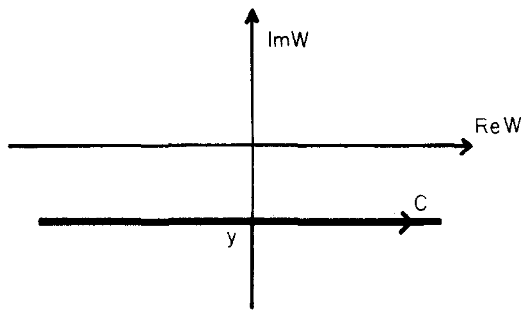

FIG. 3. The contour C.

$$\times \exp\Big[-i\Big(m_\alpha + \sum_{i=1}^{n} w_i\Big)t\Big], \tag{29}$$

where

$$\tau_{\alpha\beta}(t',t) \equiv \langle 0 \mid T(\psi_\beta(t') \prod_{j=1}^{m} a_{k_j}(t')\, \psi^+_\alpha(t) \prod_{i=1}^{n} a^+_{k_i}(t)) \mid 0\rangle. \tag{29'}$$

Because of the asymptotic condition for the unstable V particle assumed in Eq. (24), the complex mass M_v enters in the reduction formula whenever an unstable V particle is involved. For proceeding the calculation, an extended definition of the delta function with complex argument needs to be made. This can be done by considering the following integral

$$I \equiv \frac{1}{2\pi} \int_-^+ dW f(W) \int_-^+ dt\, e^{i(W-z)t}, \tag{30}$$

where $z = x - iy$ is a complex number and $f(W)$ is an analytic function or has singularities only along the real axis.

Assuming the order of integration in Eq. (30) can be interchanged, we get

$$I = \frac{1}{2\pi} \int_-^+ dt \int_-^+ dW f(W)\, e^{i(W-z)t}. \tag{31}$$

Using the analytic properties assumed for the function $f(W)$, we can lower the region of integration to the contour C (cf. Fig. 3) which runs from $W = -\infty - iy$ to $W = \infty - iy\,(y > 0)$. Equation (31) becomes

$$I = \frac{1}{2\pi} \int_-^+ dt \int_C dW f(W)\, e^{i(W-z)t}. \tag{32}$$

Define a new real variable E such that

$$E \equiv W + iy, \qquad dE = dW, \tag{33}$$

then

$$I = \frac{1}{2\pi} \int_-^+ dt \int_-^+ f(E - iy)\, e^{i(E-x)t}\, dE. \tag{34}$$

Interchanging the order of integration again, we get

$$I = \int_-^+ dE f(E - iy) \frac{1}{2\pi} \int_-^+ dt\, e^{i(E-x)t}. \tag{35}$$

Notice that

$$\frac{1}{2\pi} \int_-^+ dt\, e^{i(E-x)} \equiv \delta(E - x), \tag{36}$$

which is the regular definition of a Dirac delta function. Therefore,

$$I = f(z). \tag{37}$$

From Eqs. (30) and (37) we see that it is reasonable to define an extended delta function with complex argument as following

$$\delta(W-z) \equiv \frac{1}{2\pi} \int_-^+ dt\, e^{i(W-z)t} \tag{38a}$$

and

$$\int_-^+ dW f(W-Z) = f(Z) \tag{38b}$$

for an analytic function $f(W)$.

Nakanishi[3] discussed complex delta function with similar ideas but different method.

Using the reduction formula in Eq. (29) together with the definition of extended delta function in Eq. (38), we can calculate the various matrix elements for both decay and scattering processes.

We will now determine the renormalization constant Z_u^v defined in Eq. (25). Consider the following unstable V particle propagator

$$\hat{\tau}_u^v(W) = -i \int_{-\infty}^{\infty} dt\, e^{iWt} \langle 0 \mid T(B_u^v(t) B_u^{v+}(0)) \mid 0 \rangle. \tag{39}$$

Substituting Eqs. (23) and (25) into (39) and using Eq. (4), we get

$$\hat{\tau}_u^v(W) = \frac{1}{|Z_u^v|} \times \left(AA^+ \hat{\tau}'(W) + (AC^+ + A^+C) \int d^3k \frac{u(w)}{(2w)^{1/2}} \hat{\tau}^2(W,w) + CC^+ \int d^3k d^3k' \frac{u(w)u(w')}{(4ww')^{1/2}} \hat{\tau}^4(W,w,w') \right). \tag{40}$$

We have discussed several ways to determine the renormalization constant Z' for the field ψ_v. From among these we will now pick the condition in Eq. (21), namely,

$$\left| \operatorname*{Res}_{W=M_v} [\hat{\tau}^1(W)]^{\text{II}} \right| = 1 \tag{21}$$

and

$$\left| \operatorname*{Res}_{W=M_v} [\hat{\tau}_u^v(W)]^{\text{II}} \right| = 1. \tag{41}$$

The methods of analytical continuing the tau function in Eq. (40) are not unique. Since the higher tau functions can always be written in terms of the lower ones (c.f. Eqs. (8), and (9)], we will now analytically continue only the lowest tau function involved, i.e., $\hat{\tau}^1(W)$, for the continuation of $\hat{\tau}_u^v(W)$. Using Eq. (8) and (9) together with conditions in (21) and (41), Z_u^v can be determined to be

$$(Z_u^v)^{1/2} = \left| A + Cg' \int d^3k \frac{u(w)}{(2w)^{1/2}(M_v - m_N - w)} \times \left(1 + G \int \frac{d^3k' u^2(w')}{(2w')(m_N + w' - M_v)}\right)^{-1} \right| \tag{42}$$

for arbitrary real c-numbers A and C.

IV. EXTENDED LSZ FORMALISM FOR THE UNSTABLE V PARTICLE DECAY

By using the reduction in Eq. (29), the matrix element for the decay process

$$V_u \to N + \theta_k$$

can be written as

$$S_d = \int_{-T}^{T} \int dt\, dt'\, e^{i(m_N+w)t'} \overrightarrow{\left(i\frac{d}{dt'} - m_N - w\right)} \times \langle 0 \mid T(\psi_N(t') a_k(t') B_u^{v+}(t)) \mid 0 \rangle \overleftarrow{\left(i\frac{d}{dt} + M_v\right)} e^{-iM_v t}. \tag{43}$$

We have defined the unstable particle to be the complex pole of the analytically continued Green's function on the unphysical sheet. Therefore, we first analytically continue the matrix element as functions of the variable W onto the unphysical sheet, and then evaluate them on the energy shell. Among many ways of analytical continuing the tau functions, we again choose to analytically continue only the lowest tau function, i.e., $\hat{\tau}^1(W)$. With the help of Eqs. (4), (8), (9), (23), (25) and (38), Eq. (43) becomes

$$S_d = \frac{2\pi}{(Z_u^v)^{1/2}} \delta(M_v - m_N - w) \times \frac{u(w)}{(2w)^{1/2}} \{(W - M_v)[\hat{\tau}^1(W)]^{\text{II}}\}_{W=M_v} \times \left[A + C\frac{g'}{4\pi^2} \int_\mu^\infty \frac{dw'(w'^2-\mu^2)^{1/2} u^2(w')}{(M_v - m_N - w')} \times \left(1 + \frac{G}{4\pi^2} \int_\mu^\infty \frac{dw'' u^2(w'')(w''^2-\mu^2)^{1/2}}{(m_N + w'' - M_v)}\right)^{-1}\right] \times g' \left(1 + \frac{G}{4\pi^2} \int_\mu^\infty \frac{dw''' u^2(w''')(w'''^2-\mu^2)^{1/2}}{(m_N + w''' - M_v)}\right)^{-1}. \tag{44}$$

From this decay matrix element, we can calculate the total probability per unit time, of the unstable elementary V particle decaying into the continuum $|N\theta_k\rangle\rangle$ for all momentum $\mathbf{k}$, which by uncertainty principle is the width of the decay.

Because the extended delta function with complex argument appeared in Eq. (44), we will now modify slightly the conventional formula for calculating the width of the decay as follows:

$$E = \left| \int_{\text{all } k} \frac{S_d^2}{T} \times \frac{d^3k}{(2\pi)^3} \right|, \tag{45}$$

where T is a period of time and $d^3k/(2\pi)^3$ is the phase volume factor.

Notice that

$$[2\pi\delta(M_v - m_N - w)]^2 = 4\pi^2 \delta(0)\delta(M_v - m_N - w) = 2\pi T \delta(M_v - m_N - w) \tag{46}$$

$$\because \delta(0) \underset{T\to\text{large}}{=\!=\!=} \frac{1}{2\pi} \int_{-T/2}^{T/2} dt = \frac{T}{2\pi}. \tag{46'}$$

Substituting Eqs. (44) and (46) into (45), the width of the decay can be calculated to be

$$E = g'^2 \mid u^2(M_v - m_N) [(M_v - m_N)^2 - \mu^2]^{1/2} \mid \Big/ \left(2\pi \left| 1 + \frac{G}{4\pi^2} \int_\mu^\infty \frac{dw u^2(w)(w^2-\mu^2)^{1/2}}{(m_N + w - M_v)} \right|^2\right)^{-1} \tag{47}$$

which is independent of the form of the field operator for the unstable V particle. The same result occurred for all S-matrices in the stable case of the Lee model.[10,12,13,14]

If the complex part of the mass of the unstable elementary particle can be neglected, then to the first order in the four-point coupling G, Eq. (47) becomes

$$E = \frac{g'^2}{2\pi} u^2(m_v' - m_N)[(m_v' - m_N)^2 - \mu^2]^{1/2} \times \left(1 - \frac{G}{2\pi^2} P \int_\mu^\infty \frac{dw u^2(w)(w^2-\mu^2)^{1/2}}{(m_N + w - m_v')}\right). \tag{48}$$

This is the result for width Γ obtained in Eq. (16) under this same approximation. Recall that width Γ was defined to be the complex part of the pole of the analytically continued Green's function $\hat{\tau}^1(W)$ on the unphysical Riemann sheet. From Eqs. (16) and (48) we see now that the decay width E calculated by our LSZ formalism agrees with the width determined by the complex pole of the Green's function when the complex part of the mass of the unstable elementary V particle is neglected. They differ from each other in the higher order terms which is expected from the uncertainty principle explained in Sec. I.

By using the reduction formula and definition of the extended delta function, the S matrix for all the unstable V particle scattering processes can be obtained.

V. UNSTABLE ($V\theta$) COMPOSITE STATE

First, let us review some results related to the ($V\theta$) bound state in the Lee model. The S matrix for the elastic scattering process

$$V + \theta_k \rightarrow V + \theta_{k'}$$

in the Lee model is[6]

$$S^{V\theta}_{kk'} = \delta_{kk'} + 2\pi i\, \delta(w - w')\, \frac{u^2(w)}{2w}\, g^2 \times \frac{1 + h(w)A(w)}{h(w)[1 - h(w)A(w)]}, \tag{49}$$

where

$$h(w) \equiv w[1 - \beta(w)] \equiv w\left(1 + \frac{g^2}{4\pi^2} \int_\mu^\infty \frac{dw' u^2(w')(w'^2 - \mu^2)^{1/2}}{w'^2(w' - w - i\epsilon}\right) \tag{50}$$

and

$$A(w) \equiv -\frac{1}{\pi} \int_\mu^\infty dw'\, \mathrm{Im}\left(\frac{1}{1 - \beta(w')}\right) \times \frac{1}{w'(w' - w)\{1 - \beta(w - w')\}}. \tag{51}$$

For simplification, we assume $m_v = m_n = m$.

It was shown that $D(w)$ defined as

$$D(w) \equiv 1 - h(w)A(w) \tag{52}$$

has a real zero w_B below the threshold μ for sufficiently large coupling constant g.[6] The zero corresponds to a stable ($V\theta$) bound state with total energy $m_B = m + w_B$.

The condition on the coupling constant g for having a ($V\theta$) bound state is

$$g^2 > g_B^2 \equiv \left(\frac{\mu}{4\pi^2} \int_\mu^\infty \frac{dw'(w'^2 - \mu^2)^{1/2} u^2(w')}{w'^2(w' - \mu)}\right)^{-1} \tag{53}$$

If the condition in Eq. (53) is not fulfilled, i.e., if $g < g_B$, then $D(w)$ will not have any zero for $w < \mu$. As $w > \mu$, write

$$D(w) = h(w)\{[1/h(w)] - A(w)\}. \tag{54}$$

From Eqs. (50) and (51), we can get

$$\mathrm{Im}[h(w)]^{-1} = \left[-\frac{g^2}{4\pi}\, u^2(w)(w^2 - \mu^2)^{1/2}\right] \Big/ |h(w)|^2 \tag{55}$$

and

$$\mathrm{Im}A(w) = \frac{1}{\pi} \int_\mu^{w-\mu} dw'\, \mathrm{Im}\left(\frac{1}{1 - \beta(w')}\right) \times \frac{\mathrm{Im}[1 - \beta(w - w')]}{w'(w' - w)\,|1 - \beta(w - w')|^2}. \tag{56}$$

From Eqs. (55) and (56), we see that $D(w)$ has a nonvanishing imaginary part for $w > \mu$. Therefore, as $g > g_B$, the function $D(w)$ does not have any zeros in the entire physical sheet for all w.

In summary: (1) As we decrease the coupling constant g such that $g < g_B$, $S^{V\theta}_{kk'}$ will not have any real pole below the threshold; (2) $S^{V\theta}_{kk'}$ does not have any pole in the entire physical region.

In field theory, the S-matrix can always be calculated in terms of the Green's functions. Defining an unstable particle to be complex pole of the analytically continued Green's function is then equivalent to defining it to be complex pole of the analytically continued S-matrix on the unphysical Riemann sheet.

We now analytically continue the S-matrix $S^{V\theta}_{kk'}$ for the $V + \theta$ elastic scattering onto the unphysical sheet. First, we rewrite $S^{V\theta}_{kk'}$ in the following form

$$S^{V\theta}_{kk'} = \delta_{kk'} + 2\pi i\, \delta(w - w')\, \frac{u^2(w)}{2w}\, g^2 \times \left[w\left(\frac{2}{1 + wC(w)} - 1 + \beta(w)\right)\right]^{-1} \tag{57}$$

where $C(w)$ is defined as

$$C(w) \equiv -\int_{C_1} \frac{dZ}{[1 - \beta(Z)]} \times \frac{\beta(w - Z)}{Z(w - Z)[1 - \beta(w - Z)]}. \tag{58}$$

The contour C_1 is shown in Fig. 4.

The method of analytical continuation of the function $C(w)$ to the unphysical sheets is not unique.[15] Here, we arbitrarily choose to expand $C(w)$ into a Taylor series about the point $w = \mu$ and neglect higher order terms

$$C(w) = C(\mu) + (w - \mu)\, C'(\mu). \tag{59}$$

$C(\mu)$ and $C'(\mu)$ can be calculated by contour integration which gives

$$C(\mu) = \beta(\mu)/h(\mu) \tag{60}$$

and

$$C'(\mu) = \frac{\beta(\mu)}{\mu h(\mu)} - \left(\frac{g^2}{4\pi^2} \int_\mu^\infty \frac{dw' u^2(w')(w'^2 - \mu^2)^{1/2}}{w'(w' - \mu)^2} \Big/ h(\mu)[1 - \beta(\mu)]\right). \tag{61}$$

We can now analytically continue the S-matrix $S^{V\theta}_{kk'}$ in Eq. (57) onto the second Riemann sheet as

$$(S^{V\theta}_{kk'})^{\mathrm{II}} = \delta_{kk'} - 2\pi i\, \delta(w - w') g^2\, \frac{u^2(w)}{2w^2} \times \left[1 - \beta^{\mathrm{II}}(w) - \frac{2}{1 + w(C(\mu) + (w - \mu)C'(\mu))}\right]^{-1}, \tag{62}$$

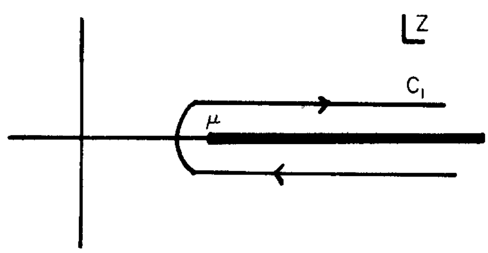

FIG. 4. The contour C_1.

where

$$1-\beta^{\mathrm{II}}(w)=1-\beta(w)+2i\,\mathrm{Im}[1-\beta(w)]. \qquad (63)$$

We now define the unstable $(V\theta)$ bound state to be the complex pole of Eq. (62) at

$$z_0=w'_B-i\Gamma B/2. \qquad (64)$$

If we denote the complex mass of this unstable $(V\theta)$ bound state to be M_B, then

$$M_B=m+z_0=m'_B-i\Gamma B/2, \qquad (65)$$

where

$$m'_B\equiv m+w'_B \qquad (66)$$

is the "observed" mass of this unstable $(V\theta)$ bound state, Γ_B is the inverse of the lifetime of this unstable $(V\theta)$ bound state.

The value of m'_B and Γ_B are determined by the real and imaginary parts of the following equation

$$1-\beta^{\mathrm{II}}(z_0)-2\{1+z_0[C(\mu)+(z_0-\mu)C'(\mu)]\}^{-1}=0. \qquad (67)$$

VI. DECAYS OF THE UNSTABLE $(V\theta)$ COMPOSITE STATE

In this section, we will calculate the decay amplitudes for the unstable $(V\theta)$ composite state by the extended LSZ formalism constructed in Sec. III.

The most general local interpolating field operator for the unstable $(V\theta)$ composite state with quantum numbers $q_1=1$, $q_2=2$ can be written as

$$B_0^{V\theta}(t)=A'\psi_v(t)\int d^3k\,a_k(t)+C'\psi_N(t)\iint d^3k_1d^3k_2a_{k_1}(t)\,a_{k_2}(t), \qquad (68)$$

where A' and C' are real c-numbers.

The renormalized field operator $B_u^{V\theta}(t)$ is defined to be

$$B_u^{V\theta}(t)=B_0^{V\theta}(t)/(Z_u^{V\theta})^{1/2}, \qquad (69)$$

where $Z_u^{V\theta}$ is the renormalization constant which can be determined by calculating the following unstable $(V\theta)$ composite state propagator

$$\hat{\tau}_u^{V\theta}(W)=-i\int_{-\infty}^{\infty}dt\,e^{iWt}\langle 0\,|\,T(B_u^{V\theta}(t)B_u^{V\theta+}(0))\,|\,0\rangle. \qquad (70)$$

Substituting Eqs. (68) and (69) into Eq. (70), we can express $\hat{\tau}_u^{V\theta}(W)$ in terms of the tau functions defined in Eqs. (A1).

Analogous to the unstable elementary V particle case, we require the following condition

$$\left|\operatorname*{Res}_{W=M_B}[\hat{\tau}_u^{V\theta}(W)]^{\mathrm{II}}\right|=1. \qquad (71)$$

As we said once previously, there are many ways to continue the propagator $\hat{\tau}_u^{V\theta}(W)$ onto the unphysical Riemann sheet. Same as before, we will not analytically continue only the lowest tau function $\hat{\tau}^5$ as a function of the variable W onto the unphysical sheet. By using the Eqs. (A2-A4) and (71), $Z_u^{V\theta}$ can be determined to be

$$(Z_u^{V\theta})^{1/2}=\left|\int\frac{d^3k u(w)F(M_B,w)}{(2w)^{1/2}(M_B-m-w)}\times\left(A'+2gc'\int\frac{d^3k'u(w')}{(2w')^{1/2}(M_B-m-w-w')}\right)\right|, \qquad (72)$$

where (c.f. Eq. A5)

$$\operatorname*{Res}_{W=M_B}[\hat{\tau}^5(W,w,w')]^{\mathrm{II}}\equiv\frac{F(M_B,w)F(M_B,w')}{(M_B-m-w)(M_B-m-w')}. \qquad (73)$$

The asymptotic condition for the unstable $(V\theta)$ composite state operator $B_u^{V\theta}(t)$ is assumed to be

$$\lim_{t\to\mp T}\langle\langle\beta\,|\,e^{-iM_Bt}B_u^{V\theta+}(t)\,|\,\alpha\rangle\rangle=\langle\langle\beta\,|\,B_{u_{\substack{\mathrm{in}\\ \mathrm{out}}}}^{V\theta+}\,|\,\alpha\rangle\rangle. \qquad (74)$$

The in and out fields are related to the Heisenberg field $B_u^{V\theta}(t)$ at time $t=\pm T$ where T is some very large value. An unstable $(V\theta)$ composite state is created by operating with the in field operator $B_{u_{\mathrm{in}}}^{V\theta+}$.

We are now going to calculate the decay amplitudes for the following two processes:

(a) $(V\theta)_u\to V+\theta_k$,

(b) $(V\theta)_u\to N+\theta_k+\theta_{k'}$.

Case (a)

$$(V\theta)_u\to V+\theta_k.$$

By using the asymptotic conditions and the reduction formula, the decay matrix element can be written as

$$S_d^{(a)}=\frac{1}{(Z_vZ_u^{V\theta*})^{1/2}}\int_{-T}^{T}\int dtdt'\,e^{i(m+w)t}\left(i\frac{\overrightarrow{d}}{dt'}-m-w\right)\times\langle 0\,|\,T(B_0^V(t)\,a_k(t)B_0^{V\theta+}(0))\,|\,0\rangle\left(i\frac{d}{dt'}+M_B\right)e^{-iM_Bt'}, \qquad (75)$$

where Z_v is defined in Eq. (A7) and $Z_u^{V\theta}$ was defined in Eq. (69).

Substituting Eqs. (A6), (68) into Eq. (75) and using Eqs. (A1-A4), S-matrix can be expressed in terms of $\hat{\tau}^5(-)$. We then analytically continue $\hat{\tau}^5(-)$ onto the unphysical Riemann sheet. With the help of Eq. (73), $S_d^{(a)}$ can be reduced to

$$S_d^{(a)}=\frac{2\pi i}{(Z_u^{V\theta*})^{1/2}}\,\delta(M_B-m-w)\,\frac{u(w)}{(2w)^{1/2}}\times\int\frac{d^3k''u(w'')F(M_B,w)F(M_B,w'')}{(2w'')^{1/2}(M_B-m-w'')}\times\left(A'+2gC'\int\frac{d^3k'u(w')}{(2w')^{1/2}(M_B-m-w'-w'')}\right), \qquad (76)$$

where $\sqrt{Z_v}$ was cancelled by using Eq. (A8).

In analogy to the unstable elementary V particle case, the total probability per unit time of this unstable $(V\theta)$ composite state decays into the continuum $|\,V\theta\rangle\rangle$ for all momentum $\mathbf{k}$ can be calculated to be

$$E^{(a)}=\frac{1}{2\pi}\left|u^2(M_B-m)[(M_B-m)^2-\mu^2]^{1/2}F^2(M_B,M_B-m)\right|, \qquad (77)$$

where $(Z_u^{V\theta*})^{1/2}$ was cancelled out by using Eq. (72).

Case (b)

$$(V\theta)_u\to N+\theta_k+\theta_{k'}.$$

The width of this decay process can be calculated by the same way as we did in the case (a). Omitting the detailed calculations, we will only give the result:

$$E^{(b)} = \frac{g^2}{2\pi} \times \left| \int \frac{d^3k u^2(M_B - m - w) u^2(w)[(M_B - m - w)^2 - \mu^2]^{1/2}}{(2\pi)^3(2w)} \times \left(\frac{F(M_B, w)}{M_B - m - w} + \frac{F(M_B, M_B - m - w)}{w} \right)^2 \right| \tag{78}$$

From Eqs. (77) and (78), we see that the widths of the decays of the unstable $(V\theta)$ composite state are again independent of the form of the field operator.

VII. UNSTABLE $(V\theta)$ COMPOSITE STATE SCATTERING

We are going to investigate the problem of scattering a θ particle off the unstable $(V\theta)$ composite state, i.e.,

$$(V\theta)_u + \theta_k \to (V\theta)_u + \theta_{k'}.$$

By using the asymptotic condition and the reduction formula, the S-matrix element for this process can be written as

$$S_{kk'}^{(V\theta)_u\theta} = \delta_{kk'} + \iint dt\, dt'\, e^{i(M_B+w)t} \overrightarrow{\left(i \frac{d}{dt} - M_B - w\right)} \times \langle 0 \mid T(B_u^{V\theta}(t) B_u^{V\theta+}(t')) \mid 0 \rangle \times \overleftarrow{\left(i \frac{d}{dt'} + M_B + w'\right)} e^{-i(M_B+w')t'}. \tag{79}$$

Substituting Eqs. (68) and (69) into Eq. (79) and using definitions of the tau functions in the V-2θ sector of the Lee Model (c. f. Eqs. (A9-A12), we can reduce the S matrix to

$$S_{kk'}^{(V\theta)_u\theta} = \delta_{kk'} + \frac{2\pi i}{|Z_u^{V\theta}|} \delta(w - w')(w - w')^2 \frac{u^2(w)}{2w} \times \iint \frac{d^3p_1 d^3p'_1 u(w_{p_1}) u(w_{p'_1})}{(4 w_{p_1} w_{p'_1})^{1/2}} \Big\{ \hat{\tau}^9(W, w_{p_1}, w, w'_{p_1}, w') \times \left(A' + 2gC' \iint \frac{d^3p_2 u(w_{p_2})}{(2w_{p_2})^{1/2}(W - m - w - w_{p_1} - w_{p_2})} \right) \times \left(A' + 2gC' \int \frac{d^3p'_2 u(w'_{p_2})}{(2w'_{p_2})^{1/2}(W - m - w' - w'_{p_1} - w'_{p_2})} \right) \Big\}_{|W = M_B + w}. \tag{80}$$

Since the result for $\hat{\tau}^9(-)$ is in terms of $\hat{\tau}^5(-)$, among many ways, we will again analytically continue only the function $\hat{\tau}^5(-)$ onto the unphysical sheet. To the lowest order term in Eq. (A13), we get

$$\left| S_{kk'}^{(V\theta)_u\theta} \right| = \delta_{kk'} + 2\pi\delta(w - w') \frac{u'(w)}{2w} \times \left| F^2(M_B, w)\, h(M_B - m - w) \right|. \tag{81}$$

The S-matrix obtained in Eq. (81) is independent of the form of the interpolating field operator for the unstable $(V\theta)$ composite state.

IX. SUMMARY AND CONCLUSION

In this article, the unstable particles were investigated. We defined the unstable elementary V particle in the Lee model II to be the complex pole of the analytically continued Green's function on the unphysical Riemann sheet. The extended LSZ formalism was developed for this unstable elementary V particle. The decay amplitude for the process $V_u \to N + \theta$ was calculated. The S matrix for the unstable V particle scattering process can also be obtained.

The essence of this extended LSZ formalism is the assumption of the asymptotic condition for the unstable particle in terms of its complex mass. The Green's functions are analytically continued onto the unphysical Riemann sheet where the unstable particle manifests itself as a pole. The formalism is exact and does not depend on the arbitrary separation of the total Hamiltonian.

By treating the unstable composite state on the equal footing as the unstable elementary particle, the extended LSZ formalism can also include the unstable composite state. We illustrated our formalism on the $(V\theta)$ composite state in the Lee model. When the coupling constant is decreased less than some critical value, this $(V\theta)$ composite state then becomes an unstable $(V\theta)$ composite state. The decay probabilities for the processes

$$(V\theta)_u \to V + \theta, \quad (V\theta)_u \to N + \theta + \theta$$

and the S matrix for the process

$$(V\theta)_u + \theta \to (V\theta)_u + \theta$$

were calculated.

Both the unstable elementary V particle in the Lee model II and the unstable $(V\theta)$ composite state served as two excellent examples for illustrating our LSZ formalism for the unstable particles.

We compared the decay width of the unstable elementary V particle calculated by our extended LSZ formalism with that determined by the imaginary part of the position of the pole on the unphysical Riemann sheet. They agreed to each other in the lowest order approximation which is expected from the uncertainty principle. In fact, our LSZ formalism results can be shown to reduce to those obtained by perturbation theory in the lowest order approximation as one would expect if our extended LSZ formalism is correct.

We also like to point out without showing the proof that our results of mass, lifetime, and renormalization constant agree in the lowest order approximation to those determined by defining the unstable particle to be the real pole of the reaction K matrix.[16]

Throughout this article, we have always used the most general local interpolating field operators. The very interesting result we obtained is that all decay and scattering amplitudes for the unstable particles are independent of the form of the interpolating fields.

The analytic continuation of the various matrix elements involving the unstable particles is not unique. Also, the determination of the renormalization constant for the unstable particle is not unique. However, the various results agree to each other in the lowest order approximation as expected from the uncertainty principle.

APPENDIX

The four appropriate tau functions in the V–θ sector of the Lee Model were defined as[6]

$$\tau^5(t, w, w') = \frac{(4ww')^{1/2}}{u(w)u(w')} \langle 0 \mid T(\psi_v(t) a_k(t) \psi_v^+(0) a_{k'}^+(0)) \mid 0 \rangle,$$

$$\tau^6(t, w, w', w'') = \frac{(8ww'w'')^{1/2}}{u(w)u(w')u(w'')} \times \langle 0 \mid T(\psi_N(t) a_k(t) a_{k'}(t) \psi_v^+(0) a_{k''}^+(0)) \mid 0 \rangle,$$

$$\tau^7(t,w,w',w'') = \frac{(8ww'w'')^{1/2}}{u(w)u(w')u(w'')} \times \langle 0 \mid T(\psi_v(t)a_k(t)\psi_N^+(0)a_{k'}^+(0)a_{k''}^+(0)) \mid 0\rangle ,$$

$$\tau^8(t,w,w',w'',w''') = \frac{(16ww'w''w''')^{1/2}}{u(w)u(w')u(w'')u(w''')} \times\langle 0 \mid T(\psi_N(t)a_k(t)a_{k'}(t)\psi_N^+(0)a_{k''}^+(0)a_{k'''}^+(0)) \mid 0\rangle . \quad \text{(A1)}$$

It was shown[6] that these tau functions satisfied the following relations

$$\hat\tau^6(W,w,w',w'') = \frac{g[\hat\tau^5(W,w,w'') + \hat\tau^5(W,w',w'')]}{W-m-w-w'}, \quad \text{(A2)}$$

$$\hat\tau^7(W,w,w',w'') = \frac{g[\hat\tau^5(W,w,w') + \hat\tau^5(W,w,w'')]}{W-m-w-w'}, \quad \text{(A3)}$$

$$\hat\tau^8(W,w,w',w'',w''') = \frac{4ww'(\delta_{kk''}\delta_{k'k'''} + \delta_{kk'''}\delta_{k'k''})}{u^2(w)u^2(w')(W-m-w-w')} + \frac{g[\hat\tau^7(W,w',w'',w''') + \hat\tau^7(W,w,w'',w''')]}{W-m-w-w'}. \quad \text{(A4)}$$

The solution of $\tau^5(W,w,w')$ was derived[6] to be

$$\begin{aligned}\tau^5(W,w,w') &= \frac{2w\,\delta_{kk'}}{u^2(w)h(W-m-w)} + \frac{g^2}{(W-m-w)(W-m-w')} \\
&\times\Big\{\frac{-2h(W-m)}{ww'[1+h(W-m)I^+(W-m)]} \\
&\times[(W-m-w)I^+(W-m-w) + (m-W)I^+(W-m)] \\
&\times[(W-m-w')I^+(W-m-w') + (m-W)I^+(W-m)] \\
&+ \frac{1}{[1-\beta(W-m)](W-m-w-w')} \\
&+ I^+(W-m)\left[\frac{m-W}{W-m-w-w'} + \frac{(m-W)^2}{ww'}\right] \\
&+ [(m+w'-W)(W-m-w-w') + w'(w-w')] \\
&\times \frac{(m-W+w')I^+(W-m-w')}{(w'-w)w'(W-m-w-w')} \\
&+ [(m+w-W)(W-m-w'-w) + w(w'-w)] \\
&\times \frac{(m+w-W)I^+(W-m-w)}{w(w-w')(W-m-w-w')}\Big\},\end{aligned}$$

where

$$I(z) \equiv \frac{1}{\pi}\int_\mu^\infty dw'\,\mathrm{Im}\left(\frac{1}{1-\beta(w')}\right)\frac{1}{w'[1-\beta(W-w')](w'-z)}. \quad \text{(A5)}$$

The most general local interpolating field operator for the stable V particle in the Lee model could be written as[10]

$$B_0^V(t) = A\psi_v(t) + C\psi_N(t)\int d^3k a_k(t) \quad \text{(A6)}$$

and the renormalized interpolating field $B^V(t)$ was defined as

$$B^V(t) \equiv B_0^V(t)/(Z_v)^{1/2}. \quad \text{(A7)}$$

Z_v is the renormalization constant and was calculated to be[10]

$$(Z_v)^{1/2} = A + Cg\int\frac{d^3k\,u(w)}{(2w)^{1/2}(-w)}. \quad \text{(A8)}$$

The appropriate four tau functions in the V-2θ sector of the Lee model were defined as[12]

$$\tau^9(t,w_1,w_2,w_3,w_4) = \prod_{i=1}^{4}\frac{(2w_i)^{1/2}}{u(w_i)} \times\langle 0 \mid T(\psi_v(t)a_{k1}(t)a_{k2}(t)\psi_v^+(0)a_{k3}^+(0)a_{k4}^+(0)) \mid 0\rangle,$$

$$\tau^{10}(t,w_1,w_2,w_3,w_4,w_5) = \prod_{i=1}^{5}\frac{(2w_i)^{1/2}}{u(w_i)} \times\langle 0 \mid T(\psi_N(t)a_{k1}(t)a_{k2}(t)a_{k3}(t)\psi_v^+(0)a_{k4}^+(0)a_{k5}(0))\mid 0\rangle,$$

$$\tau^{11}(t,w_1,w_2,w_3,w_4,w_5) = \prod_{i=1}^{5}\frac{(2w_i)^{1/2}}{u(w_i)} \times\langle 0 \mid T(\psi_v(t)a_{k1}(t)a_{k2}(t)\psi_N^+(0)a_{k3}^+(0)a_{k4}^+(0)a_{k5}(0))\mid 0\rangle,$$

$$\tau^{12}(t,w_1,w_2,w_3,w_4,w_5,w_6) = \prod_{i=1}^{6}\frac{(2w_i)^{1/2}}{u(w_i)} \times\langle 0 \mid T(\psi_N(t)a_{k1}(t)a_{k2}(t)a_{k3}(t)\psi_N^+(0)a_{k4}^+(0)a_{k5}^+(0)a_{k6}^+(0)) \mid 0\rangle. \quad \text{(A9)}$$

These tau functions satisfied the following equations

$$\hat\tau^{10}(W,w_1,w_2,w_3,w_4,w_5) = g\,\frac{[\hat\tau^9(W,w_2,w_3,w_4,w_5) + \hat\tau^9(W,w_1,w_3,w_4,w_5) + \hat\tau^9(W,w_1,w_2,w_4,w_5)]}{W-m-w_1-w_2-w_3}, \quad \text{(A10)}$$

$$\hat\tau^{11}(W,w_1,w_2,w_3,w_4,w_5) = g(W-m-w_3-w_4-w_5)^{-1} \times[\hat\tau^9(W,w_1,w_2,w_4,w_5)\,\hat\tau^9(W,w_1,w_2,w_3,w_5) + \hat\tau^9(W,w_1,w_2,w_3,w_4)], \quad \text{(A11)}$$

$$\begin{aligned}\hat\tau^{12}(W,w_1,w_2,w_3,w_4,w_5,w_6) &= \left(\prod_{i=1}^{3}\frac{2w_i}{u^2(w_i)}\right)(W-m-w_1-w_2-w_3)^{-1}[\delta_{k1\,k4}\delta_{k2\,k5}\delta_{k3\,k6} + \delta_{k1\,k4}\delta_{k2\,k6}\delta_{k3\,k5} \\
&+ \delta_{k1\,k5}\delta_{k2\,k4}\delta_{k3\,k6} + \delta_{k1\,k5}\delta_{k2\,k6}\delta_{k3\,k4} + \delta_{k1\,k6}\delta_{k2\,k4}\delta_{k3\,k5} + \delta_{k1\,k6}\delta_{k2\,k5}\delta_{k3\,k4}] \\
&+ g[\hat\tau^{11}(W,w_2,w_3,w_4,w_5,w_6) + \hat\tau^{11}(W,w_1,w_3,w_4,w_5,w_6) + \hat\tau^{11}(W,w_1,w_2,w_4,w_5,w_6)]\times(W-m-w_1-w_2-w_3)^{-1}.\end{aligned} \quad \text{(A12)}$$

The result of $\hat\tau^9(W,w_1,w_2,w_3,w_4)$ solved by an iterative expansion method[13] is

$$\hat{T}^9(W+m,w_1,w_2,w_3,w_4) = \frac{4w_1w_2(\delta_{k1k3}\delta_{k2k4}+\delta_{k1k4}\delta_{k2k3})}{u^2(w_1)u^2(w_2)h(W-w_1-w_2)} + \frac{1}{h(W-w_1-w_2)h(W-w_3-w_4)}$$

$$\times\Bigg\{\frac{2w_2\delta_{k2k4}}{u^2(w_2)}\,g^2U^-(W-w_2,w_1,w_3) + \frac{g^4U^-(W-w_2,w_1,w_3)U^-(W-w_3,w_2,w_4)}{h(W-w_2-w_3)}$$

$$+\frac{g^6}{4\pi^2}\int_\mu^\infty \frac{dwu^2(w)(w^2-\mu^2)^{1/2}U^-(W-w_2,w_1,w)U^-(W-w,w_2,w_4)U^-(W-w_4,w,w_3)}{h(W-w-w_2)h(W-w-w_4)}$$

$$+\frac{g^8}{16\pi^4}\int_\mu^\infty \frac{dwu^2(w)(w^2-\mu^2)^{1/2}U^-(W-w_2,w_1,w)}{h(W-w-w_2)}\int_\mu^\infty \frac{dw^1u^2(w')(w'^2-\mu^2)^{1/2}}{k(W-w-u')h(W-w'-w_3)}$$

$$\times\, U^-(W-w,w_2,w')U^-(W-w',w,w_2)U^-(W-w_3,w',w_4)+\cdots \begin{matrix}+\text{ terms with } w_3 \text{ and } w_4 \text{ interchanged}\\ +\text{ terms with } w_1 \text{ and } w_2 \text{ interchanged}\end{matrix}\Bigg\}, \qquad \text{(A13)}$$

where

$$U^-(W,w,w') \equiv \frac{2w\delta_{kk'}}{g^3u^2(w)}\,h(W-w') + \frac{h(W-w)h(W-u')\hat{T}^t(W+m,w,w')}{g^2}. \qquad \text{(A14)}$$

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