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Scattering, Weak Decays, and Final-State Interactions in Model Theories in a Dressed-Particle Picture*

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Elastic and inelastic collisions in the Lee model are treated in a dressed-particle picture. The procedure by which the renormalization constant Z disappears from the integral equations for the transition matrix is studied in detail. A new procedure is given for obtaining the exact transition matrix for $N - \theta$ scattering. A hypothetical fermion B is introduced and the decays $B \to N + \theta$, $B \to V + \theta$, as well as the decay in the Goldberger–Treiman model are studied in the dressed-particle picture. The iterative expansion of the $B \to V + \theta$ decay amplitude is obtained and is shown to agree with the renormalized power series for this decay, though such is not the case for $B \to N + \theta$ decay, or the decay in the Goldberger–Treiman model. It is shown that in the final-state interaction of $B \to V + \theta$ decay, there are cancellation effects between one- and two-meson contributions, which are crucial in avoiding divergences.

I. INTRODUCTION

IN an earlier paper,[1] a method was presented for eliminating the bare-particle n-meson states from their role as Hilbert space base vectors in a theory of meson scattering from a static source. By the application of a scattering formalism due to Ekstein,[2] and by the formulation of the problem in terms of the so-called "asymptotically stationary" states, a set of nonlinear integral equations for the transition matrix elements was derived. These equations were iterated to sixth order to reproduce the "renormalized" series expansion for the S matrix, in terms of physical parameters, without requiring renormalization, or for that matter, any subtractions. In this earlier work the charge states of the static source itself were represented by means of isotopic spin operators. This simplified the problem greatly, since it eliminated any formal distinction between dressed- and bare-particle operators, and in fact, obviated the necessity of speaking about "nucleon" operators at all. In spite of the advantages of this procedure from the point of view of simplicity, there are still great advantages to be had from generalizing this type of treatment by explicitly using dressed-particle operators for all particles involved in the interaction: For one, it is then possible to treat weak decays in this type of model theory, whereas no change in nucleon number can ever be incorporated into a purely isotopic spin formalism. Moreover, since in a fully relativistic, physically realistic theory, isotopic spin operators are certainly inadequate to represent fermions, it can be hoped that valuable lessons can be learned from writing even a "static source" theory[3] with dressed-particle operators for fermions as well as bosons. The theory chosen for this discussion is the Lee model.[4]

* Supported by the National Science Foundation and by the U. S. Army Research Office (Durham, North Carolina).
[1] K. Haller, Phys. Rev. **120**, 1045 (1960). This will henceforth be referred to as HI.
[2] H. Ekstein, Phys. Rev. **101**, 880 (1956).
[3] It is to be noted however, that the theory becomes less "static" and richer in content when creation and annihilation operators are used for the fermions.
[4] T. D. Lee, Phys. Rev. **95**, 329 (1954).

II. THE HAMILTONIAN

The Hamiltonian[5] for the Lee model is given by $H = H_0 + H_1$ with

$$H_0 = \sum_k a_k^\dagger a_k \omega_k + m(v^\dagger v + n^\dagger n)$$

and

$$H_1 = -g \sum_k u(k)(2\omega_k)^{-\frac{1}{2}}(v^\dagger n a_k + a_k^\dagger n^\dagger v) + \delta m v^\dagger v. \quad (1)$$

The Hamiltonian allows the primitive vertex $V \rightleftarrows N + \theta$ and the quantum number $N(V) + N(\theta)$, and (the total number of V's and θ's) is a constant of motion; the quantum number $N(V) + N(N)$ is also a constant of motion. Although in this treatment no infinite integrals ever appear so that even with $u(k) = 1$ no divergence problems would arise, $u(k)$ is explicitly included, since in this model a ghost state arises when no cutoff is introduced.[6] Since the existence or nonexistence of the ghost state is not of primary interest in this discussion, it will be assumed that $u(k)$ has the properties necessary to keep the ghost state from arising, and that $u(k) = [1; 0]$ for $[k < k_0; k > k_0]$.

We will now attempt to find a nonsingular transformation S which will be used to generate the dressed-particle operators, Ω_i from the bare-particle operators ω_i by $\Omega_i = S\omega_i S^{-1}$. The Hamiltonian will then be written in terms of the dressed instead of the bare operators as indicated by $H(\cdots \omega_i \cdots) = \mathfrak{H}(\cdots \Omega_i \cdots)$. We will admit S as a dressing operator if, for all creation operators $\Omega_i^\dagger$, $\mathfrak{H}\Omega_i^\dagger \mid 0\rangle = E_i\Omega_i^\dagger \mid 0\rangle$, so that all physical particle one-particle states are eigenfunctions of the exact Hamiltonian. Needless to say, this specification of S is not unique. Greenberg and Schweber have discussed unitary dressing transformations for the Lee model[7]. In the case of such unitary transformations, the transformed Hamiltonian has an infinite number of terms, a fact which would make it unsuitable for the treatment intended in this work.

The dressing operation to be used here is a nonunitary one and is adapted from one used by Lopuszański[8] in a discussion of the Ruijgrok–Van Hove model. It is given by $S = e^F\nu$, where

$$F = g \sum_k u(k)(2\omega_k^3)^{-\frac{1}{2}} a_k^\dagger n^\dagger v,$$

and where ν is a Hermitian operator which is defined by

$$[\nu, n] = [\nu, n^\dagger] = [\nu, a_k] = [\nu, a_k^\dagger] = 0,$$
$$\nu v = Z^{-\frac{1}{2}} v\nu, \qquad \nu v^\dagger = Z^{\frac{1}{2}} v^\dagger \nu.$$

The vacuum is taken to be an eigenfunction of ν with eigenvalue 1. Application of this transformation to the various creation and annihilation operators leads to a set of dressed operators. The various dressed operators, expressed in terms of bare operators are

$$\begin{aligned} A_k^\dagger &= a_k^\dagger, \\ A_k &= a_k - g u(k)(2\omega_k^3)^{-\frac{1}{2}} n^\dagger v, \\ N^\dagger &= n^\dagger, \\ N &= n - g \sum_\kappa u(\kappa)(2\omega_\kappa^3)^{-\frac{1}{2}} a_\kappa^\dagger v, \\ V^\dagger &= Z^{\frac{1}{2}}[v^\dagger + g \sum_\kappa u(\kappa)(2\omega_\kappa^3)^{-\frac{1}{2}} a_\kappa^\dagger n], \\ V &= Z^{-\frac{1}{2}} v. \end{aligned} \quad (2)$$

Since the transformation S is not unitary, A_k, N and V are no longer the Hermitian adjoints of $A_k^\dagger$, $N^\dagger$ and $V^\dagger$ respectively. We will denote the Hermitian adjoints of $A_k^\dagger$, $N^\dagger$ and $V^\dagger$ by $\mathfrak{A}_k$, $\mathfrak{N}$, and $\mathfrak{V}$, respectively. The Hamiltonian can now be written in terms of the dressed operators as follows:

$$H = \mathfrak{H}_0 + \mathfrak{H}_1 \quad \text{with}$$
$$\mathfrak{H}_0 = m(V^\dagger V + N^\dagger N) + \sum_k A_k^\dagger A_k \omega_k,$$

and

$$\mathfrak{H}_1 = -gZ^{-\frac{1}{2}} \sum_k u(k)(2\omega_k)^{-\frac{1}{2}} e^{-F} V^\dagger N e^{+F} A_k - \delta m V^\dagger N^\dagger V N - \delta m v^\dagger v. \quad (3)$$

Elimination of all terms in which two fermion annihilation operators follow each other at the extreme right (since only one-fermion problems will be discussed in this work) leads to

$$\mathfrak{H}_1 = -gZ^{-\frac{1}{2}} \sum_k u(k)(2\omega_k)^{-\frac{1}{2}} V^\dagger N A_k + g^2 \sum_{k,q} u(k)u(q)(4\omega_k\omega_q^3)^{-\frac{1}{2}}(N^\dagger N - V^\dagger V) A_q^\dagger A_k + g^3 Z^{\frac{1}{2}} \sum_{k,q,\kappa} u(k)u(q)u(\kappa)(8\omega_k\omega_q^3\omega_\kappa^3)^{-\frac{1}{2}} N^\dagger V A_q^\dagger A_\kappa^\dagger A_k. \quad (4)$$

At this point the mass renormalization δm has dropped out of the Hamiltonian; it is however apparent that $\mathfrak{H}_1$, even when written in terms of the renormalized coupling constant $g_\rho = gZ^{\frac{1}{2}}$, contains Z explicitly, although no physical quantity should contain any reference to Z. This persistence of the unphysical Z in the Hamiltonian has been

[5] For simplicity the N and V particles are assigned the same mass.

[6] G. Källén and W. Pauli, Medd. Dansk Mat. Fys 30, No. 7 (1955).

[7] O. Greenberg and S. Schweber, Nuovo Cimento 8, 378 (1955).

[8] J. Lopuszański, Physica 25, 745 (1959). See also reference (7).

pointed out by various authors.[7,8] It will be shown later in this paper that despite the fact that Z appears in the dressed-particle Hamiltonian $\mathcal{H}$, when the previously outlined program for deriving integral equations for the transition matrix is followed, Z systematically disappears from the integral equations in an entirely straightforward manner.

III. $N - \theta$ SCATTERING

The transition matrix for $N + \theta_{\mathbf{k}} \rightarrow N + \theta_{\mathbf{q}}$ can be written[1,2]

$$R(\mathbf{q};\mathbf{k}) = \langle \chi_N(\mathbf{q}) \mid \psi_N^{(+)}(\mathbf{k}) \rangle, \tag{5}$$

where

$$\psi_N^{(+)}(\mathbf{k}) = N_-^\dagger A_{\mathbf{k}}^\dagger \mid 0\rangle - (\mathcal{H} - E_k - i\eta)^{-1}\chi_N\,\mathbf{k}),$$

and

$$\chi_N(\mathbf{q}) = (\mathcal{H} - m - \omega_q)N^\dagger A_{\mathbf{q}}^\dagger \mid 0\rangle$$
$$= -gu(q)(2\omega_q)^{-\frac{1}{2}}[Z^{-\frac{1}{2}}V^\dagger - g\sum_{\kappa} u(\kappa)(2\omega_\kappa^3)^{-\frac{1}{2}}N^\dagger A_\kappa^\dagger] \mid 0\rangle;$$

from Eq. (2) we have

$$\chi_N^*(\mathbf{q}) = -g_\rho u(q)(2\omega_q)^{-\frac{1}{2}}\langle 0 \mid V. \tag{6}$$

The above leads to

$$R(\mathbf{q};\mathbf{k}) = g_\rho u(q)(2\omega_q)^{-\frac{1}{2}}$$
$$\times \langle 0 \mid V[\mathcal{H} - \omega_k - m - i\eta]^{-1} \mid \chi_N(\mathbf{k})\rangle, \tag{5a}$$

and, when the operator $1 = \sum_n \psi_n\rangle\langle\psi_n$ is inserted, we have

$$R(\mathbf{q};\mathbf{k}) = \frac{g_\rho u(q)}{(2\omega_q)^{\frac{1}{2}}}\sum_n \frac{\langle 0 \mid V \mid \psi_n\rangle\langle\psi_n \mid \chi_N(\mathbf{k})\rangle}{E_n - m - \omega_k - i\eta}. \tag{5b}$$

The set ψ_n here consists of dressed one-particle states and outgoing scattering states. Due to the selection rules that are operative in the Lee model, the only nonvanishing contributions to the sum are from $\psi = \mid V\rangle$, and from $N - \theta$ scattering states. Equation (5b) can be rewritten as

$$R(\mathbf{q};\mathbf{k}) = \frac{g_\rho^2 u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{1}{2}}} - \frac{1}{2\pi^2}\int \frac{\kappa^2\, d\kappa\, R(\mathbf{q};\kappa)R^*(\mathbf{k};\kappa)}{\omega_\kappa - \omega_k - i\eta}. \tag{7}$$

Incidentally, it is worth noting that in the above treatment, the use of the scattering theory discussed in (2) is quite necessary. We might try to take advantage of the fact that the asymptotically stationary states are eigenfunctions of $\mathcal{H}_0$ and invoke the more usual scattering theory[9] which leads to a linear integral equation. For $N - \theta$ scattering, the linear integral equation for $T(\mathbf{q};\mathbf{k})$, (the transition matrix in this theory) is

$$T(\mathbf{q};\mathbf{k}) = \langle 0 \mid a_{\mathbf{q}}\mathfrak{N}\mathcal{H}_1 A_{\mathbf{k}}^\dagger N^\dagger \mid 0\rangle - \sum_{\kappa}\langle 0 \mid a_{\mathbf{q}}\mathfrak{N}\mathcal{H}_1 A_{\kappa}^\dagger N^\dagger \mid 0\rangle T(\kappa;\mathbf{k})[\omega_\kappa - \omega_k - i\eta]^{-1}$$
$$+ \langle 0 \mid a_{\mathbf{q}}\mathfrak{N}\mathcal{H}_1 V^\dagger \mid 0\rangle\langle 0 \mid v\mathcal{H}_1^* A_{\mathbf{k}}^\dagger N^\dagger \mid 0\rangle\omega_k^{-1}.$$

The various vacuum expectation values in this equation are all identically 0, as long as the cutoff $u(q)$ keeps Z finite. When $Z \rightarrow \infty$ we are again faced with indeterminate expressions. We must therefore discard this approach.

Equation (7) can be iterated as was discussed in HI. In this case, however, the iteration leads to an exact solution. An exact solution of Eq. (7) can also be represented by a contour integral.

To generate the iterative solution, it is most convenient to deal with the reactance matrix $K(\mathbf{q};\mathbf{k})$ which obeys the equation

$$K(\mathbf{q};\mathbf{k}) = \frac{g_\rho^2 u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{1}{2}}} - \frac{1}{2\pi^2}\int P\frac{\kappa^2\, d\kappa\, K(\mathbf{q};\kappa)K(\mathbf{k};\kappa)}{\omega_\kappa - \omega_k}, \tag{8}$$

where P denotes the principal value of the integral. Iteration gives

$$K^{(2)}(\mathbf{q};\mathbf{k}) = \frac{g_\rho^2 u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{1}{2}}}, \quad \text{and}$$

$$K^{(4)}(\mathbf{q};\mathbf{k}) = \frac{g_\rho^2 u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{1}{2}}}\left[-\frac{g_\rho^2\omega_k}{4\pi^2}\int \frac{\kappa^2\, d\kappa\, u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_k)}\right]$$

(the P will be suppressed for the remainder of this section). By induction we will now show that the nth term is

$$K^{(2n)}(\mathbf{q};\mathbf{k}) = \frac{g_\rho^2 u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{1}{2}}} \times \left[-\frac{g_\rho^2}{4\pi^2}\omega_k\int \frac{\kappa^2\, d\kappa\, u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_k)}\right]^{(n-1)}. \tag{9}$$

If Eq. (9) is true up to n, then

$$K^{(2n+2)}(\mathbf{q};\mathbf{k}) = \frac{g_\rho^2 u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{1}{2}}}\left\{\left(-\frac{g_\rho^2}{4\pi^2}\right)^n\omega_k \times\left[n\int \frac{\omega_\kappa^{(n-1)}\kappa^2\, d\kappa\, u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_k)}\left(\int \frac{p^2\, dp\, u^2(p)}{\omega_p^3(\omega_p - \omega_\kappa)}\right)^{(n-1)}\right]\right\}. \tag{10}$$

The expression in the square bracket on the right-hand side of Eq. (10) can be written

$$I = \int \frac{\kappa^2\, d\kappa\, p^2(1)\, dp(1)\cdots p^2(n-1)\, dp(n-1)}{\omega_\kappa^3\omega_{p(1)}^3\cdots\omega_{p(n-1)}^3} \times \sum_{\mathcal{P}} \frac{\omega_\kappa^{(n-1)}}{(\omega_\kappa - \omega_k)(\omega_{p(1)} - \omega_\kappa)\cdots(\omega_{p(n-1)} - \omega_\kappa)}, \tag{11}$$

[9] e.g., B. A. Lippmann and J. Schwinger, Phys. Rev. 79, 469 (1950); M. Gell-Mann and M. L. Goldberger, Phys. Rev. 91, 398 (1953).

where $\sum_\varphi$ indicates the sum of the expression as written plus all terms obtained when κ is permuted with each $p(i)$ in turn. It is then necessary to prove that

$$\sum_\varphi \frac{\omega_\kappa^{(n-1)}}{(\omega_{p(1)} - \omega_\kappa)\cdots(\omega_{p(n-1)} - \omega_\kappa)(\omega_\kappa - \omega_k)} = \frac{\omega_k^{(n-1)}}{(\omega_{p(1)} - \omega_k)\cdots(\omega_{p(n-1)} - \omega_k)(\omega_\kappa - \omega_k)}, \quad (12)$$

or

$$\omega_k^{(n-1)} = \sum_\varphi \omega_\kappa^{(n-1)} \frac{\Pi_i^{(n-1)}(\omega_{p(i)} - \omega_k)}{\Pi_i^{(n-1)}(\omega_{p(i)} - \omega_\kappa)}. \quad (12a)$$

If we let $\kappa = p(0)$, then

$$\omega_k^{(n-1)} = \sum_{r=0}^{(n-1)} \frac{[\Pi_i(\omega_{p(i)} - \omega_k)]_r'}{[\Pi_i(\omega_{p(i)} - \omega_r)]_r'} \omega_r^{(n-1)}, \quad (12b)$$

where r is one of the set $i = 0, \cdots (n-1)$, and $[\Pi_i(\ )]_r'$ indicates the product of all i's except for the $i = r$ term which is omitted. Eq. (12b) is the Lagrange interpolation formula[10] for the representation of $\omega_k^{(n-1)}$ as a function that is identical to it at n points. Since $\omega_k^{(n-1)}$ is a polynomial of rank $(n-1)$, it is identical to this representation everywhere, and Eq. (12b) is an identity. This proves the theorem.[11] We can now write

$$K(\mathbf{q};\mathbf{k}) = \frac{g_\rho^2 u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{3}{2}}} \sum_{n=0}^{\infty} \left[-\left(\frac{g_\rho^2}{4\pi^2}\right)\omega_k \int \frac{\kappa^2\, d\kappa\, u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_k)} \right]^n$$
$$= g_\rho^2(2\omega_q^{\frac{1}{2}}\omega_k^{\frac{3}{2}})^{-1}u(q)u(k)\cdot\left[1 + \frac{g_\rho^2}{4\pi^2}\omega_k \int \frac{\kappa^2\, d\kappa\, u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_k)}\right]^{-1}. \quad (13)$$

To obtain the transition from the reactance matrix, we apply the Heitler equation which leads us to

$$R(\mathbf{q};\mathbf{k}) = g_\rho^2(2\omega_q^{\frac{1}{2}}\omega_k^{\frac{3}{2}})^{-1}u(q)u(k) \cdot\left[1 + \frac{g_\rho^2}{4\pi^2}\omega_k \int \frac{\kappa^2\, d\kappa\, u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_k - i\eta)}\right]^{-1}. \quad (14)$$

To represent $R(\mathbf{q};\mathbf{k})$ by a contour integral, we substitute $h(\omega) = \omega[r(\omega)]^{-1}$ into Eq. (7); here,

$$r(\omega_k) = 2\omega_q^{\frac{1}{2}}\omega_k^{\frac{3}{2}}R(\mathbf{q};\mathbf{k})[u(q)u(k)]^{-1}.$$

This implies that

$$\text{Im}\,[h(\omega)] = -[4\pi\omega]^{-1}(\omega^2 - m_\theta^2)^{\frac{1}{2}}\theta(\omega - m_\theta)u^2(\omega)$$

on the upper branch of the real axis. From the form of Eq. (8), we can fix bounds on the high-energy ω dependence of $h(\omega)$, and then, by performing a contour integral, the explicit form of $h(\omega)$ is easily arrived at.[12] Both these solutions are not necessarily unique, and in fact fail to be unique by the Castillejo–Dalitz–Dyson ambiguities.[13]

IV. SCATTERING IN HIGHER SECTORS

The transition matrix for $V - \theta$ scattering is

$$R_V(\mathbf{q};\mathbf{k}) = \langle\chi_V(\mathbf{q}) \mid \psi_V^{(+)}(\mathbf{k})\rangle, \quad (15)$$

where

$$\chi_V(\mathbf{q}) = (\mathfrak{H} - m - \omega_q)V^\dagger A_\mathbf{q}^\dagger\,|0\rangle; \quad (16)$$

using Eq. (6), we have

$$\chi_V(\mathbf{q}) = -\frac{g^2u(q)}{(2\omega_q)^{\frac{1}{2}}}\left\{\sum_\kappa \frac{u(\kappa)}{(2\omega_\kappa^3)^{\frac{1}{2}}} \times\left[A_\kappa^\dagger V^\dagger - g_\rho \sum_\mathbf{p} \frac{u(p)}{(2\omega_p^3)^{\frac{1}{2}}} A_\mathbf{p}^\dagger A_\kappa^\dagger N^\dagger\right]|0\rangle\right\},$$

and

$$\chi_V^*(\mathbf{q}) = -\frac{g_\rho^2 u(q)}{(2\omega_q)^{\frac{1}{2}}}\sum_\kappa \frac{u(\kappa)}{(2\omega_\kappa^3)^{\frac{1}{2}}}\langle 0|\, VA_\kappa. \quad (16a)$$

The above lead to

$$R_V(\mathbf{q};\mathbf{k}) = -g_\rho^2u(q)u(k)(2\omega_q^{\frac{1}{2}}\omega_k^{\frac{3}{2}})^{-1} - \langle\chi_V(\mathbf{q})\mid[\mathfrak{H} - m - \omega_k - i\eta]^{-1}\mid\chi_V(\mathbf{k})\rangle. \quad (17)$$

We insert $1 = |\psi_n\rangle\langle\psi_n|$ into the right-hand side of Eq. (17) and we obtain contributions from the $V - \theta$ and the $N - \theta_1$, θ_2-scattering states. In the expression for $R_V(\mathbf{q};\mathbf{k})$, the matrix element $\langle\chi_V(\mathbf{q}) \mid \psi_N^{(+)}(\boldsymbol{\kappa},\boldsymbol{\kappa}')\rangle$ appears. This quantity is the transition matrix for the inelastic process $V + \theta_\mathbf{q} \rightleftarrows N + \theta_\boldsymbol{\kappa} + \theta_{\boldsymbol{\kappa}'}$, and we will refer to it as $R_\alpha(\mathbf{q};\boldsymbol{\kappa},\boldsymbol{\kappa}')$. Eq. (17) becomes

$$R_V(\mathbf{q};\mathbf{k}) = -\frac{g_\rho^2u(q)u(k)}{2\omega_q^{\frac{1}{2}}\omega_k^{\frac{3}{2}}} - \sum_\kappa \frac{R_V(\mathbf{q};\boldsymbol{\kappa})R_V^*(\mathbf{k};\boldsymbol{\kappa})}{\omega_\kappa - \omega_k - i\eta} - \sum_{\kappa,\kappa'} \frac{R_\alpha(\mathbf{q};\boldsymbol{\kappa},\boldsymbol{\kappa}')R_\alpha^*(\mathbf{k};\boldsymbol{\kappa},\boldsymbol{\kappa}')}{\omega_\kappa + \omega_{\kappa'} - \omega_k - i\eta}. \quad (17a)$$

The same procedure can be invoked to derive an integral equation for the quantity $R_N(\mathbf{q},\mathbf{q}';\mathbf{k},\mathbf{k}')$, the transition amplitude for $N + \theta_\mathbf{k} + \theta_{\mathbf{k}'} \to N + \theta_\mathbf{q} + \theta_{\mathbf{q}'}$. In that case we have

$$R_N(\mathbf{q},\mathbf{q}';\mathbf{k},\mathbf{k}') = -\sum_{\kappa,\kappa'} \frac{R_N(\mathbf{q},\mathbf{q}';\boldsymbol{\kappa},\boldsymbol{\kappa}')R_N^*(\mathbf{k},\mathbf{k}';\boldsymbol{\kappa},\boldsymbol{\kappa}')}{\omega_\kappa + \omega_{\kappa'} - \omega_k - \omega_{k'} - i\eta} - \sum_\kappa \frac{R_\beta(\mathbf{q},\mathbf{q}';\boldsymbol{\kappa})R_\beta^*(\mathbf{k},\mathbf{k}';\boldsymbol{\kappa})}{\omega_\kappa - \omega_k - \omega_{k'} - i\eta}, \quad (18)$$

where

$$R_\beta(\mathbf{q},\mathbf{q}';\boldsymbol{\kappa}) = \langle\chi_N(\mathbf{q},\mathbf{q}') \mid \psi_V^{(+)}(\boldsymbol{\kappa})\rangle.$$

[10] E. Goursat, *A Course in Mathematical Analysis*, translated by E. Hedrick (Dover Publications, Inc., New York, 1909), Vol. I.

[11] The author is indebted to Professor A. A. Blank for pointing out the identity of Eq. (12) and the Lagrange interpolation formula.

[12] M. L. Goldberger and S. B. Treiman, Phys. Rev. **113**, 1663 (1959).

[13] L. Castillejo, R. H. Dalitz, and F. J. Dyson, Phys. Rev. **101**, 453 (1956).

Similarly we obtain

$$R_\alpha(\mathbf{q};\mathbf{k},\mathbf{k}') = -\sum_\kappa \frac{R_V(\mathbf{q};\kappa)R_\beta^*(\mathbf{k},\mathbf{k}';\kappa)}{\omega_\kappa - \omega_k - \omega_{k'} - i\eta} - \sum_{\kappa,\kappa'} \frac{R_\alpha(\mathbf{q};\kappa,\kappa')R_N^*(\mathbf{k},\mathbf{k}';\kappa,\kappa')}{\omega_\kappa + \omega_{\kappa'} - \omega_k - \omega_{k'} - i\eta}, \quad (19)$$

and

$$R_\beta(\mathbf{q},\mathbf{q}';\mathbf{k}) = -\frac{g_\rho}{2^{\frac{1}{2}}}\left[\frac{u(q)}{(2\omega_q)^{\frac{1}{2}}}\delta_{\mathbf{q}',\mathbf{k}} + \frac{u(q')}{(2\omega_{q'})^{\frac{1}{2}}}\delta_{\mathbf{q},\mathbf{k}}\right] - \sum_\kappa \frac{R_\beta(\mathbf{q},\mathbf{q}';\kappa)R_V^*(\mathbf{k};\kappa)}{\omega_\kappa - \omega_k - i\eta} - \sum_{\kappa,\kappa'} \frac{R_N(\mathbf{q},\mathbf{q}';\kappa,\kappa')R_\alpha^*(\mathbf{k};\kappa,\kappa')}{\omega_\kappa + \omega_{\kappa'} - \omega_k - i\eta}. \quad (20)$$

Equations (17a), (18), (19), and (20) are a closed set of simultaneous integral equations. They can be iterated exactly as were the integral equations in HI. As in the case of these latter, as well as in the case of $N - \theta$ scattering, there are no longer any unphysical quantities in these integral equations, and only the "renormalized" coupling constant g_ρ appears. The argument presented in HI that all iteration integrals are finite, applies equally well to this case.

IV. WEAK DECAYS AND FINAL-STATE INTERACTIONS

We will now examine the consequence of adding various additional terms to the Hamiltonian, so that the new Hamiltonian allows certain specified weak decays. We will postulate the existence of an additional fermion B, with mass $m_B > m_N + 2m_\theta$, which we will, in one case, allow to decay by the scheme $B \to N + \theta$, and, in a later section, by the scheme $B \to V + \theta$. Finally we will also discuss the Goldberger–Treiman model.[12]

(A) $B \to N + \theta$ Decay

The term $H_a + m_B b^\dagger b$, where

$$H_a = G\sum_k u(k)(2\omega_k)^{-\frac{1}{2}}(ba_\mathbf{k}^\dagger n^\dagger + n a_\mathbf{k} b^\dagger), \quad (21)$$

is added to the Hamiltonian to describe this decay. For simplicity, the momentum dependence of B is suppressed. Since this is a weak decay, only the lowest-order term in G will be considered and no attempt will be made to dress the B particle. To first order in G, the decay amplitude is given by

$$D(\mathbf{p}) = \langle\psi_N^{(-)}(\mathbf{p})\,|(\mathcal{H}_T - m_B)|\,B\rangle, \quad (22)$$

where $\mathcal{H}_T = \mathcal{H} + \mathcal{H}_a + m_B B^\dagger B$, and where we have written $B^\dagger$, B for $b^\dagger$, b respectively, to indicate that to this order in G, the bare and dressed B are identical. We have

$$(\mathcal{H}_T - m_B)B^\dagger\,|0\rangle = \mathcal{H}_a B^\dagger\,|0\rangle,$$

and

$$D(\mathbf{p}) = G\langle\psi_N^{(-)}(\mathbf{p})|\sum_\mathbf{k} u(k)(2\omega_k)^{-\frac{1}{2}}A_\mathbf{k}^\dagger N^\dagger\,|0\rangle. \quad (22a)$$

Applying Eq. (5) of HI, we have

$$D(\mathbf{p}) = G\sum_\mathbf{k} u(k)(2\omega_k)^{-\frac{1}{2}}\langle\psi_N^{(-)}(\mathbf{p})| \times [|\psi_N^{(-)}(\mathbf{k})\rangle - (\mathcal{H} - E_k + i\eta)^{-1}\,|\chi_N(\mathbf{k})\rangle] = G\sum u(k)(2\omega_k)^{-\frac{1}{2}} \times [\delta_{\mathbf{p},\mathbf{k}} - \langle\psi_N^{(-)}(\mathbf{p})|\,(\mathcal{H} - E_k + i\eta)^{-1}\,|\chi_N(\mathbf{k})\rangle], \quad (22b)$$

which becomes

$$D(\mathbf{p}) = G\left[\frac{u(p)}{(2\omega_p)^{\frac{1}{2}}} + \sum_\mathbf{k}\frac{u(k)}{(2\omega_k)^{\frac{1}{2}}}\left(\frac{R^{(-)}(\mathbf{p};\mathbf{k})}{\omega_k - \omega_p - i\eta}\right)\right]. \quad (22c)$$

Here $R^{(-)}(\mathbf{p};\mathbf{k})$ is given by $\langle\psi_N^{(-)}(\mathbf{p})\mid\chi_N(\mathbf{k})\rangle$; it is a form of the transition matrix for $N - \theta$ scattering and is identical to $R(\mathbf{p};\mathbf{k})$ on the energy shell. It is given by

$$R^{(-)}(\mathbf{p};\mathbf{k}) = g_\rho^2 u(p)u(k)(2\omega_p^{\frac{1}{2}}\omega_k^{\frac{1}{2}})^{-1} \times\left[1 + \frac{g_\rho^2}{4\pi^2}\omega_p\int\frac{\kappa^2\,d\kappa\,u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_p - i\eta)}\right]^{-1}. \quad (23)$$

Since the ω_k dependence of $R^{(-)}(\mathbf{p};\mathbf{k})$ is entirely trivial, the integrations indicated in Eq. (22a) can be immediately performed; the resulting expression for $D(\mathbf{p})$ is

$$D(\mathbf{p}) = \frac{G}{(2\omega_p)^{\frac{1}{2}}}\left\{1 - \frac{g_\rho^2}{4\pi^2\omega_p}\int\frac{k^2\,dk\,u(k)}{\omega_k(\omega_k - \omega_p - i\eta)} \times\left[1 + \frac{g_\rho^2}{4\pi^2}\omega_p\int\frac{\kappa^2\,d\kappa\,u^2(\kappa)}{\omega_\kappa^3(\omega_\kappa - \omega_p - i\eta)}\right]^{-1}\right\}. \quad (24)$$

(B) The Goldberger–Treiman Model

In the Goldberger–Treiman model, in addition to the N, V, and θ particles, an additional particle θ' is introduced. θ' participates in no strong interactions whatsoever, and interacts weakly according to the scheme

$$H_\gamma = \frac{G}{M}\sum_{\mathbf{k},\mathbf{q}}\frac{n^\dagger n[a_\mathbf{k}^\dagger\alpha_\mathbf{q} + a_\mathbf{k}\alpha_\mathbf{q}^\dagger]u(k)U(q)}{2(\omega_k W_q)^{\frac{1}{2}}}. \quad (25)$$

The decay amplitude for the decay $V \to N + \theta'$ is then computed. Since in the case treated here $m_V = m_N$, we will take the θ' to be a massless particle. The decay can then take place in the limit of zero-momentum θ' particles. The part of H_γ

which contributes to the decay amplitude for $V \to N + \theta'$ is

$$(\mathfrak{IC}_\gamma)' = \left(\frac{G}{M}\right) \sum_{\mathbf{k},\mathbf{q}} u(k)(2\omega_k)^{-\frac{1}{2}} N^\dagger [N + g_\rho \sum_{\boldsymbol{\kappa}} u(\kappa)(2\omega_\kappa^3)^{-\frac{1}{2}} A_{\boldsymbol{\kappa}}^\dagger V] \times [A_{\mathbf{k}} + g_\rho u(k)(2\omega_k^3)^{-\frac{1}{2}} N^\dagger V][\alpha_{\mathbf{q}}^\dagger (2W_q)^{-\frac{1}{2}}] U(q). \quad (25a)$$

In this decay there are no strong final-state interactions, and D_{GT}, the amplitude for $V \to N + \theta'$ decay, is

$$D_{GT}(\mathbf{p}) = \langle 0 | \, \mathfrak{N}\alpha_{\mathbf{p}}(\mathfrak{IC}_\gamma)' \, | V\rangle = \frac{G}{M} \frac{g_\rho U(p)}{(2W_p)^{\frac{1}{2}}} \sum_{\mathbf{k}} \frac{u^2(k)}{2\omega_k^2}. \quad (26)$$

Since, for the Lee Model, δm is given by

$$\delta m = -g^2 \sum_{\mathbf{k}} u^2(k)(2\omega_k^2)^{-1}, \quad (26a)$$

we can write

$$D_{GT} = -\frac{G}{M} \frac{U(p)}{(2W_p)^{\frac{1}{2}}} \frac{Z}{g_\rho} \delta m, \quad (26b)$$

which agrees with the result of Goldberger and Treiman. In the zero-frequency limit, this gives a vanishing decay rate, but that is a kinematic detail which is of no consequence to this discussion.

(C) $B \to V + \theta$ Decay

For this case we add the term $H_c + m_B b^\dagger b$, where H_c is given by

$$H_c = G_0 \sum_{\mathbf{k}} u(k)(2\omega_k)^{-\frac{1}{2}} (b a_{\mathbf{k}}^\dagger v^\dagger + v a_{\mathbf{k}} b^\dagger) \quad (27)$$

to the Hamiltonian. Because of the weakness of H_c, we again make no attempt to dress the B particle, except that we allow G to differ from its corresponding bare coupling constant G_0. D_V, the transition amplitude for $B \to V + \theta$ decay, is given, to first order in G, by $D_V(\mathbf{p}) = \langle \psi_V^{(-)}(\mathbf{p}) \mid \mathfrak{IC}_c \mid B\rangle$. Using Eq. (2), we have that

$$\mathfrak{IC}_c \, |B\rangle = \frac{G}{Z^{\frac{1}{2}}} \sum_{\mathbf{k}} \frac{u(k) A_{\mathbf{k}}^\dagger}{(2\omega_k)^{\frac{1}{2}}} \times \left[V^\dagger - g_\rho \sum_{\boldsymbol{\kappa}} \frac{u(\kappa) A_{\boldsymbol{\kappa}}^\dagger N^\dagger}{(2\omega_\kappa^3)^{\frac{1}{2}}} \right] |0\rangle, \quad (28)$$

which, in turn gives

$$D_V(\mathbf{p}) = \frac{G}{Z^{\frac{1}{2}}} \sum_{\mathbf{k}} \frac{u(k)}{(2\omega_k)^{\frac{1}{2}}} \left[\langle \psi_V^{(-)}(\mathbf{p})| \, A_{\mathbf{k}}^\dagger V^\dagger \, |0\rangle - g_\rho \sum_{\boldsymbol{\kappa}} \frac{u(\kappa)}{(2\omega_\kappa^3)^{\frac{1}{2}}} \langle \psi_V^{(-)}(\mathbf{p})| \, A_{\mathbf{k}}^\dagger A_{\boldsymbol{\kappa}}^\dagger N^\dagger \, |0\rangle \right]. \quad (29)$$

The same procedure that was followed in part (A) here leads to

$$D_V(\mathbf{p}) = \frac{G}{Z^{\frac{1}{2}}} \left[\frac{u(p)}{(2\omega_p)^{\frac{1}{2}}} - \sum_{\mathbf{k}} \frac{u(k) R_V^{(-)}(\mathbf{p};\mathbf{k})}{(2\omega_k)^{\frac{1}{2}}(\omega_k - \omega_p - i\eta)} + g_\rho \sum_{\mathbf{k},\boldsymbol{\kappa}} \frac{u(k)u(\kappa) R_\alpha^{(-)}(\mathbf{p};\mathbf{k},\boldsymbol{\kappa})}{(2\omega_k\omega_\kappa^3)^{\frac{1}{2}}(\omega_k + \omega_\kappa - \omega_p - i\eta)} \right], \quad (29a)$$

where

$$R_\alpha^{(-)}(\mathbf{p};\mathbf{k},\boldsymbol{\kappa}) = \langle \psi_V^{(-)}(\mathbf{p}) \mid \chi_N(\mathbf{k},\boldsymbol{\kappa})\rangle.$$

In an identical fashion, we obtain the following expression for $D_N(\mathbf{q},\mathbf{p})$, the amplitude for $B \to N + \theta_{\mathbf{q}} + \theta_{\mathbf{p}}$ decay:

$$D_N(\mathbf{q},\mathbf{p}) = -\frac{G}{Z^{\frac{1}{2}}} \left[\frac{g_\rho(\omega_q + \omega_p)u(q)u(p)}{(2\omega_q\omega_p)^{\frac{1}{2}}} - g_\rho \sum_{\mathbf{k},\boldsymbol{\kappa}} \frac{u(k)u(\kappa) R_N^{(-)}(\mathbf{p},\mathbf{q};\mathbf{k},\boldsymbol{\kappa})}{(2\omega_k\omega_\kappa^3)^{\frac{1}{2}}(\omega_k + \omega_\kappa - \omega_q - \omega_p - i\eta)} + \sum_{\mathbf{k}} \frac{u(k) R_\beta^{(-)}(\mathbf{p},\mathbf{q};\mathbf{k})}{(2\omega_k)^{\frac{1}{2}}(\omega_k - \omega_q - \omega_p - i\eta)} \right], \quad (30)$$

where

$$R_N^{(-)}(\mathbf{p},\mathbf{q};\mathbf{k},\boldsymbol{\kappa}) = \langle \psi_N^{(-)}(\mathbf{p},\mathbf{q}) \mid \chi_N(\mathbf{k},\boldsymbol{\kappa})\rangle,$$

and

$$R_\beta(\mathbf{p},\mathbf{q};\mathbf{k}) = \langle \psi_N^{(-)}(\mathbf{p},\mathbf{q}) \mid \chi_V(\mathbf{k})\rangle.$$

We now address ourselves to the problem of iterating the expression for $D_V(\mathbf{p})$ to the first few orders in g_ρ^2. The integral equations for $R_V^{(-)}(\mathbf{p};\mathbf{k})$ and $R_\alpha^{(-)}(\mathbf{p};\mathbf{k},\boldsymbol{\kappa})$ are:

$$R_V^{(-)}(\mathbf{p};\mathbf{k}) = -\frac{g_\rho^2 u(p)u(k)}{2\omega_p^{\frac{1}{2}}\omega_k^{\frac{1}{2}}} - \sum_{\boldsymbol{\kappa}} \frac{R_V^{(-)*}(\boldsymbol{\kappa};\mathbf{p}) R_V^{(-)}(\boldsymbol{\kappa};\mathbf{k})}{\omega_\kappa - \omega_p - i\eta} - \sum_{\boldsymbol{\kappa},\boldsymbol{\kappa}'} \frac{R_\beta^{(-)*}(\boldsymbol{\kappa},\boldsymbol{\kappa}';\mathbf{p}) R_\beta^{(-)}(\boldsymbol{\kappa},\boldsymbol{\kappa}';\mathbf{k})}{\omega_\kappa + \omega_{\kappa'} - \omega_p - i\eta}, \quad (31)$$

and

$$R_\alpha^{(-)}(\mathbf{p};\mathbf{k},\mathbf{k}') = -\frac{g_\rho}{2^{\frac{1}{2}}} \left[\frac{u(k)}{(2\omega_k)^{\frac{1}{2}}} \delta_{\mathbf{p},\mathbf{k}'} + \frac{u(k')}{(2\omega_{k'})^{\frac{1}{2}}} \delta_{\mathbf{p},\mathbf{k}} \right] - \sum_{\boldsymbol{\kappa}} \frac{R_V^{(-)*}(\boldsymbol{\kappa};\mathbf{p}) R_\alpha^{(-)}(\boldsymbol{\kappa};\mathbf{k},\mathbf{k}')}{(\omega_\kappa - \omega_p - i\eta)} - \sum_{\boldsymbol{\kappa},\boldsymbol{\kappa}'} \frac{R_\beta^{(-)*}(\boldsymbol{\kappa},\boldsymbol{\kappa}';\mathbf{p}) R_N^{(-)}(\boldsymbol{\kappa},\boldsymbol{\kappa}';\mathbf{k},\mathbf{k}')}{(\omega_\kappa + \omega_{\kappa'} - \omega_p - i\eta)}. \quad (32)$$

Similar equations can be written for all other matrix elements appearing in Eqs. (31) and (32).

Using Eqs. (31) and (32), $D_V(\mathbf{p})$ will be expanded to g_ρ^2. To lowest order (independent of g_ρ), $D_V^{(0)}(\mathbf{p}) = (G/Z^{\frac{1}{2}})u(p)(2\omega_p)^{-\frac{1}{2}}$; to the next order, there are two contributions to $D_V^{(2)}(\mathbf{p})$—one from the integral over $R_V^{(-)}$, the other from the integral over $R_\alpha^{(-)}$. We will label these $[D_V^{(2)}(\mathbf{p})]_V$ and $[D_V^{(2)}(\mathbf{p})]_\alpha$, respectively. We then have

$$[D_V^{(2)}(\mathbf{p})]_V = \left(\frac{G}{Z^{\frac{1}{2}}}\right) \frac{u(p)}{(2\omega_p)^{\frac{1}{2}}} g_\rho^2 \sum_{\mathbf{k}} \frac{u^2(k)}{\omega_k(\omega_k - \omega_p - i\eta)}, \quad (33)$$

and

$$[D_V^{(2)}(\mathbf{p})]_\alpha = -\left(\frac{G}{Z^{\frac{1}{2}}}\right)\frac{u(p)}{(2\omega_p)^{\frac{1}{2}}}\,g_\rho^2 \times\left[\sum_{\mathbf{k}}\frac{u^2(k)}{\omega_k^2}+\omega_p\sum_{\mathbf{k}}\frac{u^2(k)}{\omega_k^3}\right].$$

Although each of these integrals diverges separately at high frequencies, $D_V^{(2)}(\mathbf{p})$ (given by $D_V^{(2)}(\mathbf{p}) = [D_V^{(2)}(\mathbf{p})]_V + [D_V^{(2)}(\mathbf{p})]_\alpha$) is a convergent integral in the sense that as the integral is cut off at increasingly higher frequencies, it approaches a finite limit. $D_V^{(2)}(\mathbf{p})$ is given by

$$D_V^{(2)}(\mathbf{p}) = -\left(\frac{G}{Z^{\frac{1}{2}}}\right)u(p)\left(\frac{\omega_p}{2}\right)^{\frac{1}{2}}\frac{g_\rho^2}{4\pi^2} \times\int\frac{k^2\,dk\,u^2(k)}{\omega_k^3(\omega_k-\omega_p-i\eta)}. \tag{33a}$$

To the next highest order, $D_V^{(4)}(\mathbf{p})$, we obtain

$$[D_V^{(4)}(p)]_V = \left(\frac{G}{Z^{\frac{1}{2}}}\right)\frac{u(p)}{(2\omega_p)^{\frac{1}{2}}}\left(\frac{g_\rho^2}{4\pi^2}\right)^2 \times\int\frac{k^2\,dk\,\kappa^2\,d\kappa\,u^2(k)u^2(\kappa)}{(\omega_k\omega_\kappa^3)(\omega_k-\omega_p-i\eta)(\omega_\kappa-\omega_p-i\eta)},$$

$$[D_V^{(4)}(p)]_\alpha = -\left(\frac{G}{Z^{\frac{1}{2}}}\right)\frac{u(p)}{(2\omega_p)^{\frac{1}{2}}}\left(\frac{g_\rho^2}{4\pi^2}\right)^2 \times\int\frac{k^2\,dk\,\kappa^2\,d\kappa\,u^2(k)u^2(\kappa)(\omega_k+\omega_\kappa)}{(\omega_k^2\omega_\kappa^3)(\omega_k+\omega_\kappa-\omega_p-i\eta)(\omega_\kappa-\omega_p-i\eta)}. \tag{34}$$

Again, each of these integrals individually diverges at high frequencies. The sum of both, $D_V^{(4)}(p)$, is given by

$$D_V^{(4)}(p) = \left(\frac{G}{Z^{\frac{1}{2}}}\right)u(p)\left(\frac{\omega_p}{2}\right)^{\frac{1}{2}}\left(\frac{g_\rho^2}{4\pi^2}\right)^2 \times\int\frac{k^2\,dk\,\kappa^2\,d\kappa\,u^2(k)u^2(\kappa)}{\omega_k^2\omega_\kappa^2(\omega_k-\omega_p-i\eta)(\omega_\kappa-\omega_p-i\eta)(\omega_k+\omega_\kappa-\omega_p-i\eta)}, \tag{34a}$$

and this is a convergent integral.

(D) Discussion

For purposes of comparison, we will now develop the old-fashioned power-series expansion of $D_V(p)$. The primitive expression for the T operator is given by

$$T = H'' + H''(E-H_0+i\eta)^{-1}H'' + \cdots H''(E-H_0+i\eta)^{-1} \times H''\cdots(E-H_0+i\eta)^{-1}H''+\cdots,$$

and $\langle f \mid T \mid i\rangle$ is the primitive transition-matrix element; H'' is given by

$$H'' = H_1 + G_0\sum_{\mathbf{k}}u(k)(2\omega_k)^{-\frac{1}{2}}[va_{\mathbf{k}}b^\dagger + ba_{\mathbf{k}}^\dagger v^\dagger].$$

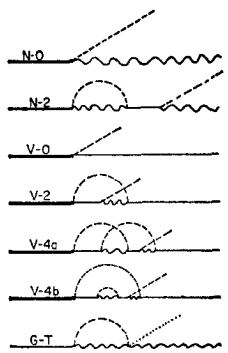

FIG. 1. Decay graphs. N graphs represent $B \to N + \theta$ decays, V graphs represent $B \to V + \theta$ decays, and the G T graph represents the $V \to N + \theta'$ decay in the Goldberger-Treiman model. The numbers designate the order of g_ρ in each diagram. The thick solid line indicates the B particle, the thin solid line the V particle, the wavy line the N particle, the dashed line the θ particle, and the dotted line the θ' particle.

In the amplitude for $B \to V + \theta$ decay, the second term in the expression for H'' is operative at the first vertex, and H_1 is operative at all other vertices. In order to express these matrix elements properly in terms of dressed-particle parameters, and in order to avoid divergent integrals (in the sense in which that term has been used in this paper), it is necessary to renormalize the theory[14]; thus the self energy can be written[4] $S(E) = ZS_f(E)$. In the case of the Lee model with $B \rightleftarrows V + \theta$ coupling, there are, beyond the graphs in the Lee model, additional decay vertex graphs (diagrams $V-0$, $V-4$). We can write the proper decay vertex part

$$\Delta(E, E') = G_0(2\omega_p)^{-\frac{1}{2}}L(E, E'),$$

and we can write the following integral equation for $L(E, E')$:

$$L(E,E') = 1 + \frac{g^2}{4\pi^2} \times\int\frac{k^2\,dk\,L(E,E-\omega_k)S(E-\omega_k)}{\omega_k(E'-\omega_k)}. \tag{35}$$

Using $S(E) = ZS_f(E)$, this becomes

$$L(E,E') = 1 + \frac{g_\rho^2}{4\pi^2} \times\int\frac{k^2\,dk\,L(E,E-\omega_k)S_f(E-\omega_k)}{\omega_k(E'-\omega_k)}. \tag{35a}$$

We now inquire whether $L(E\,E')$ can be written as $L(E, E') = \alpha L_f(E, E')$ where $L_f(E, E')$ is convergent and where $L_f(0, 0) = 1$. Assuming $L(E, E') = \alpha L_f(E, E')$, we have

$$\alpha L_f(E,E') = 1 + \frac{\alpha g_\rho^2}{4\pi^2} \times\int\frac{k^2\,dk\,L_f(E,E-\omega_k)S_f(E-\omega_k)}{\omega_k(E'-\omega_k)}. \tag{35b}$$

[14] G. Chew, Phys. Rev. **94**, 1749 (1954); A. Lenard (private communication).

Since the integral on the right-hand side of Eq. (35b) includes all finite radiative corrections inserted into the primitive skeleton (there is only one proper irreducible graph), we have

$$\frac{g_\rho^2}{4\pi^2}\int \frac{k^2\,dk\,L_f(E, E-\omega_k)S_f(E-\omega_k)}{\omega_k(E'-\omega_k)} = \Lambda_0 + \Lambda_f(E, E'),$$

where Λ_0 is the skeleton divergence.[15] Since the skeleton integral is logarithmically divergent, $\Lambda_f(E, E')$ is convergent, and the answer to the question posed above is affirmative. We have

$$\alpha[1 + \Lambda_f(E, E')] = 1 + \alpha\Lambda_0 + \alpha\Lambda_f(E, E'),$$

and

$$\alpha = (1 - \Lambda_0)^{-1}.$$

Moreover, we have the result that decay vertex graphs are renormalized precisely as are vertex graphs in any static theory. An extra factor of $Z^{-\frac{1}{2}}$ is obtained from a full complement of wave-function renormalization bubbles at the right of the $B \rightleftarrows V + \theta$ vertex. In the limit of $m_B \to m_V$, $m_\theta \to 0$, the entire decay amplitude is given by $D_V(p) = Gu(p)(2\omega_p Z)^{-\frac{1}{2}}$, where $G = \alpha G_0$. At least to this order in G we may take this to define a "physical coupling constant" $(\alpha G_0/Z^{\frac{1}{2}})$. Of course the arguments for defining the physical coupling constant by going to this limit are far less compelling than are the ones in the case of charge renormalization in quantum electrodynamics, but the procedure is as sound as the one invoked in the case of the scattering of any particles with nonvanishing rest mass.

It is now possible to apply the rules for renormalizing decay graphs and to compute the expression for the decay matrix element to all orders in g_ρ. This has been done to order g_ρ^4; to this order, the diagrams V–0, V–2, V–4a, and V–4b occur. When the renormalized expressions corresponding to these graphs are computed, they agree completely with the results obtained by iterating Eq. 29a [e.g. Eqs. 33a and 34a].

We will now address ourselves to the appearance of the weak coupling constant G in the expression for $\mathfrak{IC}_c$ in Eq. (28). There are two possible points of view that may be taken in discussing the type of model theory treated here. In one case, the cut off $u(k)$ can be adjusted so that all integrals converge primitively, all renormalization constants are well defined and, hopefully, all or most problems are exactly soluble. In such a treatment, since the values of all primitive graphs are finite, it is entirely optional and almost trivial whether the theory is renormalized or not, i.e., whether or not a finite renormalization constant is factored out explicitly from a primitive expression; this is, of course, providing the scattering theory is applied to the correct asymptotically stationary states.

To discuss the $B \to V + \theta$ decay from that point of view would require an exact solution for a Ruijgrok–Van Hove-type theory[16] with two V particles, and V_2 unstable. It is not our purpose here to find such a solution to this problem.

In the second case, a somewhat more heuristic point of view is taken. The cut off is permitted to recede to infinity without extensive inquiry as to whether this is consistent with the formal manipulations that are made in the course of developing the theory. In the absence of such a detailed inquiry which, in any case is not possible except in very simple models, the manipulations that lead to the integral equations are valid in a formal sense only, and do not follow unambiguously as they would in a calculation in which the first point of view is taken. This latter procedure was followed in HI and also here in the case of $B \to V + \theta$ decay. In particular, the relation between the bare and dressed B operators is a case in point. The dressed B operator is not well defined since the one-particle B function should not be an eigenstate of H_T. Thus the identification of $G_0 b$ with GB, obvious a choice as it is, is in the nature of an "ansatz" which constitutes part of the theory. We note that in the limit $m_B \to m_V$ only the $BA^\dagger V^\dagger$ part of $\mathfrak{IC}_c$ contributes to the decay amplitude, and only in the Born approximation. Since the expression consists of dressed operators, the $\mathfrak{IC}_c$ weak vertex must include the zero energy, zero-energy exchange contributions of the primitive proper decay vertex part, hence G, and not G_0, is the proper coefficient in $\mathfrak{IC}_c$.

We observe that just as the integral equations in HI and Eqs (7) and (17a) to (20) correctly reproduce the "renormalized" transition matrix, so also does Eq. (29a) correctly reproduce the renormalized decay amplitude without requiring subtraction or, for that matter, any thing other than straightforward iteration. In spite of the heuristic basis of some of the

[15] J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons*, (Addison-Wesley Publishing Company, Inc., Cambridge, Massachusetts, 1955), p. 212f. Note that in our Eq. 35b, we have $L(E, E') = 1 + \Lambda(E, E')$ and, later, that $L_f(E, E') = 1 + \Lambda_f(E, E')$.

[16] Th. W. Ruijgrok and L. Van Hove, Physica **22**, 880 (1956); Th. W. Ruijgrok, Physica **24**, 137 and 185 (1958); Physica **25**, 357 (1959).

manipulations that led to Eq. (29a), it is still a great improvement over the old fashioned perturbation procedures since in the present case, the integral equations themselves contain no more divergences or unphysical quantities (if $G/Z^{\frac{1}{2}}$ is properly interpreted as the physical coupling constant). In the old theory however, these problems can be solved only in a perturbative sense, order by order.

The situation with respect to the iterative expansion of the decay amplitude is quite different in the case of the $B \rightarrow N + \theta$ decay. The proper "ansatz" in that case is $b = B$, and the expansion of the decay amplitude consists of integrals that diverge as the cut off approaches infinity. In fact the "pseudo self energy" graphs (in which one vertex is weak and one strong; see N-type diagrams) when they appear in this expansion, reproduce the primitive unrenormalized expression and not the renormalized one for this term. This is perhaps not very surprising, since in this model there is no distinction between bare and dressed particles in the case of any particle participating in the interaction, and the bare- and dressed-particle picture in a sense coincide. It seems therefore that the fact that "g" is the proper coupling constant even in $\mathfrak{IC}_a$, and the associated appearance of primitive "divergent" pseudo-self energy terms in the expansion of $D_N(p)$ are outgrowths of the severely restrictive selection rules that operate in the Lee model to keep both the N and the θ bare. We would not expect this feature of the $B \rightarrow N + \theta$ decay to be duplicated in any realistic theory for elementary particle interactions.

In the case of $B \rightarrow V + \theta$ decay, although the interaction Hamiltonian when written in terms of bare-particle operators contains only a $B - V - \theta$ vertex, it contains an additional $B - N - \theta_1 - \theta_2$ vertex when written in the dressed-particle picture. In general, in more realistic models, it is reasonable to expect that such bare-particle Hamiltonians, when transcribed into the dressed-particle picture, proliferate terms to include vertices with many states to which transitions are not forbidden by the selection rules. We can separate the equation for the $B \rightarrow V + \theta$ decay into three parts:

(1) The Born term $G(2\omega_p Z)^{-\frac{1}{2}}$;

(2) The $R_V^{(-)}$ term, in which the dressed decay Hamiltonian $\mathfrak{IC}_c$ connects the B and $V - \theta$ states, and the $V - \theta$ state scatters $V + \theta \rightarrow V + \theta$;

(3) The $R_\alpha^{(-)}$ term in which $\mathfrak{IC}_c$ connects the B and the $N - \theta - \theta$ states (though there is no such coupling in the bare-particle picture) and the $N - \theta - \theta -$ state scatters $N + \theta + \theta \rightarrow V + \theta$.

In spite of obvious differences,[17] there is a strong resemblance between Eq. (29a) and equations for the decay amplitude which arise in dispersion theoretic treatments.[18] The following observations about Eq. (29a) may therefore have relevance to dispersion theoretic calculations: The R_α^- contributions (two-meson states) may not be dropped with respect to R_V^- (one-meson states). In fact, since elimination of the two-meson relative to the one-meson contributions lends to spurious divergences, this would seem to be a particularly pernicious mistake. Moreover, the Hamiltonian $\mathfrak{IC}_c$ dictates the relative magnitude of the one-meson and two-meson contributions. Any but the correct relation between the one-meson and two-meson contributions would again lead to spurious divergences.

V. ACKNOWLEDGMENTS

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[17] For example, Eq. (29a) involves the scattering transition amplitudes off the energy shell, though in the case of the one-meson processes, the energy parameter that is "off" the shell is trivial.

[18] For example, J. D. Jackson, *On the Equivalence of Different Treatments of Two-Body Final State Interactions* (preprint).

Mechanical Model for Quantum Field Theory*

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We consider two harmonic oscillators, coupled during a finite time. Initial and final states can be defined unambiguously, and if the duration of the coupling is sufficiently short, the S matrix can be computed explicitly. The coupling gx^2y is investigated in detail, for complex values of g. It is found that, along the real axis, the S matrix behaves smoothly as a function of g and tends to the unit matrix for $g \to 0$, as it should. However, the S matrix has a line of essential singularities along the imaginary g axis, including the origin, so that it cannot be expanded into powers of g. If such an expansion is sought by means of a perturbation procedure, it is found that each term of the series is finite (no need of renormalization), but the series as a whole diverges.

IT is well known that quantum field theory is fraught with considerable mathematical difficulties, among which the divergences play a prominent role. Recently, Bialynicki-Birula[1] suggested that the origin of these divergences is a singular behavior of the S matrix at zero coupling constant. The renormalization procedure would essentially be the removal of that singular part. The purpose of the present paper is to show, by means of a simple model, that the problem of the singular behavior of the S matrix at zero coupling constant is entirely distinct from the problem of ultraviolet divergences.

Let us consider two identical harmonic oscillators, coupled during a finite time. The Hamiltonian of the system is, with suitable units,

$$H = \tfrac{1}{2}(p_x^2 + p_y^2 + x^2 + y^2) + g(t)f(x, y). \tag{1}$$

Since $g(t)$ vanishes outside a finite time interval, the definition of the initial and final states Ψ_i and Ψ_f is unambiguous[2] and the S matrix, defined by $\Psi_f = S\Psi_i$, is given as usual, by

$$S = T\,[\exp \int -ig(t)f(x, y)\,dt]. \tag{2}$$

The time ordering of the operators is necessary, because, although x and y commute at any time, we have, e.g.,

$$[x(t'), x(t'')] = -i \sin (t' - t''). \tag{3}$$

(This relation readily follows from the solution of the Heisenberg equations of motion for x and p_x

$$x = x_0 \cos t + p_{x0} \sin t,$$

$$p_x = p_{x0} \cos t - x_0 \sin t,$$

where x_0 and p_{x0} are the initial values of the operators x and p_x, satisfying the usual commutation relations.)

It is now formally possible to represent (2) as a sum of Feynman diagrams, using (3) as a propagator.[3] However, for the sake of simplicity, we shall here consider only the special case where $g(t) \neq 0$ during a time much shorter than the period of the oscillators, so that we can make

$$g(t) \to g\ \delta(t), \tag{4}$$

where g is now a constant. Thus we obtain from (2):

$$S = e^{-igf(x,y)}, \tag{5}$$

which could also have been obtained directly from (1) and (4), by integrating the Schrödinger equation $i\dot{\Psi} = H\Psi$ about $t = 0$.

We can consider (5) as the q representation of the S matrix. However, to make the correspondence with quantum field theory, we need the energy representation

$$S_{mn} = \iint \Psi_m^*(x, y)e^{-igf(x,y)}\Psi_n(x, y)\,dx\,dy, \tag{6}$$

where the $\Psi_m(x, y)$ are the eigenfunctions of the free Hamiltonian.

As an illustration, we shall compute the vacuum–vacuum transition amplitude in the special case

$$f(x, y) = x^2y, \tag{7}$$

so that one type of oscillator appears linearly and one quadratically, as in quantum electrodynamics. Here, the "vacuum" is given by

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[1] I. Bialynicki-Birula, Phys. Rev. **122**, 1942 (1961).

[2] An essential difference from quantum field theory is that here, ψ_i and ψ_f can be arbitrary linear combinations of the various eigenstates of the oscillators, while in quantum field theory, the initial and final numbers of particles must be integers, because of superselection rules.

[3] J. Weinberg (private communication).

$$\Psi_0(x, y) = \pi^{-\frac{1}{2}} \exp[-\tfrac{1}{2}(x^2 + y^2)], \quad (8)$$

so that

$$S_{00} = \pi^{-1} \iint e^{-x^2-y^2-igx^2y}\, dx\, dy, \quad (9)$$

$$= 2\pi^{-\frac{1}{2}} \int_0^\infty \exp[-x^2 - \tfrac{1}{4}g^2x^4]\, dx. \quad (10)$$

With $z = \frac{1}{2}gx^2$, $p = 2/g$, this becomes

$$S_{00} = \left(\frac{p}{\pi}\right)^{\frac{1}{2}} \int_0^\infty z^{-\frac{1}{2}} e^{-pz-z^2}\, dz$$

$$= \pi^{-\frac{1}{2}} g^{-1} e^{1/2g^2} K_{\frac{1}{4}}(1/2g^2), \quad (11)$$

where K is the modified Bessel function of the third kind.[4] This function behaves quite smoothly for all real values of g and tends to unity when $g \to 0$, as can easily be seen from (10) and as should be expected on physical grounds. However, it is also easily seen from (10) that S_{00} diverges badly for purely imaginary g. This result is reminiscent of Dyson's heuristic argument,[5] according to which the electromagnetic vacuum would explode spontaneously into a large number of pairs, if $e^2 \to -e^2$.

On the other hand, we may ask how a perturbation treatment of this problem (i.e. a power series in g) would display the essential singularity of the S matrix at $g = 0$. The answer is readily obtained by expanding (9) or (10) into powers of g. The result is

$$S_{00} = \sum [(-1)^m (4m)!/2^{6m} m!\,(2m)!] g^{2m}, \quad (12)$$

and can also be obtained from the known asymptotic behavior of $K(z)$ for $z \to \infty$.[6] Note that each term is finite, even without renormalization (contrary to Bialynicki-Birula's conjecture[1]). This is related to the fact that the propagator (3) has no singularity.

For large m, the ratio of consecutive terms of (12) is $-mg^2$, so that this series has a zero radius of convergence. A similar result was obtained long ago by Hurst[7] and Thirring[8] for a simple model of field theory. The present "mechanical" model has the advantage of being still simpler, so that the *explicit* value of the S matrix can also be obtained and compared with the result of perturbation theory.

Although a rigorous proof seems difficult, there are indications that a similar situation prevails in quantum electrodynamics[9] and probably in all other nontrivial field theories. Roughly speaking, this is due to the fact that the number of distinct Feynman diagrams of order n behaves approximately like $n!$,[10] so that any perturbation expansion is at best asymptotic, i.e. of limited accuracy. We may wonder whether this inability to achieve exact results is due only to a temporary weakness of our mathematical tools, or perhaps reflects an underlying and yet undiscovered indeterminacy of nature.

The author is indebted to Professors R. L. Arnowitt and P. G. Bergmann for the warm hospitality of Syracuse University, and to the U. S. Educational Foundation in Israel for the award of a Fulbright travel grant.

[4] A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Tables of Integral Transforms* (McGraw-Hill Book Company, Inc., New York, 1954), Vol. I, p. 146, Eq. (23).

[5] F. J. Dyson, Phys. Rev. **85**, 631 (1952).

[6] A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 86, Eq. (7).

[7] C. A. Hurst, Proc. Cambridge Phil. Soc. **18**, 625 (1952).

[8] W. Thirring, Helv. Phys. Acta, **26**, 33 (1953).

[9] S. Frautschi, Prog. Theoret. Phys. (Kyoto) **22**, 882 (1959).

[10] For instance, in quantum electrodynamics, there are $(n - f)!2k!/2^k k!n!$ topologically distinct Feynman diagrams of order n, with $2f$ external fermion lines and $n - 2k = p$ external photon lines. (This is most easily proved by counting the number of pairings in the Wick theorem.) The number of diagrams thus increases approximately n-fold, for large n, when $n \to n + 2$.

Approximate Solution of a Nonlinear Field Equation

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Variational principles for obtaining the eigensolutions ψ_i of the equation $\nabla^2\psi - \psi + \psi^3 = 0$ are developed. Variational solutions to the first two spherically symmetric eigenstates are obtained. Variational solutions of odd parity are also obtained.

1. INTRODUCTION

THERE has recently been some interest in nonlinear field theories of elementary particles.[1] These theories represent attempts to avoid the difficulties connected with singularities arising in the usual linear field theories. A complete theory of elementary particles must be a spinor theory. However several authors have devoted their attention to obtaining particle-like solutions of nonlinear scalar differential equations which might have some relevance to spin-zero particles and are presumably easier to solve. The nonlinear scalar equation most commonly considered[2] is the generalization of the Klein–Gordon equation

$$\Box\varphi - (\mu^2 - \lambda\varphi^*\varphi)\varphi = 0, \tag{1.1}$$

where λ is a coupling constant measuring the strength of the self-coupling of the field. After separating off a plane-wave factor by writing $\varphi = e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\chi(\mathbf{r})$, the equation becomes

$$\nabla^2\chi - \alpha^2\chi + \lambda\chi^3 = 0, \tag{1.2}$$

with $\alpha^2 = \mu^2 + k^2 - \omega^2/c^2$.[3] By changing variables to $\varrho = \alpha\mathbf{r}$ and $\psi = \alpha^{-1}(\lambda)^{\frac{1}{2}}\chi$, both the constants can be eliminated from (1.2).[4] Throughout the remainder of this paper, the standard form

$$\nabla^2\psi(\varrho) - \psi(\varrho) + \psi^3(\varrho) = 0 \tag{1.3}$$

will be used.

Three trivial solutions to (1.3) are $\psi = 0, \pm 1$. For the spherically symmetric case it has been shown by Finkelstein, Lelevier, and Ruderman,[5] by a phase-plane analysis, that (1.3) possesses a set of eigensolutions analytic everywhere, with zero slope at the origin and asymptotic to zero at infinity for a discrete set of initial values, $\psi_i(0)$. For the intervening ranges of initial values of ψ, solutions are asymptotic to $+1$ and -1 alternately. We shall assume that there exists also a discrete set of nonspherically symmetric eigensolutions asymptotic to zero. The eigensolutions will be called one-particle, two-particle, etc. solutions, according to whether they are substantially different from zero in one, two, etc. regions of space infinitely far from one another.

2. VARIATIONAL PRINCIPLE FOR PARTICLE STATES

Equation (1.3) arises as the Euler equation for the Lagrangian:

$$L = +\tfrac{1}{2}\int [(\nabla\psi)^2 + \psi^2 - \tfrac{1}{2}\psi^4]\, d\varrho. \tag{2.1}$$

The possibility then of obtaining approximate solutions to (1.3) by a variational principle using (2.1) is immediately suggested. The difficulty arises because of the indefinite sign of L, and there is no assurance that the variational solution will provide an upper or a lower bound to L; indeed the integrand does not satisfy the Legendre condition.[6]

In order to develop a variational principle without this defect, we first note that if we multiply (1.3) by ψ, integrate over all space and use Green's theorem, the integral relation

$$\int \psi^4\, d\varrho = \int [(\nabla\psi)^2 + \psi^2]\, d\varrho \tag{2.2}$$

is established.

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[1] W. Heisenberg, Rev. Mod. Phys. **29**, 269 (1947); L. I. Schiff, Phys. Rev. **84**, 1 (1951); R. J. Finkelstein, Phys. Rev. **75**, 1079 (1949); R. J. Finkelstein, C. Fronsdal, and P. Kaus, Phys. Rev. **103**, 1571 (1956); T. H. R. Skyrme, Proc. Roy. Soc. (London) **A247**, 260 (1958).

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[3] Equation (1.2) has also been obtained by one of the authors in a nonlinear electromagnetic theory: H. Schiff, Proc. Roy. Soc. (London) **A269**, 277 (1962).

[4] This conformal invariance has been exploited by D. F. Kurdgelaidze, Soviet Phys.—JETP **11**, 339 (1960).

[5] R. J. Finkelstein, R. LeLevier, and M. Ruderman, Phys. Rev. **83**, 326 (1951).

[6] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers Inc., New York, 1953) First English Edition, p. 214.

Consider now the variational problem of extremizing

$$L = \tfrac{1}{2}\int [(\nabla\psi)^2 + \psi^2]\, d\varrho, \tag{2.3}$$

subject to (2.2) as a subsidiary condition. We use the Lagrange multiplier method and extremize

$$L' = \tfrac{1}{2}\int \{(1-\mu)[(\nabla\psi)^2 + \psi^2] + \mu\psi^4\}\, d\varrho. \tag{2.4}$$

The Euler equation which makes L' an extremum then becomes

$$-(1-\mu)\nabla^2\psi + (1-\mu)\psi + 2\mu\psi^3 = 0. \tag{2.5}$$

Now multiply by ψ, integrate over all space and use Green's theorem to obtain

$$\int \psi^4\, d\varrho = \frac{\mu - 1}{2\mu}\int [(\nabla\psi)^2 + \psi^2]\, d\varrho;$$

but since (2.2) must also be satisfied, $\mu = -1$, and (2.5) becomes (1.3) as desired.

Now however, $\frac{1}{2}\int[(\nabla\psi)^2 + \psi^2]\, d\varrho$ satisfies the Legendre condition and has a minimum. The application of subsidiary conditions can only serve to raise the value of this minimum.[7] Thus, determining a minimum of (2.3) subject only to (2.2), is equivalent to finding the ground-state solution of (1.3).

To obtain excited states by the variational method we must apply further subsidiary conditions. Let ψ_i and ψ_j be two different eigensolutions of (1.3). They then satisfy

$$\nabla^2\psi_i - \psi_i + \psi_i^3 = 0, \tag{2.6}$$

$$\nabla^3\psi_j - \psi_j + \psi_j^3 = 0. \tag{2.7}$$

Multiply (2.6) by ψ_j, (2.7) by ψ_i, subtract and integrate over all space using the symmetrical form of Green's theorem to obtain

$$\int \psi_i^3\psi_j\, d\varrho = \int \psi_j^3\psi_i\, d\varrho. \tag{2.8}$$

Relation (2.8) is in some ways analogous to the usual orthogonality relation between eigensolutions of a linear differential equation.

For the first excited state, consider the variational problem of minimizing L of (2.3) subject to (2.2) and

$$\int \psi^3\psi_1\, d\varrho = \int \psi\psi_1^3\, d\varrho, \tag{2.9}$$

where ψ_1 is the ground state solution of (1.3) or the solution of the first variational problem. Again we use the Lagrange-multiplier method and minimize

$$L'' = \tfrac{1}{2}\int [(\nabla\psi)^2 + \psi^2]\, d\varrho + \frac{\mu}{2}\int [\psi^4 - (\nabla\psi)^2 - \psi^2]\, d\varrho + \nu\int [\psi^3\psi_1 - \psi\psi_1^3]\, d\varrho. \tag{2.10}$$

The Euler equation is

$$-(1-\mu)\nabla^2\psi + (1-\mu)\psi + 2\mu\psi^3 + \nu(3\psi^2\psi_1 - \psi_1^3) = 0. \tag{2.11}$$

Now the Lagrangian is invariant under the operation $\psi \to -\psi$ and so are the subsidiary conditions (2.2) and (2.9). Therefore, if $\psi = \psi_2$ minimizes the Lagrangian subject to the subsidiary conditions, so must $\psi = -\psi_2$. Thus if ψ_2 is a solution to the Euler equation, so must $-\psi_2$ be a solution. This is true of (2.11) only if $\psi_2 = \pm\psi_1(3)^{-\frac{1}{2}}$ or if $\nu = 0$. In any case, (2.11) becomes identical to (2.5) and thus as before, finally becomes (1.3). But clearly $\psi_2 = \pm\psi_1(3)^{-\frac{1}{2}}$ does not satisfy the Euler equation so ν must equal zero. The variational principle in a similar way leads to (1.3) again as the Euler equation for minimization of L, subject to further subsidiary conditions such as

$$\int \psi^3\psi_2\, d\varrho = \int \psi\psi_2^3\, d\varrho.$$

3. VARIATIONAL SOLUTIONS FOR SPHERICALLY SYMMETRIC STATES

The procedure in applying the variational method to the solution of (1.3) is now little different from that used for linear differential equations. In order to ensure obtaining an upper bound to the Lagrangian, all variational trial functions must satisfy

$$\int \psi^4\, d\varrho = \int [\psi^2 + (\nabla\psi)^2]\, d\varrho, \tag{A}$$

and

$$\int \psi\psi_i^3\, d\varrho = \int \psi^3\psi_i\, d\varrho, \tag{B}$$

for all lower states ψ_i. [*Note added in proof.* It is clear that condition (B) is necessary but may not be sufficient to ensure an upper bound to the Lagrangian for excited states, because it is satisfied identically for $\psi = \psi_i$.] In order to make the trial

[7] Reference 6, p. 407.

TABLE I. Variational approximations to the ground state of Eq. (1.3).

	Function	Conditions satisfied exactly	Optimum parameter values						$\frac{1}{16\pi}\int \psi^4 \, d\varrho$
			A	p	α	s	b	c	
	Teshima's solution								1.503
1.	$A/(p^2+\rho^2)$	(A), (E)	$2\sqrt{2}/3$	$1\sqrt{6}$	···	···	···	···	1.715
2.	$Ae^{-\alpha\rho}$	(A), (E)	$4\sqrt{2}$	···	$\sqrt{3}$	···	···	···	1.540
3.	$Ae^{-\alpha\rho^1}$	(A), (E)	5.66	···	1.73	1.00	···	···	1.540
4.	$A(1+c\rho)e^{-\alpha\rho}$	(A), (E)	5.17	···	2.27	···	···	0.908	1.536
5.	$A[(e^{-\rho}-e^{-\alpha\rho})/\rho+be^{-\alpha\rho}]$	(A), (C), (D)	2.7397	···	5.2	···	−2.50	···	1.5071
6.	$A[(e^{-\rho}-e^{-\alpha\rho})/\rho+(b+c\rho)e^{-\alpha\rho}]$	(A), (C), (D)	2.6060	···	4.10	···	−1.360	2.33	1.5058
7.	$A[(e^{-\rho}-e^{-\alpha\rho})/\rho+be^{-\alpha\rho}]$	(A), (C)	2.7094	···	5.491	···	−2.950	···	1.5045

functions more like the true solutions, they may also be made to satisfy

$$\psi(\rho) \to f(\theta,\varphi)e^{-\rho}/\rho \qquad \rho \to \infty\,, \tag{C}$$

and for spherically symmetric states,

$$\left.\frac{d\psi}{d\rho}\right|_{\rho=0} = 0. \tag{D}$$

Actually for any trial function having a variable amplitude factor A, minimization of L with respect to A automatically satisfies condition (A). The exact particle-like solutions to (1.3) also have been shown[3] to satisfy the relation

$$4\int(\nabla\psi)^2\,d\varrho = 12\int\psi^2\,d\varrho = 3\int\psi^4\,d\varrho. \tag{E}$$

The satisfaction of this relation is not demanded in the variational method, but occurs automatically in functions where ρ is everywhere multiplied by a variational scale parameter. The relation (E) does guarantee the proportionality of the Lagrangian (2.1) or (2.3) to the energy or mass of the localized states according to the usual expressions.[2,3]

For the spherically symmetric ground state, the various variational approximations are listed in Table I. Table II gives corresponding results for the first excited spherically symmetric state.

Teshima[8] has also found the first three spherically symmetric solutions of (1.3) numerically. Using his results, the values for the ratio $\int\psi^4\,d\varrho/\int\psi^2\,d\varrho$ for the first three solutions are 4.00004, 4.002 and 3.999 respectively. We take this as evidence of the accuracy of his numerical solutions and so his values of $(1/16\pi)\int\psi^4\,d\varrho$ are also included in Tables I and II.

In Table I, a succession of trial functions are seen to give values which approach Teshima's value for $(1/16\pi)\int\psi^4\,d\varrho$ more and more closely from above than expected. Indeed, function 7 gives a value only 0.1% higher than Teshima's. It can be seen that the requirement of zero slope at the origin for function 5 is disadvantageous as regards obtaining an upper bound to the Lagrangian. Thus we have not applied condition (D) in the variational calculations for the second spherically symmetric state.

Table II contains two three-parameter trial solutions, both of which give values for $(1/16\pi)\int\psi^4\,d\varrho$ about 5% higher than Teshima's. Functions 8 and 9 have been orthogonalized with respect to functions 4 and 7, respectively. A better value for the Lagrangian could no doubt be obtained by using more flexible trial functions, or by using functions 8 and 9 in the Green's function method described in reference 3.

4. VARIATIONAL SOLUTIONS OF ODD PARITY

The variational method should be of great advantage in seeking nonspherically symmetric solu-

TABLE II. Variational approximations to the first excited spherically symmetric state of Eq. (1.3).

	Function	Conditions Satisfied	Optimum parameter values				$\frac{1}{16\pi}\int\psi^4\,d\varrho$
			A	α	b	c	
8.	$A(1+c\rho)e^{-\alpha\rho}$	(A), (B), (E)	14.38	1.802	···	−1.876	9.9712
9.	$A\left(\frac{e^{-\rho}-e^{-\alpha\rho}}{\rho}+be^{-\alpha\rho}\right)$	(A), (B), (C)	20.36	2.535	···	−2.3	10.02
	Teshima's solution						9.460

[8] R. K. Teshima, M.Sc. Thesis, University of Alberta, Edmonton, Alberta, Canada (1960, unpublished).

TABLE III. Variational approximations to the lowest odd-parity one-particle state of Eq. (1.3).

Function	Conditions satisfied exactly	Optimum parameter values						$\frac{1}{16\pi}\int \psi^4 \, d\varrho$
		A	α	β	γ	s	b	
9. $Az \exp(-\alpha\rho)$	(A), (B), (E)	$32/\sqrt{3}$	$\sqrt{3}$	...	...	...	...	5.47
10. $Az \exp(-\alpha\rho^s)$	(A), (B), (E)	3.03	2.76	...	...	1.8	...	4.72
11. $A(z \exp\{-[\alpha^2(x^2+y^2)+\gamma^2z^2]^{\frac{1}{2}}\} + b(5\gamma^2z^3 - 3[\alpha^2(x^2+y^2)+\gamma^2z^2]z) \exp\{-\beta[\alpha^2(x^2+y^2)+\gamma^2z^2]^{\frac{1}{2}}\})$	(A), (B), (E), (F)	11.37	1.76	2.12	1.37	...	1.65	4.115

tions to (1.3), because rough variational estimates of the energy can be obtained very quickly.

We now seek a solution of odd parity employing a sequence of trial functions having this property. Note that the "orthogonality" conditions (B) with respect to all spherically symmetric solutions are then satisfied exactly by symmetry. There is now, however, an additional relation [Eq. (5.1) of reference 3] valid for all particle-like solutions of (1.3), which the variational functions may be made to satisfy; namely

$$\int \left(\frac{\partial\psi}{\partial z}\right)^2 d\varrho = \int \left(\frac{\partial\psi}{\partial x}\right)^2 d\varrho. \qquad \text{(F)}$$

Suppose $\psi_0(\rho)$ is the lowest spherically symmetric solution of (1.3) corresponding to an energy E_0. Then clearly $\psi = \psi_0(|\varrho + \mathbf{R}|) - \psi_0(|\varrho - \mathbf{R}|)$ for R tending toward infinity is an odd-parity two-particle solution with an energy $E = 2E_0(< 3.01)$. We believe that this is indeed the lowest odd-parity solution. Hence in seeking variationally the lowest odd-parity one-particle solution, one must be careful that the lower two-particle solution is not being approached. The results of the variational approximations to the lowest one-particle and two-particle states respectively are contained in Tables III and IV.

Functions 9 and 10 are well localized and when used in the variational principle seem to give rough approximations to the energy of the lowest one-particle odd-parity state. Functions 12 and 13 are able to approximate, for certain limiting values of their parameters, a two-particle state, and the only minimum they give is of this nature.

Function 11 is a very flexible five-parameter function. Its form derives from the function

$$A[\rho P_1(\cos\theta)e^{-\alpha\rho} + b\rho^3 P_3(\cos\theta)e^{-\beta\rho}]$$

by including an additional cartesian scale parameter. In practice, however, it becomes a two-parameter function after satisfying relations (A), (E), and (F). The lowest extremum obtained using function 11 is a minimum representing a one-particle solution. Indeed the form of the function is such that for no values of the parameters could it approximate a two-particle state. The use of a trial function with more than five parameters in order to get a still better approximation to the lowest odd-parity one-particle state would involve an appreciable amount of labor. However, we believe that the energy of this state must be quite close to (4.11). We know of no other calculations to compare with ours for odd-parity states.

5. CONCLUSION

We have developed a variational principle for the eigensolutions of the most commonly considered nonlinear scalar field equation. The field equation appears as the Euler equation for the minimization of a Lagrangian subject to one or more subsidiary conditions.

The variational principle allows us to obtain approximate solutions to the nonlinear equation, and upper bounds to the corresponding values of the Lagrangian. Such solutions and bounds were ob-

TABLE IV. Variational approximations to the lowest odd-parity two-particle state of Eq. (1.3).

Function	Conditions satisfied exactly	Optimum parameter values				$\frac{1}{16\pi}\int \psi^4 \, d\varrho$
		A	α	n	R	
12. $Az^{2n+1} \exp(-\alpha\rho)$	(A), (B), (E)	$\to 0$	$\to\infty$	$\to\infty$	...	3.56
13. $A\{\exp(-\alpha\lvert\varrho - \mathbf{R}\rvert) - \exp(-\alpha\lvert\varrho + \mathbf{R}\rvert)\}$	(A), (B), (E), (F)	$4\sqrt{2}$	$\sqrt{3}$	...	$\to\infty$	3.08
Function constructed from Teshima's one-particle solution						3.01

tained for a set of trial functions for the first two spherically symmetric eigenstates. The best trial functions give energy values in good agreement with those of Teshima, which were obtained by numerical solution of the nonlinear equation.

The variational method is well suited to obtaining approximations to nonspherically symmetric eigensolutions of the nonlinear equation. We have obtained one variationial solution of odd parity. We expect that other nonspherically symmetric single-particle solutions exist.

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Generalized Momentum Operators in Quantum Mechanics*

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The usual form P_0 for the quantum-mechanical operator P conjugate to a generalized coordinate q_1 is, in atomic units,

$$P_0 = -ig^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}),$$

where g is the Jacobian of the transformation from Cartesian coordinates to the generalized coordinates. However, in some cases, this plusible form for P is not Hermitian with respect to physically acceptable bound-state wavefunctions, as it must be if it is to represent a real observable quantity. In this paper, the general form

$$P = -i(\mathbf{A}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{A})$$

is justified. Here $\mathbf{A} = h_1\hat{\mathbf{q}}_1$, where h_1 is the metric scale factor corresponding to q_1, and $\hat{\mathbf{q}}_1$ is the unit vector in the direction of increasing q_1. This general form reduces to P_0 if the usual formula for the divergence is applied. In the cases where P_0 is not Hermitian, it transpires that $\hat{\mathbf{q}}_1$ is ill-defined at one or both of the end points α and β of the range of q_1, and the divergence formula is thus invalid at such points. It is shown that, in order to obtain a Hermitian form for P, certain terms involving delta functions similar to Dirac's must be added to the usual formula for div $\mathbf{A}$. These terms can be regarded as implicit in div $\mathbf{A}$. If $\hat{\mathbf{q}}_1$ is ill-defined at the lower limit $q_1 = \alpha$, then the resulting new Hermitian form for P, which we propose as the correct one, is

$$P = -i[g^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}) + \tfrac{1}{2}\delta_+(q_1 - \alpha)].$$

If $\hat{\mathbf{q}}_1$ is, in addition, ill-defined at the upper limit $q_1 = \beta$, then the extra term $+\frac{1}{2}i\,\delta_-(\beta - q_1)$ must be added. Corresponding new forms are obtained for the Laplacian operator. In addition, the new formulas for P are applied to hypervirial relations. In the Appendix, Charles Goebel obtains a similar expression for the momentum operators by replacing the metric scale function by θg where θ is a step function, unity inside and zero outside the range of definition of the generalized coordinates. The differentiation of θ then produces the delta functions.

I. INTRODUCTION

THE usual form for the quantum-mechanical momentum operator which is conjugate to a generalized coordinate is, in some cases, not Hermitian with respect to physically acceptable bound-state wavefunctions. In such cases we propose, and seek to justify, that the correct Hermitian form is obtained by the addition of certain terms involving delta functions similar to Dirac's.

One of the basic assumptions of quantum mechanics is that to the classical observable p_x, the Cartesian x component of the momentum of a system, there corresponds the quantum-mechanical operator $P_x = -i\hbar\,\partial/\partial x$; we shall employ atomic units where $\hbar = 1$, so that $P_x = -i\,\partial/\partial x$. The P_x satisfies the necessary commutation rules, and it is Hermitian with respect to physically acceptable

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tained for a set of trial functions for the first two spherically symmetric eigenstates. The best trial functions give energy values in good agreement with those of Teshima, which were obtained by numerical solution of the nonlinear equation.

The variational method is well suited to obtaining approximations to nonspherically symmetric eigensolutions of the nonlinear equation. We have obtained one variationial solution of odd parity. We expect that other nonspherically symmetric single-particle solutions exist.

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Generalized Momentum Operators in Quantum Mechanics*

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The usual form P_0 for the quantum-mechanical operator P conjugate to a generalized coordinate q_1 is, in atomic units,

$$P_0 = -ig^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}),$$

where g is the Jacobian of the transformation from Cartesian coordinates to the generalized coordinates. However, in some cases, this plusible form for P is not Hermitian with respect to physically acceptable bound-state wavefunctions, as it must be if it is to represent a real observable quantity. In this paper, the general form

$$P = -i(\mathbf{A}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{A})$$

is justified. Here $\mathbf{A} = h_1\hat{\mathbf{q}}_1$, where h_1 is the metric scale factor corresponding to q_1, and $\hat{\mathbf{q}}_1$ is the unit vector in the direction of increasing q_1. This general form reduces to P_0 if the usual formula for the divergence is applied. In the cases where P_0 is not Hermitian, it transpires that $\hat{\mathbf{q}}_1$ is ill-defined at one or both of the end points α and β of the range of q_1, and the divergence formula is thus invalid at such points. It is shown that, in order to obtain a Hermitian form for P, certain terms involving delta functions similar to Dirac's must be added to the usual formula for div $\mathbf{A}$. These terms can be regarded as implicit in div $\mathbf{A}$. If $\hat{\mathbf{q}}_1$ is ill-defined at the lower limit $q_1 = \alpha$, then the resulting new Hermitian form for P, which we propose as the correct one, is

$$P = -i[g^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}) + \tfrac{1}{2}\delta_+(q_1 - \alpha)].$$

If $\hat{\mathbf{q}}_1$ is, in addition, ill-defined at the upper limit $q_1 = \beta$, then the extra term $+\frac{1}{2}i\,\delta_-(\beta - q_1)$ must be added. Corresponding new forms are obtained for the Laplacian operator. In addition, the new formulas for P are applied to hypervirial relations. In the Appendix, Charles Goebel obtains a similar expression for the momentum operators by replacing the metric scale function by θg where θ is a step function, unity inside and zero outside the range of definition of the generalized coordinates. The differentiation of θ then produces the delta functions.

I. INTRODUCTION

THE usual form for the quantum-mechanical momentum operator which is conjugate to a generalized coordinate is, in some cases, not Hermitian with respect to physically acceptable bound-state wavefunctions. In such cases we propose, and seek to justify, that the correct Hermitian form is obtained by the addition of certain terms involving delta functions similar to Dirac's.

One of the basic assumptions of quantum mechanics is that to the classical observable p_x, the Cartesian x component of the momentum of a system, there corresponds the quantum-mechanical operator $P_x = -i\hbar\,\partial/\partial x$; we shall employ atomic units where $\hbar = 1$, so that $P_x = -i\,\partial/\partial x$. The P_x satisfies the necessary commutation rules, and it is Hermitian with respect to physically acceptable

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bound-state wavefunctions. The eigenfunctions of P_x, $(2\pi)^{-\frac{1}{2}} \exp[i\lambda x]$, are orthogonal for different λ over $-\infty \leq x \leq \infty$, and Fourier analysis shows that an arbitrary bound-state wavefunction $\psi(x)$ can be expanded in terms of them.

It is natural to inquire whether a similar correspondence

$$p \leftrightarrow P = -i\,\partial/\partial q_1 \tag{1}$$

exists for p, the generalized classical momentum (assumed to be real) which is conjugate to any generalized coordinate q_1. Here p is defined as $\partial L/\partial \dot{q}_1$, where L is the classical Lagrangian. Such a correspondence is often asserted in texts on quantum mechanics, with the proviso that the operator $-i\,\partial/\partial q_1$ be Hermitian. Usually, however, this operator is not Hermitian as it stands. It is the object of this paper to show that a function $F(q_1)$ can always be chosen so that the operator

$$P = -i\,\partial/\partial q_1 + F(q_1) \tag{2}$$

is Hermitian with respect to acceptable bound-state wavefunctions. We observe that the inclusion of $F(q_1)$ does not affect the commutation relation

$$[P, q_1] = -i. \tag{3}$$

The operator P is actually restricted to the form (2) in order that the various commutation rules be satisfied.[1]

The status of momentum operators in quantum mechanics has always been somewhat obscure. Even the simplest one, P_x, is not a proper operator in Hilbert space, since its eigenfunctions are not quadratically integrable over the full range $-\infty \leq x \leq \infty$ (as a result it is convenient to introduce the concept of "eigendifferentials").[2] However, if a generalized momentum operator P is to represent a real observable p, then it is easily shown (see Sec. II) that P must be Hermitian with respect to acceptable bound-state wavefunctions. We realize that if one prefers not to regard a certain p as necessarily being an observable, then one does not need to assume that there exists a corresponding operator P with this Hermitian property. Nevertheless, it seems reasonable to us to suppose that real classical generalized momenta are in fact observables, and so we seek a general form for P which has the necessary Hermitian character.

What might be termed the "usual" form for P, which we call P_0, is

$$P_0 = -ig^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}\ ) = -i\,\partial/\partial q_1 - (i/2g)(\partial g/\partial q_1). \tag{4}$$

Here g is the magnitude of the Jacobian of the transformation from Cartesian coordinates to the generalized coordinates. The form (4) is discussed and justified by Kemble.[2] However, in some cases, even this plausible form is not Hermitian as required. In this paper we show that this shortcoming can be remedied by the addition of terms involving delta functions.

Firstly, however, the Hermitian character which must be imposed upon P is discussed. Next, the general form

$$P = -i(\mathbf{A}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{A}) \tag{5}$$

is justified. Here $\mathbf{A} = h_1\hat{\mathbf{q}}_1$, where $\hat{\mathbf{q}}_1$ is the unit vector in the direction of increasing q_1, and h_1 is the metric scale factor corresponding to the coordinate q_1. It is shown that the usual form P_0 [as given by (4)] is derivable from (5) by a straightforward application of the divergence formula. In the cases where P_0 is not Hermitian, it transpires that the vector $\hat{\mathbf{q}}_1$ is not well-defined at certain points, which are singularities of the coordinate system. The delta-function terms which must now be added to P_0 can be regarded as being implicit in div $\mathbf{A}$. We thus postulate that (5) is the true form for P, provided that the special interpretation of div $\mathbf{A}$ is made whenever necessary. If $\hat{\mathbf{q}}_1$ is ill-defined at the lower limit of q_1, $q_1 = \alpha$, then the explicit form of P is

$$P = -i[g^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}\ ) + \tfrac{1}{2}\,\delta_+(q_1 - \alpha)]. \tag{6}$$

If $\hat{\mathbf{q}}_1$ is also ill-defined at the upper limit $q_1 = \beta$, then we have

$$P = -i[g^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}\ ) + \tfrac{1}{2}\,\delta_+(q_1 - \alpha) - \tfrac{1}{2}\,\delta_-(\beta - q_1)] \tag{7}$$

(the delta-functions are discussed in Sec. IV). Even now, P is not in general Hermitian with respect to a pair of its own eigenfunctions. Such a property is equivalent to the orthogonality of the pair of eigenfunctions. In the following paper,[3] it is demonstrated that, although these eigenfunctions are not usually orthogonal to each other, an arbitrary bound-state wavefunction can nevertheless be expanded in terms of them.

Generalized momentum operators like P have recently come into prominence in connection with

[1] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, Oxford, England, 1947), 3rd Ed., Chap. 4.

[2] E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* (Dover Publications, Inc., New York, 1958).

[3] P. D. Robinson, J. Math. Phys. 4, 348 (1963).

the hypervirial relations introduced by Hirschfelder,[4,5,6] which have applications in a wide class of problems. The present paper is completed by a discussion of the relevance of the new form for P in this context. The new form is useful, since it is desirable that the operators which are employed be Hermitian. In a similar manner, a new form for the Laplacian operator is obtained involving delta functions. However, the delta-function terms rarely would have any effect on the theoretically predicted physical properties of a system.

In the Appendix, Charles Goebel approaches the determination of the momentum operator in a somewhat different manner. He extends the range of definition of the generalized coordinates by using a step function θ which is unity inside and zero outside the range of definition of the generalized coordinates. He then uses the "usual" form (4) for the momentum operator in which the metric scale factor g is replaced by the product θg. The differentiation of θ then produces delta functions at the usual integration limits of the coordinates. Effectively, Goebel's momentum operators are the same as our new form. His Eq. (A12) or (A13) (which are true only if his wavefunctions ϕ and ψ are bounded) agree with our Eq. (7). Thus, Goebel's treatment bolsters our conclusion.

II. THE HERMITIAN PROPERTY OF P

Since p is real, its mean value $\bar{p}$ in any bound state $\psi(q)$ of the system must also be real. Thus $\bar{p} = \bar{p}^*$, which means that

$$\int \psi^* P \psi \, d\tau = \int \psi P^* \psi^* \, d\tau. \tag{8}$$

The integration here is over the volume τ in which the system is confined (which might be the whole of space). If $\psi(q)$ were a continuum state, then it would not in general be quadratically integrable, and (8) would be replaced by a similar result involving the eigendifferentials[2] corresponding to $\psi(q)$. We shall always assume, however, that $\psi(q)$ is a bound state.

Equation (8) defines the Hermitian character which P must exhibit. P is said to be Hermitian with respect to the pair of functions ψ^* and ψ over the domain of integration τ. The stronger definition

$$\int \psi_1^* P \psi_2 \, d\tau = \int \psi_2 P^* \psi_1^* \, d\tau \tag{9}$$

for any two acceptable bound-state wavefunctions ψ_1 and ψ_2 is sometimes used. Equation (9) can be deduced from (8) if $\psi_1 + \psi_2$ and $\psi_1 + i\psi_2$ are also possible bound-state wavefunctions. Furthermore, it is asserted by Kemble[2] and others that P should be Hermitian in the sense of (9) with respect to any two of its own eigenfunctions ϕ_1 and, ϕ_2 (or, if necessary, the corresponding eigendifferentials). This requirement is equivalent to the orthogonality of ϕ_1 and ϕ_2; it can be shown[3] that such orthogonality is not usual for generalized momentum eigenfunctions, and that it is not necessary for the expansion of an arbitrary bound-state wavefunction in terms of the ϕ's. Thus (8) is the only Hermitian condition which we impose upon P.

III. THE GENERAL FORM FOR P

For simplicity, we assume that the quantum-mechanical system is merely a single particle of mass m, which is under the influence of a time-independent potential $V(q_1, q_2, q_3)$. Let the motion be described by a bound-state wavefunction $\psi(q_1, q_2, q_3)$.[7] q_1, q_2, and q_3 are three triply orthogonal, generalized coordinates with metric

$$ds^2 = h_1^2 \, dq_1^2 + h_2^2 \, dq_2^2 + h_3^2 \, dq_3^2, \tag{10}$$

and volume element

$$d\tau = h_1 h_2 h_3 \, dq_1 \, dq_2 \, dq_3 = g \, dq_1 \, dq_2 \, dq_3. \tag{11}$$

$g(= h_1 h_2 h_3)$ is the magnitude of the Jacobian of the transformation T from Cartesian coordinates (x, y, z) to the generalized coordinates (q_1, q_2, q_3). Let us fix attention on the coordinate q_1. We suppose that p is its conjugate momentum, and that P is the quantum-mechanical operator corresponding to p.

Classically, since V is independent of the $\dot{q}$'s, we have, from (10):

$$p = \partial L / \partial \dot{q}_1 = \partial / \partial \dot{q}_1 (\tfrac{1}{2} m \dot{s}^2) = m h_1^2 \dot{q}_1. \tag{12}$$

Furthermore, if $\boldsymbol{\pi}$ is the linear momentum vector of the particle ($\boldsymbol{\pi}$ has Cartesian components $p_x = m\dot{x}$, etc.), and if the vector $\mathbf{A}$ is defined by

$$\mathbf{A} = h_1^2 \operatorname{grad} q_1 = h_1 \hat{\mathbf{q}}_1, \tag{13}$$

then it follows from (12) that

$$p = \mathbf{A} \cdot \boldsymbol{\pi}. \tag{14}$$

The elementary rules for the Cartesian momentum components imply the correspondence

$$\boldsymbol{\pi} \leftrightarrow -i \operatorname{grad}. \tag{15}$$

Thus it seems reasonable to suppose that if (14) is first symmetrized to give

[4] J. O. Hirschfelder, J. Chem. Phys. **33**, 1462 (1960).
[5] S. T. Epstein and J. O. Hirschfelder, Phys. Rev. **123**, 1495 (1961).
[6] J. O. Hischfelder and C. A. Coulson, J. Chem. Phys. **36**, 941 (1962).
[7] All the wavefunctions mentioned in this paper are assumed to be time-independent.

$$p = \tfrac{1}{2}(\mathbf{A}\cdot\boldsymbol{\pi} + \boldsymbol{\pi}\cdot\mathbf{A}), \tag{16}$$

and then (15) is applied, we shall get a plausible form for P. This form is

$$P = -i[\mathbf{A}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{A}]$$
$$= -i[\partial/\partial q_1 + \tfrac{1}{2}\,\text{div}\,(h_1\hat{\mathbf{q}}_1)]. \tag{17}$$

Expression (17) is already in the required form (2), but if it is to be the true form for P, then it must exhibit the necessary Hermitian character. We can hope to establish this property with the help of Green's theorem (the divergence theorem), together with the identity

$$\psi^*(\mathbf{B}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{B})\psi$$
$$+ \psi(\mathbf{B}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{B})\psi^* \equiv \text{div}\,(\psi^*\psi\mathbf{B}), \tag{18}$$

which is true for any vector $\mathbf{B}$ and scalar ψ. We thus postulate that (17) is the true form for P, and proceed to investigate its Hermiticity. We will show that the Hermitian condition (8) is satisfied, provided that a certain interpretation (which will be explained) is placed on div $(h_1\hat{\mathbf{q}}_1)$ at points, if any, where $\hat{\mathbf{q}}_1$ is not well defined.

Setting $\mathbf{B} = \mathbf{A}$ in (18), it follows, using (17), that

$$\int \psi^* P\psi\, d\tau - \int \psi P^*\psi^*\, d\tau$$
$$= -i\int \text{div}\,(\psi^*\psi\mathbf{A})\, d\tau. \tag{19}$$

From this, we see that (8) is satisfied if and only if the volume integral

$$\int \text{div}\,(\psi^*\psi\mathbf{A})\, d\tau \tag{20}$$

vanishes. Assuming that Green's theorem can be applied to div $(\psi^*\psi\mathbf{A})$ over the whole of the region τ in which the system is confined, then, if S is the boundary surface of τ, we have

$$\int_\tau \text{div}\,(\psi^*\psi\mathbf{A})\, d\tau = \int_S \psi^*\psi\mathbf{A}\cdot d\mathbf{S}. \tag{21}$$

If the system is artificially confined, then a physically acceptable wavefunction ψ must be zero on S, and the surface integral vanishes. If τ is the whole of space, then, strictly, one should first consider Eq. (21) for a very large region τ. An acceptable ψ tends to zero sufficiently fast as S recedes to infinity to ensure that the surface integral vanishes in the limit. Thus, in order to establish that the general form (17) for P satisfies the Hermitian condition (8), we need only justify the application of Green's theorem in the form (21).

Sufficient conditions for the theorem to apply are that $\partial/\partial x(\psi^*\psi\mathbf{A}\cdot\mathbf{i})$, $\partial/\partial y(\psi^*\psi\mathbf{A}\cdot\mathbf{j})$ and $\partial/\partial z(\psi^*\psi\mathbf{A}\cdot\mathbf{k})$ be continuous in τ, and approach their values on S continuously. Here $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are unit vectors in the x, y, and z directions. These conditions can however be relaxed somewhat, and finite discontinuities in the partial derivatives are allowed across another surface which divides S into two parts. Thus the discontinuities in grad ψ which occur at nuclei will not present any difficulties. It is only the points where $\hat{\mathbf{q}}_1$ is not well-defined which should at first be excluded from the region over which Green's theorem is applied, and we will show that even such points can be included provided that the special interpretation of div $(h_1\hat{\mathbf{q}}_1)$ is made at these points whenever necessary.

Before continuing, we remark that the "usual" form (4) for P, which we call P_0, is now obtained directly from the formula for the divergence of any vector $\mathbf{B}$ in generalized coordinates, i.e.

$$\text{div}\,\mathbf{B} = \frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial q_1}(h_2h_3\mathbf{B}\cdot\hat{\mathbf{q}}_1)\right.$$
$$\left. + \frac{\partial}{\partial q_2}(h_3h_1\mathbf{B}\cdot\hat{\mathbf{q}}_2) + \frac{\partial}{\partial q_3}(h_1h_2\mathbf{B}\cdot\hat{\mathbf{q}}_3)\right]. \tag{22}$$

This gives

$$\text{div}\,(h_1\hat{\mathbf{q}}_1) = \frac{1}{g}\frac{\partial g}{\partial q_1}, \tag{23}$$

and, making use of (17), expression (4) for P_0 follows.

IV. THE INTERPRETATION OF div $(h_1\hat{\mathbf{q}}_1)$ WHEN $\hat{\mathbf{q}}_1$ IS ILL-DEFINED

It can be shown that the vector $\hat{\mathbf{q}}_1$ is only ill-defined in one of the following situations:

(i) when h_1 is zero;
(ii) when h_1 is infinite;
(iii) when h_2 or h_3 is zero.

At points where $\hat{\mathbf{q}}_1$ is ill-defined, the transformation T from (x, y, z) to (q_1, q_2, q_3) is not one-to-one. It is natural for these singular points of the transformation to correspond to extreme values of q_1, q_2 or q_3. If $\hat{\mathbf{q}}_1$ is not uniquely defined, then neither is the vector $\mathbf{A}$ $(=h_1\hat{\mathbf{q}}_1)$ or the general expression (22) for the divergence.

Let us suppose that the range of q_1 is $\alpha \leq q_1 \leq \beta$ and that $\hat{\mathbf{q}}_1$ is not defined uniquely at the lower limit $q_1 = \alpha$, which corresponds to a singularity (or singularities) in T. This means that instead of representing a *surface* of constant q_1 in (x, y, z) space, $q_1 = \alpha$ represents a degenerate form of surface, i.e. a line or a point. We will show that under certain circumstances it is necessary that

$$\text{div}\,(h_1\hat{\mathbf{q}}_1) = \frac{1}{g}\frac{\partial g}{\partial q_1} + \delta_+(q_1 - \alpha), \tag{24}$$

in order that Green's Theorem be applicable to div $(\psi^*\psi h_1\hat{\mathbf{q}}_1)$ over any region τ containing the point or line $q_1 = \alpha$. Furthermore, if the upper limit $q_1 = \beta$ also represents a degenerate surface, we must have

$$\text{div}\,(h_1\hat{\mathbf{q}}_1) = \frac{1}{g}\frac{\partial g}{\partial q_1} + \delta_+(q_1 - \alpha) - \delta_-(\beta - q_1). \quad (25)$$

[If the upper limit alone is degenerate, then the δ_+ term is omitted from (25).] The true form for P, which contains the modified expression for div $(h_1\hat{\mathbf{q}}_1)$, will now be Hermitian as required. It can be written in the form (6), or, if necessary, (7).

The functions δ_+ and δ_- in expressions (24), (25), (6), and (7) are similar to Dirac's delta functions; the only difference is that their effects inside an integral are, respectively,

$$\int_\alpha^t U(q_1)\,\delta_+(q_1 - \alpha)\,dq_1 = U(\alpha), \quad \alpha < t \leq \beta, \quad (26)$$

and

$$\int_t^\beta U(q_1)\,\delta_-(\beta - q_1)\,dq_1 = U(\beta), \quad \alpha \leq t < \beta, \quad (27)$$

for any continuous function $U(q_1)$. These delta functions have been discussed by Friedman.[8] Strictly, delta functions are meaningless unless appearing in an integrand. Thus (24) and (25) are not strict definitions of div $(h_1\hat{\mathbf{q}}_1)$ at the end points α and β; rather do they represent equalities of effect in an integration over q_1.

To justify (21), let us consider the integral of div $(\psi^*\psi h_1\hat{\mathbf{q}}_1)$ over a region τ_1 which is bounded by the surface $q_1 = t$, $\alpha < t < \beta$. If this surface is closed (e.g. a sphere or ellipsoid), then it forms the entire boundary surface S_1 of τ_1. It also surrounds the degenerate surface $q_1 = \alpha$, which must be either a point or a finite line. Alternatively, if the surface $q_1 = t$ is open (and thus extends to infinity if the system is not artificially confined), then the boundary S_1 is formed by $q_1 = t$ together with a surface or surfaces represented by extreme cases of q_2 or q_3 = constant. However, these latter surfaces will not contribute at all to the surface integral in Eq. (28) which follows, for $\hat{\mathbf{q}}_1$ is everywhere tangential to them. In this second situation, $q_1 = \alpha$ represents an infinite or semi-infinite line.

Formal application of Green's theorem gives

$$\int_{\tau_1} \text{div}\,(\psi^*\psi h_1\hat{\mathbf{q}}_1)\,d\tau = \int_{S_1} \psi^*\psi h_1\hat{\mathbf{q}}_1\cdot d\mathbf{S} = \iint (\psi^*\psi g)_{q_1=t}\,dq_2\,dq_3. \quad (28)$$

The usual divergence formula (22) implies that

$$\text{div}\,(\psi^*\psi h_1\hat{\mathbf{q}}_1) - \frac{1}{g}\,\partial/\partial q_1(\psi^*\psi g) = 0. \quad (29)$$

But

$$\int_{\tau_1} \frac{1}{g}\frac{\partial}{\partial q_1}(\psi^*\psi g)\,d\tau = \iiint \frac{\partial}{\partial q_1}(\psi^*\psi g)\,dq_1\,dq_2\,dq_3 = \iint [(\psi^*\psi g)_{q_1=t} - (\psi^*\psi g)_{q_1=\alpha}]\,dq_2\,dq_3. \quad (30)$$

Thus, from (28) and (30),

$$\int_{\tau_1}\left[\text{div}\,(\psi^*\psi h_1\hat{\mathbf{q}}_1) - \frac{1}{g}\frac{\partial}{\partial q_1}(\psi^*\psi g)\right]d\tau = \iint (\psi^*\psi g)_{q_1=\alpha}\,dq_2\,dq_3. \quad (31)$$

Equation (29) certainly holds for $\alpha < q_1 \leq t$, and so the integrand on the left-hand side of (31) can only be nonvanishing if $q_1 = \alpha$. Neither $\psi^*\psi$ nor g is ever negative. Thus, unless

$$(\psi^*\psi g)_{q_1=\alpha} = 0 \quad \text{for all} \quad q_2 \quad \text{and} \quad q_3, \quad (32)$$

it follows that the right-hand side of (31) is positive. Consequently, Eq. (31) can only hold for all acceptable ψ's which do not satisfy (32) if

$$\text{div}\,(\psi^*\psi h_1\hat{\mathbf{q}}_1) - \frac{1}{g}\frac{\partial}{\partial q_1}(\psi^*\psi g) = \psi^*\psi\,\delta_+(q_1 - \alpha). \quad (33)$$

Remembering that $h_1\hat{\mathbf{q}}_1\cdot$grad is $\partial/\partial q_1$, the ψ dependence now disappears to give

$$\text{div}\,(h_1\hat{\mathbf{q}}_1) - \frac{1}{g}\frac{\partial g}{\partial q_1} = \delta_+(q_1 - \alpha). \quad (24)$$

With this interpretation of div $(h_1\hat{\mathbf{q}}_1)$, Green's theorem can always be applied to div $(\psi^*\psi h_1\hat{\mathbf{q}}_1)$ over the region τ_1. Similarly it can be shown that regions containing points where $q_1 = \beta$ are always allowable when the $\delta_-(\beta - q_1)$ term is included in div $(h_1\hat{\mathbf{q}}_1)$, as in (25). Thus it is possible to apply Green's theorem in the form (21) over the whole of the region τ in which the system is confined, and the necessary Hermiticity of P follows.

Perhaps the simplest case where (32) does not hold (and thus delta functions are needed to make P Hermitian) arises when ψ is a σ-type hydrogen atom wavefunction expressed in terms of the parabolic coordinates $u = r(1 - \cos\theta)$, $v = r(1 + \cos\theta)$ and ϕ (see, for example, Schiff[9]). The limits on the coordinates are $0 \leq u \leq \infty$, $0 \leq v \leq \infty$, and $0 \leq \phi \leq 2\pi$; g takes the value $(u + v)/4$. The expressions $\psi^*(0, v, \phi)\psi(0, v, \phi)v/4$ and $\psi^*(u, 0, \phi)\psi(u, 0, \phi)u/4$

[8] B. Friedman, *The Principles and Techniques of Applied Mathematics* (John Wiley & Sons, Inc., New York, 1956), Chap. III.

[9] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd Edition, Chap. IV.

are generally not zero. Indeed, ψ would have to vanish along the entire semi-axes $\theta = 0$ and $\theta = \pi$ if they were. Thus (32) is not satisfied with $q_1 = u$ or with $q_1 = v$. A similar situation arises when the prolate spheroidal coordinates $\xi = (r_a + r_b)/R$, $\eta = (r_a - r_b)/R$ and ϕ are employed in the wavefunctions for a diatomic ion with nuclei at A and B. Here r_a and r_b are the respective distances of the electron from A and B; $AB = R$; $g = (\xi^2 - \eta^2)R^3/8$; and the limits on ξ and η are $1 \leq \xi \leq \infty$ and $-1 \leq \eta \leq 1$.

It sometimes happens that condition (32) is satisfied because of the nature of g. For example, in spherical polar coordinates (r, θ, ϕ) where $g = r^2 \sin\theta$, $\psi^*\psi g$ is zero at $r = 0$ (the lower limit of r) for all values of θ and ϕ. $\psi^*\psi g$ also vanishes at both the limits of θ, $\theta = 0$ and $\theta = \pi$, for all values of r and ϕ. In such cases, the need for P to be Hermitian does not lead to the introduction of delta functions, and the usual form P_0 given by (4) exhibits the required Hermitian character. Even so, it is reasonable to regard (24) or (25) as a sound interpretation[10] of div $(h_1\hat{\mathbf{q}}_1)$. Equation (24) can be rewritten as

$$g \operatorname{div} [(h_1/g)\hat{\mathbf{q}}_1] = \delta_+(q_1 - \alpha). \tag{34}$$

It can be seen, using Green's theorem [or formula (22)], that the volume integral of div $[(h_1/g)\hat{\mathbf{q}}_1]$ vanishes when taken over any region not containing points where $q_1 = \alpha$ or β. But formal application of Green's theorem over the region τ_1 gives [cf. (28)]

$$\int_{\tau_1} \operatorname{div}\left(\frac{h_1}{g}\,\hat{\mathbf{q}}_1\right) d\tau \equiv \iiint g \operatorname{div}\left(\frac{h_1}{g}\,\hat{\mathbf{q}}_1\right) dq_1\, dq_2\, dq_3 = \iint dq_2\, dq_3, \tag{35}$$

which is only consistent if (34) holds.

There is an analogy here with electrostatics. To take a simple example, the field $\mathbf{E}$ of a unit point charge situated in vacuo at the origin $r = 0$ is

$$\mathbf{E} = (1/r^2)\hat{\mathbf{r}}. \tag{36}$$

$\mathbf{E}$ must satisfy div $\mathbf{E} = 0$ in regions where there is no charge, and div $\mathbf{E} = 4\pi\rho$ if there is a charge density ρ. Both these conditions can be expressed in the single relation

$$r^2 \operatorname{div} [(1/r^2)\hat{\mathbf{r}}] = \delta_+(r), \tag{37}$$

which is the form of (34) in polar coordinates with $q_1 = r$.

[10] The delta-function interpretation of div $(h_1\hat{\mathbf{q}}_1)$ is an extension of a one-dimensional result of Friedman (reference 8), which states: "The symbolic derivative of a piecewise differentiable function with jumps is the ordinary derivative, where it exists, plus the sum of δ-functions at the jumps multiplied by the magnitude of the jumps."

We conclude this section by listing the forms of P which contain delta functions in the four most frequently used coordinate systems (Cartesian coordinates excepted).

General form:

$$P = -i[\partial/\partial q_1 + \tfrac{1}{2} \operatorname{div} (h_1\hat{\mathbf{q}}_1)]. \tag{17}$$

(i) Spherical polar coordinates (r, θ, ϕ), $g = r^2 \sin\theta$:

$$P_r = -i[\partial/\partial r + 1/r + \tfrac{1}{2}\,\delta_+(r)], \tag{38}$$

$$P_\theta = -i[\partial/\partial\theta + \tfrac{1}{2}\cot\theta + \delta_+(\theta) - \delta_-(\pi - \theta)]. \tag{39}$$

(ii) Cylindrical polar coordinates (u, ϕ, z), $g = u$:

$$P_u = -i\{\partial/\partial u + \tfrac{1}{2}[1/u + \delta_+(u)]\}. \tag{40}$$

(iii) Parabolic coordinates (u, v, ϕ), $g = (u + v)/4$:

$$P_u = -i\{\partial/\partial u + \tfrac{1}{2}[1/(u + v) + \delta_+(u)]\}, \tag{41}$$

$$P_v = -i\{\partial/\partial v + \tfrac{1}{2}[1/(u + v) + \delta_+(v)]\}. \tag{42}$$

(iv) Prolate spheroidal coordinates (ξ, η, ϕ), $g = (\xi^2 - \eta^2)R^3/8$:

$$P_\xi = -i[\partial/\partial\xi + \xi/(\xi^2 - \eta^2) + \tfrac{1}{2}\,\delta_+(\xi - 1)], \tag{43}$$

$$P_\eta = -i[\partial/\partial\eta - \eta/(\xi^2 - \eta^2) + \tfrac{1}{2}\,\delta_+(\eta + 1) - \tfrac{1}{2}\,\delta_-(1 - \eta)]. \tag{44}$$

In the polar systems (i) and (ii), the appropriate condition (32) is satisfied and it is not necessary to include the delta functions in order that P should be Hermitian with respect to acceptable bound-state wavefunctions. As we have shown, however, the delta functions occur naturally in the div $(h_1\hat{\mathbf{q}}_1)$ contribution to P, and so it seems reasonable to include them in P itself.

As Epstein points out,[11] it is possible to change the parametrization of a coordinate system so that the new g vanishes at the integration limits. Thus even if ψ is not required to vanish there, the new condition like (32) will still be satisfied and the corresponding P will not require delta functions for its Hermiticity. For example, in (iv) above, ξ and η can be replaced by λ and μ where $\xi = \cosh\lambda$ and $\eta = \cos\mu$. With this parametrization, the new form for g is $g = (\cosh^2\lambda - \cos^2\mu)\sin\lambda\sin\mu$, which vanishes at the new integration limits $\lambda = 0$ and $\mu = 0$ or π. In such cases, because the singularities in the coordinate system are not removed, we believe that delta-function terms should still be included in P, but that their effect inside an integral is usually nullified by the new form for g. This is the same situation which arises directly with the polar systems (i) and (ii) above. An "inverse" example is provided by the spherical polar system (i) if r and θ are replaced by new coordinates $s = \frac{1}{3}r^3$

[11] S. T. Epstein, private communication (22 May 1962).

and $t = \cos\theta$. The new g is unity, and the delta-function terms are now certainly necessary for the Hermiticity of the operators P_s and P_t.

V. THE EFFECT OF THE DELTA FUNCTIONS ON THE EIGENFUNCTIONS OF P

The eigenfunctions ϕ of P_0, the usual form (4) for P, are

$$\phi(q_1, q_2, q_3; \lambda) = N(q_2, q_3)g^{-\frac{1}{2}} \exp(i\lambda q_1), \qquad \alpha \leq q_1 \leq \beta, \tag{45}$$

where λ is the eigenvalue and $N(q_2, q_3)$ is an arbitrary function of q_2 and q_3. If instead P takes the new form, which amounts to

$$P = P_0 - \tfrac{1}{2}i\,\delta_+(q_1 - \alpha) + \tfrac{1}{2}i\,\delta_-(\beta - q_1), \tag{7}$$

then the new eigenfunctions Φ are still given by expression (45) at all internal points $\alpha < q_1 < \beta$, since the delta functions vanish unless $q_1 = \alpha$ or $q_1 = \beta$ as the case may be. The only effect of the delta functions is to introduce discontinuities in the eigenfunctions at the end points α and β. The nature of these discontinuities can be derived in a formal manner from the eigenvalue equation, which is

$$g^{-\frac{1}{2}}\,\partial/\partial q_1(g^{\frac{1}{2}}\Phi) + \tfrac{1}{2}[\delta_+(q_1 - \alpha) - \delta_-(\beta - q_1)]\Phi = i\lambda\Phi. \tag{46}$$

Equation (46) has the solution

$$\Phi = Q(q_1)\phi, \tag{47}$$

provided that

$$dQ/dq_1 + \tfrac{1}{2}[\delta_+(q_1 - \alpha) - \delta_-(\beta - q_1)]Q = 0. \tag{48}$$

Thus, formally,

$$Q(q_1) = C \exp\left\{\tfrac{1}{2}\int_\alpha^{q_1} [\delta_+(q - \alpha) - \delta_-(\beta - q)]\,dq\right\}, \tag{49}$$

which means that

$$Q(q_1) = Ce^{\frac{1}{2}}, \qquad \alpha < q_1 < \beta, \tag{50}$$

and

$$Q(\alpha) = Q(\beta) = C. \tag{51}$$

The choice of $C = e^{-\frac{1}{2}}$ for the constant of integration enables us to take $\Phi = \phi$ at all internal points $\alpha < q_1 < \beta$, and $\Phi = e^{-\frac{1}{2}}\phi$ at the end points.

Because of these discontinuities in the eigenfunctions Φ at the end points, Eqs. (26) and (27), which define the effects of the delta functions inside an integral, are not satisfied with $U = \Phi$. As a result, it can be shown[12] that even the new form for P is not Hermitian in the sense of (9) with respect to a pair of its own eigenfunctions $\Phi_1(\lambda_1)$ and $\Phi_2(\lambda_2)$. Since

$$0 \neq \int \Phi_1^* P \Phi_2\,d\tau - \int \Phi_2 P^* \Phi_1^*\,d\tau = (\lambda_2 - \lambda_1)\int \Phi_1^*\Phi_2\,d\tau,$$

the non-Hermiticity is equivalent to the non-orthogonality of Φ_1 and Φ_2. This is not a new situation, as the eigenfunctions ϕ of the usual form P_0 are not in general orthogonal either. In fact,

$$\int_\alpha^\beta \Phi_1^*\Phi_2 g\,dq_1 = \int_\alpha^\beta \phi_1^*\phi_2 g\,dq_1, \tag{52}$$

since the discontinuities in Φ have no effect on the integral here. As already mentioned, the non-orthogonality of the eigenfunctions is discussed in the following paper.

VI. APPLICATION TO HYPERVIRIAL OPERATORS

In classical mechanics, the time-average value of the Poisson Bracket of the Hamiltonian H with a function w of the coordinates and momenta is zero, provided that the function w remains finite throughout the trajectory. Hence,[4] letting the bar indicate the time average,

$$\overline{(H, w)} = 0. \tag{53}$$

Correspondingly, in quantum mechanics, the diagonal elements of the Heisenberg equation of motion in the energy representation state that[4,5,6,13]

$$\langle\psi\,|i[H, W]|\,\psi\rangle = 0. \tag{54}$$

Here ψ is a bound-state energy eigenfunction and W is the quantum-mechanical operator corresponding to w. If $w = \sum_i \mathbf{r}_i\cdot\boldsymbol{\pi}_i$, Eq. (53) is the classical virial theorem and (54) is the quantum-mechanical virial theorem. For other choices of w, Eqs. (53) and (54) give the hypervirial relations.

The quantum-mechanical hypervirial relations can be used to improve approximate wavefunctions. Suppose, for example, that $\psi(\mathbf{q}, a)$ is an approximate wavefunction with an imbedded variational parameter a. The $\mathbf{q}$ denotes the dependence on the generalized coordinates $q_1, q_2, \cdots, q_n$. Further let us suppose that

$$\partial\psi/\partial a = iW\psi, \tag{55}$$

[12] See Appendix where Goebel, using a different sort of derivation, reaches a different conclusion.

[13] Equation (54) requires that H be Hermitian with respect to $W\psi$ as well as to ψ. S. T. Epstein points out in University of Wisconsin Theoretical Chemistry Report WIS-AEC-37 (June 1962), for hydrogen atom bound S states, if $W = p_r$ (the radial momentum), then H is not Hermitian with respect to $W\psi$ and (54) must be corrected accordingly. As is shown in this same report and also by P. D. Robinson and J. O. Hirschfelder, in University of Wisconsin Theoretical Chemistry WIS-NASA-1 (August 1962), the hypervirial relations may be modified so as to apply to continuum wavefunctions and scattering problems.

where W is a Hermitian operator. Then, if $\psi(\mathbf{q}, a_0)$ satisfies (54), it is easy to show that[5] the approximate energy E is stationary with respect to variations of a around a_0, that is $(\partial E/\partial a)_{a=a_0} = 0$. In this proof, the Hermitian nature of W was required first in showing that

$$\langle iW\psi \mid H\psi\rangle + \langle \psi \mid iHW\psi\rangle = \langle \psi \mid i[H, W] \mid \psi\rangle, \quad (56)$$

and second in showing that

$$\langle iW\psi \mid \psi\rangle + \langle \psi \mid iW\psi\rangle = 0. \quad (57)$$

The most useful hypervirials are generated by functions of the form

$$w = \tfrac{1}{2}(fp + pf). \quad (58)$$

Here f is a function of the generalized coordinates and p is the momentum conjugate to q_1. In accordance with the discussion in Secs. III and IV, the corresponding Hermitian quantum-mechanical operator is

$$W = -i(\mathbf{B}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{B}). \quad (59)$$

Here $\mathbf{B} = fh_1\hat{\mathbf{q}}_1 = f\mathbf{A}$. Then since $\text{div}\,\mathbf{B} = f\,\text{div}\,\mathbf{A} + \mathbf{A}\cdot\text{grad}\,f$, it follows that

$$W = -if(\mathbf{A}\cdot\text{grad} + \tfrac{1}{2}\,\text{div}\,\mathbf{A}) - \tfrac{1}{2}i\mathbf{A}\cdot\text{grad}\,f. \quad (60)$$

Making use of (17), Eq. (60) becomes

$$W = fP - \tfrac{1}{2}i\,\partial f/\partial q_1. \quad (61)$$

Finally, using the new form for the momentum operator (7), we have

$$W = -i\{f^{\frac{1}{2}}g^{-\frac{1}{2}}\,\partial/\partial q_1(f^{\frac{1}{2}}g^{\frac{1}{2}}\ \ ) + \tfrac{1}{2}f[\delta_+(q_1 - \alpha) - \delta_-(\beta - q_1)]\}. \quad (62)$$

Here, as before, the delta functions are required only when the coordinate transformation from curvilinear to Cartesian is ill-defined at the extreme values α and β of q_1. If the delta functions were omitted from W, Eqs. (56) and (57) might not be satisfied.

Let us consider an example. In a discussion[6] of the diatomic hydrogen ion H_2^+, the hypervirial (in prolate spheroidal coordinates)

$$w = \tfrac{1}{2}(\xi p_\xi + p_\xi\xi) + \tfrac{1}{2}(\eta p_\eta + p_\eta\eta) \quad (63)$$

was used. The usual formula for the quantum-mechanical momentum operator then led to

$$W_0 = -i(\xi\,\partial/\partial\xi + \eta\,\partial/\partial\eta + 2). \quad (64)$$

The new form for the momentum operator, or (62), leads to

$$W = W_0 - \tfrac{1}{2}i[\xi\,\delta_+(\xi - 1) + \eta\,\delta_+(\eta + 1) - \eta\,\delta_-(1 - \eta)]. \quad (65)$$

Since Σ-type H_2^+ wavefunctions are not zero along the entire internuclear axis, the addition of the delta functions makes an appreciable contribution to the various integrals. In reference (6), W_0 was used erroneously in place of W. Fortunately, none of the conclusions were affected. However, subsequently, Leon Jones found that Eq. (57) was not satisfied when he used W_0. Indeed, it was the investigation of this seeming paradox that led to the present paper.

By a transformation of the coordinates, a hypervirial operator (linear in the momentum) can be expressed in the form of a momentum operator in a new coordinate set. Let W be given by (62) and define the new coordinate S by the relation

$$S = \int \frac{dq_1}{f}. \quad (66)$$

In this integration, all of the q's except q_1 are held fixed. Then W may be written in the form

$$W = -i\{(fg)^{-\frac{1}{2}}\,\partial/\partial S((fg)^{\frac{1}{2}}\ \ ) + \tfrac{1}{2}[\delta_+(S - \alpha') - \delta_-(\beta' - S)]\}, \quad (67)$$

where α' and β' are the extreme values of S. The expression (67) now corresponds to a momentum operator in an orthogonal coordinate system where fg is the product of the metric scale factors. It is easy to show that

$$[W, S] = -i, \quad (68)$$

and therefore S is the coordinate conjugate to W. Provided that W is independent of a, the explicit solution to (55) is found to be[5]

$$\psi(\mathbf{q}, a) = g^{-\frac{1}{2}}(\partial\sigma/\partial q_1)^{\frac{1}{2}}\Phi(\sigma, q_2, \cdots, q_n). \quad (69)$$

Here $q_1 \to \sigma(\mathbf{q}, a)$ is a point transformation such that

$$S(\sigma) = a + S(q_1). \quad (70)$$

In order that the functional form for $\psi(\mathbf{q}, a)$ be suitable to represent a bound-state wavefunction, the following criteria for f have been found:

(1) f must be finite and continuous for all interior points.

(2) At any interior point where $f = 0$, the value of $\partial f/\partial q_1$ must be finite.

(3) At the integration limits for q_1, the value of f/q_1 must be finite.

With the use of delta functions, the third condition can now be relaxed at integration limits where the value of q_1 is finite.

VII. A NEW FORM FOR THE LAPLACIAN

Corresponding to the new forms for P and div $(h_1\hat{\mathbf{q}}_1)$ given by expressions (6) and (24) [or, if necessary, by (7) and (25)], it is possible to find a new form for the Laplacian ∇^2. If $U(q_1)$ is a function of q_1 alone, then

$$\nabla^2 U = \text{div grad } U = \text{div } (h_1\hat{\mathbf{q}}_1 \cdot h_1^{-2}\,\partial U/\partial q_1)$$

$$= [\text{div } (h_1\hat{\mathbf{q}}_1)]h_1^{-2}\,\partial U/\partial q_1 + \partial/\partial q_1(h_1^{-2}\,\partial U/\partial q_1). \quad (71)$$

From (24), this becomes

$$\nabla^2 U = [g^{-1}\,\partial/\partial q_1(gh_1^{-2}\,\partial/\partial q_1) + \delta_+(q_1 - \alpha)h_1^{-2}\,\partial/\partial q_1]U. \quad (72)$$

If, in addition, U is a function of q_2 and q_3, then the appropriate terms in $\partial/\partial q_2$ and $\partial/\partial q_3$ must be added to the new expression (72) for ∇^2.

If we are guided merely by the requirement that ∇^2, being proportional to the kinetic energy operator, is Hermitian with respect to acceptable bound-state wavefunctions, then we are led to the form

$$\nabla^2 U = [g^{-1}\,\partial/\partial q_1(gh_1^{-2}\,\partial/\partial q_1) + \delta_+(q_1 - \alpha)(h_1^{-2}\,\partial/\partial q_1 + G)]U, \quad (73)$$

where G is an arbitrary real function. The choice $G = 0$ makes (73) agree with (72).

There is a third approach. In terms of the usual form P_0 for P, the usual form for $\nabla^2 U$ is $-g^{-\frac{1}{2}}P_0 g h_1^{-2} P_0 g^{-\frac{1}{2}}U$. With the new form (6) for P, we find that, in order to arrive at (72), it is necessary to require the convention

$$\delta_+^2(q_1 - \alpha) = -2h_1^2 g^{-1}\,\partial/\partial q_1[gh_1^{-2}\,\delta_+(q_1 - \alpha)] \quad (74)$$

for the meaning of δ_+^2. With the aid of this convention, expressions for powers of P can be derived directly from (6).

If the $\delta_-(\beta - q_1)$ term is needed, as in (7) and (25), then we must have $\delta_+(q_1 - \alpha) - \delta_-(\beta - q_1)$ in Eqs. (72), (73), and (74) instead of $\delta_+(q_1 - \alpha)$.

It should be observed that the delta-function terms in ∇^2 do not often have any effect. Usually the $\delta_+(q_1 - \alpha)$ in (72) is nullified, either by the h_1^{-2} which may be zero at $q_1 = \alpha$, or by the g which appears in the volume element for an integration.

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APPENDIX. A FORMAL TREATMENT OF DIFFERENTIAL OPERATORS IN A FINITE REGION.

(This treatment is by Charles J. Goebel, Department of Physics, University of Wisconsin, Madison, Wisconsin.)

We shall consider the derivative operator in a one-dimensional space. It is well known that if the inner product of two functions is defined as

$$(\phi, \psi) = \int g(x)\,dx\phi^*(x)\psi(x), \quad (A1)$$

where $g(x)$ is a real "weight function", then the real anti-Hermitian derivative operator D, with the properties

$$D^* = D, \qquad D(x\ ) = [x\,D + 1](\ ), \qquad (\phi, D\psi) = -(\psi, D\phi)^* \quad (A2)$$

is given by

$$D = g^{-\frac{1}{2}}\,\partial_x(g^{\frac{1}{2}}\ \ ) = \partial_x + \tfrac{1}{2}g^{-1}g'. \quad (A3)$$

The eigenfunctions $\varphi_\lambda(x)$ of D, satisfying

$$D\varphi_\lambda = i\lambda\varphi_\lambda\ , \quad (A4)$$

are given by

$$\varphi_\lambda = (2\pi g)^{-\frac{1}{2}}e^{i\lambda x}, \quad (A5)$$

the constant factor being chosen so that they are orthonormal

$$\int g(x)\,dx\varphi_\lambda^*(x)\varphi_{\lambda'}(x) = \delta(\lambda - \lambda') \quad (A6)$$

and complete

$$\int d\lambda\varphi_\lambda^*(x)\varphi_\lambda(y) = \frac{\delta(x - y)}{g(x)}. \quad (A7)$$

We now want to consider the case in which the integration in the definition of the inner product, Eq. (A1), extends only over a finite region, say $\alpha < x < \beta$. Formally, the results (A3)–(A7) will continue to hold if the limitations on the range of integration are effected by the vanishing of the weight function g outside the range α to β.

For instance, suppose that

$$(\phi, \psi) = \int_\alpha^\beta dx\phi^*\psi, \quad (A8)$$

i.e. of the form (1) with

$$g(x) = \theta(\beta - x)\theta(x - \alpha), \quad (A9)$$

where $\theta(x)$ is the "step function" defined by

$$\theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0, \end{cases} \quad (A10)$$

with the derivative

$$\theta'(x) = \delta(x). \tag{A11}$$

The anti-Hermitian derivative D, as given by (A3), is then

$$D = \partial_x + \frac{\delta(x-\alpha)}{2\theta(x-\alpha)} - \frac{\delta(x-\beta)}{2\theta(\beta-x)}, \tag{A12}$$

i.e.

$$\begin{aligned}(\phi, D\psi) &= \int_\alpha^\beta dx\phi^*(x)\Big[\theta(\beta-x)\theta(x-\alpha)\,\partial_x \\ &\quad + \frac{\delta(x-\alpha)}{2} - \frac{\delta(x-\beta)}{2}\Big]\psi(x) \\ &= \int_\alpha^\beta dx\phi^*\psi' + \frac{\phi^*(\alpha)\psi(\alpha)}{2} \\ &\quad - \frac{\phi^*(\beta)\psi(\beta)}{2}.\end{aligned} \tag{A13}$$

Here (A13) agrees with Eq. (7) of the text. The eigenfunctions of D, as given by (A5), are

$$\varphi_\lambda(x) = (2\pi\theta(\beta-x)\theta(x-\alpha))^{-\frac{1}{2}}e^{i\lambda x}; \tag{A14}$$

they are orthogonal and complete, according to (A6) and (A7), although the orthogonality, and the completeness for x and y outside the interval α to β, is only formal, because of the infiniteness of the negative powers of the step function. Of course the expansion in these eigenfunctions of a function defined in the interval α to β,

$$\psi(x) = \int d\lambda a(\lambda)\varphi_\lambda(x), \qquad \alpha < x < \beta,$$

$$\text{where} \quad a(\lambda) = \int g(x)\,dx\varphi_\lambda^*(x)\psi(x),$$

is identical to the expansion in "plane waves" $(2\pi)^{-\frac{1}{2}}\,e^{i\lambda x}$ because the $\varphi_\lambda(x)$ are identical to these in the region where the function $g(x)\psi(x)$ is nonzero.

On the Nonorthogonality of Generalized Momentum Eigenfunctions in Quantum Mechanics*

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The orthogonality requirement usually specified for the eigenfunctions ϕ of a quantum-mechanical operator P which has a continuous spectrum of eigenvalues λ, is $\int \phi^*(\lambda)\phi(\lambda')\,d\lambda = \delta(\lambda - \lambda')$. The derivation of this result is examined; it is seen to be merely a sufficient, but not a necessary condition for the consistent expansion of a bound-state wavefunction ψ in the form $\int a(\lambda)\phi(\lambda)\,d\lambda$. The situation when P is a generalized momentum operator is investigated in detail. Such operators were discussed in the preceding paper. It is shown that any two of the corresponding momentum eigenfunctions are not usually orthogonal. Nevertheless, with the help of Fourier analysis, a consistent expansion $\psi = \int a(\lambda)\phi(\lambda)\,d\lambda$ is established. The theory is illustrated with the familiar examples of a "particle in a box" and a ground-state hydrogen atom.

When a space coordinate has a finite range, a quantum condition can be imposed on the generalized momentum eigenvalues so that the momentum eigenfunctions form a complete discrete orthogonal set. We attempt to justify the belief that such quantization is not essential unless it is necessary to ensure single-valued eigenfunctions.

I. INTRODUCTION

IT is frequently implied in texts on quantum mechanics that, if a quantum-mechanical operator P has a continuous spectrum of eigenvalues λ, then any two of its appropriately normalized eigenfunctions $\phi(\lambda)$ and $\phi(\lambda')$ are orthogonal to each other by virtue of a relation

$$\int \phi^*(\lambda)\phi(\lambda')\,d\tau - \delta(\lambda - \lambda'). \tag{1}$$

Here δ is the Dirac delta function, and the integration is over the whole of the space to which the system is confined. This relation is sometimes specified as being a necessary condition for the consistent expansion of an arbitrary, physically acceptable bound-state wavefunction ψ in the form

$$\psi = \int a(\lambda)\phi(\lambda)\,d\lambda. \tag{2}$$

In this paper, the situation when P is a generalized momentum operator is examined. These operators were discussed in the preceding paper.[1] It is shown that any two of the corresponding generalized momentum eigenfunctions ϕ are *not* usually orthogonal. The only exception occurs with such functions as $\phi = (2\pi)^{-\frac{1}{2}} \exp[i\lambda x]$, where x is a Cartesian coordinate; in this case,

$$(2\pi)^{-1} \int_{-\infty}^{\infty} \exp[i(\lambda' - \lambda)x]\,dx$$

is a possible definition of $\delta(\lambda - \lambda')$, and condition (1) is automatically satisfied.

This apparent paradox of nonorthogonal eigenfunctions is resolved. First we study a "proof" of the orthogonality requirement (1), and it is seen that (1) is merely a *sufficient*, but not a *necessary* condition to be met in order that a consistent expansion (2) be possible. The relevant equations involving the momentum eigenfunctions are next discussed. With the help of Fourier analysis, a consistent expansion like (2) is established even though condition (1) is not usually satisfied. The theory is then illustrated with the familiar examples of a "particle in a box" and a ground-state hydrogen atom. When a space coordinate has a finite range, a quantum condition can be imposed on the generalized momentum eigenvalues so that the momentum eigenfunctions form a complete discrete orthogonal set. In conclusion, we attempt to justify the belief that such quantization is not essential unless it is necessary to ensure single-valued eigenfunctions.

II. THE PLAUSIBILITY OF THE ORTHOGONALITY RELATION

For simplicity, we consider the quantum-mechanical system corresponding to a particle in a bound state described by a wavefunction ψ which is a function of a single noncyclic coordinate q. We suppose that the range of q is $\alpha \leq q \leq \beta$, and that ψ is normalized with the help of an appropriate

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[1] P. D. Robinson and J. O. Hirschfelder, J. Math. Phys. 4, 338 (1963).

weighting factor $w(q)$, so that

$$\int_\alpha^\beta \psi^*(q)\psi(q)w(q)\,dq = 1. \tag{3}$$

Thus the particle may either have only one degree of freedom, or it may have more degrees of freedom which are not represented in ψ for reasons of symmetry (e.g. an s-state electron in a hydrogen atom). It is assumed that $w(q)$ is not zero or infinite in the open interval $\alpha < q < \beta$, but it may be so at the end points α and β. (A zero or infinity in $w(q)$ is a natural boundary for q).

According to the Principle of Superposition of States, $\psi(q)$ can be "expanded" as in (2) in terms of the eigenfunctions $\phi(q, \lambda)$ of an operator P, viz:

$$\psi(q) = \int_{\text{all }\lambda} a(\lambda)\phi(q, \lambda)\,d\lambda. \tag{4}$$

Here $a^*(\lambda)a(\lambda)\,d\lambda$ is the probability that λ has a value in the interval $(\lambda, \lambda + d\lambda)$, and it follows that

$$\int_\alpha^\beta \psi^*(q)\psi(q)w(q)\,dq = \int a^*(\lambda)a(\lambda)\,d\lambda. \tag{5}$$

Substitution for ψ^* from the conjugate of (4) into (5) yields

$$\int_\alpha^\beta \psi(q)\left[\int a^*(\lambda)\phi^*(q, \lambda)\,d\lambda\right]w(q)\,dq = \int a^*(\lambda)a(\lambda)\,d\lambda. \tag{6}$$

Assuming that the order of integration in (6) can be inverted, we obtain

$$\int a^*(\lambda)\left[a(\lambda) - \int_\alpha^\beta \phi^*(q, \lambda)\psi(q)w(q)\,dq\right]d\lambda = 0, \tag{7}$$

which implies that $a(\lambda)$ is uniquely[2] defined by

$$a(\lambda) = \int_\alpha^\beta \phi^*(q, \lambda)\psi(q)w(q)\,dq. \tag{8}$$

Now substitute for ψ from (4) into (8), and invert the order of integration, giving

$$a(\lambda) = \int a(\lambda')\left[\int_\alpha^\beta \phi^*(q, \lambda)\phi(q, \lambda')w(q)\,dq\right]d\lambda'. \tag{9}$$

It is often argued that since (9) must hold for any $a(\lambda)$ which is consistent with the expansion of an arbitrary acceptable $\psi(q)$ in the form (4), then it must follow that a delta-function orthogonality relation

$$\int_\alpha^\beta \phi^*(q, \lambda)\phi(q, \lambda')w(q)\,dq = \delta(\lambda - \lambda') \tag{10}$$

(similar to (1), with $d\tau = w\,dq$) is satisfied by the ϕ's. Clearly (10) is a *sufficient* condition for (9) to hold, for then the delta-function property ensures that the right-hand side of (9) is also $a(\lambda)$; however, as we shall see, it is not *necessary* that (10) be true in order that (9) should be.

A relation similar to (9) which must exist between the ψ's and the ϕ's is found by substituting for $a(\lambda)$ from (8) into (4), viz:

$$\psi(q) = \int_{q'=\alpha}^\beta \psi(q') \times \left[\int \phi^*(q', \lambda)\phi(q, \lambda)\,d\lambda\right]w(q')\,dq'. \tag{11}$$

We now go on to discuss the equations of this section in the case where $\phi(q, \lambda)$ is the generalized momentum eigenfunction corresponding to the coordinate q.

III. THE GENERALIZED MOMENTUM EIGENFUNCTIONS AND FOURIER TRANSFORM THEORY

In the preceding paper,[1] it is shown that:

(i) the usual form P_0 for the generalized momentum operator P conjugate to the coordinate q is

$$P_0 = -iw^{-\frac{1}{2}}\,d/dq(w^{\frac{1}{2}}); \tag{12}$$

(ii) if an acceptable bound-state wavefunction ψ exists for which

(a) $(\psi^*\psi w)_{q=\alpha} \neq 0$ and/or (b) $(\psi^*\psi w)_{q=\beta} \neq 0$,

then it is necessary to add to P_0 the corresponding delta-function terms

(a) $-\frac{1}{2}i\,\delta_+(q - \alpha)$ and/or (b) $+\frac{1}{2}i\,\delta_-(\beta - q)$,

in order to obtain a form for P which is Hermitian with respect to ψ^* and ψ. Here we have assumed that $\hbar = 1$, and the more general weighting factor $g(q_1, q_2, q_3)$ of the preceding paper has been replaced by $w(q)$.

If no delta functions are needed in P, then the eigenfunctions of P are those of P_0 [as given by (12)], i.e.

$$\phi(q, \lambda) = Nw^{-\frac{1}{2}} \exp[i\lambda q], \qquad \alpha \leq q \leq \beta. \tag{13}$$

Here N is a kind of normalizing factor which is determined later. If either delta-function term is present, however, it can be formally shown[1] that a finite discontinuity in ϕ is caused at the appropriate end point. Even so, integrals like

[2] Alternatively, one might deduce from (7) that $a(\lambda) = \int \phi^*\psi w\,dq + b(\lambda)$, where $\int a^*(\lambda)b(\lambda)\,d\lambda = 0$, but it would then follow from (4) and (5) that $\int b^*(\lambda)b(\lambda)\,d\lambda = 0$, i.e. $b(\lambda) = 0$.

$$\int_{q=\alpha}^{\beta} f(q)\phi(q, \lambda)\, dq$$

can still be evaluated using the ϕ given by Eq. (13) if $f(q)$ is finite in the neighborhood of α and β. We have assumed that q is noncyclic, and that the generalized momentum eigenvalues λ form a continuous spectrum from $-\infty$ to $+\infty$. (If q were a cyclic coordinate, then the singlevaluedness of ϕ would impose a quantum condition on λ).

Equations (4) and (8) now become, from (13),

$$w^{\frac{1}{2}}\psi(q) = N \int_{-\infty}^{\infty} a(\lambda) \exp [i\lambda q]\, d\lambda, \qquad (14)$$

and

$$a(\lambda) = N \int_{q=\alpha}^{\beta} w^{\frac{1}{2}}\psi(q) \exp [-i\lambda q]\, dq, \qquad (15)$$

respectively. The similarity between (14) and (15) and formulas for the Fourier transform and inverse Fourier transform is apparent. The Fourier transform $A(\lambda)$ of a function $F(q)$ may be defined as

$$A(\lambda) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} F(q) \exp [-i\lambda q]\, dq. \qquad (16)$$

It now follows from a theorem of Titchmarsh[3] that, if $F(q')$ is quadratically integrable over $-\infty \leq q' \leq \infty$, and is of bounded variation in the neighborhood of $q' = q$, then

$$\tfrac{1}{2}\{F(q + 0) - F(q - 0)\} = (2\pi)^{-\frac{1}{2}} \lim_{t\to\infty} \int_{-t}^{t} A(\lambda) \exp [i\lambda q]\, d\lambda. \qquad (17)$$

The function $w^{\frac{1}{2}}\psi(q)$ is, however, only meaningful in the physically relevant range of the system $\alpha \leq q \leq \beta$. Thus, to establish the identification with Fourier-transform theory when α and β are both finite, we must define $F(q)$ as follows:

$$\begin{aligned}
&\text{(i)} && F(q) = 0, && q < \alpha;\\
&\text{(ii)} && F(q) = \tfrac{1}{2}w^{\frac{1}{2}}(\alpha)\psi(\alpha), && q = \alpha;\\
&\text{(iii)} && F(q) = w^{\frac{1}{2}}(q)\psi(q), && \alpha < q < \beta;\\
&\text{(iv)} && F(q) = \tfrac{1}{2}w^{\frac{1}{2}}(\beta)\psi(\beta), && q = \beta;\\
&\text{(v)} && F(q) = 0, && q > \beta.
\end{aligned} \qquad (18)$$

If β is $+\infty$ but α is finite, then (iii) is extended to the range $\alpha < q \leq \infty$ and (iv) and (v) are omitted. Similarly, if α is $-\infty$ but β is finite, then (iii) is extended to $-\infty \leq q < \beta$ while (i) and (ii) are omitted. If α is $-\infty$ and β is $+\infty$, then we simply define $F(q)$ as $w^{\frac{1}{2}}(q)\psi(q)$ for all q. The normalization condition (3) ensures that $F(q)$ is quadratically integrable, and we can safely assume that it is of bounded variation, for $w^{\frac{1}{2}}\psi(q)$ is neither infinite nor wildly oscillatory if ψ is an acceptable bound-state wavefunction. With the above definitions of $F(q)$, it therefore follows from (17) that

$$F(q) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} A(\lambda) \exp [i\lambda q]\, d\lambda, \qquad (19)$$

the limiting process in (17) being understood. Finally, if we set

$$N = (2\pi)^{-\frac{1}{2}}, \qquad (20)$$

then we see from (15), (16), and (18) that

$$a(\lambda) \equiv A(\lambda). \qquad (21)$$

We can thus invoke Fourier-transform theory and assert that, provided N is taken to be $(2\pi)^{-\frac{1}{2}}$, then Eqs. (14) and (15) are mutually consistent; Eq. (14) becomes the same as (19), and Eq. (15) the same as (16). Furthermore, we note that Eq. (11), with substitution from (13), (18), and (20), is now just the exponential form of Fourier's integral formula, i.e.,

$$F(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(q') \exp [i(q - q')\lambda]\, d\lambda\, dq'. \qquad (22)$$

Also Parseval's theorem for Fourier transforms

$$\int_{-\infty}^{\infty} F^*(q)F(q)\, dq = \int_{-\infty}^{\infty} A^*(\lambda)A(\lambda)\, d\lambda \qquad (23)$$

can be identified with the probability equivalence relation (5).

IV. THE NONORTHOGONALITY OF THE MOMENTUM EIGENFUNCTIONS

We turn our attention to the crucial equation (9), upon which claims of orthogonality of the ϕ's are based. Using Eqs. (16), (18), (19), and (21), we can establish the relation

$$a(\lambda) = (2\pi)^{-1} \int_{q=\alpha}^{\beta} \exp [-i\lambda q]\, dq \int_{-\infty}^{\infty} a(\lambda') \times \exp [i\lambda' q]\, d\lambda'. \qquad (24)$$

This relation (24), if the order of integration is inverted, is precisely the form taken by equation (9) when we substitute for the ϕ's from (13). Thus

[3] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford University Press, Oxford, England, 1948), 2nd Ed., Chap. III.

Fourier-transform theory has shown that there is no necessity for the ϕ's to be orthogonal in order that (9) should hold. Consequently an expansion like (4), for $\psi(q)$ in terms of generalized momentum eigenfunctions, is possible without such orthogonality.

It is interesting to examine the various forms of the integral

$$\int_\alpha^\beta \phi^*(q, \lambda)\phi(q, \lambda')w(q)\, dq, \tag{25}$$

which, from (13) and (20), is the same as

$$(2\pi)^{-1} \int_\alpha^\beta \exp\,[i(\lambda' - \lambda)q]\, dq. \tag{26}$$

There are three different cases to consider: (a) α and β both finite; (b) one finite and one infinite; (c) $\alpha = -\infty$ and $\beta = +\infty$. The results are:

$$\text{(a)}\quad (2\pi)^{-1} \int_\alpha^\beta \exp\,[i(\lambda' - \lambda)q]\, dq = \frac{\exp\,[i(\lambda' - \lambda)\beta] - \exp\,[i(\lambda' - \lambda)\alpha]}{2\pi i(\lambda' - \lambda)}; \tag{27}$$

$$\text{(b)}\quad (2\pi)^{-1} \int_\alpha^\infty \exp\,[i(\lambda' - \lambda)q]\, dq = (2\pi)^{-1} \exp\,[i(\lambda' - \lambda)\alpha] \times [\pi\delta(\lambda - \lambda') + i(\lambda' - \lambda)^{-1}], \tag{28}$$

(there is a similar result here if $\alpha = -\infty$ and β is finite);

$$\text{(c)}\quad (2\pi)^{-1} \int_{-\infty}^\infty \exp\,[i(\lambda' - \lambda)q]\, dq = \delta(\lambda - \lambda'). \tag{29}$$

It is only in case (c), where the range of q is from $-\infty$ to $+\infty$, that the eigenfunctions $\phi(q, \lambda)$ are always orthogonal for different λ's. It should be observed that the integrals are not strictly convergent in cases (b) and (c). The right-hand sides of (28) and (29) are really Cesàro sums of order unity.[4] In (28), $(\lambda' - \lambda)^{-1}$ is to be interpreted as zero (the mean of its limits as $\lambda \to \lambda' + 0$ and $\lambda \to \lambda' - 0$) when $\lambda = \lambda'$. As regards the equality of effect inside the integral over λ' in (9), it is perfectly legitimate to employ these Cesàro sums.

In the two cases (a) and (b) where the consistency of Eq. (9) is not obvious, it is possible to demonstrate this consistency without appeal to Fourier-transform theory. The appropriate result (27) or (28) is first inserted for the integral (25) on the right-hand side of (9), and then the calculus of residues is employed in conjunction with (15) to show that the right-hand side of (9) does in fact simplify to $a(\lambda)$.

We have seen that any two generalized momentum eigenfunctions with the same q but different λ's are not usually orthogonal to one another. However, they are always orthogonal with respect to integration over λ if they have the same λ but different q's. Using (13) and (20), we obtain

$$\int_{-\infty}^\infty \phi^*(q', \lambda)\phi(q, \lambda)\, d\lambda = (2\pi)^{-1} w^{-\frac{1}{2}}(q')w^{\frac{1}{2}}(q) \int_{-\infty}^\infty \exp\,[i(q' - q)\lambda]\, d\lambda = w^{-\frac{1}{2}}(q')w^{\frac{1}{2}}(q)\, \delta(q - q'). \tag{30}$$

This directly ensures the consistency of Eq. (11).

V. TWO SIMPLE EXAMPLES

To illustrate the above theory, we quote two familiar examples from elementary quantum mechanics where the generalized momentum eigenfunctions are not orthogonal, and yet a consistent expansion of a wavefunction in terms of them is possible.

(a) "Particle in a Box"

A particle of unit mass is restricted to the section $0 \leq x \leq L$ of the x axis, where it can move freely. Here we have

$$\psi_n(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi x}{L}\right), \qquad n = 1, 2, 3 \cdots;$$

$$w(x) = 1;$$

$$\phi(x, \lambda) = (2\pi)^{-\frac{1}{2}} \exp\,(i\lambda x);$$

$$\int_0^L \phi^*(x, \lambda)\phi(x, \lambda')\, dx = \frac{\exp\,[i(\lambda' - \lambda)L] - 1}{2\pi i(\lambda' - \lambda)} \neq 0$$

(unless $(\lambda' - \lambda)L = 2k\pi$ where k is an integer);

$$a(\lambda) = \int_0^L \phi^*(x, \lambda)\psi_n(x)\, dx = n(L\pi)^{\frac{1}{2}}(n^2\pi^2 - \lambda^2L^2)^{-1}[1 + (-)^{n+1} \exp\,(-i\lambda L)].$$

It can be verified that $\psi_n(x) = \int_{-\infty}^{+\infty} a(\lambda)\phi(x, \lambda)\, d\lambda$.

(b) Ground-State Hydrogen Atom

For a hydrogen atom in its ground state, we have, in atomic units,

[4] The integral $\int_0^\infty f(t)\, dt$ is said to be summable by Cesàro's means of order $\gamma \geq 0$ to the sum I if

$$\lim_{T\to\infty} \int_0^T (1 - t/T)^\gamma f(t)\, dt = I.$$

$$\psi(r) = \pi^{-\frac{1}{2}} \exp[-r], \quad 0 \leq r \leq \infty;$$

$$w(r) = 4\pi r^2;$$

$$\phi(r, \lambda) = (2\pi 2^{\frac{1}{2}} r)^{-1} \exp[i\lambda r];$$

$$\int_0^\infty \phi^*(r, \lambda)\phi(r, \lambda')w(r)\, dr = \tfrac{1}{2}\,\delta(\lambda - \lambda') + \frac{i}{2\pi(\lambda' - \lambda)} \neq 0;$$

$$a(\lambda) = \int_0^\infty \phi^*(r, \lambda)\psi(r)w(r)\, dr = \left(\frac{2}{\pi}\right)^{\frac{1}{2}}(1 + i\lambda)^{-2}.$$

Again it can be verified that $\psi(r) = \int_{-\infty}^{\infty} a(\lambda)\phi(r, \lambda)\, d\lambda$.

VI. CONCLUSION AND DISCUSSION

We have seen that any acceptable bound-state wavefunction $\psi(q)$ can be expanded in the form

$$\psi(q) = \int_{-\infty}^{\infty} a(\lambda)\phi(q, \lambda)\, d\lambda, \tag{4'}$$

where the functions $\phi(q, \lambda)$ are the eigenfunctions of the generalized momentum operator P which is conjugate to q, i.e.,

$$\phi(q, \lambda) = (2\pi w)^{-\frac{1}{2}} \exp[i\lambda q]. \tag{13'}$$

The expansion coefficients are determined uniquely from the expression

$$a(\lambda) = \int_\alpha^\beta \phi^*(q, \lambda)\psi(q)w(q)\, dq. \tag{8'}$$

The functions $\phi(q, \lambda)$, although not necessarily orthogonal, nevertheless form a complete continuum set for the expansion of acceptable ψ's. This completeness is a direct consequence of Plancherel's theorem for complex Fourier transforms, which establishes the convergence *in mean* of such an expansion to any quadratically integrable function. From (17) and (18), it follows that the integral in (4') is convergent to $\psi(q)$ in the open interval $\alpha < q < \beta$. If the end points $q = \alpha$ and/or $q = \beta$ are finite, then Eq. (4') only holds at these points when $w^{\frac{1}{2}}\psi$ is zero there. We should not expect (4') to be true otherwise, for then it is necessary to include the delta-function terms in the operator P, with the resultant uncertainty in its eigenfunctions at the end points.

An interesting situation arises when the range of q from α to β is a finite one. The functions $\phi(q, \lambda)$ can then be made orthogonal to one another for different λ by imposing a quantum condition on λ. The orthogonality integral (25) takes the form (27), which always vanishes if

$$\lambda' - \lambda = 2k\pi/(\beta - \alpha), \quad k = \pm 1, \pm 2, \cdots. \tag{31}$$

Condition (31) is satisfied provided that the momentum eigenvalues are

$$\lambda = C + 2k\pi/(\beta - \alpha), \quad k = 0, \pm 1, \pm 2, \cdots, \tag{32}$$

where C is an arbitrary constant. Any two members of the countably infinite subset $\{\phi_k(q)\}$ of the continuum set $\{\phi(q, \lambda)\}$, where

$$\phi_k(q) = (2\pi w)^{-\frac{1}{2}} \exp\{iq[C + 2\pi k/(\beta - \alpha)]\}, \quad k = 0, \pm 1, \pm 2, \cdots, \tag{33}$$

thus satisfy the orthogonality relationship

$$\int_\alpha^\beta \phi_k^*(q)\phi_{k'}(q)w(q)\, dq = (2\pi)^{-1}(\beta - \alpha)\,\delta_{kk'}. \tag{34}$$

We can see that the set of functions $\{\phi_k(q)\}$ is also complete. There can exist no normalized function $G(q)$ orthogonal to all the $\phi_k(q)$'s, for this would imply the existence of a function $(2\pi w)^{\frac{1}{2}}G(q) \exp[-iqC]$ with all its Fourier coefficients over $\alpha \leq q \leq \beta$ equaling zero, which in turn would imply that $G(q)$ is zero.[5] The set $\{\phi_k(q)\}$ is thus closed, and therefore complete.[5]

The functions $\phi_k(q)$, which are normalized if multiplied by $(2\pi)^{\frac{1}{2}}(\beta - \alpha)^{-\frac{1}{2}}$, form a complete orthogonal set of discrete generalized momentum eigenfunctions. Von Neumann[6] would insist that the quantum condition (31) is necessary, and that the $\phi_k(q)$'s are in fact the only true momentum eigenfunctions, for they are mutually orthogonal and the operator P is thus Hermitian with respect to any pair of them. However, we have seen that the orthogonality is unnecessary for the expansion of an acceptable $\psi(q)$, and in the preceding paper[1] it was shown that on physical grounds, P need only be Hermitian with respect to acceptable bound-state wavefunctions. Thus there would seem to be no direct need for the quantum condition (31). Furthermore, when one or other of the limits α and β is infinite, such a quantum condition is not possible. In this case, if one insists on the orthogonality of eigenfunctions, one must reject P as a quantum-mechanical operator which represents an observable quantity. We are inclined to believe that this orthogonality is not essential, and accordingly that the quantum condition (31) is not necessary. The condition is indeed rather a strange one, because of the arbitrariness of the constant C which is introduced into the eigen-

[5] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1953), Vol. I, Chap. II.

[6] J. Von Neumann, *Mathematical Foundations of Quantum Mechanics*, translated by R. T. Beyer (Princeton University Press, Princeton, New Jersey, 1955), Chap. II.

values. We think that the only occasion on which a generalized momentum eigenvalue is quantized is when this is necessary to ensure that the eigenfunction is single valued. This happens if q is a cyclic coordinate, for example an azimuthal angle.

The situation discussed above for a finite range of q is curious, but does not lead to any obvious paradoxes. $\psi(q)$ can either be expanded as in (4′) in terms of the complete continuum set $\{\phi(q, \lambda)\}$, or it can be expanded as an infinite sum in terms of the complete discrete set $\{\phi_k(q)\}$. In the latter case, we have

$$\psi(q) = \sum_{k=-\infty}^{\infty} a_k \phi_k(q), \tag{35}$$

where

$$a_k = 2\pi(\beta - \alpha)^{-1} \int_{\alpha}^{\beta} \phi_k^*(q)\psi(q)w(q)\, dq. \tag{36}$$

The series (35) is effectively a Fourier-series expansion for a function of period $(\beta - \alpha)$ which takes the form $(2\pi w)^{+\frac{1}{2}} \exp[-iqC]\psi(q)$ when $\alpha \leq q \leq \beta$. Like the integral in (4′), this series is convergent in the open interval $\alpha < q < \beta$, but not at the end points unless $w^{\frac{1}{2}}\psi$ is zero there. An apparent paradox arises if we expand an arbitrary momentum eigenfunction $\phi(q, \lambda)$ in terms of the set $\{\phi_k(q)\}$, i.e.

$$\phi(q, \lambda) = \sum_{k=-\infty}^{\infty} c_k \phi_k(q), \tag{37}$$

and then apply the operator P. This gives, formally,

$$\lambda\phi(q, \lambda) = \sum_{k=-\infty}^{\infty} [C + 2\pi k/(\beta - \alpha)]c_k\phi_k(q). \tag{38}$$

If (38) were true, it would follow from the orthogonality of the ϕ_k's that $\lambda = C + 2\pi k/(\beta - \alpha)$ for all k. However, to obtain (38) we have effectively differentiated (37), term by term, with respect to q, and the explicit form of c_k shows that this is not allowed because the series in (38) is divergent.

Finally we remark that, although for simplicity we have discussed merely a one-dimensional system in this paper, the extension to include more dimensions is not difficult. For instance, in a system described by three generalized coordinates (q_1, q_2, q_3), the eigenfunctions of the momentum operator P_1 conjugate to the variable q_1 are[1]

$$\phi(q_1, q_2, q_3; \lambda) = N(q_2, q_3)g^{-\frac{1}{2}}(q_1, q_2, q_3) \exp[i\lambda q_1]. \tag{39}$$

Here g is the Jacobian of the transformation from Cartesian coordinates to the generalized coordinates, and N is an arbitrary function of q_2 and q_3. $\phi(q_1, q_2, q_3; \lambda)$ can be made a suitably normalized, simultaneous eigenfunction of P_1, q_2, and q_3, if we take N to be[7] $(2\pi)^{-\frac{1}{2}}\, \delta(q_2 - q_2')\, \delta(q_3 - q_3')$. With this choice for N, an arbitrary bound-state wavefunction $\psi(q_1, q_2, q_3)$ can be expanded in the form

$$\psi(q_1, q_2, q_3) = \iiint a(\lambda)\phi(q_1, \lambda; q_2, q_2'; q_3, q_3')\, d\lambda\, dq_2'\, dq_3', \tag{40}$$

where

$$a(\lambda) = \iiint \phi^*(q_1, \lambda; q_2, q_2'; q_3, q_3') \times \psi(q_1, q_2, q_3)g(q_1, q_2, q_3)\, dq_1\, dq_2\, dq_3. \tag{41}$$

The delta-function factors in $N(q_2, q_3)$ now effectively reduce the system to a one-dimensional one.

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[7] E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* (Dover Publications, Inc., New York, 1958), Chap. VIII.

Electrostatic Interactions in Complex Electron Configurations*

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Simplified expressions for the matrix elements of electrostatic interactions both within and between several types of complex electron configurations have been obtained by the application of angular-momenta recoupling techniques. The use of these recoupling techniques avoids the usual extensive calculation of the sums of products of the matrix elements of tensors of the types $V^{\kappa k}$ and U^k. The derived expressions involve the sums of products of coefficients of fractional parentage and $n-j$ symbols, and as such, are amenable to machine computation.

INTRODUCTION

STUDIES of the complex spectra of rare-earth and actinide ions are complicated by the frequent requirement of a detailed knowledge of the structure of quite complex electron configurations, and in some cases a knowledge of the electrostatic interactions between the configurations is necessary. The configurations of greatest interest are typified by f^n, $f^n l'$, $f^n l' l''$, and $f^n l'^2$. The electrostatic matrices of all the f^n configurations are well known and will not be discussed. Of primary interest will be the interactions of the electrons outside the f^n core with those of the f^n core. The number of states occurring for these configurations is very large, and hence it is desirable to be able to compute the matrix elements on a high-speed computer. However, before calculations such as these are attempted, it is essential that the expressions for the matrix elements be put in as simple a form as is possible.

Racah[1] and Arima *et al.*[2] have given general procedures for calculating the matrix elements of direct and exchange-type interactions between outer electrons and an equivalent electron core. Their treatment of exchange-type interactions requires the expanding of the exchange interactions into the sums of direct interactions. This approach—although equivalent, in its final results, to the method outlined in this paper—is complicated by the appearance of sums of products of tensors of the types $V^{\kappa k}$ and U^k. In seeking simplifications of their formulas and in making the formulas amenable to machine computation, it is desirable to avoid having to evaluate the matrix elements of several tensorial quantities prior to the actual evaluation of the electrostatic matrix elements. In the present formulation of the problem, the need to evaluate the matrix elements of the double tensors $V^{\kappa k}$ is overcome by suitably recoupling the angular momenta of the electrons involved in the electrostatic interactions. As a result, the formulas may be expressed in a concise manner that displays clearly the properties of the angular momenta involved by the use of $n-j$ symbols.[3]

$l^n l' l''$ CONFIGURATIONS

It will be assumed that the two inequivalent electrons are coupled together and then coupled to the l^n core to form a total-orbital and a total-spin quantum number. For complete generality, consider the matrix elements of the angular part of the electrostatic interaction between a configuration $l^n l' l''$ and a second configuration $l^n l''' l^{i v}$. We may write, for the matrix elements of the electrostatic interactions of the inequivalent electrons with the l^n equivalent electron core,

$$
\begin{aligned}
&(l^n S_1 L_1 (sl', sl'') S_1' L_1'; S_2 L_2 \\
&\quad \times |\sum_{i<j} (C_i^k \cdot C_j^k)| \; l^n S_3 L_3 (sl''', sl^{iv}) S_3' L_3'; S_4 L_4) \\
&\quad = n \sum_{\psi} (\psi_1 \{| \bar{\psi}) (\psi_3 \{| \bar{\psi}) (l^{n-1} \bar{\alpha} \bar{S} \bar{L}, sl, S_1 L_1 \\
&\quad \times (sl', sl'') S_1' L_1'; S_2 L_2 \; |(C_i^k \cdot C_j^k)| \; l^{n-1} \bar{\alpha} \bar{S} \bar{L}, sl, \\
&\quad \times S_3 L_3 (sl''', sl^{iv}) S_3' L_3'; S_4 L_4), \qquad (1)
\end{aligned}
$$

where the $(\psi \{| \bar{\psi})$ are the usual coefficients of

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[1] G. Racah, Phys. Rev. **62**, 438 (1942).

[2] A. Arima, H. Horie, and Y. Tanabe, Progr. Theoret. Phys. (Kyoto) **11**, 143 (1954).

[3] M. Rotenberg, R. Bivins, N. Metropolis, and J. K. Wooten, *The 3-j and 6-j Symbols* (Technology Press, Cambridge, Massachusetts, 1959).

fractional parentage[4,5] and the scalar products, $(C_i^k \cdot C_j^k)$, are tensorial sets of spherical harmonics.[6] The matrix element in (1) may now be examined. First a series of recouplings[6] of the type

$$((\bar{S}s)S_1, (ss)S_1'; S_2 \mid \bar{S}(sS_1')\sigma; S_2)$$
$$= (-1)^{\bar{S}+s+S_1'+S_2}([S_1][\sigma])^{\frac{1}{2}}\begin{Bmatrix} S_1' & S_2 & S_1 \\ \bar{S} & s & \sigma \end{Bmatrix} \quad (2)$$

is made, where $[\sigma]$, etc., are understood as $(2\sigma + 1)$, etc. Upon recoupling in both spin and orbital space, the matrix element in right-hand side (rhs) of (1) becomes

$$\sum_{\substack{\sigma\lambda \\ \sigma'\lambda'}} (-1)^{S_1'+S_2'+L_1'+L_2'} \times \delta(\sigma, \sigma')\ \delta(\lambda, \lambda')\ \delta(S_2, S_4)\ \delta(L_2, L_4) \times ([S_1][S_3][L_1][L_3])^{\frac{1}{2}}[\sigma][\lambda]\begin{Bmatrix} S_1' & S_2 & S_1 \\ \bar{S} & s & \sigma \end{Bmatrix}\begin{Bmatrix} S_2' & S_4 & S_3 \\ \bar{S} & s & \sigma' \end{Bmatrix} \times \begin{Bmatrix} L_1' & L_2 & L_1 \\ \bar{L} & l & \lambda \end{Bmatrix}\begin{Bmatrix} L_3' & L_4 & L_3 \\ \bar{L} & l & \lambda' \end{Bmatrix}(\sigma\lambda \mid (C_i^k \cdot C_j^k) \mid \sigma'\lambda'), \quad (3)$$

where

$$(\sigma\lambda \mid (C_i^k \cdot C_j^k) \mid \sigma'\lambda') = ((sS_1')\sigma, (lL_1')\lambda \mid (C_i^k \cdot C_j^k) \mid (sS_3')\sigma', (lL_3')\lambda'). \quad (4)$$

Thus there remains only to evaluate the matrix elements in (4) for three electrons, and then perform the sum over σ and λ in (3). For direct interactions the calculation is quite straightforward,[6] and after application of the Biedenharn–Elliott sum rule[3] to the sum over λ, the matrix element on the rhs of Eq. (1) becomes, for direct interactions,

$$(-1)^{L_1'+L_2+L_2+l+k}[l]\begin{Bmatrix} l & k & l \\ 0 & 0 & 0 \end{Bmatrix}(L_1' \mid\mid C_i^k \mid\mid L_3') \times \begin{Bmatrix} L_3' & k & L_1' \\ L_1 & L_2 & L_3 \end{Bmatrix}(\psi_1 \mid\mid U^k \mid\mid \psi_3), \quad (5)$$

where

$$(\psi_1 \mid\mid U^k \mid\mid \psi_3) = n([L_1][L_3])^{\frac{1}{2}} \sum_{\bar{\psi}} (\psi_1\{\mid\bar{\psi})(\psi_3\{\mid\bar{\psi}) \times (-1)^{\bar{L}+L_1+l+k}\begin{Bmatrix} l & L_1 & \bar{L} \\ L_3 & l & k \end{Bmatrix}. \quad (6)$$

If the coefficients of the radial integral $R^k(ll'; ll''')$ are required, the matrix element in (5) is evaluated by putting

$$(l'l''L_1' \mid\mid C_1^k \mid\mid l'''l^{iv}L_3') = (-1)^{l'''+L_3'+k}([l'][l'''][L_1'][L_3'])^{\frac{1}{2}} \times \begin{bmatrix} l' & k & l''' \\ 0 & 0 & 0 \end{bmatrix}\begin{Bmatrix} L_1' & L_3' & k \\ l''' & l' & l'' \end{Bmatrix}\delta(l'', l^{iv}), \quad (7)$$

whereas if the coefficients of $R^k(ll''; ll^{iv})$ are required, we write

$$(l'l''L_1' \mid\mid C_2^k \mid\mid l'''l^{iv}L_3') = (-1)^{l'+l'''+l^{iv}+L_1'+k}([l''][l^{iv}][L_1'][L_3'])^{\frac{1}{2}} \times \begin{bmatrix} l'' & k & l^{iv} \\ 0 & 0 & 0 \end{bmatrix}\begin{Bmatrix} L_1' & L_3' & k \\ l^{iv} & l'' & l' \end{Bmatrix}\delta(l', l'''). \quad (8)$$

The coefficients of $R^k(l'l''; l'''l^{iv})$ are trivial and need not be considered here.[6] If the electrons external to the core are equivalent, we need only replace the matrix element $(L_1' \mid\mid C_i^k \mid\mid L_3')$ in (5) by

$$(-1)^{l'}[l']\begin{bmatrix} l' & k & l' \\ 0 & 0 & 0 \end{bmatrix}(L_1' \mid\mid U^k \mid\mid L_3'), \quad (9)$$

where

$$(L_1' \mid\mid U^k \mid\mid L_3') = 2([L_1'][L_3'])^{\frac{1}{2}}(-1)^{L_1'+k} \times \begin{Bmatrix} L_1' & L_3' & k \\ l' & l' & l' \end{Bmatrix}. \quad (10)$$

If the direct interactions between $l^n l'^2$ and $l^n l'''l^{iv}$ are of interest, we may evaluate the coefficients of the radial integrals $R^k(ll'; ll''')$ and $R^k(ll'; ll^{iv})$ by putting $l' \equiv l''$ in Eqs. (7) and (8).

The exchange-type interactions may be treated by performing a recoupling of the angular momentum such as to interchange the positions of two particles. The angular part of the interactions will give rise to the coefficients of three basic types of radial integrals: $R^k(ll'; l'''l)$, $R^k(ll''; l^{iv}l)$, and $R^k(l'l''; l^{iv}l'')$. The third type is amenable to the usual two-electron treatment[6] and will not be discussed. The calculation of the matrix elements of the exchange interactions proceeds, in a manner similar to that used for the direct interactions, by first performing a recoupling on the rhs of (4), summing over and eliminating the new angular momenta (spin and orbit) that enter the expression, returning the result to Eq. (3), and performing the summation over σ and λ. The procedure is lengthy though quite straightforward, and hence only the results are given.

For $R^k(ll'; l'''l)$, the matrix elements on the rhs of Eq. (1) are given by

$$n[l]([l'][l'''][L_1][L_3][L_1'][L_3'] \times [S_1][S_3][S_1'][S_3'])^{\frac{1}{2}}(-1)^{l'''+k+l'}$$

[4] G. Racah, Phys. Rev. **63**, 367 (1943).
[5] G. Racah, Phys. Rev. **76**, 1352 (1949).
[6] U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press Inc., New York, 1959).

$$\times \begin{Bmatrix} l & k & l' \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l''' & k & l \\ 0 & 0 & 0 \end{Bmatrix} \delta(l'', l^{i\nu})$$

$$\times \sum_{\bar{\psi}} (\psi_1\{|\bar{\psi})(\psi_3\{|\bar{\psi})\begin{Bmatrix} \bar{S} & S_3 & \frac{1}{2} \\ S_1 & S_2 & S_1' \\ \frac{1}{2} & S_3' & \frac{1}{2} \end{Bmatrix}\begin{Bmatrix} l'' & l''' & L_3' & L_3 \\ l' & k & l & L_1 \\ L_1' & l & L_2 & \bar{L} \end{Bmatrix}, \tag{11}$$

while for $R^k(ll''; l^{i\nu}l)$, the matrix elements on the rhs of Eq. (1) are given by

$$n[l]([l'']...[L_1][L_3][L_1'][L_3'][S_1][S_3][S_1'][S_3'])^{\frac{1}{2}}$$

$$\times (-1)^{S_1'+S_3'+L_1'+L_3'+k}\begin{Bmatrix} l & k & l'' \\ 0 & 0 & 0 \end{Bmatrix}\begin{Bmatrix} l^{i\nu} & k & l \\ 0 & 0 & 0 \end{Bmatrix}\delta(l', l''')$$

$$\times \sum_{\bar{\psi}} (\psi_1\{|\bar{\psi})(\psi_3\{|\bar{\psi})\begin{Bmatrix} \bar{S} & S_3 & \frac{1}{2} \\ S_1 & S_2 & S_1' \\ \frac{1}{2} & S_3' & \frac{1}{2} \end{Bmatrix}\begin{Bmatrix} l' & l^{i\nu} & L_3' & L_3 \\ l'' & k & l & L_1 \\ L_1' & l & L_2 & \bar{L} \end{Bmatrix}, \tag{12}$$

where the last factor in each expression is a standard 12–j symbol.[3]

In the case in which the electrons added to the l^n core are all equivalent (though $l' \neq l$), the expression

$$2n[l][l']([L_1][L_3][L_1'][L_3']$$

$$\times [S_1][S_3][S_1'][S_3'])^{\frac{1}{2}}(-1)^k\begin{Bmatrix} l & k & l' \\ 0 & 0 & 0 \end{Bmatrix}^2$$

$$\times \sum_{\bar{\psi}} (\psi_1\{|\bar{\psi})(\psi_3\{|\bar{\psi})\begin{Bmatrix} \bar{S} & S_3 & \frac{1}{2} \\ S_1 & S_2 & S_1' \\ \frac{1}{2} & S_3' & \frac{1}{2} \end{Bmatrix}\begin{Bmatrix} l' & l' & L_3' & L_3 \\ l' & k & l & L_1 \\ L_1' & l & L_2 & \bar{L} \end{Bmatrix} \tag{13}$$

results.

For the interaction between $l^n l'^2$ and $l^n l''' l^{i\nu}$, we put $l' \equiv l''$ in Eqs. (11) and (12).

These formulas undergo considerable simplification when one or more of the angular momenta in the n–j symbols are zero.

CONFIGURATION INTERACTION BETWEEN $l^n l'$ AND $l^n l''$

Judd[7] has already treated the electrostatic interaction within the configuration $l^n l'$. His expressions may be readily generalized to give for the direct interaction the coefficients of $R^k(ll'; ll'')$ as

$$(l^n S_1 L_1 s l'; S_2 L_2 \,|\sum_{i<j}(C_i^k \cdot C_j^k)|\, l^n S_3 L_3 s l''; S_4 L_4)$$

$$= ([l'][l''])^{\frac{1}{2}}[l](-1)^{L_3+l+L_3}\,\delta(S_2, S_4)\,\delta(L_2, L_4)$$

$$\times \begin{Bmatrix} l & k & l \\ 0 & 0 & 0 \end{Bmatrix}\begin{Bmatrix} l' & k & l'' \\ 0 & 0 & 0 \end{Bmatrix}\begin{Bmatrix} l'' & k & l' \\ L_1 & L_2 & L_3 \end{Bmatrix}(\psi_1 \,||U^k||\, \psi_3), \tag{14}$$

whereas for the exchange interaction the coefficients of $R^k(ll'; l''l)$ are given by

$$n[l]([l']...[S_1][S_3][L_1][L_3])^{\frac{1}{2}}$$

$$\times (-1)^{S_1+S_3}\begin{Bmatrix} l' & k & l \\ 0 & 0 & 0 \end{Bmatrix}\begin{Bmatrix} l'' & k & l \\ 0 & 0 & 0 \end{Bmatrix}$$

$$\times \sum_{\bar{\psi}} (\psi_1\{|\bar{\psi})(\psi_3\{|\bar{\psi})\begin{Bmatrix} s & \bar{S} & S_3 \\ s & S_2 & S_1 \end{Bmatrix}\begin{Bmatrix} \bar{L} & l & L_3 \\ l & k & l'' \\ L_1 & l' & L_2 \end{Bmatrix}. \tag{15}$$

CONFIGURATION INTERACTION BETWEEN l^n AND $l^{n-1}l'$

Racah[1] has obtained an expression for the matrix elements of the electrostatic interaction between d^n and $d^{n-1}s$. This result may be considerably simplified to give, for the coefficients of $R^k(ll; ll')$,

$$(l^n S_2 L_2 \,|\sum_{i<j}(C_i^k \cdot C_j^k)|\, l^{n-1} S_3 L_3 l' S_4 L_4)$$

$$= (-1)^{L_2+L_3+l}\,\delta(S_1, S_3)\,\delta(S_2, S_4)\,\delta(L_2, L_4)$$

$$\times [l](n[l][l'])^{\frac{1}{2}}\begin{Bmatrix} l & k & l \\ 0 & 0 & 0 \end{Bmatrix}\begin{Bmatrix} l & k & l' \\ 0 & 0 & 0 \end{Bmatrix}$$

$$\times \sum_{\psi_1} (\psi_2\{|\psi_1)(\psi_1 \,||U^k||\, \psi_3)\begin{Bmatrix} L_3 & k & L_1 \\ l & L_2 & l' \end{Bmatrix}, \tag{16}$$

where ψ_1 are the parents of the $S_2 L_2$ state of l^n.

CONCLUSIONS

The application of simple recoupling techniques results in formulas which are considerably more amenable to machine calculation. The appearance of the 9–j and 12–j symbols in (9) and (10) need not disturb us, as they may be readily evaluated by standard programming techniques. The present formulas possess the advantage of requiring a minimum use of the sums over coefficients of fractional parentage with the emphasis placed on the coupling of the electrons. It might be hoped that these formulas could be further simplified. However, except for the trivial cases in which one (or more) of the inequivalent electrons is an s electron, no fundamental simplification seems possible without explicit formulas for the coefficients of fractional parentage.

These results are presented with hope that they will eventually lead to the machine computation of the energy matrices of many of the configurations discussed in this paper.

ACKNOWLEDGMENT

The work reported in this paper was greatly aided by a communication from Dr. B. R. Judd, to whom the author expresses his appreciation.

[7] B. R. Judd, Phys. Rev. 125, 613 (1962).

Partial Wave Analysis of the Scattering of Charged Spinless Particles

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The partial wave series for a relativistic charged spinless particle is not uniformly convergent and is difficult to evaluate numerically in the forward direction. The singularity in the scattering amplitude at the forward direction which leads to this nonuniform convergence is separated and given explicitly in a closed form so that the partial wave series may be accurately evaluated numerically.

THE author has recently carried out a partial wave analysis of the potential scattering of relativistic spinless charged particles.[1] For both the relativistic and nonrelativistic Schrödinger equation, the long-range nature of Coulomb scattering gives rise to a Faxén–Holtsmark series which does not converge satisfactorily in the forward direction. Nonrelativistically, this problem is solved[2] by dividing the scattering amplitude into a point Coulomb part and a "nuclear" part. The point Coulomb part is known in a closed form and the nuclear part is the difference of the original Faxén–Holtsmark series and the Faxén–Holtsmark series for the point Coulomb scattering.

In the relativistic case, however, the scattering amplitude for the point Coulomb potential is not known in a closed form. To circumvent this difficulty, we have found a series which (a) has a sum known in a closed form and (b) has a behavior for large l such that when it is subtracted from the Faxén–Holtsmark series, a difference series results which is absolutely convergent and can be summed numerically. In notation similar to that of Schiff, the Faxén–Holtsmark series for *relativistic* point Coulomb scattering is

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \exp(2i\eta_l + 2i\delta_l) P_l(\cos\theta), \quad (1)$$

where the δ_l are the "nuclear" phase shifts, calculated using relativistic Coulomb wavefunctions, and where the η_l are the relativistic Coulomb phase shifts,

$$\eta_l = \arg[\Gamma(l+1+i\lambda-\tau_l)] + \tfrac{1}{2}\pi\tau_l,$$

$$\tau_l = \tfrac{1}{2}(2l+1)\left[1 - \left(1 - \frac{4\gamma^2}{(2l+1)^2}\right)^{\frac{1}{2}}\right].$$

Here $\gamma = z_1 z_2 e^2$ in units such that $\hbar = c = 1$, z_1 and z_2 being the charge on the particle and on the nucleus; and $\lambda = \gamma/\beta$, β being the relative velocity of the particle and nucleus in the center-of-mass system.

The following considerations lead to the separation of (1) in a manner analogous to the familiar nonrelativistic separation. In Eq. (1), the δ_l approach zero rapidly for large l so that the properties of the η_l alone determine the nature of the convergence of the series. The factor $(2l+1)\exp(2i\eta_l)$ can be expanded as follows:

$$(2l+1)\exp(2i\eta_l) = (2l+1)\frac{\Gamma(l+1+i\lambda)}{\Gamma(l+1-i\lambda)} + \pi i\gamma^2 \frac{\Gamma(l+1+2i\lambda)}{\Gamma(l+1)} - (4i\gamma^2\lambda + \tfrac{1}{2}\pi^2\gamma^4)\frac{1}{2l+1} + O\left(\frac{1}{l^2}\right) + \cdots. \quad (2)$$

The first term in this expansion is the nonrelativistic Coulomb part of the series. The next two terms in (2) have been chosen to include everything of order l^0 and l^{-1} and still have a known closed form for their sums with $P_l(\cos\theta)$. Equation (1) may then be rewritten in analogy with Schiff's equation [reference 2, Eq. (20.24), p. 120]:

$$f(\theta) = f_c(\theta) + f_1(\theta) + f_2(\theta) + \frac{1}{2ik}\sum_{l=0}^{\infty}\Bigg[(2l+1)\exp(2i\eta_l + 2i\delta_l) - (2l+1)\frac{\Gamma(l+1+i\lambda)}{\Gamma(l+1-i\lambda)} - i\pi\gamma^2\frac{\Gamma(l+1+2i\lambda)}{\Gamma(l+1)} + (4i\lambda\gamma^2 + \tfrac{1}{2}\pi^2\gamma^4)\frac{1}{2l+1}\Bigg]P_l(\cos\theta), \quad (3)$$

where

[1] R. D. Hill, J. H. Hetherington, and D. G. Ravenhall, Phys. Rev. **122**, 267 (1961).
[2] See for example, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Co. Inc., New York, 1955), 2nd Ed., Sec. 20.

$$f_c(\theta) = -\frac{\lambda}{2k}\frac{1}{(\sin\frac{1}{2}\theta)^{2+2i\lambda}}\frac{\Gamma(1+i\lambda)}{\Gamma(1-i\lambda)}$$

$$= \frac{1}{2ik}\sum_{l=0}^{\infty}\frac{\Gamma(l+1+i\lambda)}{\Gamma(l+1-i\lambda)}P_l(\cos\theta),$$

as in the nonrelativistic case, and where

$$f_1(\theta) = \frac{\pi\gamma^2}{2k}\Gamma(1+2i\lambda)\frac{P_{2i\lambda}(\sin\frac{1}{2}\theta)}{(2\sin\frac{1}{2}\theta)^{1+2i\lambda}}$$

$$= \frac{i\pi\gamma^2}{2ik}\sum_{l=0}^{\infty}\frac{\Gamma(l+1+2i\lambda)}{\Gamma(l+1)}P_l(\cos\theta),$$

and

$$f_2(\theta) = \frac{i}{4k}\left(4i\lambda\gamma^2 + \frac{\pi^2\gamma^4}{2}\right)K(\cos\tfrac{1}{2}\theta)$$

$$= \frac{-1}{2ik}\sum_{l=0}^{\infty}\left(4i\lambda\gamma^2 + \frac{\pi^2\gamma^4}{2}\right)\frac{1}{2l+1}P_l(\cos\theta).$$

Here $P_{2i\lambda}(\sin\frac{1}{2}\theta)$ is a Legendre function of imaginary order and $K(\cos\frac{1}{2}\theta)$ is the complete elliptic integral of the first kind. The indicated summation of the series for $f_1(\theta)$ is accomplished by writing $P_l(\cos\theta)$ in its integral form and interchanging the summation and the integration, while $f_2(\theta)$ can be found by integration of a modified form of the generating function for Legendre polynomials.

It should be emphasized that Eq. (3) is exact; the series in this equation being just the difference between the exact expression and the terms $f_c + f_1 + f_2$. This series is absolutely convergent (and therefore its sum is finite) for every angle θ. Thus the expressions $f_c(\theta)$, $f_1(\theta)$, and $f_2(\theta)$ contain all parts of the amplitude which tend to infinity as θ approaches zero, since it is this property of the amplitude which causes the Faxén–Holtsmark series to be not uniformly convergent. The series in Eq. (3) can be summed numerically and the expressions $f_c(\theta)$, $f_1(\theta)$, and $f_2(\theta)$ can be evaluated from the closed expressions given, so that an accurate partial wave analysis can be made.

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Regge Poles and Branch Cuts for Potential Scattering

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The analytic properties of partial wave amplitudes are studied for complex energy and angular momentum. The properties of the wavefunctions are first obtained by standard methods in the theory of differential equations for general classes of potentials, and the effects of the dominant singular term in the potential near the origin are investigated. These include the appearance of branch cuts in the angular-momentum variable for potentials which are singular like z^{-2}, and the location of Regge poles for more singular potentials. The trajectories of Regge poles are also studied with particular reference to their behavior in the angular-momentum plane as the energy tends to infinity. An example is given of a singular potential in which the trajectories move to infinity in a complex direction, contrary to the normal behavior for which they tend to negative integers. The real sections of Regge surfaces are also briefly discussed.

1. INTRODUCTION

THE theory of potential scattering with complex energy and angular momentum has been described in a detailed paper by Bottino, Longoni and Regge.[1] Their work is based on the integral equations for the wavefunctions and the Jost scattering solutions. For some purposes however, it is more convenient to use the general theory of differential equations to study the wavefunctions. This was first used in this context by Mandelstam[2] and forms the basis of the first part of this paper.

In Sec. 2 we study the wavefunctions for various types of potential V with particular reference to the form of the potential near the origin. When $V(z) = o(z^{-2})$ near the origin, we obtain the usual analyticity of the wavefunctions $\phi(\lambda, k, z)$. When $V(z) = O(z^{-2})$ the indicial equation clearly exhibits a branch cut fixed in the λ plane, and this result is not altered if $V(z)$ itself has a branch cut at the origin. We study also the situation when $V(z)$ is more singular than z^{-2} at the origin and the Schrödinger equation has solutions of normal or subnormal type.[3] Then the wavefunctions have an essential singularity at the origin.

In Sec. 3 we obtain the corresponding properties and symmetries of the Jost functions and the S matrix. When there is a branch cut in the angular-momentum plane (λ), we find that there is symmetry between the right half-plane and the left half-plane through the branch cut on to the next sheet. For a singular potential (more than z^{-2}) this symmetry is on one sheet only and there are an infinite number of poles in the right half-λ plane.[4,5,6] The properties of Regge surfaces and trajectories (the paths of poles of the S matrix) are studied in Sec. 4. The fact that they are defined by analytic functions follows from the implicit function theorem.[7,8,9] By finding the asymptotic form of the Jost functions as the energy increases through real values to infinity, we show that the trajectories tend either to $\lambda_1 + i\infty$ or to negative half integers in the λ plane. In Sec. 5 we see that the former possibility occurs for the singular potential of Wannier[4,5]; it is probable that the latter is always valid for nonsingular potentials.[10] In Secs. 6 and 7 we note the example of relativistic Coulomb scattering which illustrates our general results, and we indicate the main features of the real sections of Regge surfaces.

2. WAVEFUNCTIONS FOR NONRELATIVISTIC POTENTIAL SCATTERING

In this section we show that the analytic properties of the wavefunctions for complex energy and complex orbital momenta follow from general theorems on differential equations. In particular, we study the occurrence of branch cuts in the complex angular-momentum variable and the distribution of poles in relation to the behavior of the potential at the origin.

The Schrödinger equation for the radial part

[1] A. Bottino, A. M. Longoni, and T. Regge, Nuovo Cimento **23**, 954 (1962); T. Regge, Nuovo Cimento **14**, 951 (1959); *ibid.*, **18**, 947 (1960).
[2] S. Mandelstam, University of Birmingham preprint (February 1962).
[3] A. R. Forsyth, *Theory of Differential Equations* (Cambridge University Press, Cambridge, England, 1902), Vol. 3.
[4] E. Vogt and G. H. Wannier, Phys. Rev. **95**, 1190 (1954).
[5] G. H. Wannier, Quart. Appl. Math., **11**, 33 (1953).
[6] E. Predazzi and T. Regge, Nuovo Cimento **24**, 518 (1962).
[7] E. Hilb, Encyclyclopedie der Mathematik Wissenschaft (B. G. Teubner, Leipzig, Germany, 1915), Vol. 2, Part 2.
[8] S. Bochner and W. T. Martin, *Several Complex Variables* (Princeton University Press, Princeton, New Jersey, 1948).
[9] Similar results have been obtained by J. R. Taylor, Phys. Rev. **127**, 2257 (1962).
[10] A. Ahmadzadeh, P. G. Burke, and C. Tate, *UCRL*, **10140**, March 1962.

$R(z) = \psi(z)/z$ of the wavefunction for a spherically symmetric potential $\hbar^2V(z)/2m$, can be written

$$\psi''(z) + k^2\psi(z) - [(\lambda^2 - \tfrac{1}{4})/z^2]\psi(z) - V(z)\psi(z) = 0, \qquad (2.1)$$

where $\lambda = l + \frac{1}{2}$ and $E = \hbar^2k^2/2m$. When the potential is zero, the solutions behaving like $z^{\pm\lambda+\frac{1}{2}}$ at the origin are

$$\phi_0(\pm\lambda, k, z) = 2^{\pm\lambda}\Gamma(1 \pm \lambda)z^{\frac{1}{2}}k^{\mp\lambda}J_{\pm\lambda}(kz). \qquad (2.2)$$

At integer values of λ, these two solutions are no longer independent; however the relation

$$W[\phi_0(\lambda, k, z)\phi_0(-\lambda, k, z)] = \phi_0(\lambda, k, z)\phi_0'(-\lambda, k, z) - \phi_0'(\lambda, k, z)\phi_0(-\lambda, k, z) = -2\lambda \qquad (2.3)$$

is still true.

For $kz \neq 0$, $J_\lambda(kz)$ is an entire function of λ and k. Then the functions $\phi_0(\pm\lambda, k, z)$ have simple poles in λ at the negative and positive integers, respectively, and are entire functions of k^2. In the z plane, the origin is an algebraic singularity whose type depends upon λ. In considering the corresponding properties for $V \neq 0$, Poincare's[7] theorem for linear differential equations implies that the λ dependence of the Jost functions, and hence of the S matrix, will be determined by these wavefunctions.

The Jost functions are given by the Wronskians of the wavefunctions ϕ with scattering solutions of (2.1) which behave like $\exp[\mp ikz]$ as $z \to \infty$. For $V = 0$ these functions are

$$f_0(\lambda, +k, z) = (\pi kz/2)^{\frac{1}{2}}H_\lambda^{(2)}(kz) \times \exp[-i\pi(\lambda + \tfrac{1}{2})/2], \qquad (2.4)$$

$$f_0(\lambda, -k, z) = (\pi kz/2)^{\frac{1}{2}}H_\lambda^{(1)}(kz) \times \exp[i\pi(\lambda + \tfrac{1}{2})/2]. \qquad (2.5)$$

The properties of $f(\lambda, \pm k, z)$ have been studied by Bottino, Longoni, and Regge[1] (when the potential is nonzero) from the Green's function integral equation

$$f(\lambda, \pm k, z) = f_0(\lambda, \pm k, z) + \frac{i\pi(z)^{\frac{1}{2}}}{4}\int_z^\infty d\xi(\xi)^{\frac{1}{2}}V(\xi)f(\lambda, \pm k, \xi) \times [H_\lambda^{(1)}(\pm k\xi)H_\lambda^{(2)}(\pm kz) - H_\lambda^{(1)}(\pm kz)H_\lambda^{(2)}(\pm k\xi)]. \qquad (2.6)$$

For z in some neighborhood of the origin but not actually zero, the analytic properties of $f(\lambda, \pm k, z)$ in λ will not depend upon the behavior of the potential at the lower limit. We can then admit a large class of potentials with strong singularities at the origin, provided only, that the integral in (2.6) is convergent at infinity. Under these conditions, if $V(z)$ is analytic for $\mathrm{Re}\, z > 0$ and continuous on $\mathrm{Re}\, z = 0$, Bottino *et al.*[1] have shown that: $f(\lambda, \pm k, z)$ is analytic in $\{\lambda \mid \lambda \neq \infty\} \times \{k \mid \pm \mathrm{Im}\, k < 0\}$ and is continuous on $\{\lambda \mid \lambda \neq \infty\} \times \{k \mid \mathrm{Im}\, k = 0\}$ for all z outside some immediate neighborhood of the origin.

They show that these domains can be united to give the whole finite k plane with branch cuts along the imaginary axis; the latter are only kinematic in character for $|\mathrm{Im}\, k| < \frac{1}{4}\mu$ for a potential with an exponential tail of range $1/\mu$. These properties do not depend on the nature of $V(z)$ near zero, and will carry over to the Jost functions.

To obtain the behavior of $\phi(\pm\lambda, k, z)$ in λ, we study this function for z near the origin by the standard method of solving (2.1)—by a power series. (This method was first used in this context by Mandelstam.)[2] In the following, we shall require of $V(z)$ that the interior points of the interval $(0, \infty)$ be ordinary points of (2.1), and the point at infinity an irregular point of grade one.[3] Specific requirements concerning $V(z)$ at zero will be stated as they arise. By standard theorems in the theory of differential equations, this series will be uniformly convergent in any finite domain of the $\lambda \times k$ product plane for z in a region determined by the nearest singularity of $z^2V(z)$, except at certain isolated points in λ. It is necessary only that $|z^2V(z)|$ be bounded in this region.[3] First consider potentials having an expansion

$$z^2V(z) = \sum_{m=0}^{\infty} a_m z^m. \qquad (2.7)$$

This excludes $V(z) \sim z^{p/q}$ near the origin, which will be considered below. Substituting (2.7) and the expansion

$$\phi(\sigma, k, z) = \sum_{n=0}^{\infty} z^{\sigma+n}c_n, \qquad c_0 \neq 0 \qquad (2.8)$$

into the Schrödinger equation, we obtain recurrence relations for the coefficients c_n. The roots of the indicial equation are

$$\sigma_1, \sigma_2 = \tfrac{1}{2} \pm (\lambda^2 + a_0)^{\frac{1}{2}}, \qquad (2.9)$$

while the coefficients $c_n = c_n(\sigma, k)$ are given by

$$c_n = \frac{(-1)^n c_0 F_n(\sigma, k)}{f_0(\sigma + 1)f_0(\sigma + 2) \cdots f_0(\sigma + n)}, \qquad (2.10)$$

where σ denotes σ_1 or σ_2, $f_0(\sigma + n) = n(2\sigma + n - 1)$, and

$$F_n(\sigma, k) = \begin{vmatrix} -a_1 & k^2 - a_2 & -a_3 & \cdots & -a_n \\ f_0(\sigma + n - 1) & -a_1 & k^2 - a_2 & & -a_{n-1} \\ 0 & f_0(\sigma + n - 2) & -a_1 & & -a_{n-2} \\ \vdots & 0 & & & \vdots \\ & \vdots & & & \\ & & & & k^2 - a_2 \\ 0 & \cdots & 0 & f_0(\sigma + 1) & -a_1 \end{vmatrix}. \tag{2.11}$$

Clearly, $c_n(\sigma, k)$ is a rational function of σ and an entire function of k^2. Further, c_n is continuous in the parameters a_n of the potential. The zeros of the denominator occur for those values of σ at which the power-series solutions are no longer linearly independent, i.e.

$$\sigma_1, \sigma_2 = -\tfrac{1}{2}(n - 1) \qquad n = 1, 2, \cdots . \tag{2.12}$$

Except for these points, $\phi(\pm\lambda, k, z)$ is represented by a uniformly convergent power series (2.8) for z inside the circle of convergence determined by $z^2V(z)$. It is therefore an entire function of k^2 and a meromorphic function of λ, the poles being given by (2.12). This result can be extended by analytic continuation to the holomorphy domain of $z^2V(z)$ for an energy independent potential.

For $a_0 = 0$; $\sigma_1, \sigma_2 = \frac{1}{2} \pm \lambda$, and the poles of $\phi(\pm\lambda, k, z)$ correspond to $\lambda = \mp\frac{1}{2}n$. When $a_0 \neq 0$, σ_1, σ_2 given by (2.9) have branch points at $\lambda = \pm[(-a_0)]^{\frac{1}{2}}$, the poles of the wavefunction occurring for $\lambda = \mp\frac{1}{2}[(n^2 - 4a_0)]^{\frac{1}{2}}$.

We conclude that the solutions $\phi(\pm\lambda, k, z)$ of (2.1) can be continued in λ for all z within the domain of holomorphy of $V(z)$, provided that $|z^2V(z)|$ is bounded in the circle of convergence of (2.7). Within this region, the wavefunction may be represented by the series (2.8) such that:

(i) when $z^2V(z) \to 0$ as $z \to 0$, $\phi(\pm\lambda, k, z)$ is analytic for all finite λ, k except for simple poles at $\lambda = \mp\frac{1}{2}n$, $n = 1, 2, \cdots$.

(ii) when $z^2V(z) \to a_0$ as $z \to 0$, $\phi(\pm\lambda, k, z)$ is analytic for all finite λ, k except for branch points at $\lambda = \pm[-a_0]^{\frac{1}{2}}$ and simple poles at $\lambda = \mp\frac{1}{2}[(n^2 - 4a_0)]^{\frac{1}{2}}$. If $V(z)$ is independent of k, so are these branch points and poles.

Consider next the class of potentials for which

$$\lim_{z \to 0} z^{p/q}V(z) = \text{constant}, \tag{2.13}$$

where p/q is a rational number, $p \leq 2q$. Substitute $z = x^q$ in (2.1) to give

$$x^2\psi''(x) + (1 - q)x\psi'(x) - (\lambda^2 - \tfrac{1}{4})q^2\psi(x) + k^2q^2x^{2q}\psi(x) - q^2x^{2q}V(x^q)\psi(x) = 0, \tag{2.14}$$

and let the expansion of $V(z)$ for small $|x|$ take the form

$$x^{2q}V(x^q) = \sum_{m=0}^{\infty} b_m x^{m+2q-p}. \tag{2.15}$$

Note that $b_0 \neq 0$ implies $p = 2q$. The point $x = 0$ is now a regular singular point of (2.14) and a power-series solution in x may be written as before. The indicial equation in this case has the roots

$$\sigma_1, \sigma_2 = q[\tfrac{1}{2} \pm (\lambda^2 + b_0)^{\frac{1}{2}}]. \tag{2.16}$$

As one would expect, the branch points at $\lambda = \mp(-b_0)^{\frac{1}{2}}$ are independent of q and arise in exactly the same way as in (ii) above. The recurrence relations for this case indicate that the coefficients in the power series have simple poles when $\sigma = \frac{1}{2}(q - n)$; as in (2.16), these lead to simple poles in the function $\phi(\pm\lambda, k, z)$ at $\lambda = \mp\frac{1}{2}(n^2/q^2 - 4b_0)^{\frac{1}{2}}$. The poles of $\phi(+\lambda, k, z)$ lie to the left of the line $\text{Re}\ \lambda = 0$, and those of $\phi(-\lambda, k, z)$ to the right unless b_0 is positive. In this case the branch cut can be taken along the imaginary axis, and for $b_0 > \frac{1}{4}q^2$, one or more of the poles lies on the cut.

Let us consider how the coefficients in the series for $\psi(x)$ depend on p and q. Substituting the expansion

$$\psi(x) = \sum_{n=0}^{\infty} d_n x^{\sigma+n}$$

into Eq. (2.14), we obtain

$$x^\sigma \sum \{(\sigma + n)(\sigma + n - 1) + q^2k^2x^{2q} + (1 - q)(\sigma + n) - (\lambda^2 - \tfrac{1}{4})q^2 - q^2x^{2q-p}b_m x^m\} d_n x^n = 0. \tag{2.17}$$

The first nonvanishing coefficient d_n after d_0 is d_{2q-p} ($p < 2q$). When q is increased relative to p, the number of vanishing coefficients increases and the poles corresponding to them at $\lambda = \mp\frac{1}{2}(n^2/q^2 - 4b_0)^{\frac{1}{2}}$ therefore disappear. This is perhaps contrary to a possible expectation that they might have moved in towards the origin. This vanishing of certain poles is analogous to the fact that for $p = 2q$, if $V(z)$ is an even function of z, then all the odd coefficients in the wavefunction vanish and their corresponding poles disappear.

The preceding paragraphs were concerned solely with the case in which the origin is a regular singular point of (2.1). By allowing "singular" potentials, i.e. $V(z)$ more singular than $1/z^2$ at the origin, the differential equation will have two irregular points and the wavefunction $\phi(\lambda, k, z)$ has an essential singularity at this point. A systematic classification of such solutions has not been given except for the case of normal or subnormal solutions (3). Here the wavefunction assumes the form

$$\phi(\lambda, k, z) = u(\lambda, k, z) \exp [\Omega(\lambda, k, z)], \qquad (2.18)$$

where $u(\lambda, k, z)$ is a regular integral of the form (2.8) and $\Omega(\lambda, k, z)$ a polynomial in $1/z$. The subnormal case requires that z occur raised to some rational power in Ω.

Substituting (2.18) into (2.1) gives a linear equation for $u(\lambda, k, z)$:

$$u'' + 2\Omega' u' + [\Omega'' + \Omega'^2 + k^2 - (\lambda^2 - \tfrac{1}{4})/z^2 - V_S(z) - V_R(z)]u = 0, \qquad (2.19)$$

where $V(z) = V_S(z) + V_R(z)$, $V_S(z)$ being the singular part. The choice of $\Omega(\lambda, k, z)$ is dictated by the requirement that (2.19) should have at least one regular integral near $z = 0$. Giving u a series development (2.8) we have

$$\sum_{n=0}^{\infty} c_n z^{\sigma+n}[(\sigma + n)(\sigma + n - 1) + 2(\sigma + n)z\Omega' + z^2(\Omega'' + \Omega'^2 + k^2 - V_s - V_R - \lambda^2 + \tfrac{1}{4})] = 0. \qquad (2.20)$$

The indicial equation for σ is found from the coefficients of the dominant terms for small z when $n = 0$, hence Ω must be so chosen that these terms are not independent of σ. In the above equation, a necessary condition for this is that $V(z)$ should be at least as singular as $1/z^4$. We shall also take the leading term in $V(z)$ to be an even power. For $1/z^3$ or any odd power, a change of variable leads to a subnormal integral and gives the case considered. If Ω is of degree s, the leading s terms in $\Omega'^2 - V_S(z)$ must vanish by choice of the coefficients in Ω. The indicial equation will then be taken from the remaining coefficients of

$$2\sigma z\Omega' + z^2(\Omega'' + \Omega'^2 - V_s), \qquad (2.21)$$

which is a linear relation for σ, independent of λ. The coefficients c_n determined by appropriate recurrence relations must terminate, a condition which requires l to be able to take on integer values. By Poincare's theorem, $u(\lambda, k, z)$ will be an entire function of λ, since the boundary condition at the origin no longer involves λ. It then follows that (2.18) will be an entire function in the product of the $\lambda \times k$ planes for all z lying in the region of convergence of the series for u, excluding the origin.

If the coefficient of the leading term in $V_S(z)$ is g, then for small z, $\phi \sim z^\sigma \exp [\pm(g)^{\frac{1}{2}}/z^S]$. For a repulsive potential the negative root must be chosen, while for the attractive case we take the positive root. The origin then becomes a sink, leading to a capture probability in addition to the usual scattering. Further, in (2.11) we have seen that the wavefunction was continuous in the potential. Generally the wavefunction will not be analytic in the leading term of the potential for small z, the origin being a singular point. The reason is that this coupling constant determines the character of singularity in the solution at the origin, and there is no way of giving a continuous classification of these. Lastly, from (2.20), u will be a function of λ^2 only; hence, in (2.18), ϕ is symmetric in λ. This property is very useful since ϕ is also an entire function of λ. With reservations concerning the cut, this is also true in (2.8) when $a_0 \neq 0$. As we shall see, this symmetry has interesting consequences for the distribution of Regge poles in the λ plane. The particular case of the $1/z^4$ potential has been studied by Wannier,[4,5] and in less detail by Predazzi and Regge.[6]

3. PROPERTIES OF THE JOST FUNCTIONS AND S MATRIX

Let us first consider the case $z^2V(z) \to 0$ as $z \to 0$. The wavefunctions here have poles only in the finite λ plane. These are shown explicitly by writing $\phi(\pm\lambda, k, z)$ in the form

$$\phi(\pm\lambda, k, z) = \phi_0(\pm\lambda, k, z) + \Gamma(1 \pm 2\lambda)\theta(\pm\lambda, k, z), \qquad (3.1)$$

where $\theta(\pm\lambda, k, z)$ is an entire function of λ (Appendix 1). The Jost functions are

$$f(\pm\lambda, \pm k) = W[f(\lambda, \pm k, z), \phi(\pm\lambda, k, z)]$$
$$= W[f(\lambda, \pm k, z), \phi_0(\pm\lambda, k, z)]$$
$$+ \Gamma(1 \pm 2\lambda) W[f(\lambda, \pm k, z),$$
$$\times \theta(\pm\lambda, k, z)]. \tag{3.2}$$

The first Wronskian has only the poles of $\Gamma(1 \pm \lambda)$, while the second is an entire function of λ. Therefore, for some z in the circle of convergence of (2.8), we may evaluate these expressions with the result that the Jost functions are analytic in the product plane $\{k \mid \pm \operatorname{Im} k < 0\} \times \{\lambda \mid \lambda \neq \infty$ and not a pole of $\Gamma(1 \pm 2\lambda)\}$. The imaginary axis in the k plane contains the usual kinematic and dynamic cuts of $f(\lambda, \pm k, z)$.

The S matrix, defined by

$$S(\lambda, k) = \exp[2i\,\delta(\lambda, k)]$$
$$= f(\lambda, k)/f(\lambda, -k) \exp[i\pi(\lambda - \tfrac{1}{2})], \tag{3.3}$$

is a meromorphic function of λ [in general for finite k regular at the poles of (3.2)] with the usual cuts in k. The Regge poles lie on the analytic surface in the $\lambda \times k$ space given by the zeros of $f(\lambda, -k)$, defining some transcendental relation between λ and k, which we shall call the Regge surface. Actually the paths of these poles in the λ plane are of principal interest when k^2 is real.

The S matrix possesses certain discrete symmetries valid for any k; however the method used to obtain them does not allow us to be sure that the same symmetries hold without modification for points on the Regge surface. From the conjunct identity between the solutions of (2.1),

$$f(\lambda, -k)f(-\lambda, k) - f(\lambda, k)f(-\lambda, -k) = 4ik\lambda, \tag{3.4}$$

we can write the following relation between $S(\lambda, k)$ and $S(-\lambda, k)$:

$$e^{-i\pi\lambda}S(\lambda, k) - e^{i\pi\lambda}S(-\lambda, k)$$
$$= -4k\lambda/f(\lambda, -k)f(-\lambda, -k), \tag{3.5}$$

and we obtain

$$S(\lambda, k) = S(-\lambda, k)$$
$$\lambda = \pm n, \qquad n = 0, 1, 2, \cdots,$$
$$S(\lambda, k) = -S(-\lambda, k) \qquad \lambda = \tfrac{1}{2} \pm n. \tag{3.6}$$

When $V(z)$ has the behavior (2.13) with $b_0 \neq 0$, these relations must be replaced by

$$f(\lambda, -k)f(-\lambda, k) - f(\lambda, k)f(-\lambda, -k)$$
$$= 4ik(\lambda^2 + b_0)^{\frac{1}{2}}, \tag{3.7}$$

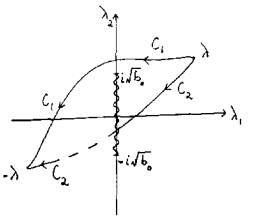

FIG. 1. λ plane, $b_0 > 0$. C_1 goes from λ to $-\lambda$ on the same sheet; C_2 goes from λ to $-\lambda$ on the second sheet. Along C_1, $(\lambda^2 + b_0)^{\frac{1}{2}} \to -(|\lambda|^2 + b_0)^{\frac{1}{2}}$, and along C_2, $(\lambda^2 + b_0)^{\frac{1}{2}} \to (\lambda^2 + b_0)^{\frac{1}{2}}$.

the symmetries being

$$S(\lambda, k) = S(-\lambda, k) \quad \text{for} \quad \lambda = 0,$$
$$S(\lambda, k) = S(-\lambda, k) \exp[\pm i\pi(\lambda^2/q^2 - 4b_0)^{\frac{1}{2}}], \tag{3.8}$$
$$\lambda = 1, 2, \cdots.$$

On the other hand, these symmetries also indicate, for physical values of λ, which terms are present in the odd part of the expansion for the potential.

When $z^2V(z) \to a_0$ at the origin, the S matrix is a meromorphic function of the angular momentum on a two-sheeted Riemann surface, the sheets hinged along a cut running in the finite λ plane between the two branch points $\lambda = \pm ia_0^{\frac{1}{2}}$. By examining (2.9) along the two paths shown in Fig. 1, we see that the reflection symmetry $\lambda \leftrightarrow -\lambda$ mentioned in Sec. 2 holds, provided the reflection is taken through the cut onto the other sheet. This property indicates directly how the Regge poles are distributed on the Riemann surface.

Finally, for the singular potentials under the restriction (2.18), the $f(\pm\lambda, \pm k)$ are entire functions of λ with complete symmetry under λ to $-\lambda$. Thus $S(\pm\lambda, k)$ is also meromorphic in λ with cuts in k as before. Further $S(\lambda, k)e^{-2\pi i\lambda} = S(-\lambda, k)$ for all λ and k, In Sec. 5, a further discussion of this case is given for Wannier's example.

The distribution of poles in the two halves of the λ plane for a fixed k on the physical boundary can be readily obtained for the three cases. For the regular potential without the $1/z^2$ term, Regge[1] has shown that, for k in the $s + i\epsilon$ limit of the physical sheet, the poles for $\operatorname{Re}\lambda > 0$ lie in a bounded region of the upper half-plane. Consequently, there can only be a finite number in this region; any point of accumulation must occur at infinity in the left half-plane. When the energy lies below threshold, the poles are real, clustering at infinity along the negative real axis. Including the a_0 term does not change the situation for $\operatorname{Re}\lambda > 0$. Regge's proof extends trivially; the integrability of the wave-function at the origin follows from (2.9), and the Jost relation

$$\phi(\pm\lambda, k, z) = [f(\lambda, -k)f(\lambda, k, z) - f(\lambda, k)f(\lambda, -k, z)](2ik)^{-1} \quad (3.9)$$

gives the continuation of (2.8) from its circle of convergence to positive real values of z. The possibility that the poles might cluster at the branch points $\lambda = \pm ia_0^{\frac{1}{2}}$ from Re $\lambda < 0$, is readily dismissed by taking the limit $\lambda \to \pm ia_0^{\frac{1}{2}}$ in (3.7), and using the properties of the zeroes of $f(-\lambda, -k)$ for k^2 real which follow from the continuity equation. There are then a finite number of poles in the right half-plane, but an infinite number to the left as before. Upon crossing to the next sheet, this distribution is reversed.

In the case of a singular potential, on the physical sheet the poles lie entirely in the first and third quadrants of the λ plane, symmetrically placed with respect to the origin. Unless $f(\lambda, -k)$ is a pure exponential or is polynomial bounded in λ, there will be an infinite number extending to infinity in some complex direction. The motion of these poles at large values of k will determine the fate of the Mandelstam representation for this class of potential.

4. PROPERTIES OF THE REGGE TRAJECTORY

Consider now the task of establishing analytic properties of the position of the Regge pole as a function of energy, together with the general shape of the trajectory. From the conjunct identity in the case $a_0 = 0$, the resonance poles and zeroes of $f(-\lambda, k)$ must satisfy an implicit equation

$$\lambda(k) = i\frac{f(\lambda, k)f(-\lambda, -k)}{4k} = i\frac{g(\lambda, k)}{4k}. \quad (4.1)$$

Any general properties obtained from this relation will necessarily hold on the Regge trajectory though are not unique to it. The function $g(\lambda, k)$, a given function of energy at the position of the resonance pole, satisfies

$$\begin{aligned} g(\lambda, k) &= g(-\lambda, -k), \\ g(\lambda, -k) &= g(-\lambda, k), \\ g(\lambda, k) &= g^*(\lambda^*, -k^*). \end{aligned} \quad (4.2)$$

From these, $\lambda(k)$ and $\lambda(-k)$, are both consistent with (4.1); while unitarity $f(\lambda, k) = f^*(\lambda^*, -k^*)$ implies that if $\lambda(k)$ is a pole, so is $\lambda^*(-k^*)$.

The right-hand side of (4.1) is analytic in k except for the cuts along the imaginary axis. Applying the implicit function theorem[8,9] to the zeroes of $f(\lambda, -k)$ with $\partial f(\lambda, -k)/\partial\lambda \neq 0$, one sees immediately that $\lambda(k)$ has a unique single-valued continuation in the k plane. The Regge pole as a function of s has the usual two-sheeted behavior near threshold, but the left-hand cut starting at $s = 0$ and running along the negative real axis lies in the unphysical sheet. The portion of this cut from $-\mu^2/4 < s < 0$ has been shown by Bottino *et al.*[1] to be purely kinematic. From Watson[11] and Appendix B,

$$\begin{aligned} f(\lambda, ke^{-2\pi i}) &= f(\lambda, k) - \alpha f(\lambda, -k), \\ f(-\lambda, -ke^{-2\pi i}) &= (1 + \alpha^2)f(-\lambda, -k) - \alpha f(-\lambda, k) \end{aligned} \quad (4.3)$$

(where $\alpha = 2i \cos \pi\lambda$), wherever these functions are analytic. Then

$$\begin{aligned} \lambda(ke^{-2\pi i}) &= (i/4k)[(1 + \alpha^2)f(\lambda, k)f(-\lambda, -k) - \alpha f(\lambda, k)f(-\lambda, k)] \\ &= (1 + \alpha^2)\lambda(k) - (i\alpha/4k)f(\lambda, k)f(-\lambda, k). \end{aligned} \quad (4.4)$$

For the zeroes of $f(-\lambda, k)$,

$$\lambda(ke^{-2\pi i}) = (1 + \alpha^2)\lambda(k) - [i\alpha(1 + \alpha^2)/4k]f(\lambda, -k)f(-\lambda, -k). \quad (4.5)$$

The discontinuity across this portion of the unphysical cut will then be given by

$$\text{disc } \lambda(k) = \alpha\lambda(k)[\alpha - e^{i\pi(\lambda+\frac{1}{2})}S(-\lambda, k)], \quad (4.6)$$

vanishing at physical values of λ.

The behavior of $\lambda(k)$ for large $|k|$ follows from (4.1) together with the result of Appendix A, viz. that the Born approximation dominates at high energies for all λ except the negative half-odd integers. Let us assume that the resonance poles do not tend to these exceptional points at large energies. We can then apply the Born approximation by making an asymptotic expansion of (4.1) in inverse powers of $|k|$, that is

$$\lim_{k\to\infty} \lambda(k) = \frac{if_0}{4k}(\lambda, k)f_0(-\lambda, -k) \times \left[1 + O\left(\frac{1}{|k| \ln |k|}\right)\right], \quad (4.7)$$

the error term going uniformly to zero off the cuts. From this we can obtain a consistency relation which must be satisfied in the limit $k \to \infty$. Substitute (A.8) from appendix A into (4.7) and use the relation $\Gamma(\lambda)\Gamma(1 - \lambda) = \pi/\sin \pi\lambda$; this gives

$$\exp 2\pi i\lambda = 0(1/|k| \ln |k|) \quad \text{as} \quad k \to \infty. \quad (4.8)$$

[11] G. N. Watson, *Bessel Functions* (Cambridge University Press, Cambridge, England, 1922).

This will be true only if $\lambda \to \lambda_1 + i\infty$ as $k \to \infty$, where for nonsingular potentials Regge[1] has shown that λ_1 must be less than zero. This is the consistency condition for the Regge trajectory which must be satisfied if λ does not tend to the poles of the wave-function ϕ. To establish that in fact $\lambda \to -(n + \frac{1}{2})$, it is therefore necessary to prove that Im λ is bounded for large k. When $k^2 \to -\infty$ on the physical sheet, the absence of a left-hand cut for the Regge trajectory requires that Im $\lambda = 0$. However we have not been able to establish this for the physical region, though it has been verified numerically for Yukawa potentials.[10] For potentials that give rise to a Schrödinger equation of singular type, the limit $\lambda \to \lambda_1 + i\infty$ can actually occur with $\lambda_1 > 0$.

In Fig. 2, a typical bounded Regge trajectory is drawn for values of s on the real axis. The nth pole for $a_0 = 0$ starts at $-\frac{1}{2}(2n - 1)$ for large negative s, becoming complex at threshold and bending back to this value via the upper half-plane as s takes the $+i\epsilon$ limit along the physical cut. The turning points in the trajectory are a manifestation of the complexity of the potential. If the poles are isolated, the trajectory will remain in the upper half-plane. This places a severe restriction on the scattering amplitude, which may not be true when production thresholds are present. For $a_0 = 0$, we may then write

$$\lambda_n(s) = -\tfrac{1}{2}(2n - 1) + \frac{1}{\pi}\int_0^\infty \frac{ds'\ \text{Im}\ \lambda_n(s')}{(s' - s)} \qquad (4.9)$$

for the bounded trajectory.

Lastly, let us turn to the case when the $1/z^2$ term is present. The conjunct identity gives the consistency condition in the form

$$(\lambda^2(k) + a_0)^{\frac{1}{2}} = (i/4k)f(\lambda, k)f(-\lambda, -k), \qquad (4.10)$$

the right-hand side being a meromorphic function of $\sigma(k) = (\lambda^2(k) + a_0)^{\frac{1}{2}}$ in accordance with section 2(ii). By our preceding arguments, $\sigma(k)$ has analyticity in k except for the imaginary axis, the lower part being relevant to the resonance pole. Thus $\lambda(k)$ can have additional branch points occurring at conjugate points for an attractive potential at short range. In general these will be isolated square-root branch points at complex values of s.

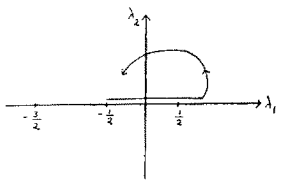

FIG. 2. λ plane $a_0 = 0$.

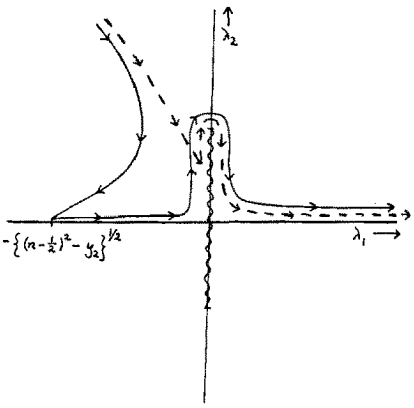

FIG. 3. Regge trajectories in the λ plane ($a_0 > 0$).

The high-energy limit also differs in this case, as the Born-approximation argument breaks down at $\lambda = -\frac{1}{2}(n^2 - 4a_0)^{\frac{1}{2}}$. The Regge poles have been shifted by the $1/z^2$ term—some becoming complex for an attractive potential—and lie in the cut on the imaginary axis. In the next section we shall see how these poles move further through the cut into the right half-plane as the potential becomes singular. On the other hand, as the potential becomes less singular at the origin, these poles representing the high-energy limit, move further to the left. Finally, when $V(z)$ has only even terms, at large energy there will be no resonance poles remaining in the finite plane. Instead they move to infinity, possibly in a direction parallel to the negative real axis.

An example of a trajectory when the cut is present is given by the potential $V(z) = g_2/z^2 - g_1/z$; $g_1, g_2 > 0$; for which

$$S(\lambda, k) = \frac{\Gamma[(\lambda^2 + g_2)^{\frac{1}{2}} + \frac{1}{2} - ig_1/2k]}{\Gamma[(\lambda^2 + g_2)^{\frac{1}{2}} + \frac{1}{2} + ig_1/2k]}, \qquad (4.11)$$

with the position of the poles

$$\lambda_n(s) = \pm[(ig_1/2k - n + \tfrac{1}{2})^2 - g_2]^{\frac{1}{2}}$$
$$n = 1, 2, \cdots. \qquad (4.12)$$

The path is shown in Fig. 3, where $-\infty < s + i\epsilon < \infty$, the points $(\lambda_1, \lambda_2) = (-\epsilon, \epsilon)$; $(\theta, Na_0 + \epsilon)$; (ϵ, ϵ); correspond, respectively, to

$$s_1 = \frac{-g_1^2}{[2n - 1 - 2(g_2)^{\frac{1}{2}}]^2}; \qquad s_2 = \frac{-g_1^2}{[2n - 1]^2};$$
$$s_3 = \frac{-g_1^2}{[2n + 2(g_2)^{\frac{1}{2}} - 1]^2}. \qquad (4.13)$$

The solid curve is for $g_2 < \frac{1}{4}$, when all the poles

start off at real values. For $g_2 > \frac{1}{4}$, a finite number start at points on the imaginary axis; these are indicated by the dotted path. In both cases none of the poles go through the cut onto the next sheet for real values of the energy.

5. THE $1/z^4$ POTENTIAL

The $1/z^4$ potential is a ready example for examining the behavior of the Regge poles in the singular case. This potential, which occurs in the polarization of gas molecules by a stream of charged particles, was first examined in this connection by Vogt and Wannier.[4] The Mathieu equation which arises in the course of this work has been studied in detail by Wannier,[5] with specific application to the problem of polarization. As we shall make free use of this work with reference to the Mandelstam representation, we refer the reader to reference 5 and to the appendix of reference 4.

For the case of scattering, the repulsive potential is of greater interest in that it approximates to the "hard core" effect at small distances, which so far seems to be characteristic of potentials obtained from relativistic theories. Consider then a potential

$$V(z) = g^2/z^4, \tag{5.1}$$

where g is taken real and positive. In (2.1) make the following set of substitutions:

$$\psi(z) = z^{\frac{1}{2}}\phi(z); \quad x = \ln(z/z_0); \quad z_0^2 = ig/k, \tag{5.2}$$

reducing to Mathieu's equation for ϕ,

$$\phi''(x) - (\lambda^2 - 2igk\cosh 2x)\phi(x) = 0. \tag{5.3}$$

The solutions of this equation and the Jost-type of connection formulas between them will be found in reference 5. For small z, (2.1) indicates $\psi(z) \sim \exp[\pm g/z]$, while at large distances from the origin, $\psi(z) \sim \exp[(\pm ikz)/z]$. The solution of (5.3) satisfying the hard-core boundary condition in Wannier's notation is

$$\psi(z) \sim (ig/z)^{\frac{1}{2}} e^{-i\pi/4} h_{\lambda-\frac{1}{2}}(i\ln(z/z_0)), \tag{5.4}$$

where in applying these formulas, analytic continuation is carried out in k from the positive imaginary axis. By making use of the connection formulas of reference 5 and following reference 4, one easily finds the following expression for the scattering amplitude:

$$f(k,\theta) = \frac{i}{2k} \times \sum_{l=0}^{\infty} \frac{(-1)^l P_l(\cos\theta)(2l+1)\exp(\Phi)}{i\exp(\Phi)\cos\pi\beta - \cos\pi\gamma}. \tag{5.5}$$

The parameter γ may be eliminated by using $\exp(\Phi) = i\sin\pi\gamma/\sin\pi\beta$ with the result that the partial wave amplitude assumes the form

$$a(\lambda, s) = \frac{\exp(i\pi\lambda)}{2[i\cos\pi\beta - (\exp(-2\Phi) + \sin^2\pi\beta)^{\frac{1}{2}}]}. \tag{5.6}$$

The analytic surface in the $\lambda \times k$ space leading to the Regge poles is given by solutions to the transcendental equation

$$\Phi(\lambda, k) = (m + \tfrac{1}{2})\pi i \qquad m = \cdots, -1, 0, 1, \cdots. \tag{5.7}$$

Wannier's approximation to the phase function $\Phi = \Phi_0$ may be written

$$\Phi_0(\lambda, k) = 2(\lambda^2 - 2igk) \times \int_0^1 \frac{(1-t^2)^2\,dt}{(1+t^2)^2[\lambda^2 t^2 + igk(1+t^4)]^{\frac{1}{2}}} = \frac{\pi(\lambda^2 - 2ikg)}{2(\lambda^2 + 2ikg)^{\frac{1}{2}}} F\left(\tfrac{3}{2}, \tfrac{1}{2}; 2; \frac{\lambda^2 - 2ikg}{\lambda^2 + 2ikg}\right). \tag{5.8}$$

The Floquet parameter β is given implicitly[12] by the roots of

$$\cos\pi\beta = 1 - 2\,\Delta(0)\sin^2(\tfrac{1}{2}\pi\lambda), \tag{5.9a}$$

where $\Delta(0)$ is the Hill determinant for Mathieu's equation,

$$\Delta(0) = \begin{vmatrix} 1 & \frac{ikg}{4^2 - \lambda^2} & 0 & \cdots \\ \frac{ikg}{2^2 - \lambda^2} & 1 & \frac{ikg}{2^2 - \lambda^2} & 0 \cdots \\ 0 & \frac{-igk}{\lambda^2} & 1 & \frac{-ikg}{\lambda^2}\ 0 \cdots \end{vmatrix}. \tag{5.10a}$$

(5.9a) indicates that $\cos\pi\beta$ is an entire function of λ, with exponential behavior at infinity. The proof of the absolute convergence of $\Delta(0)$ for finite values of k can readily be extended to uniform convergence. The alternative form of (5.9a) gives the exponential behavior in k,

$$\cos\pi\beta = 1 - 2\,\bar{\Delta}(0)\sin^2\tfrac{1}{2}\pi(-ikg)^{\frac{1}{2}}, \tag{5.9b}$$

[12] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, England, 1927), Chap. 19.

where

$$\bar{\Delta}(0) = \lim_{p\to\infty} \prod_{n=1}^{p} \frac{(4n^2 - \lambda^2)^2}{(4n^2 + ikg)^2} \times \Delta(0) \frac{\lambda^2}{-ikg}. \quad (5.10b)$$

Consider now $a(\lambda, s)$ for some fixed physical value of λ and examine the behavior for large values of k on the physical sheet. From (5.8),

$$\Phi_0 \sim \omega(|k|\ g)^{\frac{1}{2}} \exp\ [\tfrac{1}{2}i(\arg k - \tfrac{3}{2}\pi)],$$

where ω is a positive number. (5.10b) indicates that $\bar{\Delta}(0)$ is bounded for large k with leading term unity. $\cos \pi\beta$ will be bounded along $\arg k = \frac{1}{2}\pi$, but increases exponentially in any other direction in the physical sheet. Consequently, $a(\lambda, s)$ will tend to zero in any direction except along the negative real axis. A dispersion relation for this function will then require one subtraction in the s variable. For a complex potential, i.e., g complex, $\arg g$ can be chosen so that an unsubtracted dispersion relation holds on the physical sheet. Whether or not a Mandelstam representation is valid for the total amplitude $f(s, \theta)$ will depend upon the behavior of the poles (5.7) as functions of the energy. We examine this next.

The asymptotic behavior of the denominator in (5.6) for large $|\lambda|$ indicates that the counterpart of the Jost function $f(\lambda, -k)$ is not polynomial bounded nor is it a pure exponential. There will then be an infinite number of poles in each quadrant of the λ plane. For the physical sheet, the first and third quadrants are relevant. The presence of an infinite number of poles in the right half-plane is the complication which casts doubt on the validity of the Mandelstam representation. In appendix C we discuss (5.7) in some detail. The result of this work shows that the poles all lie outside the circle $|\lambda|^2 = 2g\ |k|$. When $k = ik_2$, $k_2 > 0$, the poles come in from infinity along the imaginary axis as k_2 is decreased through positive values to zero. The behavior at $k = 0$ is highly nonanalytic, the poles tending to zero roughly as $k_2 \to 0$ as $|\lambda|^2 \sim 4gk_2$ exp $[o(1/k_2)]$. (This is an essential singularity.)

For physical values of k, the poles are all confined, say, to the lower half of the first quadrant. For finite energy they may not cross the line $\arg \lambda = \pi/4$, but approach this line asymptotically as k tends to infinity;

$$\lambda_M^2 \approx 2igk[1 \pm (2m + 1)(gk)^{-\frac{1}{2}}].$$

The implication of this behavior is that for large energies, at least the real part of the pole becomes unbounded. In terms of Regge's representation for the scattering amplitude, this would imply an infinite number of subtractions in $\cos \theta$; hence we would not be able to write a dispersion relation for the amplitude directly in momentum transfer. However, even though the Mandelstam representation does not hold, the representation in terms of integrals and an infinite sum over poles in the λ plane is valid. In this particular case, the scattering amplitude reduces to an infinite sum, the integral along the line $\text{Re}\ \lambda = 0$ vanishing by virtue of the symmetry of the S matrix with respect to the origin. For a discussion of the evaluation of the cross section for this system by means of this method, we refer the reader to reference 4.

6. RELATIVISTIC POTENTIAL SCATTERING

The equation for the radial part $\psi(z)/z$ of the wavefunction for relativistic potential scattering is

$$z^2\psi''(z) - (\lambda^2 - 1/4)\psi(z) + z^2(E^2 - m^2 + V^2 - 2EV)\psi(z) = 0, \quad (6.1)$$

where $E^2 = k^2 + m^2$, $c = \hbar = 1$. The condition for $z=0$ to be a regular singular point is that $V(z)$ shall be no more singular than $1/z$ at the origin. For

$$zV(z) = \sum_{m=0}^{\infty} a_m z^m, \quad (6.2)$$

from our previous discussion, there will be branch points for the wavefunctions $\phi(\pm\lambda, k, z)$ at $\lambda = \pm a_0$, and simple poles at $\lambda = \pm\frac{1}{2}(n^2 + 4a_0^2)^{\frac{1}{2}}$ $n = 1, 2, \cdots$. These points also give the high-energy limits. We cannot, however, get rid of a finite number of these poles by dropping odd terms in (6.2) as in Sec. 2. Only when the odd terms in $V^2 - 2EV$ vanish will this happen. This is in general not so at finite energy. Of course when V is even, then ϕ is entire in λ.

For a potential more singular than $1/z$, the discussion on singular potentials now applies. The nature of the distribution of poles and the various asymptotic limits follows as in Sec. 5. In passing, let us mention the particular case of $V(z) = g^2/z^2$. Equation (6.1) becomes (5.3) where $k^2 = E^2 - m^2$ and λ^2 is replaced by $\lambda^2 + 2g^2E$. The solution for the poles proceeds as before only now the angle at which the poles tend to infinity at large energy is $\frac{3}{8}\pi$. Furthermore, the appearance of the energy

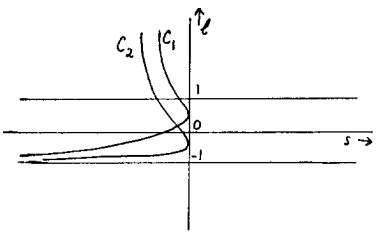

FIG. 4. The real projection of the Regge curve for examples of the neutron–proton system, C_1 in the triplet state, C_2 singlet state.

in the order of the equation introduces an energy-dependent branch point in the λ plane.

For a further, more detailed description of this case, we refer to recent papers by Oehme and Singh.[12,13]

7. REAL SECTIONS OF REGGE SURFACES

In this section we discuss some features of Regge surfaces in potential theory with a view to extending this study in a subsequent paper[13] to field theory. First we consider potentials for which explicit solutions exist. The Coulomb potential has been analyzed both for the nonrelativistic and the relativistic Schrödinger equation by Singh,[14] and for the latter also by Oehme.[15] Nonrelativistic Coulomb scattering gives Regge surfaces

$$l + n + 1 = \pm ie^2/2k \qquad n = 0, 1, 2, \cdots, \tag{7.1}$$

where a positive sign corresponds to an attractive potential. In the energy variable we have

$$E(n, l) = -e^4/4(l + n + 1)^2. \tag{7.2}$$

The algebraic curves for real (E, l) are now the same for attractive and repulsive potentials, however they refer to singularities of the partial wave amplitude on different Riemann sheets in E. The branch that intersects positive integers in l is on the physical sheet for an attractive potential, but on the unphysical sheet for the repulsive case. For the latter, the poles at the integers correspond to virtual states (sometimes called anti-bound states). The long-range character of this potential leads to bound states (or virtual states) for all l. The curve (7.2) touches the branch point at $E = 0$ asymptotically and crosses through from physical to unphysical sheet at infinity in l.

For a potential of shorter range, as between neutron and proton, the corresponding curve will meet the line $E = 0$ between $l = 0$ and $l = 1$ in the triplet states, and between $l = -1$ and $l = 0$ in the singlet state. In the former case, the part of the curve at $l = 0$ is on the physical sheet and in the latter, it is on the unphysical sheet. The real projections of the curves are illustrated in Fig. 4, where the negative integers have been taken as asymptotic values.

A similar real projection of the Regge curve can be deduced for a square-well potential by extrapolation from the work of Nussensweig,[16] (though, as is well known, the continuation to complex l is ambiguous for a square-well potential). He solves for the poles of the S matrix at $l = 0$, and $l = 1$; one can see from his solution how the tangent point on $E = 0$ moves to larger values of l as the strength of the interaction increases.

We do not know of any soluble potentials leading to resonances, but if there is a resonance, the character of the real projection of the Regge curve must be of the form shown in Fig. 5. Then by following the intersection $E = E_1$ (real) with the surface, we obtain the trajectory for the pole as E_1 increases; $l = l(E_1)$, $E = E_1$ real. This trajectory must come near to the curve $E = E(l_1)$, $l = l_1$ real, near the resonance as shown by the broken lines in Fig. 5.

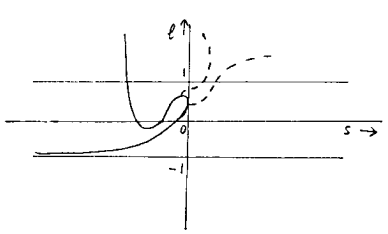

FIG. 5. The real projection of a Regge curve for a system having a resonance.

ACKNOWLEDGMENTS

We are indebted to Dr. P. W. Anderson for calling our attention to the work of Wannier and Vogt.[4] One of us (J.C.) wishes to acknowledge a grant from the Department of Scientific and Industrial Research.

APPENDIX A

In this appendix, it is shown that for the class of nonsingular potentials considered in the text, the asymptotic behavior of the wavefunctions and Jost functions for large values of the energy is given by the Born approximation for all finite λ—except,

[13] J. Challifour and R. J. Eden, *Regge Surfaces and Singularities in a Relativistic Theory*, (Cambridge University Press, Cambridge, England, preprint, 1962).
[14] V. Singh: *UCRL*, 9972, December 1961.
[15] R. Oehme, University of Chicago preprint (1962).
[16] H. M. Nussenzweig, Nucl. Phys. **11**, 499 (1959).

possibly, for a discrete set of points. By using the Phragmén–Lindelöf theorem on the remainder terms, this asymptotic development can be extended to complex values of the energy.

For the wavefunctions $\phi(\pm\lambda, k, z)$, consider the case $a_0 = 0$. By extracting the Born terms from the coefficients $c_n(\pm\sigma, k)$, we will show that $\phi_0(\pm\lambda, k, z)$ dominates the high-energy behavior and $\phi \sim \phi_0$ uniformly for all finite λ, except for the poles of $\Gamma(\frac{1}{2} \pm \lambda)$ for z in the domain of convergence of the series.

Write (2.11) as

$$F_n(\sigma, k) = F_n'(\sigma, k) + F_n''(\sigma, k), \qquad \text{(A1)}$$

where $\sigma = \sigma_1$ or σ_2, and

$$F_n'(\sigma, k) = \begin{vmatrix} 0 & k^2 & 0 & \cdots & 0 \\ f(\sigma+n-1) & 0 & k^2 & \cdots & \cdot \\ 0 & f(\sigma+n-2) & 0 & \cdots & \cdot \\ \cdot & & & 0 & k^2 \\ 0 & \cdots & 0 & f(\sigma+1) & 0 \end{vmatrix}. \qquad \text{(A2)}$$

The remainder is easily shown to be

$$F_n''(\sigma, k) = \sum_{j=1}^{n} F_{n-j}(\sigma, k) G_j(\sigma, k), \qquad \text{(A3)}$$

with a determinantal expression for $G_j(\sigma, k)$ which is of one degree lower in k^2 than F_j;

$$G_j(\sigma, k) = \begin{vmatrix} 0 & k^2 & 0 & \cdots & -a_j \\ f(\sigma+n-1) & 0 & k^2 & & \vdots \\ 0 & f(\sigma+n-2) & 0 & & \\ \vdots & 0 & & 0 & -a_2 \\ 0 & \vdots & 0 & f(\sigma+n-j+1) & -a_1 \end{vmatrix}. \qquad \text{(A4)}$$

Substituting $F_n'(\sigma, k)$ for $F_n(\sigma, k)$ in (2.10) and (2.8), we obtain

$$\phi_0(\pm\lambda, k, z) = z^{\mp\lambda+\frac{1}{2}}\Gamma(1 \pm 2\lambda) \times \sum_{n=0}^{\infty} \frac{(-z)^n F'(\sigma, k)}{n!\,\Gamma(1+n \pm 2\lambda)}. \qquad \text{(A5)}$$

Note that $F_n'(\sigma, k)$ vanished for odd values of n, and this is just the Bessel series

$$\phi_0(\pm\lambda, k, z) = 2^{\mp\lambda}\Gamma(1 \pm \lambda) k^{\mp\lambda} z^{\frac{1}{2}} J_{\mp\lambda}(kz).$$

By expanding the determinants, we find that for large k^2,

$$F_n(\sigma, k) = F_n'(\sigma, k)[1 + F_n''(\sigma, k)/F_n'(\sigma, k)] \sim F_n'(\sigma, k)[1 + 0(1/|k|^2)].$$

Each term in the series for $\phi_0(\pm\lambda, k, z)$ dominates (2.8) term by term, and the original series was uniformly convergent. Thus the asymptotic development will be true for all λ with the exception of the values given above. These are just the poles of the remainder series. This is the result stated.

The restriction on a_0 can be removed, the Born approximation constituting the leading term in an asymptotic expansion for large k. However the term $-a_0/z^2$ must be included in the centrifugal terms in calculating ϕ_0. The points at which the asymptotic development may break down in the λ plane are the counterpart of the half-odd integers as described in Sec. 2.

The case of the Jost scattering solutions is readily dealt with by making use of the following bounds in (2.6):

$$|J_\lambda(kz)| \leq K \frac{(|k|\,z)^{\lambda_1}}{(1+|k|\,z)^{\lambda_1+\frac{1}{2}}} \exp\left[|\mathrm{Im}\, k|\, z - \lambda_2 \arg k\right], \quad \lambda = \lambda_1 + i\lambda_2, \quad \lambda_1 > 0,$$

$$|H_\lambda^{(2)}(kz)| \leq K(2/\pi\,|k|\,z)^{\frac{1}{2}}\left[\frac{1+|k|\,z}{|k|\,z}\right]^{\lambda_1-\frac{1}{2}} \times \exp\left[(\mathrm{Im}\, k)z - \tfrac{1}{2}\pi\lambda_2 + \pi\,|\lambda_2|\right] \qquad \text{(A6)}$$

(and similarly for the other Hankel function), for $0 < z < \infty$, the last holding for the lower half-plane. These are readily obtained from integral representations for the Bessel functions involved, and constitute the appropriate form for complex values of the bounds given by Levinson.[17] These are less generous at the high-energy limit than those used by Bottino *et al.*[1] and give the usual $1/|k|$ bound on the kernel of (2.6);

[17] N. Levinson, Kgl. Danske Videnskab. Selskab., Mathfys. Medd. **25**, No. 9 (1949).

$$\left|\frac{i\pi}{2}(z\xi)^{\frac{1}{2}}\{J_\lambda(k\xi)H_\lambda^2(kz) - J_\lambda(kz)H_\lambda^2(k\xi)\}\right|$$

$$\leq \exp(-\lambda_2 \arg k)\frac{K}{|k|}\left(\frac{|k|\,\xi}{1+|k|\,\xi}\right)^{\lambda_1+\frac{1}{2}}\left(\frac{1+|k|\,z}{|k|\,z}\right)^{\lambda_1-\frac{1}{2}}$$

$$\times \exp\{|\mathrm{Im}\,k|\,\xi + (\mathrm{Im}\,k)z - \tfrac{1}{2}\pi\lambda_2 + \pi\,|\lambda_2|\}, \quad \text{(A7)}$$

for $\mathrm{Im}\,k < 0$, $\xi > z$. A similar bound results for $\mathrm{Im}\,k > 0$ by making use of the corresponding bound for $H_\lambda^{(1)}$; for the details of this, see reference 1.

The proof of the dominance of the Born term in (2.6) now goes for $\mathrm{Re}\,\lambda > 0$ as in the usual case,[18] and is extended to $\mathrm{Re}\,\lambda < 0$ by the symmetry $f(\lambda, \pm k, z) = f(-\lambda, \pm k, z)$. The result of these operations is that $f(\lambda, \pm k, z) \sim f_0(\lambda, \pm k, z)$ uniformly for large $|k|$ lying in the respective domains of the k plane, $\mathrm{Im}\,k < \frac{1}{2}\mu$ for all finite λ, and $0 < z_0 < z < \infty$, where

$$\int_{z_0}^{\infty} V(z)\exp(\mu z)\,dz$$

is critically convergent. By making asymptotic expansions of the wavefunctions in (3.2), we have:

In the limit $|k| \to \infty$ for $\mathrm{Im}\,k \leq 0$, $f(\lambda, k) \sim f_0(\lambda, k)$ uniformly for finite λ except at $\lambda = -\frac{1}{2}n$ when $a_0 = 0$, or $\lambda = -\frac{1}{2}(n^2 - 4a_0)^{\frac{1}{2}}$ when $a_0 \neq 0$. For $a_0 = 0$,

$$f_0(\lambda, k) = [-i2^\lambda\Gamma(\lambda+1)/k^\lambda](2k/\pi)^{\frac{1}{2}} \times \exp[-i\pi\tfrac{1}{2}(\lambda+\tfrac{1}{2})]. \quad \text{(A8)}$$

APPENDIX B

Here we just wish to add a note on the extension of the rule for the transformation of the Jost functions on going around the branch point at $k = 0$, to all values of λ in the plane except for the poles of $f(\pm\lambda, \pm k)$. Since ϕ is an entire function of k^2, the rule follows once established for $f(\lambda, \pm k, z)$.

The bounds in Appendix A can be used to extend the proof of Bottino *et al.*[1] of the convergence of the Born series to all finite values of λ. Analytic continuation in k extends each term in

$$f(\lambda, \pm k, z) = \sum_{n=0}^{\infty} f_n(\lambda, \pm k, z) \quad \text{(B1)}$$

to the domain of Sec. 2. From Watson,[11]

$$H_\lambda^{(1)}(k\omega e^{m\pi i})H_\lambda^{(2)}(kze^{m\pi i}) - H_\lambda^{(1)}(kze^{m\pi i})H_\lambda^{(2)}(k\omega e^{m\pi i}) = H_\lambda^{(1)}(k\omega)H_\lambda^{(2)}(kz) - H_\lambda^{(1)}(kz)H^{(2)}(k\omega); \quad \text{(B2)}$$

hence by induction on n, the law of transformation of f_0 extends to each f_n, and then, by convergence of the resulting series, to the sum f. We are then justified in using (5.3) for other than real positive values of λ.

[18] R. G. Newton, J. of Math. Phys. 1, 319 (1960).

APPENDIX C

The general restrictions imposed upon the location of the resonance poles for a real potential may be deduced from the continuity equation as used by Regge.[1] Taking the particular case of a singular potential with a wavefunction satisfying the hard-core boundary condition, we may write the following relation valid for all λ, k on the Regge surface with $\mathrm{Im}\,k > 0$:

$$\mathrm{Re}\,k\,\mathrm{Im}\,k\int_0^\infty |\psi(z)|^2\,dz = \mathrm{Re}\,\lambda\,\mathrm{Im}\,\lambda\int_0^\infty\left|\frac{\psi(z)}{z}\right|^2 dz. \quad \text{(C1)}$$

Allowed regions of the λ–k planes for the poles of the S matrix are then

$$\left.\begin{matrix}\mathrm{Im}\,k > 0 & \mathrm{Im}\,\lambda < 0\\ \mathrm{Re}\,k \gtrless 0 & \mathrm{Re}\,\lambda \lesseqgtr 0\end{matrix}\right\}, \text{ and } \left.\begin{matrix}\mathrm{Im}\,\lambda > 0\\ \mathrm{Re}\,\lambda \gtrless 0\end{matrix}\right\}. \quad \text{(C2)}$$

When k is physical, the contribution depending upon the energy becomes the Wronskian of ϕ and ϕ^*, so that (C1) is replaced by

$$k = 2\,\mathrm{Re}\,\lambda\,\mathrm{Im}\,\lambda\int_0^\infty dz\left|\frac{\psi(z)}{z}\right|^2,$$

and poles are allowed in $k \gtrless 0$, $\mathrm{Im}\,\lambda\,\mathrm{Re}\,\lambda \gtrless 0$. Finally when $\mathrm{Re}\,k = 0$, $\mathrm{Im}\,k > 0$, the poles must lie on the lines given by $\mathrm{Re}\,\lambda\,\mathrm{Im}\,\lambda = 0$.

A more detailed picture of the distribution of poles in the λ plane can be found by considering the possible values of λ for which (5.7) may have a solution. In Wannier's first approximation, this equation reads

$$F(\tfrac{3}{2}, \tfrac{1}{2}; 2; z) = (2m+1)i/[z(\lambda^2 + 2igk)^{\frac{1}{2}}], \quad \text{(C3)}$$

where k will be taken real and positive;

$$z = (\lambda^2 - 2igk)/(\lambda^2 + 2igk), \quad z = z_1 + iz_2. \quad \text{(C4a)}$$

The positive branch of the square root in (C3) is the one relevant for our purposes, and we shall also regard m as positive. It will be useful to have a picture of the mapping λ to z for a given fixed k defined by (C4). Setting

$$\lambda = |\lambda|\exp(i\phi); \qquad 2igk/\lambda^2 = \exp(-2\theta), \qquad \theta = \theta_1 + i\theta_2,$$

one finds

$$z = (\sinh 2\theta_1 - i\cos 2\phi)/(\cosh 2\theta_1 + \sin 2\phi). \quad \text{(C4b)}$$

This correspondence is shown in Fig. 6, the z plane being covered twice. The line $\phi = \frac{1}{4}\pi$ is taken into a segment of the real axis $-1 < z < 1$, while $\phi = -\frac{1}{4}\pi$ corresponds to the remainder of the real axis. Circles in the λ plane, i.e., θ_1 constant, are mapped into circles in the z plane given by

$$(z_1 - \coth 2\theta_1)^2 + z_2^2 = 1/\sinh^2 2\theta_1. \qquad \text{(C5)}$$

Similarly, the lines ϕ constant become circles with center $z_1 = 0$, $z_2 = \tan 2\phi$, and radius $\cos 2\phi$. The imaginary axis Re $z = 0$, is the map of the circle $|\lambda|^2 = 2gk$; the inside of this circle for $|\phi| < \frac{1}{4}\pi$ arises from points in the third quadrant of z, while the outside arises from points in the fourth. For lines in the wedge $\frac{1}{4}\pi < \phi < \frac{3}{4}\pi$, the relationship is the same only in the upper half of the z plane.

Our procedure will be to match the signs of real and imaginary parts on both sides of (C3), and in this way implement the information obtained from the continuity equation. The work of Van Vleck[19] shows that the hypergeometric function $F(\frac{3}{2}, \frac{1}{2}; 2; z)$ has no zero except possibly at infinity. Hence on the real axis $-\infty < z < 1$, $F(\frac{3}{2}, \frac{1}{2}; 2; z)$ is positive. Further, the hypergeometric function is real analytic in the plane cut along the positive real axis from one to infinity. The sign of its real and imaginary parts may be obtained by using the representation

$$F(\tfrac{3}{2}, \tfrac{1}{2}; 2; z) = \frac{2}{\pi}\int_0^1 \frac{(1-t)^{\frac{1}{2}}\,dt}{t^{\frac{1}{2}}(1-zt)^{\frac{3}{2}}} \quad |\arg(1-z)| < \pi,$$

the branch of $(1 - tz)^{-\frac{3}{2}}$ determined by requiring $(1 - tz)^{-\frac{3}{2}} \to 1$ as $z \to 0$. Setting $1 - tz = Me^{i\alpha}$, $z = |z|\, e^{i\mu}$ gives the real and imaginary parts in the form

$$\begin{aligned} \text{Re } F(\tfrac{3}{2}, \tfrac{1}{2}; 2; z) &= \frac{2}{\pi}\int_0^1 \frac{(1-t)^{\frac{1}{2}}\,dt}{t^{\frac{1}{2}}M^{\frac{3}{2}}}\cos(\tfrac{3}{2}\alpha), \\ \text{Im } F(\tfrac{3}{2}, \tfrac{1}{2}; 2; z) &= -\frac{2}{\pi}\int_0^1 \frac{(1-t)^{\frac{1}{2}}\,dt}{t^{\frac{1}{2}}M^{\frac{3}{2}}}\sin(\tfrac{3}{2}\alpha), \end{aligned} \qquad \text{(C6)}$$

where $\tan\alpha = -t|z|\sin\mu/1 - t|z|\cos\mu$, $|\alpha| < \frac{1}{2}\pi$. For arg $k = 0$, the mapping (C4) is such that we may always take $|z| \leq 1$ for $0 < \phi < \frac{1}{2}\pi$, so that $\tan\alpha$ can maintain a uniform sign along the contour of integration for a given z. Thus for z within the unit circle, $\sin(3\alpha/2)$ has one sign; hence Im $F \gtrless 0$ for Im $z \gtrless 0$. Similarly, in the second and third

[19] E. B. Van Vleck, Trans. Am. Math. Soc. 3, 110 (1902).

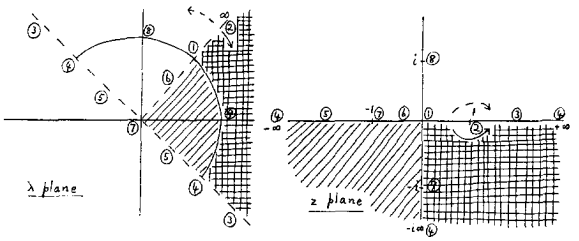

FIG. 6. The λ–z correspondence for equation (C.4).

quadrants, $\cos(\frac{3}{2}\alpha)$ is positive definite and Re $F > 0$. In the right half-plane all z inside the domain $|z| \leq 1$ with $|z| \leq 3^{\frac{1}{2}}/(|\sin\mu| + (3)^{\frac{1}{2}}\cos\mu)$ have Re $F > 0$, while outside, Re $F < 0$. This region cuts the unit circle at $\mu = 0$, $\mu = \pm\frac{1}{3}\pi$ and requires $|z| \leq 1$ $|z| \geq \frac{3}{4}$.

Lastly, rewrite the right-hand side of (C3) as

$$[(2m+1)/|z|\,N^{\frac{1}{2}}]i\,\exp[-i(\mu + \tfrac{1}{2}\gamma)],$$

with N the modulus of the root, and

$$\tan\gamma = (|\lambda|^2\sin 2\phi + 2gk)/(|\lambda|^2\cos 2\phi), \quad 0 < \gamma < \pi,$$

for the positive branch of the square root. It is now straightforward to consider the following cases:

(i) $\phi = \frac{1}{4}\pi$, $-1 < z < 1$. In (C3) the left-hand side is real and positive, while the right-hand side is complex. Hence for finite λ and $k \neq 0$, poles may not occur anywhere along this line.

(ii) $\frac{1}{4}\pi < \phi < \frac{1}{2}\pi$. Here $\frac{1}{2}\pi < \gamma < \pi$, and there can be no matching of real and imaginary parts.

(iii) $0 < \phi < \frac{1}{4}\pi$. In this case for $|\lambda|^2 > 2gk$, $0 < \gamma < \frac{1}{2}\pi$, hence (C3) may have solutions in the range $0 < \mu + \gamma/2 < \frac{1}{2}\pi$.

(iv) $\phi = 0$, $|z| = 1$. $0 < \gamma < \frac{1}{4}\pi$, $0 < \frac{1}{2}\gamma + \mu < \frac{1}{2}\pi$. The matching of the imaginary parts requires $-\frac{1}{2}\pi < \mu < 0$, which is in the region for Re $F < 0$. There are then no solutions along this line.

Consider now the high-energy limit $k \to \infty$. It is seen immediately that $|\lambda|$ cannot remain finite for a solution. We can satisfy (C3) asymptotically for large k by requiring

$$[(2m+1)i][(\lambda^2 + 2igk)^{\frac{1}{2}}/(\lambda^2 - 2igk)] \to 1.$$

The poles then must lie in the sector $0 < \phi < \frac{1}{4}\pi$ outside the circle $|\lambda|^2 = 2gk$, tending asymptotically to the line $\lambda^2 = 2gk\, e^{i(\frac{1}{2}\pi)}$ as k becomes infinite.

The configuration in the λ plane for complex values of energy can be obtained from the above by rotation through an angle $\frac{1}{2}(\arg k)$.

Potential Scattering

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The potential-scattering model is discussed from the point of view of analyticity properties of the scattering amplitude. Dynamical schemes based on the Mandelstam representation and the use of Regge poles are reviewed. Consequences for strong interaction physics are also briefly reviewed.

I. INTRODUCTION

THE present paper is primarily a review article on recent research concerning potential scattering. Particular emphasis is placed on Regge's theorem and its application to the Mandelstam representation. We hope that this paper will be useful as an introduction to recent research on dynamical calculations in the realm of the strong interactions.

II. POTENTIAL SCATTERING

1. Limitations

Potential scattering is concerned with nonrelativistic scattering according to quantum mechanics, using the Schrödinger equation. One must guard against simply equating quantum mechanics with the solution of the Schrödinger equation; even in classical mechanics, we must use field theory to describe electromagnetic radiation. Quantum field theory is a particular formulation of quantum mechanics which allows us to deal with systems of many particles, taking into account the exclusion principle, and it permits the description of particle creation and annihilation.

The general acceptance of the Schrödinger equation in atomic physics is based mainly on the successful explanation of the complicated atomic spectra. In nuclear physics, only the symmetries, but not the dynamics contained in the Schrödinger equation have led to useful results. This is reflected in the complicated form of the nucleon–nucleon potential that must be assumed in a phenomenological approach.

Quantum mechanics was originally invented to deal with bound states, since the calculation of binding energies of atoms was important for the theoretical interpretation of atomic spectra. The wavefunctions of the bound states span a Hilbert space, that is, a complete linear space with an inner product.

In dealing with scattering states, we have to allow wavefunctions which are not normalizable, and hence do not belong to the Hilbert space. To deal with these states it is customary to enclose the system in a large box. This procedure is very annoying and leads to incorrect conclusions in dispersion theory. Hunziker and Jost[1] have shown that it is possible to formulate potential scattering in terms of the Banach space of bounded functions, which seems very natural. Nevertheless, there is no physical principle to decide the issue, so we prefer to remain rather vague in the following on this point.

In the following, we consider the collision at nonrelativistic energies, in the center-of-mass system, of two distinguishable spinless particles, interacting via a time-independent, local, spherically symmetric potential $V(r)$, depending only on the relative separation $r = |\mathbf{x}| = |\mathbf{x}_1 - \mathbf{x}_2|$ of the two particles. We set $\hbar = 2m = 1$, where m is the reduced mass of the two particles. The Schrödinger equation is

$$(\nabla^2 + k^2)\psi = V\psi,$$

where $s = k^2$ is the kinetic energy of the particles at the beginning of the scattering process.

Boundary conditions are imposed to pick out the physically acceptable solutions. Solutions of the Schrödinger equation, which are bounded and continuous and have positive energy, correspond to scattering states, while square-integrable solutions for negative energy correspond to bound states.

Two different complete sets of scattering wavefunctions, the incoming and outgoing solutions are used; these require an additional asymptotic boundary condition. The incoming solutions represent the

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[1] W. Hunziker, Helv. Phys. Acta **34**, 593 (1961).

physical state in which a plane wave is incident and all possible final states are formed. The outgoing states are obtained from the incoming states by motion reversal.

2. The Lippmann-Schwinger Equation

The incoming and outgoing states will be denoted by

$$\langle \mathbf{x} \mid \mathbf{k}^{\text{in}}_{\text{out}} \rangle,$$

and a plane wave by

$$\langle \mathbf{x} \mid \mathbf{k} \rangle = e^{i\mathbf{k}\cdot\mathbf{x}}.$$

The asymptotic boundary conditions that define these solutions may be incorporated into their dynamical equation by writing the Schrödinger equation as an integral equation

$$\langle \mathbf{x} \mid \mathbf{k}^{\text{in}}_{\text{out}} \rangle = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi} \int d^3\mathbf{y} \, \frac{e^{\mp ik|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|} V(\mathbf{y}) \langle \mathbf{y} \mid \mathbf{k}^{\text{in}}_{\text{out}} \rangle,$$

often referred to as the Lippmann-Schwinger equation. The Green's function that appears here,

$$G_{\mp}(x) = -\frac{e^{\mp ikr}}{4\pi r} = \lim_{\epsilon \to 0+} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{e^{i\mathbf{p}\cdot\mathbf{x}}}{k^2 - p^2 \pm i\epsilon},$$

satisfies the equation

$$(\nabla^2 + k^2) G_{\mp}(\mathbf{x}) = \delta(\mathbf{x}).$$

The equivalence of the integral equation with the ordinary Schrödinger equation follows immediately.

Many theorems in scattering theory, including unitarity and analyticity can be deduced from the integral equation.

In proving analyticity, one generally proceeds by writing down a formal solution—for example, the Fredholm solution—and verifying explicitly the mathematical existence (convergence) of the result, and then deducing the analytic properties simply by inspection. Thus, analyticity is more or less a byproduct of existence theorems. This method was first introduced in an extremely simple case by Poincaré.

From the Lippmann-Schwinger equation, if V is real, the motion-reversal theorem to which we have referred, follows immediately:

$$\langle \mathbf{x} \mid \mathbf{k}_{\text{in}} \rangle = \langle \mathbf{x} \mid -\mathbf{k}_{\text{out}} \rangle^*.$$

3. Scattering Amplitude

From the Lippmann-Schwinger equation, follows The asymptotic form of the wavefunction for the limit $r \to \infty$:

$$\langle \mathbf{x} \mid \mathbf{k}^{\text{in}}_{\text{out}} \rangle \xrightarrow[r\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{e^{\mp ikr}}{r} M(\mathbf{k}', \mathbf{k}),$$

where

$$M(\mathbf{k}', \mathbf{k}) = \frac{-1}{4\pi} \int d^3\mathbf{y} \, e^{-i\mathbf{k}'\cdot\mathbf{y}} V(\mathbf{y}) \langle \mathbf{y} \mid \mathbf{k}_{\text{in}} \rangle.$$

Here $\mathbf{k}'$ is a vector of length k in the direction $\mathbf{x}$, that is, $\mathbf{k}' = k\hat{\mathbf{x}}$. Using Dirac's notation, we may write

$$M(\mathbf{k}', \mathbf{k}) = (-1/4\pi) \langle \mathbf{k}' \mid V \mid \mathbf{k}_{\text{in}} \rangle.$$

The interpretation of the scattering amplitude $M(\mathbf{k}', \mathbf{k})$ is found by recalling that the probability current flux in nonrelativistic quantum mechanics is given by

$$\mathbf{S} = -i\psi^* \overleftrightarrow{\nabla} \psi,$$

The cross section $d\sigma/d\Omega$ is defined as the ratio of the outgoing current flow to the incoming flux; thus,

$$d\sigma/d\Omega = |M(\mathbf{k}', \mathbf{k})|^2.$$

An alternative derivation of this formula follows from time-dependent scattering theory, based on the relation

$$\langle \mathbf{k}'_{\text{out}} \mid \mathbf{k}_{\text{in}} \rangle = (2\pi)^3 \delta(\mathbf{k}' - \mathbf{k}) + 8\pi^2 i \delta(\mathbf{k}'^2 - \mathbf{k}^2) M(\mathbf{k}', \mathbf{k}).$$

The quantity $\langle \mathbf{k}'_{\text{out}} \mid \mathbf{k}_{\text{in}} \rangle$ is known as the S matrix. The presence of δ functions shows that the S matrix itself is not analytic, although the scattering amplitude M is.

4. Collision Theory

Heisenberg[2] in 1943 suggested that collision theory was more fundamental than the conventional form of quantum mechanics. He believed that quantum mechanics does not apply to very small distances. The statistical interpretation of the wavefunction in collision theory need only be applied at large distances, and only for noninteracting particles. For this reason, it is desirable to deal directly with the scattering amplitude. It should become unnecessary even to admit the existence of wavefunctions or potentials.

Blankenbecler, *et al.*[3] have shown that the Mandelstam representation of the scattering amplitude, together with unitarity, provides a complete

[2] W. Heisenberg, Z. Physik **120**, 513, 673 (1943); Z. Naturforsch. **1**, 608 (1946).

[3] R. Blankenbecler, M. L. Goldberger, N. Khuri, and S. Treiman, Ann. Phys. **10**, 62 (1960).

dynamical scheme, fully equivalent to the Schrödinger equation whenever the latter is valid. We therefore study potential scattering only as a correspondence principle from which we may infer certain features of the pure scattering amplitude theory. Whether or not this inductive argument leads to a superior form of quantum mechanics for strong interaction physics, is an experimental question which remains open.

5. Unitarity

One of the essential features of our theory will be the unitarity condition. Stapp[4] has particularly emphasized the importance of unitarity, and gone so far as to deduce the analyticity properties more or less as a consequence.

The condition

$$\nabla \cdot \mathbf{S} = 0,$$

where $\mathbf{S}$ is the probability current flux, simply states the conservation law of particles. Glauber[5] has given a derivation of unitarity starting from a slight generalization of this identity, namely,

$$\nabla \cdot [\langle \mathbf{x} \mid \mathbf{k}_{\text{in}} \rangle \overleftrightarrow{\nabla} \langle \mathbf{x} \mid \mathbf{k}'_{\text{in}} \rangle^*] = 0.$$

This identity holds provided

$$|\mathbf{k}| = |\mathbf{k}'|.$$

If we integrate Glauber's identity over a large spherical volume and apply Green's theorem, and finally insert the asymptotic forms of the wavefunctions for large r, we directly obtain the unitarity condition

$$\frac{1}{2i}\,[M(\mathbf{k}', \mathbf{k}) - M^*(\mathbf{k}, \mathbf{k}')]$$

$$= \frac{k}{4\pi} \int d\Omega_{\hat{\mathbf{k}}''}\, M^*(\mathbf{k}'', \mathbf{k}') M(\mathbf{k}'', \mathbf{k}).$$

For the forward-scattering case $\mathbf{k} = \mathbf{k}'$, this reduces to the optical theorem

$$\text{Im}\, M(\mathbf{k}, \mathbf{k}) = (k/4\pi)\sigma_{\text{tot}}.$$

III. THE MANDELSTAM REPRESENTATION

1. Analytic Properties

The analyticity properties of the scattering amplitude may be deduced from the Fredholm solution of the Schrödinger equation.[6,7] The simpler formal solution provided by the Born series may be used only in the absence of bound states, since otherwise, the Born series fails to converge.

The Lippmann-Schwinger equation as it stands is not an integral equation of the Fredholm type, but by simply iterating once we do obtain a Fredholm intergral equation. The solution has the form

$$\langle \mathbf{x} \mid \mathbf{k}_{\text{in}} \rangle = F(\mathbf{x}) + \frac{1}{D(k)} \int d^3\mathbf{y}\, N(k; \mathbf{x}, \mathbf{y}) F(\mathbf{y}),$$

where

$$F(\mathbf{x}) = \langle \mathbf{x} |\, (1 + G_+ V)\, |\mathbf{k}\rangle,$$

and N, D are the usual Fredholm numerator and denominator functions.

Khuri's analysis[7] of the analytic properties of the scattering amplitude is based on the equation

$$M = (-1/4\pi)\langle \mathbf{k}' |\, V[1 + K + K^2 + KR + KRK]\, |\mathbf{k}\rangle,$$

where $K = G_+V$, and $R = N/D$. This equation follows immediately from the Fredholm solution

$$|\mathbf{k}_{\text{in}}\rangle = (1 + R)(1 + K)\, |\mathbf{k}\rangle,$$

and the original Lippmann-Schwinger equation

$$|\mathbf{k}\rangle = (1 - K)\, |\mathbf{k}_{\text{in}}\rangle.$$

One need only write the identity

$$|\mathbf{k}\rangle = (1 - K)(1 + R)(1 + K)\, |\mathbf{k}\rangle.$$

The actual derivation of the analytic properties is rather tedious, but consists only of investigating the convergence of the various integrals involved in our formal solution.

The scattering amplitude—$M(\mathbf{k}', \mathbf{k})$ in the case of a spherically symmetric potential—is a function of the following scalar products only:

$$s = k^2,$$

$$s' = k'^2,$$

$$t = -(\mathbf{k}' - \mathbf{k})^2.$$

Although the scattering amplitude is nonzero even when s, s' are not equal, it is sufficient for our theory to consider the case $s = s'$ corresponding to the physical requirement of the conservation of energy. We shall allow the energy s and the momentum transfer t to assume arbitrary un-

[4] H. P. Stapp, Phys. Rev. **125**, 2139 (1962).
[5] R. J. Glauber, *Lectures in Theoretical Physics at Boulder, Colorado* (Interscience Publishers, Inc., New York, 1958), Vol. 1, p. 315.
[6] R. Jost and A. Païs, Phys. Rev. **82**, 840 (1951).
[7] N. Khuri, Phys. Rev. **107**, 1148 (1957); S. Gasiorowicz and H. P. Noyes, Nuovo Cimento **10**, 78 (1958); T. Regge, Nuovo Cimento **8**, 671 (1958).

physical and even complex values in the following, and distinguish separately the physical region

$$s > 0,$$
$$-4s < t < 0,$$

corresponding to actual scattering processes.

2. Bound-State Poles

Clearly, the scattering amplitude may have poles wherever the Fredholm denominator $D(k)$ vanishes. According to the Fredholm alternative, when the denominator D vanishes for a particular energy s_n, there exists a solution ψ_n (not identically zero) of the homogeneous equation

$$\psi_n(\mathbf{x}) = \int K(\mathbf{x}, \mathbf{y})\psi_n(\mathbf{y})\, d^3\mathbf{y}.$$

Hence $\psi_n(x)$ satisfies the Schrödinger equation, and has the boundary condition

$$\psi_n \xrightarrow[r\to\infty]{} M\frac{e^{ik_n r}}{r}.$$

Moreover, from the equation $\nabla\cdot\mathbf{S} = 0$, integrating over a large sphere, we obtain

$$(\mathrm{Re}\ k_n)\int d\Omega\ |M|^2 = 0,$$

and hence $\mathrm{Re}\ k_n = 0$. This suggests very strongly that a pole in the scattering amplitude corresponds to a bound state, with ψ_n the wavefunction of the bound state, and binding energy $s_n = k_n^2 < 0$. This fact may be explicitly demonstrated for the Coulomb potential and the exponential potential. We note that the boundary condition guarantees square-integrability if $\mathrm{Im}\ k_n > 0$.

3. The Mandelstam Representation

By the methods outlined, one may show that $M(s, t)$ is analytic in the upper half k plane, except for the bound-state poles mentioned above. Therefore $M(s, t)$ is analytic in the entire complex s plane, except for these same poles, and a cut, $0 < s < \infty$, which arises from the fact that $k = s^{\frac{1}{2}}$.

One may show that the first Born approximation is valid at large energies:

$$M(s, t) \xrightarrow[s\to\infty]{} v(t).$$

Therefore, with an appropriate contour of integration, it follows from Cauchy's theorem that

$$M(s, t) = v(t) + \sum_B \frac{\Gamma_B(t)}{s - s_B} + \int_0^\infty \frac{ds'}{\pi}\frac{\mathrm{Im}\, M(s', t)}{s' - s - i\epsilon}.$$

The term $v(t)$, given explicitly by

$$v(t) = (-1/4\pi)\langle \mathbf{k}'\ |V|\ \mathbf{k}\rangle,$$

arises from a portion of the contour at $|s| = \infty$. The line integral represents the discontinuity across the cut. The residues $\Gamma_B(t)$ are polynomials in t whose order equals the highest angular momentum at which a bound state of energy s_B occurs.

This one-dimensional dispersion relation exhibits the analytic properties of the scattering amplitude for complex s and also the asymptotic properties of the scattering amplitude for large s.

The Mandelstam representation is a generalization of this dispersion relation which exhibits, in addition, the analytic properties of the scattering amplitude as a function of complex t. However, it does not accurately represent the behavior for $t \to \infty$.

Under the condition that the potential be a superposition of Yukawa potentials,

$$V(r) = \int_{\mu^2}^\infty dm^2\, \frac{\sigma(m^2)e^{-mr}}{\pi r},$$

Blankenbecler, *et al.*[3] have shown that the Mandelstam representation is

$$M(s, t) = v(t) + \sum_B \frac{\Gamma_B(t)}{s - s_B} + \int_0^\infty \frac{ds'}{\pi}\int_{(2\mu)^2}^\infty \frac{dt'}{\pi}\frac{\rho(s', t')}{(s' - s)(t' - t)} + \sum_n t^n \int_0^\infty \frac{ds'}{\pi}\frac{g_n(s')}{s' - s},$$

where $v(t)$ may be written

$$v(t) = -\int_{\mu^2}^\infty \frac{dm^2}{\pi}\frac{\sigma(m^2)}{m^2 - t}.$$

The limits of integration are somewhat symbolic. In fact, the spectral function $\rho(s', t')$ vanishes outside the domain

$$s'(t' - 4\mu^2) > \mu^4.$$

4. The Dynamical Scheme

Unitarity, together with dispersion relations, form the basis of a computational scheme that may be used in place of the Schrödinger equation. That is, given a potential $V(r)$, we may compute the scattering cross section and the binding energies of all bound states.

The unitarity condition derived thus far is valid only in the physical region. The Mandelstam

dynamical scheme is based on an extension of unitarity outside the physical region. This is accomplished by substituting the Mandelstam representation into the unitarity condition.

As the scattering amplitude depends only on the scalars s and t rather than on the vectors $\mathbf{k}$ and $\mathbf{k}'$, it is convenient to write the angular integral involved in the unitarity condition in another way. We wish to integrate an expression of the form

$$\int d\Omega'' \, \mathfrak{F}[\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'', \hat{\mathbf{k}}'\cdot\hat{\mathbf{k}}''].$$

If we let

$$x = \hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'', \qquad y = \hat{\mathbf{k}}'\cdot\hat{\mathbf{k}}'', \qquad z = \hat{\mathbf{k}}\cdot\hat{\mathbf{k}}' = \cos\theta,$$

we may obtain the desired formula

$$\int d\Omega'' = 2\int dx \int dy \, \Delta^{-\frac{1}{2}}\theta(\Delta),$$

where

$$\Delta(x, y, z) = \begin{vmatrix} 1 & x & y \\ x & 1 & z \\ y & z & 1 \end{vmatrix},$$

and θ is the step function

$$\theta(\Delta) = \begin{cases} 0 & \text{if } \Delta < 0 \\ 1 & \text{if } \Delta > 0. \end{cases}$$

An easy way to derive this result is to go to the Lehmann coordinate system in which $\mathbf{k}$ and $\mathbf{k}'$ are taken to lie in the XY plane, with $\mathbf{k}$ along the X axis. If (α, β) are polar coordinates of $\mathbf{k}''$ in this system, we may write $d\Omega'' = d\alpha \sin\beta d\beta$, and the Jacobian is $\partial(x, y)/\partial(\alpha, \beta) = -\sin\beta\cos\beta\sin\theta$. We then need only note that $\Delta = (\cos\beta\sin\theta)^2$. The factor 2 in our formula occurs because each value of (x, y) corresponds to two different points on the sphere related by reflection in the XY plane.

We may write $M(s, t)$ as $M(s, z)$ with $z = \cos\theta$; here θ is the scattering angle, and

$$t = -2s(1 - \cos\theta).$$

The use of the same letter M to denote different mathematical functions should not cause any confusion.

The unitarity condition may then be written in the form

$$\frac{1}{2i}[M(s + i\epsilon, z) - M(s - i\epsilon, z)] = \frac{1}{2\pi} s^{\frac{1}{2}} \iint dx\, dy \, \Delta^{-\frac{1}{2}}\theta(\Delta) M^*(s, x) M(s, y).$$

When we now substitute the Mandelstam representation into unitarity, we must, consistent with our policy in this section of writing the scattering amplitude as a function of (s, z) instead of (s, t), rewrite the denominators $(t' - t)$ appearing in the Mandelstam representation as $-2s(\lambda - z)$, where

$$\lambda = 1 + t'/2s.$$

We then typically encounter the integral

$$\int d\Omega'' \frac{1}{(\lambda_1 - \hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'')} \frac{1}{(\lambda_2 - \hat{\mathbf{k}}'\cdot\hat{\mathbf{k}}'')} = 2\pi \int_0^\infty \frac{d\lambda}{\lambda - z} \frac{\theta[-\Delta]}{[-\Delta(\lambda, \lambda_1, \lambda_2)]^{\frac{1}{2}}}.$$

The derivation of this formula is a beautiful illustration of the type of technique involved in the actual proof of the Mandelstam representation,[3] and we have therefore devoted an appendix to this problem.

Upon taking the discontinuity of the resulting unitarity equation across the t cut, we obtain the Mandelstam bootstrap equation,

$$\rho(s, t) = \int_{\mu^2}^\infty \frac{dt'}{\pi} \int_{\mu^2}^\infty \frac{dt''}{\pi} K(s; t, t', t'')\sigma(t')\sigma(t'')$$
$$- \int_{\mu^2}^\infty \frac{dt'}{\pi} \int_{(2\mu)^2}^\infty \frac{dt''}{\pi} K(s; t, t', t'')\sigma(t')[\varphi(t'') + \varphi^*(t'')]$$
$$+ \int_{(2\mu)^2}^\infty \frac{dt'}{\pi} \int_{(2\mu)^2}^\infty \frac{dt''}{\pi} K(s; t, t', t'')\varphi(t')\varphi^*(t''),$$

with

$$\varphi(t') \equiv \varphi(s, t') = \int_0^\infty \frac{ds'}{\pi} \frac{\rho(s', t')}{s' - s - i\epsilon}.$$

The function $K(s; t, t', t'')$ is an abbreviation for

$$K(s; t, t', t'') = (\tfrac{1}{4}\pi)s^{-\frac{1}{2}}(-\Delta)^{-\frac{1}{2}}\theta(-\Delta),$$

with

$$\Delta \equiv \Delta(1 + t/2s, 1 + t'/2s, 1 + t''/2s),$$

and is therefore known.

The Mandelstam bootstrap equation, also known as the extended unitarity condition, may be solved by iteration. One may divide the (s, t) plane into strips, the Nth of which is given by

$$(N\mu)^2 \leq t \leq [(N + 1)\mu]^2.$$

Given the potential, and hence the potential spectral function $\sigma(t)$, we may obtain ρ in the first strip by inspection of the Mandelstam bootstrap equation, which then reduces simply to

$$\rho = K\sigma\sigma,$$

in an obvious symbolic notation. After N interations, the bootstrap equation gives ρ and hence φ in the Nth strip.

5. Infinite-Momentum Transfers

Our dynamical scheme as it stands is not yet complete, for a glance at the Mandelstam representation shows that we need also know the bound-state poles and the single-dispersion functions $g_n(s')$. These functions are not determined because of the incompleteness of the Mandelstam representation with respect to the asymptotic properties of the scattering amplitude for $t \to \infty$. A study of this asymptotic limit will in fact lead to a dynamical scheme which is complete.

IV. REGGE POLES

1. Complex Angular Momentum

It is possible to make a heuristic argument as to why the asymptotic properties of the scattering amplitude in the limit $t \to \infty$ are related to the analyticity properties of the partial-wave amplitudes as a function of complex orbital angular momentum. We offer it only to clear up the aura of mystery usually associated with Regge analysis, and do not claim it to be at all rigorous. We do put everything on a more rigorous basis later on, although all our conclusions will have already followed from the crude heuristic argument.

Consider then the well known formula

$$\psi(k, r, z) \xrightarrow[r\to\infty]{} e^{ikrz} + M(s, z)\frac{e^{ikr}}{r},$$

and suppose that we are allowed to take the limit $z \to \infty$. We suppose, in this limit, that $M \to \infty$. Actually, of course, the limits $r \to \infty$ and $z \to \infty$ do not commute, but all we need do is fix r at some large value and let only $z \to \infty$.

Since $M \to \infty$, and since the term e^{ikrz} remains bounded, the wavefunction factorizes into a product of a function of z only, and a function of r only:

$$\psi(k, r, z) \xrightarrow[z\to\infty]{} M(k, z)\frac{e^{ikr}}{r} \quad \text{(large } r\text{)}.$$

This important conclusion may also be obtained in another way. The Schrödinger equation

$$(\nabla^2 + k^2)\psi = V\psi$$

may be rewritten in polar coordinates r, θ, ϕ. Since the scattering solution is cylindrically symmetric, we may write it as a function of r and $z = \cos\theta$. The Schrödinger equation is then

$$\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\frac{\partial}{\partial z}\left((1 - z^2)\frac{\partial}{\partial z}\right) + k^2\right]\psi(k, r, z) = V(r)\psi(k, r, z).$$

The asymptotic behavior of ψ for $z \to \infty$ is determined by this equation. One solves partial differential equations by separation of variables; thus we expect to find

$$\psi(k, r, z) = \sum_n r^{-1}R_n(r)Z_n(z).$$

For large z, a single one of these terms will dominate so that again,

$$\psi(k, r, z) \xrightarrow[z\to\infty]{} r^{-1}R(r)Z(z),$$

the wavefunction factors. The Schrödinger equation now may be used to imply that

$$Z(z) \xrightarrow[z\to\infty]{} (\text{const})\, z^\alpha,$$

where α is determined by an eigenvalue problem

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{\alpha(\alpha + 1)}{r^2} - V(r)\right)R(r) = 0,$$

with the boundary conditions

$$R(r) \xrightarrow[r\to 0]{} 0$$

$$R(r) \xrightarrow[r\to\infty]{} e^{ikr}.$$

We note that since the limit $z \to \infty$ is unphysical, the wavefunction is not required to be single valued. Therefore α does not have to be a real integer. In fact, we must allow α to be arbitrary complex. Moreover, $Z(z)$ does not have to be a Legendre function of the first kind. It may be an arbitrary linear combination of $P_\alpha(z)$ and $Q_\alpha(z)$.

The boundary conditions on $R(r)$ follow from our first argument concerning what happens to the wavefunction as $z \to \infty$ when r is large. (The limit as $r \to 0$ is found in a similar way.) From this we may also now conclude that

$$M(k, z) \xrightarrow[z\to\infty]{} (\text{const})\, z^\alpha.$$

This is the Regge theorem.[8]

We have been led to the radial equation that one also encounters by partial-wave analysis, but as our derivation clearly shows, the angular momentum α involved must be taken as complex. Moreover, we have an additional boundary condition imposed on the radial function $R(r)$, which is precisely why

[8] T. Regge, Nuovo Cimento **14**, 951 (1959); *Ibid.* **18**, 947 (1960).

this equation is an eigenvalue problem for α. The absence of the term proportional to e^{-ikr} that usually appears in the radial wavefunction will be seen later to be only the condition that the scattering amplitude have a pole at angular momentum α.

2. Jost Functions

We wish now to put Regge's theorem on a more rigorous basis, and to derive a few related results. We therefore study the radial equation in somewhat greater detail. A good review of some parts of this subject has been given by Newton.[9,10]

The asymptotic form of the expansion of a plane wave in Legendre polynomials is given by

$$e^{i\mathbf{k}\cdot\mathbf{x}} \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} (2l+1)\frac{(-)^{l+1}}{2ikr} \times P_l(\cos\theta)[e^{-ikr} + (-)^{l+1}e^{+ikr}].$$

We may interpret the term proportional to e^{-ikr} as an incoming wave, and e^{ikr} as outgoing wave. The conservation of probability allows only a phase change in the outgoing wave for a given angular-momentum channel in the physical wavefunction. We may therefore write

$$\langle \mathbf{x} \mid \mathbf{k}_{in}\rangle \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} (2l+1)\frac{(-)^{l+1}}{2ikr} \times P_l(\cos\theta)[e^{-ikr} + (-)^{l+1}e^{2i\delta_l}e^{+ikr}],$$

where the δ_l are the physical phase shifts. The scattering amplitude is given by

$$M(s,z) = \sum_{l=0}^{\infty} (2l+1)P_l(z)M(l,k),$$

with

$$M(l,k) = (1/2ik)[e^{2i\delta_l} - 1].$$

Again we use the same letter M to denote entirely distinct functions.

For arbitrary r, but for physical values of z, we may write

$$\langle \mathbf{x} \mid \mathbf{k}_{in}\rangle = \sum_{l=0}^{\infty} (2l+1)\frac{(-)^{l+1}}{2ikr}\psi(l,k,r)P_l(\cos\theta),$$

where $\psi(l, k, r)$ satisfies the radial Schrödinger equation

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

with the boundary condition

$$\psi(l,k,r) \xrightarrow[r\to\infty]{} 0.$$

The phase shift is determined by the limit $r \to \infty$:

$$\psi(l,k,r) \to e^{-ikr} + (-)^{l+1}e^{2i\delta_l}e^{+ikr}.$$

In addition to the physical solution ψ, it is convenient to work with two other mathematical solutions of the radial Schrödinger equation, commonly known as the Jost solutions.[11] They satisfy the boundary conditions

$$\varphi(l,k,r) \xrightarrow[r\to 0]{} r^{l+1},$$

$$f(l,k,r) \xrightarrow[r\to\infty]{} e^{ikr}.$$

It is clear that since the radial equation is invariant under the interchanges $k \rightleftarrows -k$, and $l \rightleftarrows -l-1$, that $f(l, -k, r)$ and $\varphi(-l-1, k, r)$ are two further solutions, provided the proper analytic continuations exist.

The Jost solution φ is defined *uniquely* by the boundary condition only if Re $(2l+1) \geq 0$, which we call the right half l plane. In the left-hand plane we define φ by analytic continuation. Similarly, the solution f is defined by the boundary condition only if Im $k \geq 0$, and in the lower half plane only by analytic continuation. Although the boundary conditions are still true outside of these restricted half planes, they are no longer defining equations.

The Wronskian of any two solutions of the radial equation is a constant, independent of r, and may therefore be evaluated in one of the two limits $r \to 0$ or $r \to \infty$. Thus,

$$\varphi(-l-1,k,r)\overleftrightarrow{\frac{d}{dr}}\varphi(l,k,r) = 2l+1$$

$$f(l,-k,r)\overleftrightarrow{\frac{d}{dr}}f(l,k,r) = 2ik,$$

where

$$f\overleftrightarrow{\frac{d}{dr}}g \equiv fg' - gf'.$$

Jost defined the two Wronskians

$$(2l+1)f(l,\pm k) = f(l,\pm k,r)\overleftrightarrow{\frac{d}{dr}}\varphi(l,k,r).$$

[Actually, Jost writes $f(l, -k)$ for our $f(l, +k)$.] Clearly, one may write

$$\varphi(l,k,r) = -[(2l+1)/2ik][f(l,k)f(l,-k,r) - f(l,-k)f(l,k,r)].$$

[9] R. G. Newton, J. Math. Phys. **1**, 319 (1960).
[10] R. G. Newton, J. Math. Phys. **3**, 867 (1962).
[11] R. Jost, Helv. Phys. Acta **20**, 256 (1947).

For integer l, we have

$$\psi(l, k, r) = -\frac{2ik}{2l+1}\frac{\varphi(l, k, r)}{f(l, k)}.$$

Hence, comparing these two equations with the definition of the phase shift, we have

$$S(l, k) \equiv e^{2i\delta_l} = (-)^l f(l, -k)/f(l, k).$$

This formula holds so far only for integer l. In extending this formula to complex l, we may choose arbitrarily to replace $(-)^l$ by $e^{+i\pi l}$. This is purely a matter of convenience, and any other choice would lead to the same physical results. We must also define $f(l, -k)$ more accurately as there are several possible different analytic continuations from $+k$ to $-k$.[12]

3. Analyticity of $\varphi(l, k, r)$

The analytic properties of the solution φ of the radial equation as a function of complex l and k may be obtained most simply by using power series. We shall assume that $rV(r)$ is entire. This large class of potentials includes the Yukawa potential $\lambda e^{-\mu r}/r$. We may therefore write

$$-r^2(k^2 - V) = \sum_{n=1}^{\infty} a_n r^n.$$

The coefficients must satisfy the following condition as a consequence of the fact that rV is entire. Given any R, arbitrarily large, there exists a number M, such that

$$|a_n| < M/R^n,$$

for all n.

The solution $\varphi(l, k, r)$ is obtained as a power series

$$\varphi(l, k, r) = r^{l+1}\sum_{n=0}^{\infty} A_n r^n.$$

The leading coefficient is $A_0 = 1$. The radial differential equation imposes the many-term recursion relation

$$A_n = \frac{1}{n(n+2l+1)}\sum_{p=0}^{n-1} a_{n-p}A_p,$$

which may be solved iteratively for the A_n.

It is immediately clear from the recursion relation that poles occur in the function φ when $2l + 1 = -n$, with $n = 1, 2, \cdots \infty$. Moreover, all these poles are simple. The function $(2l + 1)!$ is an analytic function of l with poles at the same points, and thus the ratio

$$\varphi(l, k, r)/(2l + 1)!$$

will be entire.[13]

Aside from these simple poles, we may show now that the function φ defined by the power series is an analytic function in the entire l plane and the entire k plane. We must prove that, except for the points $2l + 1 = -n$, the power series $\sum A_n r^n$ converges.

Having chosen M such that $|a_n| \leq M/R^n$, we now choose, for fixed l, a sufficiently large number N such that

$$|M/(N + 2l + 1)| \leq 1.$$

Since the first N terms of the power series are certainly finite, we may find finally a large number Q such that $|A_n| \leq Q/R^n$ for $n = 1, 2 \cdots (N - 1)$. We may now show that the inequality

$$|A_n| \leq Q/R^n$$

in fact holds for all $n \geq N$ as well, using only the pedestrian method of proof by induction. We suppose that the identity has been established for $n = 1, \cdots, m - 1$, with $m \geq N$, and then apply the recursion relation to establish the identity for $n = m$. Since R is arbitrary, we have now proved the series converges for all r. Q.E.D.

A brief inspection shows that the coefficients $A_n(l, k)$ are analytic in l and k. In fact the coefficients A_n are polynomials in k^2 and rational functions of l.

The power series provides the necessary analytic continuation of $\varphi(l, k, r)$ in the left-hand l plane. All statements about φ in the left-hand plane in the following are based on the explicit power-series solution.

For example, the theorem

$$\varphi^*(l^*, k^*, r) = \varphi(l, k, r)$$

may be proved in this way.

4. Analytic Properties of $f(l, k, r)$

We study the analytic properties of the solution $f(l, k, r)$ by the method of Poincaré, based on the integral equation

$$f(l, k, x) = e^{ikx} + \frac{1}{k}\int_x^{\infty} dy \sin k(y - x) \times \left[V(y) + \frac{l(l+1)}{y^2}\right] f(l, k, y).$$

Since

$$G(k; x, y) = (1/k)\sin k(y - x)\theta(y - x)$$

[12] A. Bottino, A. M. Longoni, and T. Regge, Nuovo Cimento **23**, 954 (1962).

[13] R. Blankenbecler and M. L. Goldberger, Phys. Rev. **126**, 766 (1962).

is a Green's function

$$(d^2/dx^2 + k^2)G(k; x, y) = \delta(x - y),$$

we may readily show that this integral equation is completely equivalent to the radial Schrödinger equation. The boundary condition on f is, of course, built in automatically.

It is convenient to separate our study into two parts. We first study the easiest case, Im $k \geq 0$, and later the more involved case Im $k \leq 0$.

Iterating the integral equation, we obtain the Neumann series solution

$$f(l, k, x) = \sum_{n=0}^{\infty} f_n(l, k, x),$$

with

$$f_0(l, k, x) = e^{ikx}.$$

The nth term of the series is

$$f_n(l, k, x) = \frac{1}{k^n} \int_x^\infty dy_1 \cdots \int_{y_{n-1}}^\infty dy_n \times \sin k(y_1 - x) \cdots \sin k(y_n - y_{n-1}) \times e^{iky_n} \prod_{j=1}^{n} \left[V(y_j) - \frac{l(l+1)}{y_j^2} \right].$$

By inspection, the integrand of the nth term is entire in both l and k. The analytic properties of the integrals are therefore determined by the convergence properties. The factor $\sin k(y - x)$ diverges as $y \to \infty$ when k is complex. Therefore the integral can be convergent only if e^{iky} can damp out this divergence, which is the case for Im $k \geq 0$. Since

$$|\sin k(y - x)| \leq e^{+(\mathrm{Im}\, k)(y-x)},$$

and

$$|e^{iky}| = e^{-(\mathrm{Im}\, k)y},$$

when Im $k \geq 0$ and $y \geq x$, one can indeed show that the integrals converge, and we can place the bound

$$|f_n| \leq e^{-(\mathrm{Im}\, k)x} \cdot \frac{1}{n!} \left[\frac{1}{|k|} \int_x^\infty dy \left| V(y) - \frac{l(l+1)}{y^2} \right| \right]^n.$$

Convergence is assured if we postulate the inequality

$$|V(y)| < M/y^2$$

to be satisfied by the potential. The majorant series obtained in this bound is an exponential series, and hence the Neumann series converges. We have thus proved that the solution $f(l, k, x)$ is analytic in the product of the entire l plane and the upper half k plane.

Having disposed of this trivial case, we now proceed to investigate analyticity in the lower half k plane. The technique we use is a generalization of one extensively used in the researches of Martin.[14,15] The main idea is to write the potential as a superposition of exponential potentials

$$V(r) + \frac{l(l+1)}{r^2} = \int_0^\infty d\lambda\, g(\lambda) e^{-\lambda r}.$$

The value of this is easily understood from the work of Ma[16] which shows that the analytic structure of the scattering amplitude is particularly simple for an exponential potential, and consists merely of poles. These poles will here be spread out and become cuts.

The Yukawa potential may be written as such a superposition:

$$\frac{e^{-\mu r}}{r} = \int_\mu^\infty d\lambda\, e^{-\lambda r},$$

as may be the centrifugal potential

$$\frac{1}{r^2} = \int_0^\infty \lambda\, d\lambda\, e^{-\lambda r}.$$

We shall assume in general that the weight function $g(\lambda)$ satisfies

$$|g(\lambda)| < G\lambda.$$

Our procedure is to substitute the representation of the potential as a superposition of exponential potentials into the Neumann series, and integrate over $y_1 \cdots y_n$. It is convenient to introduce a set of variables

$$\zeta_j = \lambda_n + \lambda_{n-1} + \cdots + \lambda_j.$$

Then we may write the nth term of the Neumann series as

$$f_n(l, k, x) = e^{ikx} \int_0^\infty d\zeta_1\, e^{-\zeta_1 x} \rho_n(l, k, \zeta_1),$$

where

$$\rho_n = \int_0^{\zeta_1} d\zeta_2 \cdots \int_0^{\zeta_{n-1}} d\zeta_n \times \frac{g(\zeta_1 - \zeta_2) \cdots g(\zeta_{n-1} - \zeta_n) g(\zeta_n)}{\prod_{j=1}^{n} \zeta_j(\zeta_j - 2ik)}.$$

This representation clearly shows the existence

[14] A. Martin, Nuovo Cimento 14, 403 (1959); J. Math. Phys. 1, 41 (1960).
[15] D. I. Fivel and A. Klein, J. Math. Phys. 1, 274 (1960).
[16] S. T. Ma, Phys. Rev. 69, 668 (1946); H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. 8, 111 (1936).

of a cut along the negative imaginary k axis, $0 \leq 2ik \leq \infty$.

To show that, apart from this cut, the function $f(l, k, x)$ is analytic in the lower half plane, we need only argue that (1) the integrals defining f_n converge, and (2) the Neumann series itself converges.

We use the postulated bound on $g(\lambda)$ and

$$\frac{1}{|\zeta_i - 2ik|} \leq \frac{1}{2\,|\mathrm{Re}\, k|}.$$

The following integral is then encountered:

$$\int_0^{\zeta_1} d\zeta_2 \cdots \int_0^{\zeta_{n-1}} d\zeta_n \frac{(\zeta_1 - \zeta_2) \cdots (\zeta_{n-1} - \zeta_n)}{\zeta_1 \cdots \zeta_{n-1}}.$$

This integral may be carried out by induction. We then obtain

$$|\rho_n| \leq \left(\frac{G}{2\,|\mathrm{Re}\, k|}\right)^n \frac{(\zeta_1)^{n-1}}{n!(n-1)!}.$$

We also obtain the bound

$$|f_n| \leq e^{+|\mathrm{Im}\, k|x} \left(\frac{G}{2\,|\mathrm{Re}\, k|\, x}\right)^n \frac{1}{n!}.$$

Thus the convergence of the integrals is proved for nonzero x, and the majorant series for the Neumann series is an exponential series. Q.E.D.

We shall now discuss $f(l, k, x)$ as a function of k on a Riemann surface. In the preceding we have restricted ourselves to one sheet

$$-\tfrac{1}{2}\pi \leq \arg k \leq +\tfrac{3}{2}\pi$$

of the full Riemann surface.

The discontinuity of $f(l, k, x)$ across the branch cut is independent of the potential for $0 \leq 2ik \leq \mu$. We may extend the function $f(l, k, x)$ onto new Riemann sheets by winding around the branch point $k = 0$. In winding around, we agree to avoid the nonkinematic part of the cut $\mu \leq 2ik < \infty$. Any point of the Riemann surface so defined may be represented in the form

$$k = |k|\, e^{i\varphi},$$

where the phase φ tells us how many times we have wound around the kinematic branch point.

On this Riemann surface we may define an operation of complex conjugation by

$$k^* = |k|\, e^{-i\varphi}.$$

This operation applied to a value of k on the principal sheet, $-\frac{1}{2}\pi \leq \arg k \leq +\frac{3}{2}\pi$, yields points on other sheets. If k is on the principal sheet, then $k^* e^{\pi i}$ is again on the principal sheet.

Let us now confine our attention to the principal sheet, and actually compute the discontinuity across the part of the cut $0 \leq 2ik \leq \mu$. The Neumann series is

$$f(l, k, x) = e^{ikx}\Bigg[1 + \sum_{n=1}^{\infty} \int_0^{\infty} d\lambda_1 \cdots \int_0^{\infty} d\lambda_n \times g(\lambda_1) \cdots g(\lambda_n) e^{-(\lambda_1 + \cdots + \lambda_n)x} \times \prod_{i=1}^{n} \frac{1}{(\lambda_1 + \cdots + \lambda_i)(\lambda_1 + \cdots + \lambda_i - 2ik)}\Bigg].$$

It is convenient to write a partial fraction expansion

$$\prod_{i=1}^{n} \frac{1}{(\lambda_1 + \cdots + \lambda_i)(\lambda_1 + \cdots + \lambda_i - 2ik)} = \sum_{s=1}^{n} \frac{\Gamma_s(\lambda_1, \cdots, \lambda_n)}{\lambda_1 + \cdots + \lambda_s - 2ik}.$$

The discontinuity may be computed by the identity

$$1/(x \pm i\epsilon) = \mathcal{P}/x \mp i\pi\delta(x).$$

We then obtain

$$f(l, k + \epsilon, x) - f(l, k - \epsilon, x) = 2\pi i e^{ikx} \sum_{n=1}^{\infty} \sum_{s=1}^{n} \int_0^{\infty} d\lambda_1 \cdots \int_0^{\infty} d\lambda_n \times g(\lambda_1) \cdots g(\lambda_n) \cdot e^{-(\lambda_1 + \cdots + \lambda_n)x} \times \Gamma_s \delta(\lambda_1 + \cdots + \lambda_s - 2ik).$$

The δ function here requires that $\lambda_1, \cdots, \lambda_s$ be less than $2ik$, and hence less than μ. Therefore,

$$g(\lambda_1) \cdots g(\lambda_s) = [l(l+1)]^s \lambda_1 \cdots \lambda_s.$$

We may carry out the integral over λ_s, eliminating this variable wherever it appears by use of the δ function. Finally, we may interchange the sumations over s and n, and thus obtain

$$f(l, k + \epsilon, x) - f(l, k - \epsilon, x) = B(l, k) f(l, -k, x),$$

with

$$B(l, k) = \sum_{s=1}^{\infty} \frac{\pi}{k} [l(l+1)]^s \times \int_0^{2ik} d\lambda_1 \cdots \int_0^{2ik} d\lambda_{s-1}\, \lambda_s \theta(\lambda_s) \times \prod_{t=1}^{s-1} \frac{\lambda_t}{(\lambda_1 + \cdots + \lambda_t)(\lambda_1 + \cdots + \lambda_t - 2ik)}.$$

We note that $B(l, k)$ is independent of $g(\lambda)$, and hence of the potential $V(r)$, and also $B(l, k)$ is independent of x. Therefore,

$$B(l, k) = \frac{f(l, k + \epsilon, x) - f(l, k - \epsilon, x)}{f(l, -k, x)} = \frac{f_0(l, k + \epsilon, x) - f_0(l, k - \epsilon, x)}{f_0(l, -k, x)},$$

where $f_0(l, k, x)$ is the solution of the radial equation in the case $V = 0$:

$$f_0(l, k, x) = e^{i(l+1)\pi/2}\left(\frac{\pi kx}{2}\right)^{\frac{1}{2}}[J_{l+\frac{1}{2}}(kx) + iN_{l+\frac{1}{2}}(kx)].$$

Since B is independent of x, we may evaluate it by examining just the limit $x \to 0$:

$$f_0(l, k, x) \xrightarrow[x\to 0]{} \left(\frac{2}{-ik}\right)^l \frac{1}{x^l} \frac{\Gamma(l + \frac{1}{2})}{\pi^{\frac{1}{2}}}.$$

We then obtain

$$B(l, k) = 2i \sin \pi l.$$

In particular, for l = real integer, the kinematic cut is simply absent.[12]

The Wronskians $f(l, k)$ satisfy the same type of relation. We may remove our restriction to the principal sheet and write

$$f(l, k) - f(l, ke^{2\pi i}) = 2i \sin \pi l f(l, ke^{\pi i}).$$

Our explicit solution also implies a reality condition which we may write as

$$f^*(l^*, k^*e^{\pi i}) = f(l, k).$$

Now that the analytic structure is clear, we may for the first time extend the definition of the S matrix, previously given only for real-integer angular momentum, to arbitrary complex l:

$$S(l, k) = [f(l, ke^{\pi i})/f(l, k)]e^{i\pi l}.$$

5. Regge Poles

It is clear from the definition of $f(l, k)$ as a Wronskian that it possesses whatever analytic properties are common to both $\varphi(l, k, r)$ and $f(l, k, r)$ and to their first derivatives. It follows therefore that

$$D(l, k) \equiv f(l, k)/(2l)!$$

is entire in l and in k except for a branch cut along the negative imaginary k axis. The S matrix, being the ratio of two entire functions of l, is itself a meromorphic function of l, the poles of S being the zeros of $f(l, k)$. These are called Regge poles.[8] If $l = \alpha$ is the position of a Regge pole, then $f(\alpha, k) = 0$, and hence,

$$\varphi(l, k, r) \xrightarrow[r\to\infty]{} \frac{2l + 1}{2ik} f(l, -k)e^{ikr}.$$

This is precisely the boundary condition we found necessary to impose in our heuristic considerations. We note that as the energy varies, a given pole $\alpha(s)$ will move continuously, sweeping out a trajectory. If $\alpha(s)$ is a real integer for some negative energy, we obviously have a bound state at that energy and angular momentum. If Re $\alpha(s)$ = real integer, and Im α is small for some positive energy, we have a resonance state at that energy.

6. The N/D Method

In order to understand and appreciate the economy of dynamical schemes based on Regge poles, it is appropriate to review the status of the older N/D method. We have already derived all the analytic properties we need.[17] We restrict ourselves, therefore, to the case of just one bound state of no spin. Our aim will be to calculate the binding energy of this bound state in the $l = 0$ channel by dispersion theory.

The S matrix in the $l = 0$ channel is given by $f(0, -k)/f(0, k)$, and hence the scattering amplitude may be written as

$$M(0, k) = N(s)/D(s),$$

with

$$N(s) = (1/2ik)[f(0, -k) - f(0, k)],$$

and

$$D(s) = f(0, k).$$

Since N is invariant under the interchange $k \rightleftarrows -k$, it possesses no right-hand cut in s. Since D has no singularities in the upper half k plane, there is no left-hand cut in s. Moreover, we may show[9] that $N \to 0$ and $D \to D(\infty)$ = const as $s \to \infty$. For convenience we may change the normalization of both N and D by dividing by $D(\infty)$.

These properties of N and D imply the pair of dispersion relations

$$N(s) = \int_{-\infty}^{-\mu^2/4} \frac{ds'}{\pi} \frac{\text{Im } N(s')}{s' - s - i\epsilon};$$

$$D(s) = 1 + \int_0^\infty \frac{ds'}{\pi} \frac{\text{Im } D(s')}{s' - s - i\epsilon}.$$

From the relation $f^*(0, k^*) = f(0, -k)$, which expresses the unitarity of the S matrix, we may derive

$$\text{Im } \frac{1}{M(0, k)} = (-s)^{\frac{1}{2}}.$$

[17] G. F. Chew and S. Mandelstam, Phys. Rev. **119**, 467 (1960).

for $s > 0$; and since N is real for $s > 0$, we have Im $D = N$ Im M^{-1}, or,

$$\text{Im } D(s) = (-s)^{\frac{1}{2}}N(s)\theta(s).$$

Similarly, for $s < 0$, we have D = real, and hence,

$$\text{Im } N(s) = D(s) \text{ Im } M(0, k)\theta(-s - \mu^2/4).$$

Inserting these two relations into the dispersion relations for N and D, and eliminating N, we obtain the integral equation

$$D(s) = 1 + \int_{-\infty}^{-\frac{1}{4}\mu^2} \frac{ds'}{\pi} \frac{D(s') \text{ Im } M(s')}{(-s')^{\frac{1}{2}} + (-s)^{\frac{1}{2}}},$$

which may be transformed to a Fredholm equation by a change of variable, $x = (-s')^{-\frac{1}{2}}$. Given Im $M(s')$ for $s' < 0$, we may solve this equation, and obtain the bound states as the solutions of $D(s) = 0$. The problem of obtaining the bound states is thus reduced to obtaining the discontinuity of the partial-wave $M(0, s)$ along the left-hand cut.

We have seen that one may determine $\rho(s, t)$ iteratively by the Mandelstam dynamical scheme, but so far Γ and $g(s)$ remain undetermined.

Now suppose we write down the Mandelstam representation, allowing for a single bound state, and project out the S-wave amplitude

$$M(0, s) = \int_{-1}^{1} \frac{dz}{2} M(s, t).$$

We recall here that $t = -2s(1 - z)$. The left-hand cut in $M(0, s)$ has as its source the denominators $(t' - t)$ of the Mandelstam representation. The $(s' - s)$ denominators, such as appear in the single-dispersion term, contribute only the right-hand cut. Thus when we take the discontinuity across the left-hand cut, the unwanted terms very conveniently drop out, and we obtain

$$[\text{Im } M(0, s')]_L = -\int_{-1}^{1} \frac{dz}{2}\left[\sigma(t)\theta(t - \mu^2) + \int_0^\infty \frac{ds'}{\pi} \frac{\rho(s', t)\theta(t - 4\mu^2)}{s' - s}\right].$$

This equation completes the dynamical scheme.

To sum up, the complete dynamical scheme is the following. We are given the potential $V(r)$ and hence $\sigma(t)$. We begin the calculation by computing the spectral function $\rho(s, t)$ using the Mandelstam bootstrap equation, symbolically

$$\rho = K\sigma\sigma + K\rho\sigma + K\rho\rho.$$

The second step is to compute the left-hand discontinuity Im $M(l, s)$ for the channels containing bound states, and the third is to use this result to solve the integral equation for D. Finally, we may locate the zeros of D to obtain the bound states.

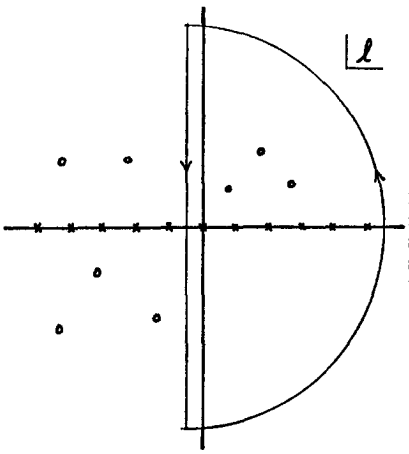

FIG. 1. Contour for Regge representation. x represents poles due to sin πl; 0 represents poles due to $M(l, k)$.

7. The Regge Theorem

The Regge theorem follows immediately by the application of the Sommerfeld–Watson transformation[18] to the Legendre series:

$$M(s, t) = \sum_{l=0}^{\infty} (2l + 1)M(l, k)P_l(z).$$

Consider the integral

$$\text{I} = \frac{1}{2i}\oint dl \frac{(2l + 1)M(l, k)P_l(-z)}{\sin \pi l},$$

where the contour is a semicircle in the right half l plane (cf. Fig. 1.) The Legendre function $P_l(z)$ is entire in l; thus by Cauchy's theorem, the integral is the sum of residues of the poles of $M(l, k)$ and of

$$\frac{1}{\sin \pi l} = \sum_{n=-\infty}^{+\infty} \frac{(-)^n}{\pi} \frac{1}{l - n}.$$

These poles at $l = 0, 1, \cdots \infty$ yield the partial-wave series.

We may write

$$M(l, k) = M_0(l, k) + \sum_n \frac{\beta_n(s)}{l - \alpha_n(s)},$$

where M_0 is analytic in the right half l plane.

We thus obtain Regge's representation for the scattering amplitude:

$$M(s, t) = -\pi \sum_n \frac{\beta_n(2\alpha_n + 1)}{\sin \pi\alpha_n} P_{\alpha_n}(-z) + \frac{i}{2}\int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty} dl \frac{(2l + 1)M(l, k)P_l(-z)}{\sin \pi l}.$$

[18] P. M. Morse and H. Feshbach *Methods of Theoretical Physics* (McGraw-Hill Book Company Inc., 1953), Vol. 1, p. 413.

We have already omitted the contribution from the semicircle at $|l| = \infty$, which is justified only if s is real and positive. For negative energies, a different representation must be chosen.

For Re $(2\alpha + 1) \geq 0$, the asymptotic behavior of the Legendre function is given by[19]

$$P_\alpha(z) \xrightarrow[z\to\infty]{} \binom{2\alpha}{\alpha}(z/2)^\alpha,$$

while in the left-hand plane we may use the relation $P_\alpha = P_{-\alpha-1}$. For this reason, Legendre functions are not very convenient for Regge analysis in the left-hand plane.

The Regge representation immediately implies that the asymptotic behavior of the scattering amplitude for $t \to \infty$ is given by

$$M(s, t) \xrightarrow[t\to\infty]{} b(s)t^{\alpha(s)},$$

where $\alpha(s)$ is the leading Regge trajectory, that is, the Regge pole furthest to the right in the complex l plane.

It must be remarked that the Regge theorem has been proved only for real, positive energies. It also is true for real, negative energies. For complex energies we have no proof, although the theorem is probably true.

8. Infinite Angular Momentum

The behavior of $M(l, k)$ for $l \to \infty$ is required in the above proof of the Regge representation. We shall here prove that when $l \to \infty$ along any ray in the right half plane, we have

$$M(l, k) \xrightarrow[l\to\infty]{} C(k)e^{-\alpha l},$$

where

$$\cosh \alpha = 1 + \mu^2/2k^2.$$

It is interesting to remark on a kind of duality that exists between the variables l and z. Just as the analytic properties in l imply the asymptotic properties for large z, so also are the asymptotic properties for large l closely related to the analytic properties of the scattering amplitude as a function of complex z. In fact, for l = real integer, but arbitrary complex z, we have[20]

$$|P_l(z)| \leq |z + (z^2 - 1)^{\frac{1}{2}}|^l,$$

and hence, using the Weierstrass majorization test, the Legendre series

$$M(s, t) = \sum_{l=0}^{\infty} (2l + 1)M(l, k)P_l(z)$$

converges in the region

$$|z + (z^2 - 1)^{\frac{1}{2}}| < e^\alpha.$$

This is precisely the Lehmann ellipse.[21] Perhaps this observation is the germ of an alternative proof of the Mandelstam representation.

We start from the Schrödinger equation, and for simplicity, we choose a Yukawa potential. We introduce the operator G^{-1}:

$$G^{-1} = \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2},$$

so that the Schrödinger equation can be written

$$G^{-1}\,|\varphi\rangle = \pi g(e^{-\mu r}/r)\,|\varphi\rangle.$$

Following Favella and Reineri[22], we introduce the Hankel transform representation

$$\langle r \mid \xi\rangle \equiv (r\xi)^{\frac{1}{2}}J_{l+\frac{1}{2}}(r\xi).$$

These form an orthogonal set of functions because they are the eigenfunctions of the operator G^{-1}:

$$G^{-1}\,|\xi\rangle = (k^2 - \xi^2)\,|\xi\rangle,$$

and the normalization

$$\langle \xi \mid \xi'\rangle = \delta(\xi' - \xi)$$

is equivalent to the well known Hankel transform theorem[23]; if

$$f(\xi) = \int_0^\infty dr\,(r\xi)^{\frac{1}{2}}J_{l+\frac{1}{2}}(r\xi)g(r),$$

then

$$g(r) = \int_0^\infty d\xi\,(r\xi)^{\frac{1}{2}}J_{l+\frac{1}{2}}(r\xi)f(\xi).$$

The solution $\varphi(l, k, r)$ is, except for a normalization factor, given by the solution of the Schrödinger equation, written in integral equation form:

$$|\varphi\rangle = |k\rangle + GV\,|\varphi\rangle,$$

where $G^{-1} \mid k\rangle = 0$. The Yukawa potential in this representation is given by[24]

$$\langle \xi\,|V|\,\xi'\rangle = gQ_l\left(\frac{\xi^2 + \xi'^2 + \mu^2}{2\xi\xi'}\right).$$

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[19] Bateman Manuscript Project, edited by A. Erdélyi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., 1953), Vol. I, p. 164.

[20] E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics* (Cambridge University Press, 1931), p. 60.

[21] H. Lehmann, Nuovo Cimento **10**, 579 (1958).

[22] L. Favella and M. T. Reineri, Nuovo Cimento **23**, 616 (1962).

[23] Cf. reference 18, p. 944.

[24] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, 1944), p. 389.

We shall, in the following, abbreviate the Legendre function of the second kind appearing here by writing $Q_l(\xi, \xi')$.

The Schrödinger equation

$$\langle \xi \mid \varphi \rangle = \delta(\xi - k) + \frac{g}{k^2 - \xi^2 + i\epsilon} \int_0^\infty d\xi'\, Q_l(\xi, \xi') \langle \xi' \mid \varphi \rangle,$$

may be written as a Fredholm equation, viz.

$$y(l, k, \xi) \equiv \frac{(k^2 - \xi^2)\langle \xi \mid \varphi \rangle}{g \int_0^\infty d\xi' \, \langle \xi' \mid \varphi \rangle}.$$

Then the Schrödinger equation may be written as

$$y(l, k, \xi) = Q_l(\xi, k) + g \int_0^\infty d\xi'\, K(\xi, \xi') y(l, k, \xi')$$

with the kernel

$$K(\xi, \xi') \equiv \frac{Q_l(\xi, \xi') - Q_l(\xi, k)}{k^2 - \xi'^2 + i\epsilon}.$$

Favelli and Reineri have shown that for sufficiently large l, the kernel becomes arbitrarily weak; in fact,

$$A^2 \equiv \int_0^\infty d\xi \int_0^\infty d\xi' \, |K(\xi, \xi')|^2 \xrightarrow[l\to\infty]{} \frac{M}{l^3}.$$

The proof is very simple. We note that[25]

$$Q_l(z) \xrightarrow[l\to\infty]{} (\tfrac{1}{2}\pi)^{\frac{1}{2}}(l+1)^{-\frac{1}{2}}(z^2-1)^{-\frac{1}{4}}[z + (z^2-1)^{\frac{1}{2}}]^{-(l+\frac{1}{2})}.$$

Thus Q_l depends exponentially on l except when $z = 1$. Since the argument of $Q_l(\xi, \xi')$ tends to unity as $\xi \to \infty$ and $\xi/\xi' \to 1$, we may conclude that the dominant contribution of the integral A^2 comes from such values of ξ and ξ'. We thus obtain the estimate

$$A^2 \xrightarrow[l\to\infty]{} \int_R^\infty d\xi \int_{(1-\alpha)\xi}^{(1+\alpha)\xi} d\xi' \, \frac{Q_l(\xi, \xi')^2}{\xi'^4},$$

where R may be chosen to be any arbitrary finite number, and α any (small) nonzero number. If we note that

$$Q_l(\xi, (1 \pm \beta)\xi) \xrightarrow[l\to\infty]{\xi\to\infty} l^{-\frac{1}{2}}(1+\beta)^{-l},$$

the integration becomes trivial and yields the result quoted. (It is convenient to use $1/\xi$ and ξ'/ξ as new integration variables.)

Since $A^2 < M/l^3$ for large l, it follows[26] that the series

$$y = Q + KQ + K^2Q + \cdots$$

is a uniformly (with respect to ξ) asymptotic (for large l) series. The uniformity is important because we wish to extract information about the phase shifts, which requires an interchange in limits. In fact, we obtain

$$\varphi(l, k, r) \xrightarrow[l\to\infty]{} \int_0^\infty d\xi \, (r\xi)^{\frac{1}{2}} J_{l+\frac{1}{2}}(r\xi) \frac{Q_l(\zeta, k)}{k^2 - \xi^2 + i\epsilon},$$

and the phase shift may be obtained by considering the limit $r \to \infty$. Finally we obtain

$$M(l, k) \xrightarrow[l\to\infty]{} -\frac{\pi g}{2k^2} Q_l(k, k),$$

or, $M \to e^{-\alpha l}$, as $l \to \infty$, with $\alpha = 1 + \mu^2/2k^2$.

9. Dynamical Schemes Based on Regge Poles

Several schemes have been set up which employ Regge poles in one way or another. The simplest and clearest calculational scheme based on Regge poles is that proposed by Chew, Frautschi, and Mandelstam.[27] In this scheme, we start as before by computing the spectral function $\rho(s, t)$, using the Mandelstam bootstrap equation. Having accomplished this, however, we do not solve the integral equation for D as in the old-fashioned N/D scheme, but instead simply extrapolate to large-momentum transfers.

For simplicity, we shall concentrate on the leading trajectory. Since the Regge theorem provides us with an asymptotic expansion for large t, we may also obtain all the others by subtracting out the leading trajectory. In numerical work it of course becomes increasingly difficult to obtain the trajectories after the first.

By Regge's theorem, we have

$$M(s, t) \xrightarrow[t\to\infty]{} b(s) t^{\alpha(s)},$$

where $\alpha(s)$ is the leading trajectory. If we take the discontinuity of this equation across the cut in the t plane:

$$\varphi(s, t) = \frac{1}{2i}[M(s, t + i\epsilon) - M(s, t - i\epsilon)],$$

we obtain

$$\varphi(s, t) \xrightarrow[t\to\infty]{} -b(s) \sin \pi\alpha(s) \cdot (-t)^{\alpha(s)}.$$

It is this equation, rather than the Regge theorem

[25] B. Jeffreys and H. Jeffreys, *Methods of Mathematical Physics* (Cambridge University Press 1950), pp. 655–6.

[26] T. M. Apostol, *Mathematical Analysis* (Addison-Wesley Publishing Company, Inc., 1957), p. 407, Theorem 13-19.

[27] G. F. Chew, S. C. Frautschi, and S. Mandelstam, Phys. Rev. **126**, 1202 (1962).

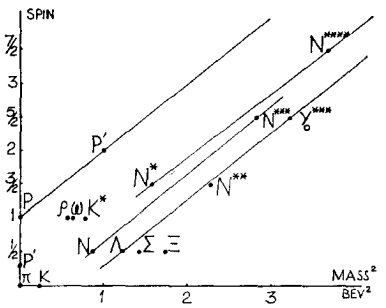

FIG. 2. Known Regge trajectories.

itself that must be used, since

$$\varphi(s, t) = \sigma(t) + \int_0^\infty \frac{ds'}{\pi} \frac{\rho(s', t)}{s' - s - i\epsilon}$$

may be computed from $\varphi(s, t)$, while $M(s, t)$ may not. The point of course is that unknown pole terms and subtractions occur in the Mandelstam representation for $M(s, t)$ which do not appear in the above dispersion relation for $\varphi(s, t)$.

The scheme proposed by Chew, Frautschi, and Mandelstam thus achieves an enormous simplification in calculating binding energies from the S-matrix dynamical scheme compared to using the Mandelstam representation and the N/D method.

Attempts have been made to free the scheme from the remaining obstacle—the bootstrap equation itself. One possibility would be to replace the bootstrap equation by a scheme based on the N/D technique. Another is to write dispersion relations for the position $\alpha(s)$ and residue $\beta(s)$ of the Regge poles, and apply unitarity directly in their dispersion relations. These alternative schemes however are not yet sufficiently worked out to report on here.

10. Applications

The actual calculation of binding energies by the scheme of Chew, Frautschi, and Mandelstam is clearly rather difficult because of the necessity of using the bootstrap equation. Instead, therefore, most people have attempted to bypass this task by phenomenological searches for Regge trajectories. This has led to a great deal of insight into elementary particle physics.

If crossing symmetry is valid, and if Regge trajectories may be analytically continued to negative energies, we may conclude that Regge's formula also holds for fixed negative momentum transfer and large energies rather than fixed energy and large-momentum transfer.

At large energies it is known experimentally that all total cross sections tend to constants. Moreover, Pomeranchuk's theorem (here regarded as an experimental fact) states that particle and antiparticle cross sections tend to the same constant at high energies. Finally, the differential cross sections are sharply forward-peaked and possess "exponential" diffraction tails

$$\frac{d\sigma}{d\Omega} \xrightarrow[s\to\infty]{} \left(\frac{d\sigma}{d\Omega}\right)_{t=0} e^{-\gamma t}.$$

All of these known facts may be summarized by postulating a "Pomeranchuk-Regge Trajectory." This trajectory is to have a larger value of Re $\alpha(s)$ than all others, and $\alpha(0) = 1$ for this trajectory. This ensures total cross sections constant at high energies. Particles on this trajectory must have zero isotopic spin and G parity $+1$. These assignments are necessary to ensure that particle and antiparticle cross sections become equal at high energy.

The known elementary particles and resonances, as well as the Pomeranchuk trajectories P, P' have been drawn in Fig. 2. We have omitted a few irrelevant particles to avoid cluttering up the diagram. The abscissa is taken as mass square, rather than mass, in order to make the trajectories parallel; there is no reason for believing that this parallelism is of any fundamental significance. We draw only those trajectories on which at least two points are known.

The main contribution of Regge's theorem in this type of plot is the inclusion of the Pomeranchuk points.

We may make a number of conclusions:

(1) Every high-spin baryon is preceded by a lower-spin baryon.

(2) The fourth pion–nucleon isobar ($T = \frac{1}{2}$) has a spin and parity $\frac{7}{2}^+$ and a higher mass than reported.[28]

(3) The Kerth resonance,[29] also called Y_0^{***}, has a spin and parity $\frac{5}{2}^+$.

(4) There are $T = 1$ analogs of the Kerth resonance with mass about 2 BeV, spin and parity $\frac{5}{2}^+$, which would appear as resonances in the $\Sigma\pi$ system.

We shall not go into any greater detail on the subject of experimental consequences here, as there already exist many excellent reviews on the subject.[30]

V. CONCLUSION

We have investigated the model of nonrelativistic potential scattering, based on the Schrödinger equa-

[28] V. P. Kenney, J. G. Dardis, and G. Brunhart, Phys. Rev. **124**, 1568 (1961).
[29] L. T. Kerth, Rev. Mod. Phys. **33**, 389 (1961).
[30] S. C. Frautschi, M. Gell-Mann, and F. Zachariasen, Phys. Rev. **126**, 2204 (1962); B. M. Udgaonkar, Phys. Rev. Letters **8**, 142 (1962).

tion. From this model we have deduced analytic and unitarity properties, which by themselves form a complete dynamical scheme which may be used in place of the Schrödinger equation. Two such schemes have been reviewed, one based on the N/D method, another based on Regge poles. A few experimental consequences of the hypothesis of Regge poles have been indicated.

Many unsolved problems remain, of which we mention only two. One is the problem of proving that Regge trajectories may be analytically continued to negative energies. Another important problem is to extend the treatment to many-body channels; one might hope to prove that the impulse approximation has an *exact* counterpart in the limit of infinite energies. Here one must of course use relativistic dynamics and crossing symmetry.

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APPENDIX I

The material in this appendix is related to Sec. (III.4). We are to evaluate the integral

$$I = \int d\Omega_q \frac{1}{\lambda_1 - \hat{\mathbf{p}}_1\cdot\hat{\mathbf{q}}} \frac{1}{\lambda_2 - \hat{\mathbf{p}}_2\cdot\hat{\mathbf{q}}}.$$

By Feynman techniques, using

$$\frac{1}{ab} = 2\int_{-1}^{1} \frac{dx}{[a(1+x) + b(1-x)]^2},$$

we may write the integral as

$$I = 2\pi \int_{-1}^{1} \frac{dx}{ax^2 + bx + c},$$

with

$$a = \tfrac{1}{4}(\lambda_1 - \lambda_2)^2 - \tfrac{1}{2}(1 - z),$$
$$b = \tfrac{1}{2}(\lambda_2^2 - \lambda_1^2),$$
$$c = \tfrac{1}{4}(\lambda_1 + \lambda_2)^2 - \tfrac{1}{2}(1 + z),$$

and

$$z = \hat{\mathbf{p}}_1\cdot\hat{\mathbf{p}}_2.$$

The singularities of $I(z)$ are of the type called coincident singularities by Eden,[31] and occur when the two roots of the quadratic equation $ax^2 + bx + c = 0$. This happens when the discriminant $b^2 - 4ac$ vanishes:

$$\Delta(\lambda_1, \lambda_2, z) = 0.$$

This equation is quadratic in z and there are two solutions:

$$z = \lambda_1\lambda_2 \pm [(\lambda_1^2 - 1)(\lambda_2^2 - 1)]^{\frac{1}{2}} \equiv \lambda_{\pm}.$$

The solution with the minus sign does not give a singular point (on the first sheet of the function) because the value of x at which the required coincidence of the roots occurs, lies outside the range $-1 \leq x \leq +1$ of integration. The other solution yields a branch point.

We may therefore write the dispersion relation

$$I(z) = \int_{\lambda_+}^{\infty} \frac{d\lambda}{\pi} \frac{f(\lambda)}{\lambda - z}.$$

The discontinuity across the cut is

$$f(\lambda) = \frac{1}{2i}\{I(\lambda + i\epsilon) - I(\lambda - i\epsilon)\}$$
$$= 2\pi^2 \int_{-1}^{1} dx\, \delta(ax^2 + bx + c).$$

The two roots of $ax^2 + bx + c = 0$ both lie within the range of integration $[-1, +1]$ and hence,

$$f(\lambda) = \frac{4\pi^2}{(b^2 - 4ac)^{\frac{1}{2}}} = \frac{4\pi^2}{[-\Delta(\lambda, \lambda_1, \lambda_2)]^{\frac{1}{2}}}.$$

Q.E.D.

[31] R. J. Eden, Phys. Rev. **119**, 1763 (1960).

New Approach to Low-Energy Potential Scattering*

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The problem of low-energy potential scattering is reformulated in a manner suggested by the "invariant imbedding" techniques of transport theory. The differential equations thus obtained have several conceptual and computational advantages over the Schrödinger equation. Some new bounds and approximations are derived and a rigorous investigation of the Born approximation is carried out.

1. INTRODUCTION

IN a recent paper, MacCallum[1] has applied the methods of "invariant imbedding," previously confined largely to transport theory, to the calculation of phase shifts and bound-state energies in quantum mechanics. When restricted to low-energy potential scattering, these techniques provide a formulation of the problem which is, at the same time, elegant and of considerable practical value. In this paper, we will follow the basic philosophy of "invariant imbedding" as far as the kinematics are concerned, but for lack of space and because the dynamics of the problem are well known, no attempt will be made to derive the dynamical equations from first principles. The basic idea will be to replace the Schrödinger equation by a differential equation which will couple the scattering lengths of a family of potentials with varying range. The potential with zero range will provide a boundary condition, and the solution to the original problem will be obtained by letting the range tend to infinity. Besides providing considerable physical insight, the differential equations obtained in this manner, are more convenient for numerical work than the Schrödinger equation and can be used to derive new bounds and approximations.

In general, the only restrictions placed on the potential are that it be spherically symmetric, and that the integral $\int_0^\infty |rU(r)|$ exist.

2. DIFFERENTIAL EQUATIONS

Low-energy potential scattering is usually described by two parameters—the scattering length a and the effective range b. They are defined by

$$k \operatorname{ctn} \delta = -1/a + \tfrac{1}{2}bk^2 + O(k^4), \tag{1}$$

where the S-wave phase shift δ, is determined by the radial Schrödinger equation and boundary conditions.

$$u''(x) + [k^2 - U(x)]u(x) = 0,$$
$$u(0) = 0 \quad u(x) \sim \sin(kx + \delta), \qquad x \to \infty. \tag{2}$$

Since the scattering length and effective range are the quantities of primary physical interest, we wish to formulate the problem in a manner which will not require the introduction of the wavefunction u. To this end, we introduce the family of potentials $U_r(x)$ defined by

$$U_r(x) = \begin{cases} U(x) & \text{for } 0 < x < r \\ 0 & \text{for } r < x < \infty, \end{cases}$$

and denote by $k\epsilon(r)$ the S-wave phase shift generated by the potential $U_r(x)$. Since $U_\infty(x) = U(x)$ and $U_0(x)$ is identically zero, it follows that $\epsilon(\infty) = \delta/k$, and $\epsilon(0) = 0$. Furthermore, it can be shown that ϵ satisfies the first-order differential equation

$$\epsilon'(r) = -U(r)\{\sin^2 k[\epsilon(r) + r]\}/k^2, \tag{3}$$

which, along with the initial condition $\epsilon(0) = 0$, will uniquely determine $\epsilon(r)$, and therefore δ.

The simplest proof of Eq. (3) is obtained by differentiating both sides of the identity

$$\epsilon(r) = \frac{1}{k}\tan^{-1}\left[k\frac{u(r)}{u'(r)}\right] - r, \tag{4}$$

and using the Schrödinger equation (2) to remove u'' from the right-hand side. MacCallum[1] has given, however, a more physically satisfying derivation which is based entirely on the principles of multiply reflected waves and makes no reference to the wavefunction u. Actually Eq. (3) was first used by Franchetti[2] who obtained it by making a formal

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[1] C. J. MacCallum, " 'Invariant Imbedding' and Wave Propagation in Inhomogeneous Media," Sandia Corporation, SC-4669(RR), (November 1961).
[2] S. Franchetti, Nuovo Cimento 6, 601 (1957).

change of variables in the Schrödinger equation.

It is known that,[3] unless U_r has a bound state of zero angular momentum at zero energy, $\epsilon(r)$ can be written as $-n\pi/k + \bar{\epsilon}(r)$ where n is the number of zero-angular momentum bound states of U_r, and $\bar{\epsilon}$ is an analytic function of k^2 in some neighborhood of $k = 0$. Defining α and β by the expansion

$$-\bar{\epsilon}(r) = \alpha(r) + \beta(r)k^2 + \cdots, \tag{5}$$

we immediately find that the scattering length of U_r is given by $\alpha(r)$ and a little algebra will show that the effective range of U_r is equal to $2[\frac{1}{3}\alpha(r) + \beta(r)/\alpha^2(r)]$. The scattering length and effective range of the original potential are, of course, obtained by setting $r = \infty$. The mathematically troublesome points where U_r has a zero-energy bound state are of particular physical interest. At these points, α must become infinite and it is easy to see that they are the only points where the number of bound states of U_r can change.

Our next task is to determine the differential equations satisfied by α and β. We first assume that none of the potentials U_r have bound states, and then discuss the general case. With this assumption we can expand both sides of Eq. (3) in powers of k^2 which yields

$$\alpha' = U(\alpha - r)^2 \qquad \alpha(0) = 0, \tag{6}$$

$$\beta' = 2\beta U(\alpha - r) - \tfrac{1}{3}U(\alpha - r)^4 \qquad \beta(0) = 0, \tag{7}$$

and similar equations for the coefficients of the higher powers of k^2. It is not difficult to verify that the coefficient of k^{2n} for $n > 0$ will satisfy a first-order linear differential equation so that, having found the first n coefficients, the $(n + 1)$st can be expressed by a quadrature formula. In particular, β is given by

$$\beta(r) = -\tfrac{1}{3}\int_0^r dx\, U(x - \alpha)^4 \times \exp\left[-2\int_x^r dy\, U(y - \alpha)\right]. \tag{8}$$

In the general case, an inspection of (3) will show that α and β satisfy Eqs. (6) and (7) for all values of r with the exception of those points where U_r has a zero-energy bound state. To complete the determination of α and β, it is necessary to give some prescription for continuing the solution of Eqs. (6) and (7) across these singular points. This is provided by the physical requirement that the inverse of the scattering length $1/\alpha$, and the effective range $2(\frac{1}{3}\alpha + \beta/\alpha^2)$, must be continuous at the points where U_r has a zero-energy bound state. A study of (6) and (7) will show that this additional requirement does, in fact, complete the determination of α and β.

On the other hand, if α is singular, Eq. (6) will no longer be suitable for numerical calculations. To remove this difficulty we define $\tan\mu = -\alpha$ and find that μ satisfies the differential equation

$$\mu' = -U(r\cos\mu - \sin\mu)^2 \qquad \mu(0) = 0. \tag{9}$$

Moreover, a little reflection will show that if we set

$$\mu(r) = n\pi + \bar{\mu}(r) \qquad -\tfrac{1}{2}\pi < \bar{\mu} \leq \tfrac{1}{2}\pi,$$

then the number of zero-angular momentum bound states of the potential U_r is equal to n and the scattering length of U_r is given by $(-\tan\bar{\mu})$. The number of bound states and scattering length of the original potential are, again, obtained by setting $r = \infty$.

Even in the presence of bound states, β is formally given by the quadrature formula (8). In this case, however, the integral (8) will be divergent unless the path of integration is moved into the complex plane. To circumvent this difficulty, one can remove the singularities of the integrand by subtracting off an analytically integrable function with the same singularities. The construction of such a function should not be difficult since, once it has been determined from (9) that α is singular at some point r_0, it follows from (6) that $U(r - \alpha)$ goes like $1/(r - r_0)$ near r_0.

The usual method for calculating scattering lengths is to integrate the zero-energy Schrödinger equation numerically and then examine the asymptotic form of the properly normalized solution. Equations (6) and (9), being of first order, are considerably easier to integrate numerically and, moreover, only the asymptotic value of α or μ is required. Furthermore, if the potential U does not change sign, both α and μ will be monotonic functions which will greatly facilitate numerical work. Finally, Eqs. (6) and (9) have the advantage that it is easy to obtain rigorous bounds on the error incurred by terminating the integration at a finite value of r.

3. INTEGRAL EQUATIONS AND BOUNDS

In addition to being very convenient for numerical work, Eq. (6) can be cast in the form of an integral equation–maximum principle which will provide bounds and approximations. We first assume that U is strictly repulsive, and later indicate what changes are necessary if this is not the case.

[3] R. G. Newton, J. Math. Phys. 1, 319 (1959).

Following a technique due to Kalaba,[4] one easily verifies that, for an arbitrary function g,

$$\alpha' = U(\alpha - r)^2 \geq U(g - r)^2 + 2U(g - r)(\alpha - g), \quad (10)$$

where equality holds if and only if $g = \alpha$. Integrating the differential inequality (10) yields

$$\alpha(r) \geq \int_0^r dx\, U(x^2 - g^2) \times \exp\left[2\int_x^r dy\, U(g - y)\right] \quad (11)$$

where, again, g is an arbitrary integrable function, and equality holds if and only if $g = \alpha$.

Inequality (11) can be used in a number of different ways. If one replaces g by α in the right-hand side of (11), he obtains an integral equation for α. On the other hand, one may insert an arbitrary trial function to obtain a lower bound on α. Finally, if g is chosen such that $|g - \alpha|$ is small, the integral (11) should be a very good approximation to α since the error involved will be of the second order in $|\alpha - g|$.

The simplest bound is, of course, obtained by setting $g = 0$ which yields

$$\alpha(r) > \int_0^r x^2 U \exp\left[-2\int_x^r yU\, dy\right] dx. \quad (12)$$

Integral (12) can be done analytically for the Yukawa potential $U = be^{-x}/x$, $(b > 0)$ with the result

$$a = \alpha(\infty) > \log(\gamma b) + \int_b^\infty \frac{e^{-t}}{t}\, dt = \log(\gamma b) - Ei(-b), \quad (13)$$

where $\gamma = .577\cdots$ is Euler's constant.

The above results hold, of course, only for repulsive potentials. It is easy to verify, however, that for attractive potentials with no bound states, one need only reverse the inequality signs in (10) through (13). On the other hand, for potentials which change sign, this method will not provide upper or lower bounds since, in this case the integral (11) has an inflection point at $g = \alpha$. For the interesting case of an attractive potential with a repulsive hard core, however, one can calculate the scattering length of the core alone and start the integration of inequality (10) from the edge of the core. This procedure will provide a rigorous upper bound on α, provided that the potential has no bound states. In any case, a simple integration by parts will show that α satisfies the integral equation obtained by setting $g = \alpha$ in the right-hand side of equation (11), and since the integral has a stationary point at $g = \alpha$, then if $|\alpha - g|$ is small, the error involved in equating α to the integral (11) will be of second order in $|\alpha - g|$.

Since in many cases one does not know the exact form of $U(x)$, it is convenient to have an estimate for the change in the scattering length as the potential is varied. With this in mind, we suppose that U depends on some parameter λ. Differentiating both sides of (6) with respect to λ yields

$$\left(\frac{d}{d\lambda}\alpha\right)' = \left(\frac{d}{d\lambda}U\right)(\alpha - r)^2 + 2U(\alpha - r)\frac{d}{d\lambda}\alpha,$$

which may be integrated immediately and gives

$$\frac{d}{d\lambda}\alpha(r) = \int_0^r dx \left(\frac{d}{d\lambda}U\right)(\alpha - x)^2 \times \exp\left[2\int_x^r dy\, U(\alpha - y)\right]. \quad (14)$$

As an example of how one can obtain useful results from Eq. (14), consider the case where U is strictly repulsive. It is clear physically that in this case, α' can never be zero. It then follows from (6) that $\alpha < r$, and we obtain the inequality

$$\left|\frac{d}{d\lambda}a\right| = \left|\frac{d}{d\lambda}\alpha(\infty)\right| < \int_0^\infty x^2 \left|\frac{d}{d\lambda}U\right| dx. \quad (15)$$

4. THE BORN APPROXIMATION

The results of the preceding section can be used to investigate the validity of the Born approximation in the low-energy limit. In this limit, the accuracy of any approximation will be determined by the accuracy with which it reproduces the scattering length and effective range. Thus, from the Born approximation for $\epsilon(r)$:

$$\epsilon(r) \approx -\frac{1}{k^2}\int_0^r U \sin^2 kx\, dx,$$

one obtains the conditions

$$\alpha(r) \approx \int_0^r Ux^2\, dx, \quad (16)$$

$$\beta(r) \approx -\tfrac{1}{3}\int_0^r Ux^4\, dx. \quad (17)$$

These must be satisfied if the Born approximation is to be valid at low energies.

Again, we first restrict ourselves to purely repulsive potentials and then discuss the general case.

[4] R. J. Kalaba, J. Math. and Mech. **8**, 519 (1959).

For repulsive potentials, the integral (12) gives a lower bound on α and an application of (15) will show that the Born integral (16) is an upper bound on α, a result previously derived by Kato[5] from his variational principle. Therefore, condition (16) will be satisfied if

$$\int_0^\infty Ux^2\,dx \approx \int_0^\infty Ux^2 \exp\left[-2\int_x^\infty yU\,dy\right] dx. \quad (18)$$

If Eq. (18) is to be valid, the integral in the exponential must be small as compared to unity. Using this result and integrating the Born integral (16) by parts, one finds that if Eq. (18) is satisfied then $\alpha \ll r$, which in turn implies that (17) is valid. Thus for repulsive potentials, condition (18) is a rigorous sufficient condition for the validity of the Born approximation at low energies.

For attractive potentials, it is seen that both the integral (12) and the Born approximation give an upper bound on α, so that condition (18) is a rigorous necessary condition in this case. If the potential changes sign, no such rigorous statements can be made. In any case, however, the integral (12) can be expected to be a considerable improvement over the Born approximation for the scattering length, which implies, of course, that if the latter is to be valid, Eq. (18) must hold. We may thus infer that for any potential without bound states, condition (18) should be a necessary and sufficient condition for the validity of the Born approximation in the low-energy limit.

For the repulsive Yukawa potential $U = (be^{-x}/x)$, $(b > 0)$, the integrals in (18) can be done analytically and one finds that the Born approximation will be valid if b is less than about one. In the general case, a more than sufficient condition on U, under which requirement (18) will be satisfied, is that

$$\int_0^\infty |xU|\,dx \ll 1. \quad (19)$$

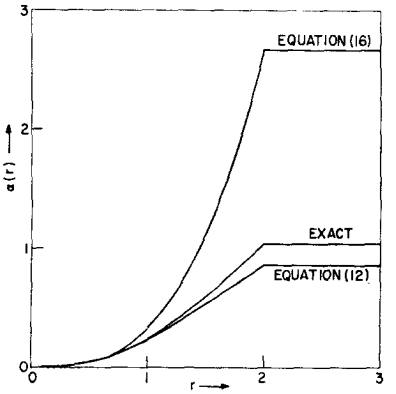

FIG. 1. Exact and approximate integrations of Eq. (6) for a spherical barrier.

5. AN EXAMPLE

We conclude with a simple example illustrating the general behavior of the function α and some of our bounds and approximations. For the spherical barrier

$$U(r) = \begin{cases} 1 & \text{for } 0 < r < 2 \\ 0 & \text{for } 2 < r < \infty, \end{cases}$$

Eq. (6) can be integrated analytically with the result

$$\alpha(r) = \begin{cases} r - \tanh r & \text{for } 0 < r < 2 \\ 2 - \tanh 2 & \text{for } 2 < r < \infty. \end{cases}$$

Figure 1 shows a plot of α and the upper and lower bounds obtained from Eq. (16) (the Born approximation), and Eq. (12).

[5] T. Kato, Prog. Theoret. Phys. (Kyoto) 6, 395 (1951).

Relativistic Coulomb Scattering*†

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Contour integration is employed to evaluate analytically the angular dependence of the relativistic correction terms to the Rutherford cross section for the scattering of electrons by nuclei at high energies. The phase shifts obtained by Mott from the solution of the Dirac equation are expanded in powers of the fine structure constant, and the resulting infinite sums are converted into integrals in the complex angular-momentum plane. In turn, these integrals are evaluated by distorting the path of integration and by the use of integral representations. In this manner, the angular dependence of the cross section is obtained in closed form up to terms of the fifth (fourth) order in the cross section (wavefunction). The form of the correction term corresponding to an arbitrary power of the fine structure constant is found in terms of two-dimensional integrals involving elementary transcendental functions. A related problem, the nonrelativistic scattering for an attractive $1/r^2$ potential is also discussed.

1. INTRODUCTION

IN recent years several investigations,[1] both theoretical and experimental, have been undertaken to determine the structure of nuclei (including the proton) from the results of the scattering of fast (i.e., relativistic) electrons by nuclei. The experimental data and the theoretical results essentially measure the deviation of the actual scattering from that due to a point nucleus and thus reveal certain details of the charge distribution. It is this scattering by a point charge that will concern us here.

In this paper we shall first present an outline of the Mott calculation,[2] carry out an expansion of phase shifts in increasing powers of the fine structure constant times the nuclear charge, and sum the resulting series involving Legendre polynomials by means of the Watson transformation. By use of this last method it is possible to evaluate in closed form all the angular coefficients of the powers of α that enter into the differential cross section to order α^5 in terms of elementary transcendental functions and the dilogarithm of Euler. We then show that the coefficient of an arbitrary power of α can be expressed in terms of sums of two-dimensional integrals whose integrands contain only elementary transcendental functions. Inasmuch as certain of the sums of Legendre functions times functions of angular-momentum quantum number contained in the papers alluded to above converge very poorly, equivalent integrals may be more amenable to calculations. Finally, we indicate the nature of the functions required to express the angular dependence of the higher-order correction terms to the cross section.

2. FORMULATION OF THE PROBLEM

2.1 The Mott Formula[3]

According to Dirac, the wave equation obeyed by electrons in a force field with a scalar potential V (vector potential $\mathbf{A} = 0$) is given by

$$([E - eV/c] + \boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc)\psi = 0, \qquad (1)$$

where ψ is the four-component spinor

$$\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}. \qquad (2a)$$

In (1), p is the momentum, m the mass, and E the energy of the particle; $\boldsymbol{\alpha}$ and β are the 4×4 matrices, one of whose possible representations is indicated symbolically by

$$\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \qquad (2b)$$

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† This paper is based upon a thesis submitted to the Department of Physics of New York University in partial fulfillment of the requirements for the Ph.D., (1959).

[1] R. Hofstadter, Rev. Mod. Phys. **28**, 214 (1956); D. G. Ravenhall, *ibid.* **30**, 430 (1958). Both of these reviews contain references to a rather extensive literature.

[2] N. F. Mott, Proc. Roy. Soc. (London) **A124**, 425 (1929).

[3] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1949), 2nd Ed., pp. 76–85.

Here σ_i are the usual 2×2 Pauli spin matrices and 1 is the 2×2 unit matrix.

Before considering the Coulomb case, one first develops the formalism for potentials which decrease at infinity at least as rapidly as $1/r^{\epsilon+1}$, $\epsilon > 0$. Consider those solutions with $E > mc^2$ that obey the following boundary conditions:

$$\psi_\lambda \text{ finite at the origin,} \tag{3a}$$

and

$$\psi_\lambda \underset{r\to\infty}{\longrightarrow} a_\lambda e^{ikr} + \frac{e^{ikz}}{r} u_\lambda(\theta, \phi), \tag{3b}$$

where r, θ, ϕ are the usual spherical coordinates and k is the momentum divided by $\hbar$. The differential cross section is given by

$$\sigma(\theta, \phi) = \sum_1^4 |u(\theta, \phi|^2 / \sum_1^4 |a_\lambda|^2. \tag{4}$$

Since it can be shown by reference to the plane wave solutions of (1) that

$$\left|\frac{a_2}{a_4}\right| = \left|\frac{a_1}{a_3}\right| \quad \text{and} \quad \left|\frac{u_2}{u_4}\right| = \left|\frac{u_1}{u_3}\right|, \tag{5}$$

the cross section simplifies to

$$\sigma(\theta, \phi) = \frac{|u_3|^2 + |u_4|^2}{|a_3|^2 + |a_4|^2}. \tag{6}$$

If the beam is initially polarized along the direction of propagation (z), then the solution desired is of the form

$$\psi_3 \underset{r\to\infty}{\longrightarrow} e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}, \tag{7a}$$

$$\psi_4 \underset{r\to\infty}{\longrightarrow} g(\theta, \phi) \frac{e^{ikr}}{r}, \tag{7b}$$

where r, θ, and ϕ are the usual spherical coordinates.

By expanding the wavefunction in spherical harmonics Darwin[4,5] found the following pairs of solutions for the partial waves:

$$\begin{aligned} (\psi_3)_n &= (n+1)P_n(\cos\theta)G_n(r), \\ (\psi_4)_n &= G_n(r)P_n^{(1)}(\cos\theta)e^{i\phi}; \end{aligned} \tag{8a}$$

$$\begin{aligned} (\psi_3)_{-n-1} &= nP_n(\cos\theta)G_{-n-1}(r), \\ (\psi_4)_{-n-1} &= -G_{-n-1}P_n^{(1)}(\cos\theta)e^{i\phi}, \end{aligned} \tag{8b}$$

where G_n is a solution of the coupled equations

$$\frac{1}{\hbar}\left(\frac{E}{c} - \frac{eV}{c} + mc\right)F_n + \frac{dG_n}{dr} - \frac{n}{r}G_n = 0, \tag{9a}$$

$$\frac{1}{\hbar}\left(\frac{E}{c} - \frac{eV}{c} - mc\right)G_n + \frac{dF_n}{dr} + \frac{n+2}{r}F_n = 0, \tag{9b}$$

after the F_n are eliminated. F_n represents the radial wavefunctions associated with ψ_1 and ψ_2. G_{-n-1} satisfies the equation corresponding to (9a, b) with n replaced by $-n-1$. If the asymptotic form ($r \to \infty$) of the G's to be taken to be

$$G_n \sim (1/r)\sin(kr - n\pi/2 + \eta_n), \tag{10a}$$

$$G_{-n-1} \sim (1/r)\sin(kr - n\pi/2 + \eta_{-n-1}), \tag{10b}$$

then $i^n e^{i\eta_n} G_n$ and $i^n e^{i\eta_{-n-1}} G_{-n-1}$ are the radial functions that will have the desired asymptotic form. Finally, then, the wavefunctions are given by

$$\psi_3 = \sum_{n=0}^{\infty} \{(n+1)e^{i\eta_n}G_n + ne^{i\eta_{-n-1}}G_{-n-1}\}i^n P_n(\cos\theta), \tag{11a}$$

$$\psi_4 = \sum_{n=0}^{\infty} \{+e^{i\eta_n}G_n - e^{i\eta_{-n-1}}G_{-n-1}\}i^n P_n^{(1)}(\cos\theta)e^{i\phi}, \tag{11b}$$

or

$$2ikf(\theta, \phi) = \sum_{n=0}^{\infty} \{(n+1)(e^{2i\eta_n} - 1) + n(e^{2i\eta_{-n-1}} - 1)\}P_n(\cos\theta), \tag{12a}$$

$$2ikg(\theta, \phi) = \sum_{n=1}^{\infty} (e^{2i\eta_n} - e^{2i\eta_{-n-1}})P_n^{(1)}(\cos\theta)e^{i\phi}. \tag{12b}$$

For the case of the Coulomb interaction, as in the nonrelativistic formalism, we keep (11a) and (11b), but the phase shift is determined by comparison of the asymptotic form of the G's with

$$(1/r)\sin(kr + \gamma \ln 2kr - n\pi/2 + \eta_n),$$

where $\gamma \equiv Ze^2/hv \equiv \alpha c/v \equiv \alpha/\beta$.

Mott[2] solves (9) to find

$$e^{2i\eta_{-n-1}} = \frac{n - i\gamma'}{\rho_n - i\gamma}\frac{\Gamma(\rho_n + 1 - i\gamma)}{\Gamma(\rho_n + 1 + i\gamma)}e^{i\pi(n-\rho_n)}, \tag{13a}$$

$$e^{2i\eta_n} = \frac{n + 1 + i\gamma'}{\rho_{n+1} - i\gamma}\frac{\Gamma(\rho_{n+1} + 1 - i\gamma)}{\Gamma(\rho_{n+1} + 1 + i\gamma)}e^{i\pi(n-\rho_{n+1})}, \tag{13b}$$

with $\rho_n = +(n^2 - \alpha^2)^{1/2}$, $\gamma' = \gamma(1 - \beta^2)^{1/2}$, and $\Gamma(x)$ is the usual Gamma function. Using the abbreviations

$$C_n = -e^{-i\pi\rho_n}\Gamma(\rho_n - i\gamma)/\Gamma(\rho_n + 1 + i\gamma), \tag{14a}$$

$$F(\theta) = (i/2) \times \sum (-1)^n\{nC_n + (n+1)C_{n+1}\}P_n(\cos\theta), \tag{14b}$$

[4] G. Darwin, Proc. Roy. Soc. (London) **A118**, 654 (1928).

[5] There is a difference in sign between the $P_n^{(1)}$'s used here and those quoted by Mott (reference 2) and Darwin. Those used by Darwin and Mott also differ by factors proportional to either n or $n+1$.

$$G(\theta) = (i/2) \times \sum (-1)^n \{n^2 C_n - (n+1)^2 C_{n+1}\} P_n(\cos\theta), \quad (14c)$$

Mott finds that[6]

$$kf(\theta) = i\gamma' F + G, \quad (15a)$$

$$kg(\theta) = \{i\gamma'(1+\cos\theta)F + (1-\cos\theta)G\}/\sin\theta, \quad (15b)$$

where he has used the relations

$$P_{n+1}(\cos\theta) = \cos\theta P_n + [\sin(\theta)/(n+1)]P_n^{(1)}(\cos\theta), \quad (16a)$$

$$P_{n-1}(\cos\theta) = \cos\theta P_n - [\sin(\theta)/n]P_n^{(1)}(\cos\theta). \quad (16b)$$

Expanding F and G in powers of α, Mott gets

$$F = F_0 + \alpha F_1 + \cdots, \quad (17a)$$

$$G = G_0 + \alpha G_1 + \cdots, \quad (17b)$$

and, corresponding to the lowest approximation,

$$\sigma(\theta) = \frac{(Ze^2)^2}{4m^2v^2}\csc^4\left(\frac{\theta}{2}\right)\left(1 - \frac{v^2}{c^2}\right)\left(1 - \frac{v^2}{c^2}\sin^2\frac{\theta}{2}\right), \quad (18a)$$

and

$$\sigma(\theta) = \frac{(Ze^2)^2}{4m^2v^2}\csc^4\left(\frac{\theta}{2}\right)\left(1 - \frac{v^2}{c^2}\right) \times \left(1 - \frac{v^2}{c^2}\sin^2\frac{\theta}{2} + \pi\alpha\frac{v}{c}\sin\frac{\theta}{2}\right), \quad (18b)$$

corresponding to the next higher approximation.

2.2 Relativistic Wavefunction

Here we consider not the phase shifts, but the wavefunctions themselves. Mott finds for the G's:

$$G_{-n-1} = \frac{1}{2}\frac{e^{-ikr}e^{\pi\gamma/2}}{r\Gamma(2\rho_n+1)}(2kr)^{\rho_n} \times \frac{|\Gamma(\rho_n+1+i\gamma)|}{(\rho_n - i\gamma)^{1/2}[-i(n-i\gamma')^{1/2}]} \times \{(\rho_n - i\gamma)\phi(\rho_n + i\gamma, 2\rho_n+1, 2ikr) - (n - i\gamma')\phi(\rho_n+1+i\gamma, 2\rho_n+1, 2ikr)\}, \quad (19a)$$

and

$$G_n = \frac{1}{2}\frac{e^{-ikr}e^{\pi\gamma/2}}{r\Gamma(2\sigma_n+1)}(2kr)^{\sigma_n} \times \frac{|\Gamma(\sigma_n+1+i\gamma)|}{(\sigma_n - i\gamma)^{1/2}(n+1+i\gamma')^{1/2}} \times \{(\sigma_n - i\gamma)\phi(\sigma_n+i\gamma, 2\sigma_n+1, 2ikr) + (n+1+i\gamma')\phi(\sigma_n+1+i\gamma, 2\sigma_n+1, 2ikr)\}, \quad (19b)$$

where $\sigma_n = \rho_{n+1}$. The ϕ's are confluent hypergeometric functions of the first kind.

It is convenient to deviate from the procedure of previous authors by splitting off the term that in the limit $c \to \infty$ yields the nonrelativistic wavefunction. For this purpose we use the identities

$$\phi(\rho_n + i\gamma, 2\rho_n+1, 2ikr) = \phi(\rho_n+1+i\gamma, 2\rho_n+1, 2ikr) - [2ikr/(2\rho_n+1)]\phi(\rho_n+1+i\gamma, 2\rho_n+2, 2ikr), \quad (20a)$$

and

$$\phi(\sigma_n + i\gamma, 2\sigma_n+1, 2ikr) = [(\sigma_n+i\gamma)/(-\sigma_n+i\gamma)]\phi(\sigma_n+1+i\gamma, 2\sigma_n+1, 2ikr) + [2\sigma_n/(-\sigma_n+i\gamma)]\phi(\sigma_n+i\gamma, 2\sigma_n, 2ikr). \quad (20b)$$

We shall use the following integral representation for the ϕ's[7]:

$$\phi(a,c,x) = \frac{\Gamma(c)}{\Gamma(c-a)}e^x x^{1/2-c/2} \times \int_0^\infty e^{-t}t^{-c/2-a-1/2}J_{c-1}[2(xt)^{1/2}]\,dt, \quad (21)$$

$$\mathrm{Re}\ c > \mathrm{Re}\ a > 0, \qquad \mathrm{Re}\ x > 0.$$

Substituting these expressions into (11a), one finds (exchanging the order of summation and integration),

$$\psi_3 = ke^{ikr+\pi\gamma/2}\int_0^\infty \frac{e^{-t}t^{-i\gamma}}{u} \times \sum_{n=0}^\infty \{nJ_{2\rho_n+1}2(u)e^{-i\pi\rho_n} - (n+1)J_{2\sigma_n-1}e^{-i\pi\sigma_n}\} \times (-1)^n P_n(\cos\theta) + \frac{i}{2}\frac{e^{\pi\gamma/2+ikr}}{r}\int_0^\infty e^{-t}t^{-i\gamma-1} \times \sum_{n=0}^\infty (-1)^n P_n(\cos\theta)\{[(n+1-\sigma_n) + (\gamma'-\gamma)] \times e^{-i\pi\sigma_n}J_{2\sigma_n}(n+1) + [(\rho_n - n) + i(\gamma'-\gamma)]ne^{-i\pi\rho_n}J_{2\rho_n}\}. \quad (22)$$

In the nonrelativistic limit ($\gamma' \to \gamma$, $\rho_n \to n$, etc.) the second term vanishes.

3. CALCULATION OF CROSS SECTION

3.1 Expansion of the Scattered Field in Powers of the Fine Structure Constant

For convenience, each component of the wave is

[6] J. H. Bartlett and R. E. Watson, Proc. Am. Acad. Arts & Sci. 74, 53 (1940).

[7] It will be assumed that $2ikr = \lim_{\epsilon\to 0}(\epsilon + 2ikr)$.

split into three parts. If a factor of k is dropped to obtain a unit incident wave, the expressions for the direct wave are

$$\psi_3^{(1)} = e^{ikr}e^{\pi\gamma/2}\int_0^\infty \frac{e^{-t}t^{-i\gamma}}{u}\sum_{k=0}^{\infty}(-1)^n P_n(\cos\theta) \times [n\exp(-i\pi\rho_n)J_{2\rho_n+1} - (n+1)J_{2\sigma_n-1}\exp(-i\pi\sigma_n)]\,dt, \quad (23a)$$

$$\psi_3^{(2)} = -\frac{(\gamma'-\gamma)}{2}\frac{e^{ikr}}{kr}e^{\pi\gamma/2} \times \int_0^\infty e^{-t}t^{-i\gamma-1}\sum_{n=0}^{\infty}(-1)^n P_n(\cos\theta) \times [\exp(-i\pi\rho_n)nJ_{2\rho_n} + (n+1)J_{2\sigma_n}\exp(-i\pi\sigma_n)]\,dt, \quad (23b)$$

$$\psi_3^{(3)} = \frac{i}{2}\frac{e^{ikr}}{kr}e^{\pi\gamma/2}\int_0^\infty e^{-t}t^{-i\gamma-1}\sum_{n=0}^{\infty}(-1)^n P_n(\cos\theta) \times \{n(\rho_n-n)J_{2\rho_n}\exp(-i\pi\rho_n) - (n+1)[\sigma_n-(n+1)]J_{2\sigma_n}\exp(-i\pi\sigma_n)\}\,dt. \quad (23c)$$

These equations are obtained directly from (22). The results for ψ_4 can be written down by inspection of (11a), (11b), and (23). One sees that the changes to be made are as follows:

(a) Replace $P_n(\cos\theta)$ by $P_n^{(1)}(\cos\theta)$ and multiply by $e^{i\phi}$.

(b) Drop the factors n and $n+1$, multiplying the Bessel functions.

(c) Reverse the sign of the factor containing $J_{2\sigma_n}$ or $J_{2\sigma_n-1}$.

The use of three separate wavefunctions is equivalent to writing (13a) and (13b) as

$$\exp[2i\eta_{-n-1}] = \frac{\Gamma(\rho_n+1-i\gamma)}{\Gamma(\rho_n+1+i\gamma)} \times \exp[i\pi(n-\rho_n)]\left[1+i\frac{\gamma-\gamma'}{\rho_n-i\gamma}+\frac{n-\rho_n}{\rho_n-i\gamma}\right], \quad (24a)$$

$$\exp[2i\eta_n] = -\frac{\Gamma(\sigma_n+1-i\gamma)}{\Gamma(\sigma_n+1+i\gamma)}\exp[i\pi(n-\sigma_n)] \times \left[1+i\frac{\gamma-\gamma'}{\sigma_n-i\gamma}+\frac{n+1-\sigma_n}{\sigma_n-i\gamma}\right]. \quad (24b)$$

The Bessel functions in Eqs. (23a, b, c) and in the corresponding ones for ψ_4 are now expanded in a power series about the integers and we obtain, for example,

$$\psi_3^{(1)} = e^{ikr}e^{\pi\gamma/2}\int_0^\infty \frac{e^{-t}t^{-i\gamma}}{u}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{(-1)^n P_n(\cos\theta)}{m!} \times \{n(\partial^m/\partial\nu^m)(J_{2\nu+1}e^{-i\pi\nu})[\rho_n-n]^m + (n+1)(\partial^m/\partial\nu^m)(J_{2\nu+1}e^{-i\pi\nu})[\rho_n-n-1]^m\}. \quad (25)$$

We consider that the factors such as $[\rho_n - n]$ are expanded in powers of α^2 and that the t integration is carried out in all terms except the coefficient of the lowest power of α^2 in each of the three parts of ψ_3 and of ψ_4. Taking the asymptotic form for large kr of the resulting expressions, with the exception of the six terms (the first three terms of ψ_3 and ψ_4 mentioned above), we find the form of the incident and scattered wave far from the nucleus. This procedure is, of course, entirely equivalent to a phase-shift expansion and as such is really the same method as that employed by previous authors[2,8] with this exception. The first terms in $\psi_3^{(3)}$ and $\psi_3^{(4)}$ contain sums of Bessel functions that are exactly summable. No further expansion of these terms (in powers of γ) is necessary. The first term of an expansion of these terms in powers of γ agrees with that of McKinley and Feshbach.[8] [Cf. their Eq. (6)ff with our Eq. (28c).]

We shall first concentrate on these six terms involved and denote them generally as ψ'. One gets

$$\psi_3'^{(1)} = e^{ikr}e^{\pi\gamma/2}\int_0^\infty \frac{e^{-t}t^{-i\gamma}}{u}\sum^{\infty}(2n+1)J_{2n+1}[2u]P_n(\cos\theta)\,dt = e^{ikr}e^{\pi\gamma/2}\int_0^\infty e^{-t}t^{-i\gamma}J_0\left(2u\sin\frac{\theta}{2}\right)dt, \quad (26a)$$

$$\psi_3'^{(2)} = -\tfrac{1}{2}(\gamma-\gamma')e^{\pi\gamma/2}\frac{e^{ikr}}{kr}\int_0^\infty\sum_0^\infty\{nJ_{2n}-(n+1)J_{2n+1}\}P_n(\cos\theta)e^{-t}t^{-i\gamma-1}\,dt = -\tfrac{1}{2}(\gamma-\gamma')e^{\pi\gamma/2}\frac{e^{ikr}}{kr}\sin\frac{\theta}{2}\int_0^\infty uJ_1\left(2u\sin\frac{\theta}{2}\right)e^{-t}t^{-i\gamma-1}\,dt, \quad (26b)$$

[8] W. A. McKinley and H. Feshbach, Phys. Rev. 74, 1759 (1948).

$$\psi_3'^{(3)} = \frac{i}{2kr} e^{\pi\gamma/2}\alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1}\left[\sum_1^\infty J_{2n}P_n(\cos\theta) + \sum_0^\infty J_{2n+1}P_n(\cos\theta)\right] dt$$

$$= -\frac{i}{2kr} e^{\pi\gamma/2}\alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1}\left[J_0\left(2u\sin\frac{\theta}{2}\right) - J_0(2u)\right] dt, \tag{26c}$$

$$\psi_4'^{(1)} = 0, \tag{26d}$$

$$\psi_4'^{(2)} = \tfrac{1}{2}(\gamma - \gamma')e^{\pi\gamma/2}\frac{e^{ikr}}{kr} e^{i\phi} \int_0^\infty \sum_0^\infty (J_{2n} + J_{2n+1})P_n^{(1)}(\cos\theta) e^{-t} t^{-i\gamma-1}\, dt$$

$$= +\tfrac{1}{2}(\gamma - \gamma')e^{\pi\gamma/2}\frac{e^{ikr}}{kr} e^{i\phi} \int_0^\infty \cos\frac{\theta}{2} J_1\left(2u\sin\frac{\theta}{2}\right) e^{-t} t^{-i\gamma-1}\, dt$$

$$= -\cot(\theta/2) e^{i\phi}\psi_3^{(2)}, \tag{26e}$$

$$\psi_4'^{(3)} = \frac{i}{2kr} e^{\pi\gamma/2}\alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1}\left[\sum_0^\infty \frac{J_{2n}P_n^{(1)}}{n} - \sum_0^\infty \frac{J_{2n+1}}{n+1} P_n^{(1)}\right] e^{-t} t^{-i\gamma-1}\, dt$$

$$= -e^{i\phi}\frac{i}{2kr}\tan\frac{\theta}{2} e^{\pi\gamma/2}\alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1}\left[J_0\left(2u\sin\frac{\theta}{2}\right) - J_0(2u)\right] dt$$

$$= +\tan(\theta/2)\psi_3^{(3)} e^{i\phi}. \tag{26f}$$

In order to obtain the asymptotic behavior of these terms for large u we use

$$\int_0^\infty e^{-t} t^{\alpha'} J_{\beta'}[2(xt)^{1/2}]\, dt \underset{x\to\infty}{\to} e^{-x} x^{\alpha'} \exp[i\pi(\beta'/2 - \alpha)] + \frac{\Gamma(\beta'/2 + 1 + \alpha')}{\Gamma(\beta'/2 - \alpha')}(x)^{-\alpha'-1}, \tag{27}$$

and thus obtain, denoting the asymptotic form of ψ_i' by u_i', $\ln\sin^2(\theta/2)$ by λ, and $\Gamma(1 - i\gamma)/\Gamma(1 + i\gamma)$ by $M(1)$:

$$u_3'^{(1)} = \exp[ikz - i\ln 2kr\sin^2(\theta/2)] + \frac{\gamma}{2k\sin^2(\theta/2)} M(1) e^{i\gamma\lambda}\frac{\exp[ikr + i\gamma\ln 2kr]}{r}, \tag{28a}$$

$$u_3'^{(2)} = -M(1)\frac{\gamma - \gamma'}{2k} e^{i\lambda}\frac{\exp[ikr + i\gamma\ln 2kr]}{r}, \tag{28b}$$

$$u_3'^{(3)} = \frac{\alpha^2}{4k} M(1)\frac{e^{i\gamma\lambda} - 1}{\gamma}\frac{\exp[i\gamma\ln 2kr + ikr]}{r}, \tag{28c}$$

$$u_4'^{(1)} = 0, \tag{28d}$$

$$u_4'^{(2)} = -\cot(\theta/2) e^{i\phi} u_3'^{(2)}, \tag{28e}$$

$$u_4'^{(3)} = +\tan(\theta/2) e^{i\phi} u_3'^{(3)}. \tag{28f}$$

The coefficients of $(\exp[ikr + i\gamma\ln 2kr])/r$ in (28a, b, c, e, f) shall be denoted by f_1', f_2', $\alpha^2 f_3'$, g_2', $\alpha^2 g_3'$, respectively. In applying (27) to obtain the behavior for large kr for $\psi_3'^{(3)}$ and $\psi_4'^{(3)}$, one should consider $J_0(2u\sin\theta/2) - J_0(2u)$ as

$$\lim_{\epsilon\to 0} J_\epsilon(2u\sin\theta/2) - J_\epsilon(2u).$$

In order to evaluate the remaining terms in the scattered waves, one applies (27) to (25), term by term, and in this manner obtains series of Lengendre functions with coefficients involving $\Gamma(n + 1 - i\gamma)/\Gamma(n + 1 + i\gamma)$. For $v \sim c$, γ is approximately equal to α and therefore terms of order $\alpha^2\gamma^2$, say, must be lumped with terms of order α^4. If we denote the resulting series of Legendre functions occurring in u_3 as S_i and those in u_4 as T_i we have, for example,

$$\begin{aligned} 2ku_3 = \{&2kf_1 + 2kf_2 + 2k\alpha^2 f_3 \\ &+ \tfrac{1}{2}\pi\alpha^2 S_1 + \tfrac{1}{2}\alpha^2\gamma[2S_3 - 2i\pi S_2] \\ &+ \tfrac{1}{2}\alpha^2(\gamma - \gamma')[S_8 + i\pi S_9] \\ &- \tfrac{1}{2}\alpha^2\gamma^2[2\pi S_4 + 4iS_5] \\ &+ \tfrac{1}{2}\alpha^2(\gamma - \gamma')\gamma[2iS_{11} - 2iS_{10} \\ &- \pi S_6 + 2\pi S_{13} + 2iS_{12}] \\ &+ \tfrac{1}{8}\alpha^4[3\pi S_6 + i\pi^2 S_7 - 2iS_{11}] + \cdots\} \\ &\times \exp[ikr + i\gamma\ln 2kr]/r. \end{aligned} \tag{29}$$

The result for u_4 is analogous with the f's replaced by the g's and the S_i's by the T_i's. The T_i's can be written down by inspection from the S_i's by a method equivalent to that by which ψ_4 was obtained from ψ_3. The series S_i and their sums as obtained by contour integration are tabulated in Table I.

The meanings of the symbols in Table I are as follows:

$$\psi_r(n + 1) = (d^r/dn^r)\ln\Gamma(n + 1),$$

$$\mathfrak{L}_2 = -\int_0^z \ln(1 + \xi)\, d\xi/\xi,$$

TABLE I. Tabulation of sums.

Part I. *Sums appearing in cross section.*

$$P_n = P_n(\cos\theta),$$

$$S_1 = \sum_1^\infty P_n + \sum_0^\infty P_n = \csc(\theta/2) - 1$$

$$S_2 = \sum_1^\infty P_n\psi_1(n+1) + \sum_0^\infty P_n\psi_1(n+1) = \psi(1)[\csc(\theta/2) - 1] - \csc(\theta/2)[\ln(1+\csc\theta/2) - \ln 4]$$

$$S_3 = \sum_1^\infty P_n\psi_2(n+1) + \sum_0^\infty P_n\psi_2(n+1) = \csc(\theta/2)[\pi^2/4 - \mathfrak{L}_2(m) + \mathfrak{L}_2(-m)] - \pi^2/6$$

$$S_4 = \sum_1^\infty P_n\psi_1^2(n+1) + \sum_0^\infty P_n\psi^2(n+1) = \csc(\theta/2)\{[\psi(1) + \ln(1+\csc\theta/2) - \ln 4]^2 + \mathfrak{L}_2(m) + \mathfrak{L}_2(-m) - \pi^2/12\} - \psi_1^2(1)$$

$$S_6 = \sum_0^\infty \frac{P_n}{n^2} + \sum_0^\infty \frac{P_n}{(n+1)^2} = 2\mathfrak{L}_2\left(\frac{1}{1+\sin\theta/2}\right) - 4\mathfrak{L}_2\left(\frac{2\sin\theta/2}{1+\sin\theta/2}\right) - 4\mathfrak{L}_2\tfrac{1}{2}(1+\sin\theta/2) - 6\mathfrak{L}_2(1-\sin\theta/2) - \ln^2(1+\sin\theta/2) + 4\ln 2\ln(1+\sin\theta/2) - 2\ln^2 2 - 2\ln\sin^2\theta/2\ln(1+\sin\theta/2) + 4\pi^2/3 + S_8$$

$$S_8 = \sum_1^\infty \frac{P_n}{n^2} - \sum_0^\infty \frac{P_n}{(n+1)^2} = -\frac{1}{2}\frac{\partial^2}{\partial\nu^2}\frac{\pi\nu}{\sin\pi\nu}P_\nu(-\cos\theta)\Big|_{\nu=0} = \mathfrak{L}_2(\cos^2\theta/2) - \pi^2/6$$

$$S_9 = \sum_1^\infty \frac{P_n}{n} - \sum_0^\infty = -2\ln(1+\sin\theta/2)$$

$$S_{13} = \sum_1^\infty \frac{P_n\psi_1(n+1)}{n} - \sum_0^\infty \frac{P_n\psi_1(n+1)}{n+1} = -4\mathfrak{L}_2\left(\frac{2\sin\theta/2}{1+\sin\theta/2}\right) - 2\mathfrak{L}_2(1-\sin\theta/2) - \mathfrak{L}_2(m) - \mathfrak{L}_2(-m) - 2\psi(1)\ln(1+\sin\theta/2) + \ln 4\ln(1+\sin\theta/2) - \ln^2(1+\sin\theta/2) + 2\ln\left(\frac{2\sin\theta/2}{1+\sin\theta/2}\right)\ln\frac{1+\sin\theta/2}{(1-\sin\theta/2)^2} + 7\pi^2/12$$

Part II. *Sums not appearing in cross section.*

$$S_5 = \psi(1)\left\{\csc\frac{\theta}{2}\left[\frac{\pi^2}{4} + \mathfrak{L}_2(-m) - \mathfrak{L}_2(m)\right] - \frac{\pi^2}{6}\right\} + 2\int_0^1 \frac{\ln|y|}{(1-y)\sqrt{\ }} \times \ln\left|\frac{2(\sqrt{\ })^2(y-\cos\theta)[(y-\cos\theta)C + \sin\theta + \sqrt{\ }]}{(\sin\theta - \sqrt{\ })y\sin\theta[(y-\cos\theta)C + \sin\theta\sqrt{\ }]}\right| dy,$$

$$\sqrt{\ } = [(y-\cos\theta)^2 + \sin^2\theta]^{1/2}, \qquad C = \tan\left(\frac{\theta}{2} - \frac{\pi}{4}\right)$$

$$S_7 = \sum_1^\infty \frac{P_n}{n} + \sum_0^\infty \frac{P_n}{n+1} = -\frac{\partial}{\partial\nu}\frac{\pi\nu}{\sin\pi\nu}P_\nu(-\cos\theta)\Big|_{\nu=0} = -\ln\sin^2\theta/2$$

$$S_{10} = \sum_1^\infty \frac{P_n\psi_1(n+1)}{n^2} - \sum_0^\infty \frac{P_n\psi_1(n+1)}{(n+1)^2} = \mathfrak{L}_2(\cos^2\theta/2) - \frac{\pi^2}{6} - \frac{\pi^2}{6}\ln(1+\sin\theta/2)^2 - \tfrac{1}{2}\psi_3(1) - \int_0^1 \frac{\mathfrak{L}_2(x)[1+(1/x)] + \ln^2|x|/2}{[(x-\cos\theta)^2 + \sin^2\theta]^{1/2}}\,dx$$

$$S_{11} = \sum_1^\infty \frac{P_n}{n^3} + \sum_0^\infty \frac{P_n}{(n+1)^3} = -\frac{1}{3!}\frac{\partial^3}{\partial\nu^3}\frac{\pi\nu}{\sin\pi\nu}P_\nu(-\cos\theta)\Big|_{\nu=0} = \int_0^1 \frac{\ln|v|\ln|1 - v\cos^2\theta/2|}{v(1-v)}\,dv$$

$$S_{12} = \sum_1^\infty \frac{P_n\psi_2(n+1)}{n} - \sum_0^\infty \frac{P_n\psi_2(n+1)}{(n+1)} = -\psi_3(1) - \frac{\pi^2}{6}\ln\sin^2\theta/2 - \frac{\pi^2}{6}\ln(1+\cos\theta/2) - \int_0^1 \frac{1/x[\pi^2/6 - \mathfrak{L}_2(1-x)] + \ln^2|x|/2 + \mathfrak{L}_2(1-x)}{[(x-\cos\theta)^2 + \sin^2\theta]^{1/2}}\,dx$$

Table I (*continued*)

Part III. *Sums appearing in* μ_1.

In general, if $$S_i = \sum_1^\infty f(n)P_n(\cos\theta) \pm \sum_0^\infty g(n)P_n(\cos\theta),$$

then $$T_i = \sum^\infty \frac{f(n)}{n} P_n^{(1)}(\cos\theta) + \sum \frac{g(n)}{n+1} P_n^{(1)}(\cos\theta),$$

$T_1 = -\tan\theta/2 S_1$
$T_2 = -\tan\theta/2 S_2 + \csc\theta S_9$
$T_3 = -\tan\theta/2 S_3 - \csc\theta S_8$
$T_4 = -\tan\theta/2 S_4 - \csc\theta S_6 + 2\csc\theta S_{13}$
$T_5 = -\tan\theta/2 S_5 + \csc\theta(S_{12} - S_{10} + S_{11})$
$T_6 = -\tan\theta/2 S_6$
$T_7 = -\tan\theta/2 S_7$
$T_8 = \cot\theta/2 S_8$
$T_9 = \cot\theta/2 S_9$
$T_{10} = \cot\theta/2 S_{10} - \csc\theta S_{11}$
$T_{11} = -\tan\theta/2 S_{11}$
$T_{12} = \cot\theta/2 S_{12} + \csc\theta S_{11}$
$T_{13} = \cot\theta/2 S_{13} - \csc\theta S_6$

the dilogarithm of Euler,

$$m = (1 - \sin\theta/2)/(1 + \sin\theta/2). \tag{30}$$

3.2 The Evaluation of the Series

As an example of the evaluation of the S_i's by contour integration, consider S_3.

$$S_3 = \sum_1^\infty \psi_2(n+1)P_n(\cos\theta) + \sum_0^\infty \psi_2(n+1)P_n(\cos\theta)$$

$$= \sum_0^\infty \psi_2(n+1)P_n(\cos\theta) - \psi_2(1), \tag{31}$$

$$\sum_0^\infty \psi_2(n+1)P_n(\cos\theta) = \frac{i}{2}\int_C \frac{P_\nu(-\cos\theta)}{\sin\pi\nu}\psi_2(\nu+1)\,d\nu$$

$$= -\frac{1}{2}\int_{-\infty}^{+\infty} \frac{P_{-1/2+i\tau}}{\cosh\pi\tau}\psi_2(\tfrac{1}{2}+i\tau)\,d\tau. \tag{32}$$

In this last step we have distorted the path C, as indicated in Fig. 1, so that the path of integration lies parallel to the imaginary ν axis after adding the circular arcs at infinity. The behavior of the integrand on these circular arcs is dominated by

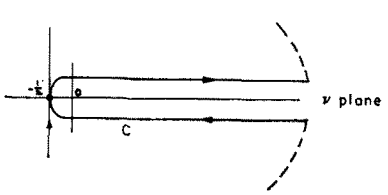

FIG. 1. The contour C.

$$\frac{P_\nu(-\cos\theta)}{\sin\pi\nu} \underset{|\operatorname{Im}\nu|\to\infty}{\longrightarrow} \exp(-\theta\,|\operatorname{Im}\nu|) \text{ for } 0 < \theta < \pi$$

and thus the integration over the circular arcs yields a vanishing small contribution to the integral. Use is made of the following integral representations:

$$P_\nu(-x) = \left(\frac{2}{\pi}\right)^{1/2} \frac{\Gamma(\frac{1}{2})}{\Gamma(\nu+1)\Gamma(-\nu)} \times \int_0^\infty \frac{\cosh[(\nu+\frac{1}{2})t]\,dt}{(\cosh t - x)^{1/2}},$$

$-1 < \operatorname{Re}(\nu) < 0$,
$+x$ not on the real axis between 1 and ∞; (33a)

$$\psi_1(z) = \psi_1(1) + \int_0^\infty \frac{e^{-t} - e^{-tz}}{1 - e^{-t}}\,dt, \quad \operatorname{Re}(z) > 0, \tag{33b}$$

$$\psi_2(z) = \frac{d\psi_1(z)}{dz} = \int_0^\infty \frac{te^{-tz}}{1 - e^{-t}}\,dt, \quad \operatorname{Re}(z) > 0, \tag{33c}$$

in the evaluation of the sums. Since

$$\int_0^\infty \frac{\cos(t\tau)\,dt}{(\cosh t - \cos\theta)^{1/2}} = \frac{1}{2}\int_{-\infty}^{+\infty} \frac{e^{it\tau}\,dt}{(\cosh t - \cos\theta)^{1/2}}, \tag{34}$$

$$\sum_{n=0}^\infty \psi_2(n+1)P_n(\cos\theta) = \frac{\sqrt{2}}{4\pi} \times \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^\infty \frac{\xi e^{-\xi/2}e^{-i\tau\xi}e^{it\tau}}{(1-e^{-\xi})(\cosh t - \cos\theta)^{1/2}}\,d\xi\,dt\,d\tau. \tag{35}$$

Interchanging the order of integration and applying the Fourier integral theorem, we have, using the successive substitutions

$$\tan v = \frac{e^{-\xi} - \cos\theta}{\sin\theta}, \qquad t = \tan\left(\frac{v-\theta}{4}\right):$$

$$\sum_0^\infty \psi_2(n+1)P_n = \frac{\sqrt{2}}{2}\int_0^\infty \frac{d\xi\,\xi e^{-\xi/2}}{(\cosh\xi - \cos\theta)^{1/2}(1-e^{-\xi})} = \frac{\csc\theta/2}{2}\int_0^{\tan(\pi-\theta)/4} \ln\left|\frac{(t-c)(t-d)}{(t+c)(t+d)}\right| \frac{dt}{t}, \quad (36)$$

where $c = \tan\theta/2 + \sec\theta/2$, $d = \tan\theta/2 - \sec\theta/2$. Finally,

$$S_3 = \csc\theta/2\left[\frac{\pi^2}{4} - \mathfrak{L}_2\left(\frac{1-\sin\theta/2}{1+\sin\theta/2}\right) + \mathfrak{L}_2\left(-\frac{1-\sin\theta/2}{1+\sin\theta/2}\right)\right] - \frac{\pi^2}{6}. \quad (37)$$

For some further details, see Appendix I.

An interesting example is

$$S_8 = \sum_1^\infty \frac{P_n(\cos\theta)}{n^2} - \sum_0^\infty \frac{P_n(\cos\theta)}{(n+1)^2} = +\frac{i}{2}\int_C \frac{P_\nu(-\cos\theta)}{\sin\pi\nu}\frac{2\nu+1}{\nu^2(\nu+1)^2}\,d\nu - \frac{i}{2\pi}\int_\Gamma \frac{P_\nu(-\cos\theta)}{\nu^3}\frac{\pi\nu}{\sin\pi\nu}\,d\nu. \quad (38)$$

Here Γ is a circular path about the origin of radius less than $\frac{1}{2}$, say, taken in a clockwise direction. When the integral over C is distorted to run parallel to the imaginary ν axis, it will have the factor

$$\int_{-\infty}^{+\infty} \frac{\tau\cosh it\tau\,d\tau}{(\tau^2+\frac{1}{4})} = 0.$$

Evaluating the residue at zero of the integral along Γ, one has

$$S_8 = -\frac{1}{2}\frac{\partial^2}{\partial\nu^2}\left(P_\nu(-\cos\theta)\frac{\pi\nu}{\sin\pi\nu}\right)\Big|_{\nu=0} = \mathfrak{L}_2(\cos^2\theta/2) - \frac{\pi^2}{6}. \quad (39)$$

3.3 The Cross Section

Since the leading term in the scattered wave amplitude is proportional to α (for $\alpha \simeq \gamma$), knowledge of the wavefunction to terms in α^4 permits the calculation of the differential cross section up to those terms proportional to α^5. However, we are actually interested in the ratio of this cross section to the Rutherford cross section,

$$\sigma_R(\theta) = \frac{\gamma^2}{4k^2\sin^4\theta/2} = \frac{(Ze^2)^2}{4m^2v^4}(1-\beta^2)\csc^4\theta/2 \text{ [Relativistic]}. \quad (40)$$

The ratio $\sigma(\theta)/\sigma_R$, commonly denoted by R, will contain terms proportional to α^{n-1} if the wavefunction and cross section are known to order α^n and α^{n+1}, respectively. We shall indicate the order in α to which the wavefunction has been calculated by a Roman numeral subscript. Then

$$R_{\rm I} = 1 - \beta^2\sin^2\theta/2, \quad (41a)$$

$$R_{\rm II} - R_{\rm I} = \pi\alpha\beta S_1\sin^2\theta/2 = \pi\alpha\beta\sin\theta/2(1-\sin\theta/2), \quad (41b)$$

$$R_{\rm III} - R_{\rm II} = (\alpha^2\lambda^2/2)\sin^2\theta/2 + \frac{\pi^2\alpha^2\beta^2}{4}S_1^2\sin^4\theta/2\sec^2\theta/2 + (\alpha^2\beta^2/4)\lambda^2\sin^4\theta/2\sec^2\theta/2 + \alpha^2\sin^2\theta/2(2S_3 + \beta^2 S_8), \quad (41c)$$

$$R_{\rm IV} - R_{\rm III} = (\pi\alpha\beta/4)Q'\lambda S_1\sec^2\theta/2\sin^4\theta/2 - (\pi\alpha^3/2\beta)Q^2S_1\sin^2\theta/2 + \pi(\alpha^3\beta/2)S_1(2S_3+S_8)\sec^2\theta/2\sin^4\theta/2 + \pi(\alpha^3\beta/2)(S_9 - 2S_2)\lambda\sin^4\theta/2\sec^2\theta/2 + (\pi\alpha^3/\beta)[2S_2 - \beta^2 S_9]\sin^2\theta/2 + 2\pi\alpha^3\beta S_{13}\sin^2\theta/2 - (2\pi\alpha^3/\beta)S_4\sin^2\theta/2 - (\pi\alpha^3\beta/4)\sin^2\theta/2 S_6. \quad (41d)$$

Here, $Q = 2\psi(1) - \lambda$, $Q' = 4\psi(1) - \lambda$, $\psi(1) = -E$ (the Euler–Mascheroni constant 0.5772) and again $\lambda = \ln\sin^2\theta/2$. It should be noted that the series S_5, S_7, S_{10}, S_{11}, and S_{12} contained in the scattering amplitude are not present in the cross section, for when $u_3u_3^*$ is calculated these series appear in terms of the form

$$\lambda i\alpha^4 S[M(1)e^{i\gamma\lambda} - M(1)e^{-i\gamma\lambda}] \sim 2\gamma^2\alpha^4 S[(\lambda - 2\psi(1)] + \cdots. \quad (42)$$

Since this calculation is exact in the limit $\alpha \to 0$, $\alpha/\gamma \simeq 1$, consistency requires that such terms be dropped unless the wavefunction (cross section) is known to order $\alpha^5(\alpha^6)$.

Using these formulas [Eqs. (43a–d)], we have calculated the cross section for scattering of electrons by lead ($Z = 82$, $\alpha = 0.598$) at a bombarding energy of 10 MeV ($\beta = 0.9976$) to order α^5. The results are plotted in Fig. 2 along with the exact results of Doggett and Spencer.[9]

[9] J. A. Doggett and L. V. Spencer, Phys. Rev. **103**, 1597 (1956).

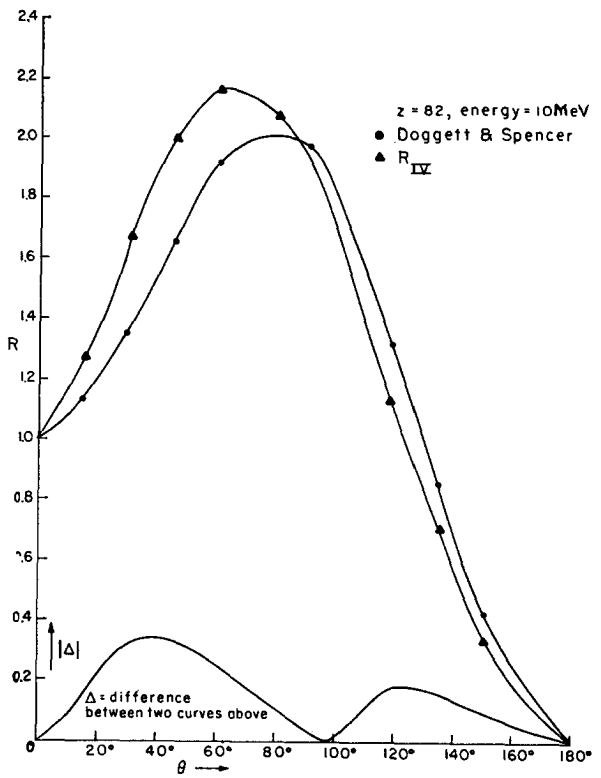

FIG. 2. Ratio of relativistic cross section to Rutherford scattering cross section.

4. THE GENERAL FORM OF THE COEFFICIENT OF α^n

In general, we can write that

$$U(\theta, \alpha, \gamma) = 2iku_3(\theta, \alpha, \beta) = \sum_{r=0}^{\infty} \sum_{S=0}^{\infty} \frac{\alpha^r \gamma^S}{r!S!} U_{r,S}(\theta, 0, 0), \quad (43)$$

where

$$U_{r,S}(\theta, 0, 0) = \frac{\partial^{r+S} U}{\partial \alpha^r \, \partial \gamma^S}(\theta, \alpha, \gamma)\Big|_{\gamma=0,\ \alpha=0}. \quad (44)$$

With an increasing amount of analytic labor, one can find the $U_{r,S}$ by expansion of the phase shifts as sums of the form

$$\sum_{n=1}^{\infty} f(n)[P_n(\cos\theta) \pm P_{n-1}(\cos\theta)].$$

This, of course, was the starting point of the work described in the previous sections. By means of contour integration, these sums were expressed in the form of integrals, some of which can be evaluated in closed form. We shall now consider an alternative approach which bypasses the intermediate step, namely, expansion of the phase shift in powers of α and γ. The total scattering amplitude will first be expressed as a contour integral in the complex ν plane; integral representations will be used for certain functions and then derivatives with respect to α and γ will be taken. The result will be that the $U_{r,S}(\theta, 0, 0)$ can be expressed in terms of two-dimensional real integrals. By a simple change in variables these integrals can be as integrals over a square in a two-dimensional space.

4.1 Nonrelativistic Scattering by an Inverse-Cube-Law Force

Before considering the relativistic Coulomb problem itself, we shall digress briefly to discuss a related problem. It is well known that the differential equation describing the motion of a relativistic classical particle moving in a Coulomb field differs from that of a nonrelativistic particle, in that the first contains an apparent force term proportional to $1/r^3$. It would appear reasonable to expect then that there will be mathematical similarities in the scattering amplitude for a particle obeying the nonrelativistic Schrödinger equation moving in an inverse-cube-law force field and the scattering amplitude dealt with in this paper.

Formally one has the following differential equation:

$$-(\hbar^2/2m)\nabla^2\chi - (\gamma'/r^2)\chi = (h^2/2m)k^2\chi, \quad (45)$$

with the boundary conditions

$$\chi \text{ finite at the origin,}$$

$$\chi \underset{r\to\infty}{\longrightarrow} e^{ikz} + h(\theta)\frac{e^{ikr}}{r}. \quad (46)$$

The solution is given by[10]

$$\chi = \sum (2n+1)P_n(\cos\theta)e^{-i\delta_n} j_{\sigma_n}(kr), \quad (47)$$

where

$$\delta_n = -\tfrac{1}{2}\pi\{[(n+\tfrac{1}{2})^2 - \eta^2]^{1/2} - (n+\tfrac{1}{2})\},$$

$$j_{\sigma_n} = (\pi/2kr)^{1/2} J_{\sigma_n+\frac{1}{2}} \quad \text{(spherical Bessel function)},$$

$$\eta^2 = 8\pi^2 m\gamma/h^2 < \tfrac{1}{4} \quad \text{(condition of regularity at origin)},$$

$$\sigma_n = [(n+\tfrac{1}{2})^2 - \eta^2]^{1/2} - \tfrac{1}{2}.$$

The scattering amplitude $h(\theta\ \eta)$ is given by

$$h(\theta, \eta) = \frac{1}{2ik}\sum_{n=0}^{\infty}(2n+1)P_n(\cos\theta)[e^{-2i\delta_n} - 1], \quad (48)$$

and we write

[10] Reference 3, pp. 40–41.

$$H(\theta, \eta) \equiv 2ikh(\theta, \eta) = \sum_{n=0}^{\infty} (2n + 1)P_n(\cos\theta)$$

$$\times \sum_{r=1}^{\infty} \frac{(i\pi)^r}{r!} \{[(n + \tfrac{1}{2})^2 - \eta^2]^{1/2} - (n + \tfrac{1}{2})\}^r$$

$$= \frac{i}{2} \int_D \frac{(2\nu + 1)P_\nu(-\cos\theta)}{\sin \pi\nu}$$

$$\times \sum_{r=1}^{\infty} \{[(\nu + \tfrac{1}{2})^2 - \eta^2]^{1/2} - (\nu + \tfrac{1}{2})\}^r \frac{(+i\pi)^r}{r!}\, d\nu. \quad (49)$$

The contour D is shown in Fig. 3; the branch line of the function $[(\nu + \frac{1}{2})^2 - \eta^2]^{1/2}$, extending from $\nu + \frac{1}{2} = -\eta$ to $\nu + \frac{1}{2} = +\eta$ is indicated by the double line. We now distort the path D so that it lies parallel to the imaginary ν axis; the contribution from the infinite semicircle (indicated by the dotted line) vanishes because the integrand approaches $e^{-|\mathrm{Im}\nu|\theta} \times [1/(\nu + \frac{1}{2})]$ for large ν. Using the variable μ, defined by $\nu + \frac{1}{2} = \mu$, and indicating the new path as Γ, we have

$$H(\theta, \eta) = \frac{\sqrt{2}}{2\pi i} \int_\Gamma \int_{-\infty}^{+\infty} \sum_r \frac{\mu e^{\mu t}}{(\cosh t - \cos\theta)^{1/2}}$$

$$\times \frac{(i\pi)^r}{r!} [K(\mu, \eta)]^r\, dt\, d\mu; \quad (50)$$

$$K(\mu, \eta) \equiv (\mu^2 - \eta^2)^{1/2} - \mu.$$

Now consider the function

$$g(\mu, \eta) = \sum_{r=1}^{\infty} \frac{(i\pi)^r}{r!} [(\mu^2 - \eta^2)^{1/2} - \mu]^r. \quad (51)$$

We desire, in general, the $2m$th derivative of this function with respect to η evaluated at $\eta = 0$. With the aid of the integral representation

$$[(\mu^2 - \eta^2)^{1/2} - \mu]^r$$

$$= r\beta^r \int_0^\infty \lambda^{-1} e^{-\mu\lambda} J_r(\beta\lambda)\, d\lambda; \quad \beta \equiv i\eta, \quad (52)$$

one finds

$$\frac{1}{(2m)!} \frac{\partial^{2m}}{\partial\eta^{2m}} g(\mu, \eta)\Big|_{\eta=0}$$

$$= \frac{1}{m!} \sum_{r=1}^{m} \frac{(-i\pi)^r (2m - r - 1)!}{(r - 1)!(m - r)!\, 2^{2m-r}} \mu^{-2m+r} \quad (53)$$

$$\equiv \sum_{r=1}^{m} D(2m, r)\mu^{-2m+r}(+i\pi)^r,$$

where

$$D(2m, r) \equiv \frac{(-1)^r (2m - r - 1)!}{m!(r - 1)!(m - r)!\, 2^{2m-r}}. \quad (54)$$

Further, then,

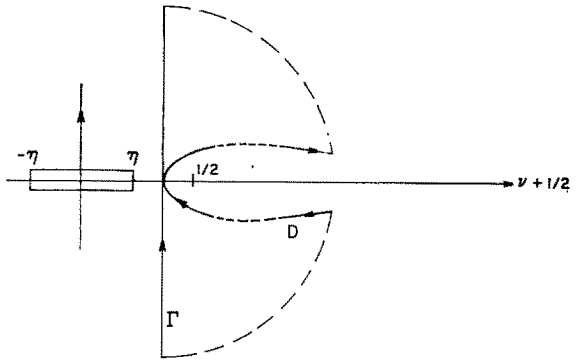

FIG. 3. The contour D.

$$\frac{\partial^{2m}}{\partial\eta^{2m}} H(\theta, \eta)\Big|_{\eta=0} = \int_\Gamma \int_{-\infty}^{+\infty} \frac{e^{+\mu t}}{(\cosh t - \cos\theta)^{1/2}}$$

$$\times \sum_{r=1}^{m} (i\pi)^r D(2m, r)\mu^{-2m+r+1}. \quad (55)$$

For the integration over μ we have, if $2m - r - 1 < 0$,

$$\int_\Gamma e^{+\mu t} \mu^{-2m+r+1}\, d\mu$$

$$= \frac{2\pi i}{(2m - r - 2)!} \frac{d^{2m-r-2}}{d\mu^{2m-r-2}} e^{+\mu t}\Big|_{\mu=0} H(t)$$

$$= \frac{2\pi i (+t)^{2m-r-2}}{(2m - r - 2)!} H(t), \quad (56a)$$

where $H(t)$ is the unit step function. If $2m - r - 1 = 0$, then

$$\int_\Gamma e^{+\mu t}\, d\mu = 2\pi i\, \delta(t). \quad (56b)$$

We can unify the results as follows:

$$\int_\Gamma e^{+\mu t} \mu^{-p}\, d\mu = 2\pi i\, \delta_p(t), \quad (57)$$

where

$$\delta_p(t) = \int_0^t \int_0^{u_1} \int_0^{u_2} \cdots \int_0^{u_{p-1}} \delta(u_p)\, du_p\, du_{p-1} \cdots du_2\, du_1.$$

(p fold)

If p is negative, the corresponding derivative of the δ function is indicated. Finally, then,

$$\frac{\partial^{2m}}{\partial\eta^2} H(\theta, \eta) = \sqrt{2}$$

$$\times \int_{-\infty}^{+\infty} \sum_{r=1}^{m} \frac{D(2m, r)\, \delta_{2m-r-1}(t)(-i\pi)^r}{(\cosh t - \cos\theta)^{1/2}}\, dt. \quad (58)$$

For the lowest-order term one finds

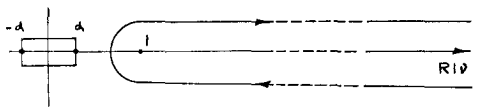

FIG. 4. The contour used in evaluation of F and G.

$$\frac{1}{2!}\frac{\partial^2 H(\theta,\eta)}{\partial\eta^2} = \sqrt{2}\,\frac{D(2,1)(i\pi)}{2(1-\cos\theta)^{1/2}} = \frac{-i\pi}{2\sin\theta/2}, \tag{59}$$

and then, to lowest order,

$$4k^2\sigma(\theta) = \pi^2\eta^4/4\sin^2(\theta/2). \tag{60}$$

4.2 The General Terms in Mott's Expansion

In treating the relativistic Coulomb scattering amplitude a procedure similar to that in Sec. 4.1 can be carried out; the exact form of the answer can be in several equivalent forms depending on the manner one uses to separate the phase shifts into distinct terms. We shall discuss the formulation used by Mott [cf. Eqs. (14) and (15)] for two reasons: First, it can be more easily compared with previous work, and second, the notation is more compact.

The functions $F(\theta)$ and $G(\theta)$ were defined in Eqs. (14a, b, c). These may be expressed as

$$F(\theta) = \frac{i}{2}\sum_{n=1}^{\infty}(-1)^n nC_n[P_n(\cos\theta) - P_{n-1}(\cos\theta)], \tag{61a}$$

$$G(\theta) = \frac{i}{2}\sum_{n=1}^{\infty}(-1)^n n^2C_n[P_n(\cos\theta) + P_{n-1}(\cos\theta)], \tag{61b}$$

Denoting by C_n^0 the function

$$-e^{-i\pi n}[\Gamma(n - i\gamma)/\Gamma(n + 1 + i\gamma)],$$

and setting

$$D_n = C_n - C_n^0, \tag{62}$$

one can rewrite (61a, b) as

$$F(\theta) = F_0 + F_1 = F_0 + \frac{i}{2} \times \sum_{n=1}^{\infty}(1-)^n nD_n[P_n(\cos\theta) - P_{n-1}(\cos\theta)], \tag{63a}$$

$$G(\theta) = G_0 + G_1 = G_0 + \frac{i}{2} \times \sum_{n=1}^{\infty}(-1)^n n^2D_n[P_n(\cos\theta) - P_{n-1}(\cos\theta)], \tag{63b}$$

where

$$F_0 = -\frac{i}{2}\frac{\Gamma(1 - i\gamma)}{\Gamma(1 - i\gamma)}e^{i\gamma\lambda}, \tag{64}$$

and

$$G_0 = i\gamma F_0\,\mathrm{ctn}^2(\theta/2). \tag{65}$$

It should be noted here that Mott drops the sum

$$-\frac{1}{2ik}\sum_{n=0}^{\infty}(2n + 1)P_n(\cos\theta),$$

which is zero if θ differs from zero. Mott obtains the values of F_0 and G_0 by demanding that, in the limit $c \to \infty$, $\alpha \to 0$, γ finite, the scattering amplitude reduces to the nonrelativistic value. Inasmuch as $C_n \to_{n\to\infty} -1/n$, and, as thus $n^2C_n \to_{n\to\infty} -n$, this sum must be retained in a formal evaluation of G_0.

We shall now find the formal expansion of the functions $F(\theta, \alpha, \gamma)$ and $G(\theta, \alpha, \gamma)$ in powers of α and γ. For convenience, we consider that α and $\gamma \equiv \alpha/\beta$ are independent variables and that the formal limit $\alpha \to 0$ need not imply $\gamma \to 0$. First, however, we need to express P_n in terms of P_{n-1} according to the relation

$$P_n(\cos\theta) = \left(\cos\theta + \frac{\sin\theta}{n}\frac{d}{d\theta}\right)P_{n-1}(\cos\theta). \tag{66}$$

This is done in order that we can use the integral representation (33a) despite a change of the path of integration. The use of this new contour is desirable because we wish to avoid both the branch line of $(\nu^2 - \alpha^2)^{1/2}$ and the poles of $\Gamma(\nu - i\gamma)/\Gamma(\nu + 1 + i\gamma)$; this contour is shown in Fig. 4. Again, the double line indicates a branch cut, this time of the function $(\nu^2 - \alpha^2)^{1/2}$.

Proceeding as in the previous section, we find that

$$\frac{1}{2m!}\frac{\partial^{2m}F_1}{\partial\alpha^2}\bigg|_{\alpha=0} = \frac{\sqrt{2}\,i}{4}\frac{1}{\Gamma(1 + 2i\gamma)}\sum_{r=1}^{m}\frac{D(2m,r)}{r!} \times \int_{\infty}^{+\infty}\int_{0}^{\infty}(i\pi + \xi)^r\exp[2i\gamma\ln(2\sinh\xi/2) - t/2] \times T(\theta, t - \xi)\frac{d\xi\,dt}{(\cosh t - \cos\theta)^{1/2}}, \tag{67}$$

and that

$$\frac{1}{2m!}\frac{1}{l!}\frac{\partial^{2m+l}F_1}{\partial\alpha^{2m}\,\partial\gamma}\bigg|_{\alpha=0,\gamma=0} = \frac{\sqrt{2}\,i(2i)^l}{4}\sum_{r=1}^{m}\sum_{s=0}^{l}\frac{D(2m,r)E(s)}{r!s!(l-s)!} \times \int_{-\infty}^{+\infty}\int_{0}^{\infty}(i\pi + \xi)^r e^{-t/2}[\ln(2\sinh\xi/2)]^{l-s} \times T(\theta, t - \xi)\frac{d\xi\,dt}{(\cosh t - \cos\theta)^{1/2}}. \tag{68}$$

In these last two equations, the operator T is given by

$$T = [\delta_{2m-r-1}(t-\xi)(1-\cos\theta) - \delta_{2m-r}(t-\xi)\sin\theta\,(\partial/\partial\theta)], \quad (69)$$

and the numbers $E(s)$ by

$$E(s) = \frac{d^s}{dx^s}\frac{1}{\Gamma(1+x)}\bigg|_{x=0}. \quad (70)$$

The first few E's are

$$E(0) = 1, E(1) = -\psi(1) = E \text{ (the Euler constant } 0.577\cdots),$$
$$E(2) = E^2 - \pi^2/6.$$

These numbers can be generated by means of the following recursion relation:

$$E(s+1) = \frac{d^s}{dx^s} - \frac{1}{\Gamma(1+x)}\psi(1+x)\bigg|_{x=0} = -\sum_{p=0}^{s}\binom{s}{p}E(s-p)\psi_{p+1}(1). \quad (71)$$

The ψ_ν's are the polygamma functions.

In obtaining the results for the derivatives of F_1, use was made of the following integral representation:

$$\frac{\Gamma(\nu-i\gamma)}{\Gamma(\nu+1+i\gamma)} = \frac{1}{\Gamma(1+2i\gamma)}B(\nu-i\gamma, 1+2i\gamma) = \frac{1}{\Gamma(1+2i\gamma)}\int_0^\infty e^{-\xi(\nu-i\gamma)}(1-e^{-\xi})^{2i\gamma}\,d\xi, \quad (72)$$

$$\text{Re}\,\nu > 0 \text{ for } \gamma \text{ real}.$$

Similar expressions for G_1 can be obtained simply by replacing T by

$$-[\delta_{2m-r-2}(t-\xi)(1+\cos\theta) + \delta_{2m-r-1}(t-\xi)\sin\theta(\partial/\partial\theta)]. \quad (73)$$

In general, the form of the integrals will be

$$\int_0^\infty\int_0^t \frac{e^{-t/2}(t-\xi)^{k_1}(i\pi-\xi)^{k_2}(\ln 2\sinh\xi/2)^{k_3}}{(\cosh t-\cos\theta)^{1/2}}\,d\xi\,dt$$

(those involving the delta function and its derivative will be simpler). The substitutions $y = e^{-\xi}$, $x = e^{-t}$ bring this into the form

$$\int_0^1\int_x^1 \frac{[\ln y/x]^{k_1}[\ln y]^{k_2}[\ln(1-y)/\sqrt{y}]^{k_3}}{[(x-\cos\theta)^2+\sin^2\theta]^{1/2}}\frac{dy}{y}\,dx.$$

As previously noted, the dilogarithm $\mathfrak{L}_2$ is defined as

$$\mathfrak{L}_2(z) = -\int_0^z \ln(1-\xi)\frac{d\xi}{\xi}. \quad (74)$$

A generalization, called the n logarithm, may be defined by

$$\mathfrak{L}_n(z) = +\int_0^z \mathfrak{L}_{n-1}(\xi)\frac{d\xi}{\xi}.$$

We may further generalize these as follows:

$$\mathfrak{L}_{2,k}(z) = -\int_0^z [\ln(1-\xi)]^k\frac{d\xi}{\xi},$$

$$\mathfrak{L}_{n,k}(z) = \int_0^z \mathfrak{L}_{n-1,k}(\xi)\frac{d\xi}{\xi}.$$

Integration by parts allows us to express $\mathfrak{L}_{n,k}(z)$ as

$$\mathfrak{L}_{n,k}(z) = \ln z\mathfrak{L}_{n-1,k}(z) = \frac{\ln^2 z}{2!}\mathfrak{L}_{n-2,k} + \cdots + (-1)^{n-1}\frac{\ln^{n-2}z}{(n-2)!}\mathfrak{L}_{2,k}(z) + \frac{(-1)^{n-1}}{(n-2)!}\int_0^z \frac{[\ln\xi]^{n-2}[\ln(1-\xi)]^k}{\xi}\,d\xi.$$

Finally then, the angular dependence of the correction terms to the scattered wave will be given by integrals of the form

$$\int_0^1 \frac{[\ln x]^{m_1}[\ln(1-x)]^{m_2}\mathfrak{L}_{n,k}(1-x)}{[(x-\cos\theta)^2+\sin^2\theta]^{1/2}}\,dx. \quad (75)$$

5. CONCLUSIONS

In this paper we have used the techniques of contour integration to obtain, in closed form, the differential cross section for relativistic Coulomb scattering up to the fifth order in the fine structure constant. The functional form of the relativistic corrections to the scattering amplitude corresponding to an arbitrary order of the fine structure constant were found in terms of two-dimensional integrals involving elementary transcendental functions.

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APPENDIX

Evaluation of the Sums

In the evaluation of the sums listed in Table I, integrals of the form

$$\int_0^\infty \frac{e^{-t/2}f(t)}{(\cosh t-\cos\theta)^{1/2}}\,dt, \quad f(t) \text{ real} \quad (A')$$

arise. The substitution $x = e^{-t}$ casts the integrals

into the form

$$\int_0^1 \frac{f(-\ln x)\,dx}{[(x-\cos\theta)^2+\sin^2\theta]^{1/2}}. \qquad (B')$$

Inasmuch as the integrals (A') are real, one must take care that no imaginary terms appear in the final result. In particular, the logarithm occurring in the integrals (B') must be considered to be $\ln|x|$. The dilogarithm and n-logarithm functions mentioned in the text require similar treatment. The following functional relations were used in simplifying the final results:

$$\mathfrak{L}_2(x)+\mathfrak{L}_2(1/x)=\tfrac{1}{3}\pi^2-\tfrac{1}{2}\ln^2|x|;$$

$$\mathfrak{L}_2(x)+\mathfrak{L}_2(1-x)=\tfrac{1}{6}\pi^2-\ln|x|\ln|1-x|.$$

These relations differ from those usually quoted, for the reasons stated.

The derivatives of the Legendre functions with respect to order were calculated by differentiating the appropriate hypergeometric series term by term. For example,

$$\begin{aligned}\left.\frac{\partial^2 P_\nu}{\partial\nu^2}\right|_{\nu=0} &= \left.\frac{\partial^2}{\partial\nu^2}F\left(-\nu,\nu+1,\frac{1+\cos\theta}{2}\right)\right|_{\nu=0}\\ &= \left.\frac{\partial^2}{\partial\nu^2}\left[1-\frac{\sin\pi\nu}{\pi}\right.\right.\\ &\quad\left.\left.\times\sum_{r=1}^{\infty}\frac{\Gamma(r+\nu+1)\Gamma(r-\nu)}{(r!)^2}(\cos^2\theta/2)^r\right]\right|_{\nu=0}\\ &= -2\sum_{r=1}^{\infty}\frac{\Gamma(r+1)\Gamma(r)}{(r!)^2}\\ &\quad\times[\psi_1(r+1)-\psi_1(r)](\cos^2\theta/2)^r\\ &= -2\sum^{\infty}\frac{(\cos^2\theta/2)^r}{r^2}=-2\mathfrak{L}_2(\cos^2\theta/2).\end{aligned}$$

Here we have used the functional relation

$$\psi_1(r+1)=\psi_1(r)+1/r.$$

The corresponding relationship for the polygamma functions follow by differentiation with respect to r.

Binary Kernel Formulation of a Heisenberg Model of Ferromagnetism*†

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An ideal Heisenberg model of a ferromagnet for spin $\frac{1}{2}$ is studied by considering the model in terms of a spin-deviation lattice gas. Utilizing the general methods of Yang and Lee, a binary kernel function is obtained in terms of which the thermodynamic properties of the lattice gas can be completely expressed. As an example, Dyson's results are rigorously obtained.

I. INTRODUCTION

IT has been demonstrated by Van Kranendonk[1] that the Heisenberg model for spin $\frac{1}{2}$ is equivalent to a lattice gas of interacting spin deviations. However, Van Kranendonk has not shown sufficient care in the handling of the interaction between spin deviations and is thus led to erroneous results. In this paper, a rigorous treatment of Van Kranendonk's spin-deviation lattice gas is given using the general methods introduced by Yang and Lee[2] in their treatment of a hard core Bose gas.

In Secs. II and III, the basic properties of the spin-deviation lattice gas are outlined and the appropriate binary kernel is obtained. In Sec. IV, we show—by obtaining Dyson's result[3,4] for the spontaneous magnetization—how the binary kernel formulation, and thus Van Kranendonk's lattice gas, can be utilized at low temperature. We thus have further confirmation that Dyson's handling of his kinematical interaction, which is not physically obvious for spin $\frac{1}{2}$, is indeed correct. In the last section we briefly discuss the possibility of using the binary kernel formulation at higher temperatures.

At this point, we should like to mention the work of Morita[5] whose approach is somewhat similar to ours. Using Van Kranendonk's lattice gas, Morita obtains Dyson's low-temperature results; but, unlike the present paper, Morita assumes in essence, part of Dyson's results.[6]

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[6] Morita's work is based on the solution of a two-particle wave equation. However, for $E = 2cJ$, his hard-core potential in the spin-$\frac{1}{2}$ wave equation is ineffective. As $E = 2cJ$ corresponds to Dyson's improper states (see Sec. 2 of reference 4), it is clear that Morita has omitted Dyson's kinematical interaction.

II. SPIN DEVIATION LATTICE GAS

The model used in this work is a cubic crystal with periodic boundary conditions. The crystal structure is taken to be simple cubic. To each lattice site $\mathbf{r}_1$, a spin vector $\mathbf{S}_{\mathbf{r}_1}$ of absolute value $\frac{1}{2}$ is attached. Each spin vector has an intrinsic magnetic moment μ, and an external magnetic field H_m is applied in the positive z direction.

The Hamiltonian for this system, assuming an isotropic exchange interaction between nearest-neighbor spin vectors, is

$$\mathcal{H} = -J \sum_{\mathbf{r}_1,\Delta} (\mathbf{S}_{\mathbf{r}_1} \cdot \mathbf{S}_{\mathbf{r}_1+\Delta} - 2\mu H_m \gamma_0^{-1} S^z_{\mathbf{r}_1}), \quad (1)$$

where the $\mathbf{r}_1$ summation is performed over all N lattice vectors and the lattice vector Δ is summed over all γ_0 nearest neighbor lattice vectors.

For spin $\frac{1}{2}$, the spin vectors satisfy the relation

$$[S^+_{\mathbf{r}_1}, S^-_{\mathbf{r}_2}] = 2\delta_{\mathbf{r}_1,\mathbf{r}_2} S^z_{\mathbf{r}_1} = \delta_{\mathbf{r}_1,\mathbf{r}_2}(1 - 2S^-_{\mathbf{r}_1} S^+_{\mathbf{r}_1}), \quad (2)$$

where

$$S^{\pm}_{\mathbf{r}_1} = S^x_{\mathbf{r}_1} \pm S^y_{\mathbf{r}_1}.$$

By combining (2) with (1), the Hamiltonian operator may be expressed as

$$\mathcal{H} = E_0 + J \sum_{\mathbf{r}_1,\Delta} (S^-_{\mathbf{r}_1} S^+_{\mathbf{r}_1} - S^-_{\mathbf{r}_1+\Delta} S^+_{\mathbf{r}_1} + S^-_{\mathbf{r}_1} S^-_{\mathbf{r}_1+\Delta} S^+_{\mathbf{r}_1} S^+_{\mathbf{r}_1+\Delta}) + 2\mu H_m \sum_{\mathbf{r}_1} S^-_{\mathbf{r}_1} S^+_{\mathbf{r}_1}, \quad (3)$$

where

$$E_0 = -\tfrac{1}{4} J N \gamma_0 - \mu H_m N. \quad (4)$$

The ground state of the system, $|0\rangle$, is defined by the condition

$$S^+_{\mathbf{r}_1} |0\rangle = 0, \quad (5)$$

for any lattice vector $\mathbf{r}_1$. That is, in the ground state, all the spin vectors are in the "up" direction, and from (3) and (5) we find the ground-state energy to be simply E_0.

A complete orthogonal set of states for the system

are the states which have a fixed number of spins in the "down" direction and these spin deviations are at specified sites. The states with one spin deviation are of the form

$$S_{\mathbf{r}_1}^- |0\rangle \equiv |\mathbf{r}_1\rangle, \tag{6}$$

where $\mathbf{r}_1$ is any one of the N lattice vectors. In general, the states with n spin deviations are of the form

$$S_{\mathbf{r}_1}^- \cdots S_{\mathbf{r}_n}^- |0\rangle \equiv |\mathbf{r}_1 \cdots \mathbf{r}_n\rangle, \tag{7}$$

where $\mathbf{r}_1 \cdots \mathbf{r}_n$ are any n lattice vectors. From (2) we find that (7) vanishes when any two lattice vectors are the same and thus, for n spin deviations there are only $\binom{N}{n}$ independent states.

Using (2) and (3), we see that the operator $\sum_{\mathbf{r}_1} S_{\mathbf{r}_1}^- S_{\mathbf{r}_1}^+$ corresponds to the total number of spin deviations and is a constant of the motion. Van Kranendonk has shown[1] that, when discussing the thermodynamic properties of the spin deviation lattice gas, the term $2\mu H_m \sum_{\mathbf{r}_1} S_{\mathbf{r}_1}^- S_{\mathbf{r}_1}^+$ in (3) is equivalent to introducing the fugacity $\mathfrak{z}$,

$$\mathfrak{z} = \exp(-2\beta\mu H_m), \tag{8}$$

into the system. Taking advantage of this equivalence, we define an effective Hamiltonian for the lattice gas as

$$\begin{aligned} H &= \mathfrak{IC} - 2\mu H_m \sum_{\mathbf{r}_1} S_{\mathbf{r}_1}^- S_{\mathbf{r}_1}^+ - E_0 \\ &= J \sum_{\mathbf{r}_1, \Delta} (S_{\mathbf{r}_1}^- S_{\mathbf{r}_1}^+ - S_{\mathbf{r}_1+\Delta}^- S_{\mathbf{r}_1}^+ \\ &\qquad - S_{\mathbf{r}_1}^- S_{\mathbf{r}_1+\Delta}^- S_{\mathbf{r}_1}^+ S_{\mathbf{r}_1+\Delta}^+). \end{aligned} \tag{9}$$

It is now a simple matter to define the wave equation for the lattice gas. Let the symmetric function $\varphi_l(\mathbf{r})$ be the probability amplitude of finding n spin deviations at lattice sites $\mathbf{r} = (\mathbf{r}_1 \cdots \mathbf{r}_n)$ while in the lth eigenstate of (9), the corresponding eigenvalue being E_l. The wave equation is then given by

$$\sum_{\mathbf{r}'} (n!)^{-1} \varphi_l(\mathbf{r}') \langle \mathbf{r} | H | \mathbf{r}' \rangle = E_l \varphi_l(\mathbf{r}) \tag{10}$$

if $\langle \mathbf{r} \mid \mathbf{r} \rangle \neq 0$, and

$$\varphi_l(\mathbf{r}) = 0 \tag{11}$$

if $\langle \mathbf{r} \mid \mathbf{r} \rangle = 0$.

For the case $n = 1$, the solutions of (10) are the usual Bloch spin waves. That is, one obtains

$$\begin{aligned} \varphi_{\lambda_1}(\mathbf{r}) &= N^{-\frac{1}{2}} \exp(i\lambda_1 \cdot \mathbf{r}_1), \\ E_{\lambda_1} &= J \sum_{\Delta} (1 - \cos \lambda_1 \cdot \Delta), \end{aligned} \tag{12}$$

where the wave vector λ_1 can assume any of the N values in the first Brillouin zone of the reciprocal lattice.

Van Kranendonk[1], and subsequently Morita[5], have shown that for spin $\frac{1}{2}$, the interaction between spin deviations is a two-body interaction. However, this interaction contains a "hard-core repulsive potential" and one has to be careful. In this work, we avoid the difficulties inherent in this singular interaction by defining a binary kernel function.

In their work, Yang and Lee[2] obtain the binary kernel from the exact two-particle solutions of the wave equation. Unfortunately, we have not been able to find a convenient set of solutions for (10) and (11) when $n = 2$.[7] However, in the next section we show that the two-particle solutions of (10) and (11) are not necessary for determining the binary kernel of the lattice gas.

III. THE BINARY KERNEL

In order to determine the binary kernel function B, we require the function U_1 as given in Yang and Lee.[2] In the coordinate representation, the U_1 function is found to be

$$\begin{aligned} U_1(\mathbf{r}_1'; \mathbf{r}_1) &= \sum_{\lambda_1} \varphi_{\lambda_1}(\mathbf{r}_1') \varphi_{\lambda_1}^*(\mathbf{r}_1) \exp(-\beta E_{\lambda_1}) \\ &= N^{-1} \sum_{\lambda_1} \exp[i\lambda_1 \cdot (\mathbf{r}_1' - \mathbf{r}_1) - \beta E_{\lambda_1}], \end{aligned} \tag{13}$$

where $\beta = (kT)^{-1}$, and use is made of (12). It is clear that U_1 can also be expressed as

$$U_1(\mathbf{r}_1'; \mathbf{r}_1) = \langle \mathbf{r}_1' | \exp(-\beta H) | \mathbf{r}_1 \rangle. \tag{14}$$

The binary kernel function is obtained by decomposing Yang and Lee's W_2^S function[2] into a sum of terms containing only the functions U_1 and B. In the coordinate representation, we find W_2^S to be given by

$$\begin{aligned} &W_2^S(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2) \\ &\quad = 2 \sum_i \varphi_i(\mathbf{r}_1'\mathbf{r}_2') \varphi_i^*(\mathbf{r}_1\mathbf{r}_2) \exp(-\beta E_i), \end{aligned} \tag{15}$$

where $\{\varphi_i\}$ is a complete orthonormal set of two-particle eigenfunctions of (10) and (11) with eigenvalues $\{E_i\}$. It is clear that W_2^S can also be written as

$$W_2^S(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2) = \langle \mathbf{r}_1'\mathbf{r}_2' | \exp(-\beta H) | \mathbf{r}_1\mathbf{r}_2 \rangle. \tag{16}$$

For the purpose of decomposing (16) we see that the states $\{|\mathbf{r}_1\mathbf{r}_2\rangle\}$ and the operators $S_{\mathbf{r}_1}^-$, $S_{\mathbf{r}_1}^+$ are rather inconvenient. That is, to decompose (16) in the manner of Yang and Lee, we must separate

[7] In Sec. III, we discuss the two-particle functions Dyson obtains in reference 3.

the free-particle motion in W_2^S from the interaction; however, as seen by the commutation relations (2), the operators $S_{\mathbf{r}_1}^-$, $S_{\mathbf{r}_1}^+$ and thus the states $\{|\mathbf{r}_1\mathbf{r}_2\rangle\}$, implicitly contain a portion of the interaction (the "hard core" part). For this reason, we introduce the Holstein and Primakoff "spin deviation" operators[8] as modified by Kubo.[9] These operators $a_{\mathbf{r}_1}^*$, $a_{\mathbf{r}_1}$ satisfy the usual relations for boson operators

$$[a_{\mathbf{r}_1}, a_{\mathbf{r}_2}] = [a_{\mathbf{r}_1}^*, a_{\mathbf{r}_2}^*] = 0,$$
$$[a_{\mathbf{r}_1}, a_{\mathbf{r}_2}^*] = \delta_{\mathbf{r}_1,\mathbf{r}_2}; \qquad a_{\mathbf{r}_1}|0\rangle = 0, \tag{17}$$

and under certain conditions are related to $S_{\mathbf{r}_1}^-$, $S_{\mathbf{r}_1}^+$ by

$$S_{\mathbf{r}_1}^+ = [1 - a_{\mathbf{r}_1}^* a_{\mathbf{r}_1}]a_{\mathbf{r}_1},$$
$$S_{\mathbf{r}_1}^- = a_{\mathbf{r}_1}^*[1 - a_{\mathbf{r}_1}^* a_{\mathbf{r}_1}]. \tag{18}$$

The conditions under which (18) applies are (i) the operator $S_{\mathbf{r}_1}^+$ acts only on states which contain at most two spin deviations, and (ii) the operator $S_{\mathbf{r}_1}^-$ acts only on states which contain at most one spin deviation. From (7) and (9) we see that these conditions are in fact satisfied in (16).

Substituting (18) into (16), and eliminating several terms which obviously vanish, we obtain

$$W_2^S(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2) = (\mathbf{r}_1'\mathbf{r}_2' |[\exp(-\beta H_2) - (2J\gamma_0)^{-1}h_3]|\, \mathbf{r}_1\mathbf{r}_2), \tag{19}$$

where

$$H_2 = \sum_{i=1}^{6} h_i, \qquad h_3 = -J \sum_{\mathbf{r}_1,\Delta} a_{\mathbf{r}_1}^* a_{\mathbf{r}_1}^* a_{\mathbf{r}_1} a_{\mathbf{r}_1},$$
$$h_1 = J \sum_{\mathbf{r}_1,\Delta} a_{\mathbf{r}_1}^* a_{\mathbf{r}_1}, \qquad h_4 = J \sum_{\mathbf{r}_1,\Delta} a_{\mathbf{r}_1}^* a_{\mathbf{r}_1}^* a_{\mathbf{r}_1} a_{\mathbf{r}_1+\Delta},$$
$$h_2 = -J \sum_{\mathbf{r}_1,\Delta} a_{\mathbf{r}_1+\Delta}^* a_{\mathbf{r}_1}, \qquad h_5 = J \sum_{\mathbf{r}_1,\Delta} a_{\mathbf{r}_1+\Delta}^* a_{\mathbf{r}_1}^* a_{\mathbf{r}_1} a_{\mathbf{r}_1},$$
$$h_6 = -J \sum_{\mathbf{r}_1,\Delta} a_{\mathbf{r}_1+\Delta}^* a_{\mathbf{r}_1}^* a_{\mathbf{r}_1+\Delta} a_{\mathbf{r}_1}. \tag{20}$$

and the states $\{|\mathbf{r}_1\mathbf{r}_2)\}$ are the two-particle states generated by the operators of (17), i.e. $\{|\mathbf{r}_1\mathbf{r}_2) = a_{\mathbf{r}_1}^* a_{\mathbf{r}_2}^*|0)\}$.

It is not difficult to convince oneself that, in the space of one- and two-particle states generated by the operators of (17),

$$H_0 = h_1 + h_2 \tag{21}$$

behaves like the free-particle Hamiltonian operator. That is, one can readily show that

$$(\mathbf{r}_1' |\exp(-\beta H_0)|\, \mathbf{r}_1) = U_1(\mathbf{r}_1'; \mathbf{r}_1), \tag{22}$$

and

$$(\mathbf{r}_1'\mathbf{r}_2' |\exp(-\beta H_0)|\, \mathbf{r}_1\mathbf{r}_2) = U_1(\mathbf{r}_1'; \mathbf{r}_1)U_1(\mathbf{r}_2'; \mathbf{r}_2) + U_1(\mathbf{r}_1'; \mathbf{r}_2)U_1(\mathbf{r}_2'; \mathbf{r}_1), \tag{23}$$

where one recognizes the right hand side of (23) as being equivalent to W_2^S for noninteracting particles.

The function $U_2(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2)$, as given by Yang and Lee, is one half the difference of (19) and (23). That is,

$$U_2(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2) = \tfrac{1}{2}(\mathbf{r}_1'\mathbf{r}_2' |[\exp(-\beta H_2) - \exp(-\beta H_0) - (2J\gamma_0)^{-1}h_3]|\, \mathbf{r}_1\mathbf{r}_2). \tag{24}$$

Finally, the binary kernel B is obtained by inserting the operator $(H_0 + \partial/\partial\beta + \delta(\beta))$ immediately preceding the square bracket in (24). We thus obtain

$$B(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2) = -\tfrac{1}{2}\left(\mathbf{r}_1'\mathbf{r}_2' \left|\left\{\sum_{i=3}^{6} h_i \exp(-\beta H_2) - (2J\gamma_0)^{-1}h_3[h_1 + h_2 + \delta(\beta)]\right\}\right| \mathbf{r}_1\mathbf{r}_2\right). \tag{25}$$

We can simplify (25) by observing that the relations

$$H_2 h_3 = 0;$$
$$(4J\gamma_0)^{-1}\left(\sum_{i=3}^{6} h_i\right)(h_1 + h_3) = h_4 + h_6,$$
$$\exp(-\beta H_2) = (4J\gamma_0)^{-1}\{(h_1 + h_3) \times \exp[-\beta(H_2 - h_3 - h_4)] - h_3\}, \tag{26}$$

are valid in the two-particle space generated by the operators of (17). Combining (25) and (26) we obtain

$$B(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2) = -\tfrac{1}{2}(\mathbf{r}_1'\mathbf{r}_2' |\{H'^* \exp[-\beta(H_0 + H')] - (2J\gamma_0)^{-1}\delta(\beta)h_3\}|\, \mathbf{r}_1\mathbf{r}_2), \tag{27}$$

where

$$H' = h_5 + h_6. \tag{28}$$

At this point we wish to emphasize that (27) was derived without any approximation and that the entire interaction between two spin deviations is found in (27).

Let us now examine the binary kernel function one obtains if Dyson's two-particle functions are used in place of the two-particle wavefunctions of (10) and (11). Dyson's two-particle functions are solutions of (10) and, in place of (11), the following equation:

$$\sum_{\mathbf{r}} \{\langle \mathbf{r}_1' |H|\, \mathbf{r}_1\rangle \delta_{\mathbf{r}_1',\mathbf{r}_2} + \langle \mathbf{r}_1' |H|\, \mathbf{r}_2\rangle \delta_{\mathbf{r}_1',\mathbf{r}_1}\} \times \varphi_l(\mathbf{r}_1\mathbf{r}_2) = E_l\varphi_l(\mathbf{r}_1'\mathbf{r}_2'). \tag{29}$$

[8] T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).
[9] R. Kubo, Phys. Rev. **87**, 568 (1952).

In Dyson's work, the scattering solutions of (10) and (29) in the low-energy limit are the only ones obtained. It is a simple matter, though, to determine the binary kernel when (10) and (29) are used with (15). One obtains

$$B_D(\mathbf{r}_1'\mathbf{r}_2'; \mathbf{r}_1\mathbf{r}_2) = -\tfrac{1}{2}(\mathbf{r}_1'\mathbf{r}_2' \,|H' \exp[-\beta(H_0 + H')]|\, \mathbf{r}_1\mathbf{r}_2), \quad (30)$$

where we note that H' has the same form as Dyson's dynamical interaction operator. By replacing (11) with (29), we have, in Dyson's terminology, neglected the kinematical interaction, and (27) differs from (30) in that the former contains the kinematical interaction while the latter does not. To be more precise, the last term in (27) comes about as a direct consequence of (11) and the difference between (30), and the first term of (27)[10] is due to the fact that though the dynamical interaction is the only contributing part of the spin deviation interaction in an ideal scattering process,[11] the binary kernel is not restricted to just these processes.

In the next section we show how the binary kernel of (27) can be used to calculate the low-temperature spontaneous magnetization and we find that the results are in agreement with those of Dyson.

IV. LOW-TEMPERATURE SPONTANEOUS MAGNETIZATION

Yang and Lee have developed[2] general cluster expansions for the thermodynamic properties of a system of interacting particles in terms of the binary kernel function. In this section we give an example of how these general relations can be applied to the spin-deviation lattice gas. That is, we will use the cluster expansion for the density of particles, given by Yang and Lee, to determine the spontaneous magnetization of the spin deviation system in the asymptotic limit of zero temperature.

The magnetization M is related to the density of spin deviations ρ by[1]

$$M = \mu(1 - 2\rho). \quad (31)$$

From Yang and Lee we find ρ to be given by

$$\rho = \sum_{\lambda_1} [m(\lambda_1) - 1] + \sum_{\lambda_1,\lambda_2} \gamma_2^S(\lambda_1\lambda_2; \lambda_1\lambda_2) \times [m(\lambda_1)]^2 m(\lambda_2) + \cdots, \quad (32)$$

when the fugacity $\mathfrak{z}$ is unity; $\mathfrak{z} = 1$ for the spin-deviation lattice gas corresponds to a vanishing external field. The function $m(\lambda_1)$, readily obtained from the Fourier transform of (13), is given by

$$m(\lambda_1) = [1 - \exp(-\beta E_{\lambda_1})]^{-1}. \quad (33)$$

The remaining functions in (32), γ_n^S with n assuming integer values greater than one, may be expressed in terms of U_1 and B, i.e. (13) and (27).

Since (32) contains an infinite number of terms, one must have some means of selecting the dominant terms in (32) for any practical calculation. The selection method we employ follows naturally from the fact that at low temperature the spin-deviation lattice gas is quite dilute. That is, at low temperature one expects the "importance" of the different terms in (32) to be inversely proportional to the number of binary kernel factors.

We now present the results of calculating ρ in ascending powers of the binary kernel function (27).[12] The zeroth-order contribution comes from those terms of (32) which do not contain any γ_n^S factor; this contribution, when evaluated in the usual low-temperature manner, is

$$\zeta(\tfrac{3}{2})\theta^{3/2} + \tfrac{3}{4}\pi\zeta(\tfrac{5}{2})\theta^{5/2} + \tfrac{3}{32}\pi^2\zeta(\tfrac{7}{2})\theta^{7/2} + O(\theta^{9/2}), \quad (34)$$

where $\theta = (4\pi J\beta)^{-1}$ and $\zeta(n)$ is the Riemann zeta function. (34) is readily recognized as the usual result for noninteracting spin deviations. The contribution due to those terms which contain only one binary kernel factor is found to be

$$2\{1 - \zeta(\tfrac{3}{2})\zeta(\tfrac{1}{2})\}\theta^3 - \{3\pi Q\zeta(\tfrac{5}{2})\zeta(\tfrac{3}{2}) + \zeta(\tfrac{1}{2})\zeta(\tfrac{5}{2}) + [\zeta(\tfrac{3}{2})]^2\}\theta^4 + O(\theta^{9/2}), \quad (35)$$

where Q is the numerical coefficient Dyson defines for a simple cubic lattice and spin $\frac{1}{2}$.[4] The next contribution, due to terms containing two binary kernel factors, is

$$2\{\zeta(\tfrac{3}{2})\zeta(\tfrac{1}{2}) - 1\}\theta^3 + \{\zeta(\tfrac{1}{2})\zeta(\tfrac{5}{2}) + [\zeta(\tfrac{3}{2})]^2\}\theta^4 + O(\theta^{9/2}). \quad (36)$$

Finally, the terms containing three binary kernel factors are found to be of order $\theta^{9/2}$ and thus, all higher-order terms are taken to be at least of order $\theta^{9/2}$. Therefore from (35) and (36) we find the total contribution to (32) due to spin-deviation interactions to be

$$-3\pi Q\zeta(\tfrac{5}{2})\zeta(\tfrac{3}{2})\theta^4 + O(\theta^{9/2}). \quad (37)$$

If (34) and (37) are combined with (31), we obtain precisely Dyson's result for the spontaneous

[10] The operator H' is non-Hermitian.

[11] See Sec. 3 of reference 3.

[12] For detailed calculations, see N. I. Greenberg, Tech. Rept. No. 222(1961), Physics Dept., University of Maryland, College Park, Maryland.

magnetization. Thus, we have established that Van Kranendonk's approach is useful in the low-temperature region and have added further confirmation to Dyson's conclusion that his kinematical interaction may be neglected in the asymptotic limit of zero temperature.

In evaluating (32) we have used the binary kernel as given in (27). Since our results are the same as Dyson's, it is clear that if we were to use (30) for the binary kernel, our results would still be the same. In fact it is obvious that once the kinematical interaction is eliminated from Dyson's cluster expansion [Eq. (156) of reference 3], one obtains essentially the binary kernel formulation with (30) as the binary kernel.

V. HIGHER TEMPERATURES

So far, we have discussed the application of the binary kernel formulation in the low-temperature region only. At higher temperatures, though the concept of a spin-deviation gas is certainly well defined, we have thus far been unable to utilize the binary kernel formulation. Our difficulty lies in the fact that the binary kernel as given in (27) is in a very awkward form for evaluating cluster expansion terms which contain a large number of binary kernel factors—such terms being obviously important at higher temperature. We feel, therefore, that a simpler form of the binary kernel must be obtained if this formulation is to be useful at higher temperatures.

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On a New Method in the Theory of Irreversible Processes*

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A new method is presented for obtaining irreversible equations describing the approach to equilibrium in systems of many particles. The basic idea is the removal of secular terms arising in a perturbation expansion by the technique used in nonlinear mechanics. The irreversible equations then appear as consistency conditions for the existence of a well behaved expansion. The method relies heavily on the existence of the natural fine-scale mixing occurring in the dynamics.

I. INTRODUCTION

In recent years much work has been devoted to the problem of obtaining equations which describe the approach to thermal equilibrium in systems of many particles. In particular, the most comprehensive of the theories presented in the past are those of Bogoliubov[1] and of Prigogine and Balescu[2,3,4] which yield kinetic equations like the Boltzmann or Fokker–Planck equations. The starting point of the Bogoliubov theory is the hierarchy of equations describing the time evolution of the one-, two-, $\cdots$ s-particle distribution functions, which is obtained from the Liouville equation by integration over part of the complete phase space. To obtain kinetic equations from the hierarchy, Bogoliubov assumes that after a time which is longer than the duration of a single collision, but short compared to the time between successive collisions, the s-particle distributions become functionals of the one-particle distribution. In the present method, we show that this relation follows from the dynamics for a certain class of initial conditions and need not be assumed. The Prigogine–Balescu theory, on the other hand, works directly with the Liouville equation whose solution is obtained by using diagrams and their topological properties. Their theory is intrinsically more complicated than the present one since it deals with much more information than is contained in the first few equations of the hierarchy.

The method presented here is similar in spirit to that of reference 1. Its basis lies in two perturbation procedures performed on the equations of the hierarchy. The first is common to all of these methods and consists of passing to the limit of large volume and many particles, keeping the spatial density in the system finite. The second expansion is peculiar to the characteristics of the interparticle potential and magnitude of the particle density, and will thus differ depending on whether the forces are long range, short range, etc. The latter perturbation expansion is not a straightforward one however, in that we demand that it hold for long times. Indeed, Bogoliubov has already demonstrated[1] that a naive expansion in a small parameter performed on the equations of the hierarchy will lead to terms growing like t in the time development of the system. This clearly indicates that a more sophisticated expansion must be used which avoids such secular behavior. Techniques for constructing expansions which avoid secular behavior in nonlinear periodic systems have been developed by van der Pol[5] and Bogoliubov and Krylov.[6] The method presented here is a generalization of this technique to systems which are not periodic in the lowest order of the expansion.

It will be seen that a characteristic feature of the method is its reliance on the fine scale or phase mixing which occurs naturally when we follow the dynamical development of the system. It is essentially this characteristic which allows information to be lost and thus yield irreversible behavior. A further point which has been emphasized by Sandri[7] and investigated in detail by him, is the description of the time development of systems which do not exhibit a kinetic regime after sufficiently long times. Thus it is possible to specify

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[1] N. Bogoliubov, *Problems of a Dynamical Theory in Statistical Physics*, Moscow, 1946, (Translated by E. K. Gora, AFCRC-TR-59-235).

[2] I. Prigogine and R. Balescu, Physica **25**, 281, (1959).

[3] I. Prigogine and R. Balescu, Physica **25**, 302, (1959).

[4] I. Prigogine and R. Balescu, Physica **26**, 145, (1960).

[5] A. Andronow and S. Chaikin, *Theory of Oscillations*, (Moscow, 1937).

[6] N. Krylov and N. Bogoliubov, *Introduction to Nonlinear Mechanics*, (Kiev, 1937).

[7] G. Sandri, (to be published).

exactly, the class of initial conditions for which a Boltzmann or Fokker–Planck equation results.

To demonstrate the theory, we apply it in this paper to a classical, weakly coupled system. We treat both the spatially homogeneous and inhomogeneous cases.

II. THE EQUATIONS OF THE HIERARCHY

We assume a classical system of N identical particles of mass m in a volume V interacting with a two-body potential energy ϕ. The Liouville equation governing the time evolution of the N-particle distribution function $f_N(\mathbf{x}_1 \cdots \mathbf{x}_N, \mathbf{v}_1, \cdots \mathbf{v}_N, t)$ is

$$\left[\frac{\partial}{\partial t} + \sum_{i=1}^{N} \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} - \frac{1}{m} \sum_{i \neq j=1}^{N} \frac{\partial \phi(\mathbf{x}_i - \mathbf{x}_j)}{\partial \mathbf{x}_i} \cdot \frac{\partial}{\partial \mathbf{v}_i}\right] f_N = 0. \tag{1}$$

We assume the normalization

$$\int f_N \prod_{i=1}^{N} d\mathbf{x}_i \, d\mathbf{v}_i = 1, \tag{2}$$

and that f_N is symmetric under interchange of the coordinates and velocities of any two particles. Reduced distribution functions are introduced[1] by defining

$$f_s(\mathbf{x}_1 \cdots \mathbf{x}_s, \mathbf{v}_1, \cdots \mathbf{v}_s, t) = V^s \int \prod_{i=s+1}^{N} d\mathbf{x}_i \, d\mathbf{v}_i \, f_N. \tag{3}$$

Upon integrating out $(N - s)$ variables in Eq. (1) and using Eq. (3), we obtain

$$\left[\frac{\partial}{\partial t} + \sum_{i=1}^{s} \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} - \frac{1}{m} \sum_{i \neq j=1}^{s} \frac{\partial \phi(\mathbf{x}_i - \mathbf{x}_j)}{\partial \mathbf{x}_i} \cdot \frac{\partial}{\partial \mathbf{v}_i}\right] f_s$$

$$= \frac{(N - s)}{mV} \int d\mathbf{x}_{s+1} \, d\mathbf{v}_{s+1} \sum_{i=1}^{s} \frac{\partial \phi(\mathbf{x}_i - \mathbf{x}_{s+1})}{\partial \mathbf{x}_i} \cdot \frac{\partial f_{s+1}}{\partial \mathbf{v}_i},$$

$$s = 1, 2, \cdots N. \tag{4}$$

This is the familiar B-B-G-K-Y hierarchy.

In the following, we pay particular attention to the equations for $s = 1$ and 2. These are

$$\frac{\partial f_1}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} = \frac{(N - 1)}{mV} \int d\mathbf{x}_2 \, d\mathbf{v}_2 \frac{\partial \phi}{\partial \mathbf{x}_1} \cdot \frac{\partial f_2}{\partial \mathbf{v}_1}, \tag{5}$$

and

$$\left[\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial}{\partial \mathbf{x}_1} + \mathbf{v}_2 \cdot \frac{\partial}{\partial \mathbf{x}_2} - \frac{1}{m} \frac{\partial \phi}{\partial \mathbf{x}_1} \cdot \frac{\partial}{\partial \mathbf{v}_1} - \frac{1}{m} \frac{\partial \phi}{\partial \mathbf{x}_2} \cdot \frac{\partial}{\partial \mathbf{v}_2}\right] f_2$$

$$= \frac{(N - 2)}{mV} \int d\mathbf{x}_3 \, d\mathbf{v}_3 \left[\frac{\partial \phi}{\partial \mathbf{x}_1} \cdot \frac{\partial f_3}{\partial \mathbf{v}_1} + \frac{\partial \phi}{\partial \mathbf{x}_2} \cdot \frac{\partial f_3}{\partial \mathbf{v}_2}\right]. \tag{6}$$

In addition, Eqs. (2) and (3) imply the relations

$$1 = \frac{1}{V} \int d\mathbf{x}_1 \, d\mathbf{v}_1 \, f_1, \tag{7}$$

and

$$f_1 = \frac{1}{V} \int d\mathbf{x}_2 \, d\mathbf{v}_2 \, f_2. \tag{8}$$

At this point it is convenient to crudely estimate the orders of magnitude of the various terms in Eqs. (5) and (6). We therefore define the following quantities:

r_0 — the range of the potential;
$\langle \phi \rangle$ — the characteristic strength of the potential;
v_{av} — the average particle velocity;
L — the characteristic scale length for macroscopic spatial gradients;
τ — a characteristic time scale for the system.

With these definitions and the use of Eq. (8), the ratios of the terms in Eq. (5) are found to be

$$1 : \frac{v_{\text{av}}\tau}{L} : (N - 1)\left(\frac{r_0^3}{V}\right)\left(\frac{\langle \phi \rangle}{m v_{\text{av}}^2}\right)\left(\frac{v_{\text{av}}\tau}{r_0}\right), \tag{9}$$

while Eq. (6) yields

$$1 : \frac{v_{\text{av}}\tau}{r_0} : \frac{v_{\text{av}}\tau}{L} : \left(\frac{\langle \phi \rangle}{m v_{\text{av}}^2}\right)\left(\frac{v_{\text{av}}\tau}{r_0}\right) :$$

$$(N - 2)\left(\frac{r_0^3}{V}\right)\left(\frac{\langle \phi \rangle}{m v_{\text{av}}^2}\right)\left(\frac{v_{\text{av}}\tau}{r_0}\right). \tag{10}$$

In obtaining Eq. (10), we introduced the relative and center-of-mass coordinates to give the estimates of the second and third terms. It is easily seen that the order-of-magnitude estimates involved in the s-particle equation follow closely from those of Eq. (10).

We now specify in detail the first of the expansions we use. We let N and $V \to \infty$ in such a way that the average density $N/V = n$ remains finite. If we introduce a formal dimensionless expansion parameter $\lambda \ll 1$, we assume that $N = 1/\lambda$ and $r_0^3/V \sim \lambda$. In this limit, the interaction of the system with the boundaries becomes negligible and, in addition, the Poincaré recurrence time of the system tends to infinity. This latter result is a useful product of the expansion since it is necessary that the recurrence time be longer than any time of interest before we can hope to find meaningful time-irreversible equations. In what follows we will be performing expansions in another small parameter, say, ϵ. In order that the characteristic times associated with the expansion in ϵ not be comparable with the recurrence time, we will assume that $\lambda \ll \epsilon$. Below, we will use only the equations which result from the lowest order of the expansion in λ.

After the lowest-order equations in the λ expansion have been obtained, we introduce for convenience the two-, three-, $\cdots$ s-particle correlation functions by means of the definitions

$$f_2(1,2) = f_1(1)f_1(2) + g(1,2), \tag{11}$$

$$f_3(1,2,3) = f_1(1)f_1(2)f_1(3) + f_1(1)g(2,3) + f_1(2)g(1,3), + f_1(3)g(1,2) + h(1,2,3), \quad \text{etc.} \tag{12}$$

Inserting these definitions in Eqs. (5) and (6), after the λ expansion has been carried out, we obtain

$$\frac{\partial f_1}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1}{\partial \mathbf{x}_1} = \frac{n}{m} \int d\mathbf{x}_2\, d\mathbf{v}_2 \frac{\partial \phi}{\partial \mathbf{x}_1} \cdot \left[\frac{\partial f_1(1)}{\partial \mathbf{v}_1} f_1(2) + \frac{\partial g}{\partial \mathbf{v}_1} \right], \tag{13}$$

and

$$\left[\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial}{\partial \mathbf{x}_1} + \mathbf{v}_2 \cdot \frac{\partial}{\partial \mathbf{x}_2} - \frac{1}{m} \frac{\partial \phi}{\partial \mathbf{x}_1} \cdot \frac{\partial}{\partial \mathbf{v}_1} - \frac{1}{m} \frac{\partial \phi}{\partial \mathbf{x}_2} \cdot \frac{\partial}{\partial \mathbf{v}_2} \right] g$$
$$= \frac{1}{m} \frac{\partial \phi}{\partial \mathbf{x}_1} \cdot \frac{\partial f_1(1)}{\partial \mathbf{v}_1} f_1(2) + \frac{1}{m} \frac{\partial \phi}{\partial \mathbf{x}_2} \cdot \frac{\partial f_1(2)}{\partial \mathbf{v}_2} f_1(1)$$
$$+ \frac{n}{m} \int d\mathbf{x}_3\, d\mathbf{v}_3 \left\{ \frac{\partial \phi}{\partial \mathbf{x}_1} \cdot \left[\frac{\partial f_1(1)}{\partial \mathbf{v}_1} g(2,3) + \frac{\partial g(1,2)}{\partial \mathbf{v}_1} f_1(3) + \frac{\partial h(1,2,3)}{\partial \mathbf{v}_1} \right] + \frac{\partial \phi}{\partial \mathbf{x}_2} \cdot \left[\frac{\partial f_1(2)}{\partial \mathbf{v}_2} g(1,3) + \frac{\partial g(1,2)}{\partial \mathbf{v}_2} f_1(3) + \frac{\partial h(1,2,3)}{\partial \mathbf{v}_2} \right] \right\}. \tag{14}$$

III. THE WEAK-COUPLING CASE

In order to proceed with the problem, we must introduce further expansions which decouple the equations of the hierarchy. Among the physical situations to which the equations apply, are three standard cases which have been extensively investigated in the past. These are dilute systems with short-range forces, systems with weak coupling, and systems with long-range forces (plasmas). We will examine here only the weak coupling case since it is analytically the simplest, yet demonstrates all the features of the theory.

We introduce a formal dimensionless expansion parameter $\epsilon \ll 1$ which measures the strength of the potential, i.e. we choose $\epsilon \sim \langle \phi \rangle / m v_{\text{av}}^2$. For this case we can choose $n r_0^3 \sim 1$ since we have in mind a moderately dense gas. There are three characteristic time scales for the system in this limit: $\tau_0 \sim r_0/v_{\text{av}}$, the duration of a collision; $\tau_1 \sim \tau_0/\epsilon^2$, the time between successive collisions; and $\tau_2 \sim L/v_{\text{av}}$, the time for an average particle to cross the macroscopic spatial gradient. To further simplify the discussion we assume, in this section, that $r_0/L \sim \epsilon^4$. This requirement means that the system is so close to spatial homogeneity that departures will be noticeable in fourth order only. We here carry the expansion through third order. Physically, we expect the system to behave quite differently on these various time scales. The expansion exploits this in that it forces the time scales to be widely disparate as far as the ordering in ϵ is concerned.

As Bogoliubov[1] pointed out, if we simply expand the distribution and correlation functions as a power series in ϵ,

$$f_1 = f_1^{(0)} + \epsilon f_1^{(1)} + \epsilon^2 f_1^{(2)} + \cdots$$
$$g = g^{(0)} + \epsilon g^{(1)} + \epsilon^2 g^{(2)} + \cdots, \quad \text{etc.}, \tag{15}$$

and solve the equations of the hierarchy, secular terms will result. If $\tau \sim \tau_0$, then the last term in Eq. (9) and the last two terms in Eq. (10) are of order ϵ compared with the first terms. However, when $\tau \sim \tau_1$, the former terms become of order $1/\epsilon$ and grow without bound. Thus, while a simple power series will describe the evolution of the system for a time comparable to the duration of a collision, the expansion will fail for times comparable to the mean free time between collisions.

We are therefore forced to adopt a different expansion; one which is similar to the procedures[5,6] used in nonlinear mechanics. These methods usually allow a more general time variation in the perturbation functions, but since the domain of definition of the functions has been enlarged, a new condition is needed to determine the additional functional dependence. This condition is merely the requirement that no secular behavior exist.

The method used here then assumes that a solution of the equations can be found in the form

$$f_1 = f_1^{(0)}(t, \epsilon\tau, \epsilon^2\theta, \cdots) + \epsilon f_1^{(1)}(t, \epsilon\tau, \epsilon^2\theta, \cdots), \tag{16}$$

with similar expressions holding for g, h, etc. The variables τ, θ, etc. are related to the original variable t by the simple equations

$$d\tau/dt = 1, \qquad d\theta/dt = 1, \quad \text{etc.} \tag{17}$$

However, the freedom in the solutions of Eqs. (17) afforded by the choice of initial conditions, allows us to treat t, $\epsilon\tau$, $\epsilon^2\theta$, etc. as independent variables in equations such as (16).

We now proceed to expand Eqs. (13) and (14) in ϵ with the above prescription. To lowest order we obtain

$$\partial f_1^{(0)}/\partial t = 0, \tag{18}$$

which simply ensures that $f_1^{(0)}$ does not vary on the short time scale, allowing, however, for a slower variation with time. Eq. (14) to lowest order in ϵ becomes

$$\frac{\partial g^{(0)}}{\partial t} + (\mathbf{v}_1 - \mathbf{v}_2)\cdot\frac{\partial g^{(0)}}{\partial \mathbf{x}} = 0. \tag{19}$$

In obtaining this equation, we have introduced $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$, the relative coordinate, and have neglected the dependence of $g^{(0)}$ on $\mathbf{x}_1 + \mathbf{x}_2$, the center-of-mass coordinate, because of our assumption that $r_0/L \sim \epsilon^4$. Similarly, the equation for $s = 3$ yields

$$\frac{\partial h^{(0)}}{\partial t} + (\mathbf{v}_1 - \mathbf{v}_2)\cdot\frac{\partial h^{(0)}}{\partial \mathbf{x}} + (\mathbf{v}_1 - \mathbf{v}_3)\cdot\frac{\partial h^{(0)}}{\partial \xi} = 0, \tag{20}$$

where $\xi = \mathbf{x}_1 - \mathbf{x}_3$.

In this section we assume that the initial values of all the correlations are zero. Therefore, the only correlations that appear will arise due to interactions. Actually this is a quite reasonable set of initial conditions to choose by virtue of Grad's theorem.[8] This restriction is removed in the next section however.

We therefore obtain from Eqs. (19) and (20),

$$g^{(0)} = 0, \tag{21}$$

$$h^{(0)} = 0. \tag{22}$$

We now proceed to next order and find

$$\frac{\partial f_1^{(1)}}{\partial t} + \frac{\partial f_1^{(0)}(\epsilon\tau)}{\partial(\epsilon\tau)} = \frac{n}{m}\int d\mathbf{x}_2\, d\mathbf{v}_2 \frac{\partial \phi}{\partial \mathbf{x}_1}\cdot\frac{\partial f_1^{(0)}}{\partial \mathbf{v}_1} f_1^{(0)}(\mathbf{v}_2) \tag{23}$$

for the one-particle distribution. The integral on the right-hand side of Eq. (23) vanishes by symmetry and we can thus integrate the left-hand side trivially. For times which are bounded by T/ϵ where T is some finite time, we find

$$f_1^{(1)}(t) = f_1^{(1)}(0) + t\,\partial f_1^{(0)}(\epsilon\tau)/\partial(\epsilon\tau). \tag{24}$$

Thus, in order to prevent secular behavior we must choose

$$\partial f_1^{(0)}(\epsilon\tau)/\partial(\epsilon\tau) = 0, \tag{25}$$

which also yields

$$\partial f_1^{(1)}(t)/\partial t = 0. \tag{26}$$

[8] H. Grad, J. Chem. Phys. **33**, 1342, (1960).

We therefore proceed to next order and obtain

$$\frac{\partial f_1^{(2)}}{\partial t} + \frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)} + \frac{\partial f_1^{(0)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)} = \frac{n}{m}\int d\mathbf{x}_2\, d\mathbf{v}_2 \frac{\partial \phi}{\partial \mathbf{x}_1}\cdot\left[\frac{\partial f_1^{(1)}}{\partial \mathbf{v}_1} f_1^{(0)}(2) + \frac{\partial f_1^{(0)}(1)}{\partial \mathbf{v}_1} f_1^{(1)}(2) + \frac{\partial g^{(1)}}{\partial \mathbf{v}_1}\right], \tag{27}$$

while Eq. (14) expanded to first order gives

$$\frac{\partial g^{(1)}}{\partial t} + (\mathbf{v}_1 - \mathbf{v}_2)\cdot\frac{\partial g^{(1)}}{\partial \mathbf{x}} = \frac{1}{m}\frac{\partial \phi}{\partial \mathbf{x}}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right) f_1^{(0)}(1) f_1^{(0)}(2). \tag{28}$$

Equation (28) is trivially solved by taking Fourier and Laplace transforms to give

$$g^{(1)}(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, p) = \frac{1}{m}\frac{\phi(k) i\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right) f_1^{(0)}(1) f_1^{(0)}(2)}{p[p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)]}, \tag{29}$$

where we have set the initial value of the correlation equal to zero. Upon taking Fourier and Laplace transforms of Eq. (27) we get

$$f_1^{(2)}(p) = \frac{f_1^{(2)}(t=0)}{p} - \frac{1}{p^2}\left[\frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)} + \frac{\partial f_1^{(0)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)}\right] + (2\pi)^3 \frac{n}{m}\int d\mathbf{k}\, \phi(k) i\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{v}_1} \times \int d\mathbf{v}_2 \frac{g^{(1)}(-\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, p)}{p}. \tag{30}$$

We now investigate the behavior of $f_1^{(2)}$ as $t \to \infty$ (again bounded by T/ϵ). We see that upon inverting the Laplace transform, the double pole at $p = 0$ will yield secular behavior. Thus we must use the freedom in $f_1^{(1)}$ and $f_1^{(0)}$ to eliminate such terms. We use the theorem that

$$\lim_{p\to 0} pf(p) = \lim_{t\to\infty} f(t)$$

to obtain the asymptotic behavior and the consistency requirement

$$\frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)} + \frac{\partial f_1^{(0)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)} = (2\pi)^3 \frac{n}{m}\int d\mathbf{k}\, \phi(k) i\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{v}_1} \times \int d\mathbf{v}_2 \lim_{p\to 0} pg^{(1)}(-\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, p). \tag{31}$$

We now use the Dirac relation

$$\lim_{\epsilon\to 0}\frac{1}{x\pm i\epsilon}=\frac{P}{x}\mp i\pi\delta(x) \tag{32}$$

to obtain

$$\frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)}+\frac{\partial f_1^{(0)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)}=8\pi^4\frac{n}{m^2}\int dk\,|\phi(k)|^2\cdot\frac{\partial}{\partial\mathbf{v}_1}\int d\mathbf{v}_2$$
$$\times\left\{\mathbf{k}\cdot\left[\frac{\partial f_1^{(0)}}{\partial\mathbf{v}_1}f_1^0(2)-\frac{\partial f_1^0}{\partial\mathbf{v}_2}f_1^0(1)\right]\delta(\mathbf{k}\cdot\mathbf{v}_1-\mathbf{k}\cdot\mathbf{v}_2)\right\}$$
$$\equiv C[f_1^0(1),f_1^0(2)]. \tag{33}$$

The argument now is similar to that following Eq. (23) and yields

$$\partial f_1^{(1)}(\epsilon\tau)/\partial(\epsilon\tau)=0, \tag{34}$$

and

$$\partial f_1^{(0)}(\epsilon^2\theta)/\partial(\epsilon^2\theta)\equiv C[f_1^0(1),f_1^0(2)]. \tag{35}$$

Equation (35) is, of course, the standard irreversible Fokker–Planck equation and can easily be manipulated into the various forms in which it appears in the literature. We see that it appears essentially as a consistency condition for the existence of a well behaved expansion on the short time scale.

The rest of Eq. (27) then gives the behavior of $f_1^{(2)}$ on the short time scale:

$$\frac{\partial f_1^{(2)}}{\partial t}=i(2\pi)^3\frac{n}{m^2}\int d\mathbf{k}\,|\phi(k)|^2\,\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{v}_1}$$
$$\times\int d\mathbf{v}_2\,\mathbf{k}\cdot\left(\frac{\partial}{\partial\mathbf{v}_1}-\frac{\partial}{\partial\mathbf{v}_2}\right)f_1^0f_1^0$$
$$\times\left[\frac{1-\epsilon^{i\mathbf{k}\cdot(\mathbf{v}_1-\mathbf{v}_2)t}}{\mathbf{k}\cdot(\mathbf{v}_1-\mathbf{v}_2)}-\frac{P}{\mathbf{k}\cdot(\mathbf{v}_1-\mathbf{v}_2)}\right.$$
$$\left.+i\pi\delta(\mathbf{k}\cdot\mathbf{v}_1-\mathbf{k}\cdot\mathbf{v}_2)\right]. \tag{36}$$

As t increases, the terms in the integrand in Eq. (36) tend to cancel. Thus $\partial f_1^{(2)}/\partial t$ tends asymptotically to zero.

To show that the method continues easily to higher order, we have obtained the next-order correction terms for the kinetic equation. This result is given in the Appendix.

IV. THE EFFECT OF INITIAL CORRELATIONS

In the previous section we assumed that all the initial correlations vanished and only correlations due to interactions arose. We now relax this condition and examine the effects of correlations which are externally imposed by choosing nonzero initial conditions. It is clear physically that if the initial conditions lead to correlations which extend over all space or have too many particles in certain velocity groups, thermal equilibrium will not be attained. Mathematically speaking, for initial correlations which are singular enough, the time to reach equilibrium can be made longer than all orders in ϵ.

To lowest order we obtain Eqs. (18), (19), and (20) again which are trivial to solve by Fourier and Laplace transforms. With initial correlations, Eq. (23) is replaced by

$$\frac{\partial f_1^{(1)}}{\partial t}+\frac{\partial f_1^{(0)}(\epsilon\tau)}{\partial(\epsilon\tau)}=\frac{n}{m}\int d\mathbf{x}_2\,d\mathbf{v}_2\,\frac{\partial\phi}{\partial\mathbf{x}_1}\cdot\frac{\partial g^{(0)}}{\partial\mathbf{v}_1}. \tag{37}$$

Using transforms again, Eq. (37) becomes

$$f_1^{(1)}(\mathbf{v}_1,p)=\frac{f_1^{(1)}(\mathbf{v}_1,t=0)}{p}-\frac{1}{p^2}\frac{\partial f_1^{(0)}(\epsilon\tau)}{\partial(\epsilon\tau)}$$
$$+(2\pi)^3\frac{n}{m}\int d\mathbf{k}\,\phi(k)ik\cdot\frac{\partial}{\partial\mathbf{v}_1}$$
$$\times\int d\mathbf{v}_2\,\frac{g^{(0)}(-\mathbf{k},\mathbf{v}_1,\mathbf{v}_2,t=0)}{p[p-i\mathbf{k}\cdot(\mathbf{v}_1-\mathbf{v}_2)]}. \tag{38}$$

It is easy to see from Eq. (38) that if the initial correlation has a delta-function behavior in $\mathbf{k}$ space, corresponding to a correlation with infinite range, the integral term will contribute a double pole in p space and therefore exhibit secular behavior. We therefore must assume that the initial correlation is limited to a finite spatial range. To investigate the asymptotic value of $f_1^{(1)}$, we again multiply by p and take the limit as $p\to 0$ through positive values. It is clear that we must choose

$$\partial f_1^{(0)}(\epsilon\tau)/\partial(\epsilon\tau)=0, \tag{39}$$

and then get

$$f_1^{(1)}(\mathbf{v}_1,t\to\infty)=f_1^{(1)}(\mathbf{v}_1,t=0)$$
$$-i(2\pi)^3\frac{n}{m}\int d\mathbf{k}\phi(k)\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{v}_1}$$
$$\times\int d\mathbf{v}_2\,g^{(0)}(-\mathbf{k},\mathbf{v}_1,\mathbf{v}_2,t=0)$$
$$\times\left[\frac{P}{\mathbf{k}\cdot(\mathbf{v}_1-\mathbf{v}_2)}-i\pi\delta(\mathbf{k}\cdot\mathbf{v}_1-\mathbf{k}\cdot\mathbf{v}_2)\right]. \tag{40}$$

In order that the integral on the right-hand side of Eq. (40) exist, $g^{(0)}$ must be sufficiently well behaved when $\mathbf{v}_1-\mathbf{v}_2\to 0$. A detailed analysis of this problem has been made by Sandri.[7]

To understand the physical meaning of Eq. (40) we first note from Eq. (19) that an initial correlation will vary slowly with time if $\mathbf{k}\cdot(\mathbf{v}_1-\mathbf{v}_2)\sim 0$.

The phase mixing or fine scale mixing of $g^{(0)}$ that occurs due to the integration over $\mathbf{v}_2$ then selects only the long-time persistent part of $g^{(0)}$, since the major contributions to the integral in Eq. (40) arise from the region where $\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2) \approx 0$. A discussion of the phenomenon of fine-scale mixing, including the asymptotic estimation of integrals similar to those appearing in Eq. (40) has been given by van Kampen[9] in connection with the problem of Landau damping of plasma oscillations. The essential point is that information can be lost from the function $g^{(0)}$ due to the integration over $\mathbf{v}_2$.

We now proceed to the next order and obtain

$$\frac{\partial f_1^{(2)}}{\partial t} + \frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)} + \frac{\partial f_1^{(0)}(\epsilon\theta)}{\partial(\epsilon^2\theta)} = \frac{n}{m}\int d\mathbf{x}_2\, d\mathbf{v}_2 \frac{\partial\phi}{\partial\mathbf{x}_1}\cdot\frac{\partial g^{(1)}}{\partial\mathbf{v}_1}, \tag{41}$$

where $g^{(1)}$ satisfies the equation

$$\begin{aligned}
&\frac{\partial g^{(1)}}{\partial t} + \frac{\partial g^{(0)}(\epsilon\tau)}{\partial(\epsilon\tau)} + (\mathbf{v}_1 - \mathbf{v}_2)\cdot\frac{\partial g^{(1)}}{\partial\mathbf{x}} \\
&- \frac{1}{m}\frac{2\phi}{\partial\mathbf{x}}\cdot\left(\frac{\partial}{\partial\mathbf{v}_1} - \frac{\partial}{\partial\mathbf{v}_2}\right)g^{(0)} \\
&= \frac{1}{m}\frac{\partial\phi}{\partial\mathbf{x}}\cdot\left(\frac{\partial}{\partial\mathbf{v}_1} - \frac{\partial}{\partial\mathbf{v}_2}\right)f_1^{(0)}(\mathbf{v}_1)f_1^{(0)}(\mathbf{v}_2) \\
&+ \frac{n}{m}\int d\mathbf{x}_3\, d\mathbf{v}_3 \left\{\frac{\partial\phi}{\partial\mathbf{x}_1}\cdot\left[\frac{\partial f_1^{(0)}}{\partial\mathbf{v}_1} g^{(0)}(2,3) + \frac{\partial h^{(0)}}{\partial\mathbf{v}_1}\right]\right. \\
&\left. + \frac{\partial\phi}{\partial\mathbf{x}_2}\cdot\left[\frac{\partial f_1^{(0)}}{\partial\mathbf{v}_2} g^{(0)}(1,3) + \frac{\partial h^{(0)}}{\partial\mathbf{v}_2}\right]\right\},
\end{aligned} \tag{42}$$

and $h^{(0)}$ satisfies Eq. (20).

Solving Eq. (42) by transforms we obtain

$$\begin{aligned}
g^{(1)}(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, p) &= \frac{g^{(1)}\,\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, t = 0)}{p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)} \\
&- \frac{1}{[p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)]^2}\frac{\partial g^{(0)}(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, t = 0, \epsilon\tau)}{\partial(\epsilon\tau)} \\
&+ \frac{1}{m}\frac{1}{p}\frac{\phi(k)i\mathbf{k}\cdot(\partial/\partial\mathbf{v}_1 - \partial/\partial\mathbf{v}_2)f_1^{(0)}(1)f_1^{(0)}(2)}{[p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)]} \\
&+ \frac{1}{m}\frac{1}{p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)}\int d\mathbf{k}'\,\phi(k')i\mathbf{k}' \\
&\cdot\left(\frac{\partial}{\partial\mathbf{v}_1} - \frac{\partial}{\partial\mathbf{v}_2}\right)\frac{g^{(0)}(\mathbf{k} - \mathbf{k}', \mathbf{v}_1, \mathbf{v}_2, t = 0)}{p + i(\mathbf{k} - \mathbf{k}')\cdot(\mathbf{v}_1 - \mathbf{v}_2)} \\
&+ (2\pi)^3\frac{n}{m}\frac{1}{p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)}\int d\mathbf{v}_3 \\
&\times\left\{\phi(k)i\mathbf{k}\cdot\left[\frac{\partial f_1^{(0)}}{\partial\mathbf{v}_1}\frac{g^{(0)}(-\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, t = 0)}{p - i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)}\right.\right. \\
&\left. - \frac{\partial f_1^{(0)}}{\partial\mathbf{v}_2}\frac{g^{(0)}(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, t = 0)}{p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_3)}\right] + \int d\mathbf{k}'\,\phi(k')i\mathbf{k}' \\
&\cdot\left[\frac{\partial}{\partial\mathbf{v}_1}\frac{h^{(0)}(\mathbf{k}, -\mathbf{k}', \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, t = 0)}{p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2) - i\mathbf{k}'\cdot(\mathbf{v}_1 - \mathbf{v}_3)}\right. \\
&\left.\left. + \frac{\partial}{\partial\mathbf{v}_2}\frac{h^{(0)}(\mathbf{k}' + \mathbf{k}, -\mathbf{k}', \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, t = 0)}{p + i(\mathbf{k}' + \mathbf{k})\cdot(\mathbf{v}_1 - \mathbf{v}_2) - i\mathbf{k}'\cdot(\mathbf{v}_1 - \mathbf{v}_3)}\right]\right\}.
\end{aligned} \tag{43}$$

We now solve Eq. (41) in the form

$$\begin{aligned}
f_1^{(2)}(\mathbf{v}_1, p) &= f_1^{(2)}(\mathbf{v}_1, t = 0) \\
&- \frac{1}{p^2}\left[\frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)} + \frac{\partial f_1^{(0)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)}\right] \\
&+ (2\pi)^3\frac{n}{m}\int d\mathbf{k}\,\phi(k)i\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{v}_1} \\
&\times\int d\mathbf{v}_2\, g^{(1)}\frac{(-\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, p)}{p},
\end{aligned} \tag{44}$$

and again investigate the asymptotic form of $f_1^{(2)}$ as $t \to \infty$. We see that $g^{(1)}$ and $h^{(0)}$ must have both a finite spatial range and regular behavior at the origin in relative velocity space for the phase mixing to take place. As far as the term in $\partial g^{(0)}(\epsilon\tau)/\partial(\epsilon\tau)$ is concerned, due to the presence of the additional free-particle propagator in the denominator, the regularity condition at the origin in velocity space must be strengthened. It is clear that we have the freedom in this expansion to choose $\partial g^{(0)}(\epsilon\tau)/\partial(\epsilon\tau)$ to be zero and thus not require this added strengthening. Under these restrictions then, all the initial correlations phase mix at a sufficient rate so that Eq. (35), the Fokker–Planck equation, again results.

We see therefore that the externally imposed correlations do not prevent the system from evolving through a kinetic stage as long as the information they contain can be lost through phase mixing. The loss of information will always occur when the physically reasonable limitations on the spatial range and velocity-space variation are imposed.

V. THE EFFECT OF SPATIAL INHOMOGENEITIES

The extension of the method outlined above to systems which are spatially inhomogeneous is straightforward. For illustration we will assume that $r_0/L \sim \epsilon^2$. This is equivalent to assuming that f_1 is a function of $\epsilon^2\mathbf{x}_1$ rather than $\epsilon^4\mathbf{x}_1$ as was assumed above. Again, for illustrative purposes, we will assume that the initial correlations vanish.

[9] N. G. Van Kampen, Physica **21**, 949, (1955).

We then find trivially that Eqs. (16)–(26) are unchanged but that Eq. (27) becomes

$$\frac{\partial f_1^{(2)}}{\partial t} + \frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)} + \frac{\partial f_1^{(0)}(\epsilon^2\theta, \epsilon^2\mathbf{x}_1)}{\partial(\epsilon^2\theta)} + \mathbf{v}_1 \cdot \frac{\partial f_1^{(0)}(\epsilon^2\theta, \epsilon^2\mathbf{x}_1)}{\partial(\epsilon^2\mathbf{x}_1)}$$
$$= \frac{n}{m}\int d\mathbf{x}_2\, d\mathbf{v}_2\, \frac{\partial\phi}{\partial\mathbf{x}_1} \cdot \left[\frac{\partial f_1^{(1)}}{\partial\mathbf{v}_1} f_1^0(2) + \frac{\partial f_1^{(0)}(1)}{\partial\mathbf{v}_1} f_1^{(1)}(2) + \frac{\partial g^{(1)}}{\partial\mathbf{v}_1}\right]. \quad (45)$$

We see that the term arising from the spatial inhomogeneity contributes a new secular term and that the arguments following Eq. (27) are only trivially modified. The analogue of Eq. (35) then becomes

$$\frac{\partial f_1^{(0)}(\epsilon^2\theta, \epsilon^2\mathbf{x}_1)}{\partial(\epsilon^2\theta)} + \mathbf{v}_1 \cdot \frac{\partial f_1^{(0)}(\epsilon^2\theta, \epsilon^2\mathbf{x}_1)}{\partial(\epsilon^2\mathbf{x}_1)} = C(f_1^{(0)} f_1^0), \quad (46)$$

where C is the collision operator given in Eq. (35). The functions of $f_1^{(0)}$ appearing in the collision operator are evaluated at $\epsilon^2\mathbf{x}_1$.

It is clear that in this method it is essential to order the ratio r_0/L in ϵ so as to enable the secular terms to be identified and removed.

VI. CONCLUSIONS

We have given a perturbation theoretic solution of the few-particle equations of the B-B-G-K-Y hierarchy for a weak coupling interaction which exhibits irreversible behavior. Further, we have seen that the basic cause of irreversibility as it appears in this method lies in the fine-scale mixing which causes a loss of information contained in the correlations arising from interactions. In addition, if initial correlations are imposed which are suitably restricted in both coordinate and velocity space, their effects will also disappear through fine-scale mixing. Thus it is possible to exactly specify the ensemble initially so that it will pass through a kinetic stage in its time evolution.

It is clear that the particular expansion in ϵ used here rules out a much wider class of dynamical solutions of the hierarchy which exhibit more complicated behavior in their time evolution. In particular, one might expect to find solutions which are non-Markoffian in nature and for which no clear cut distinction between the streaming and kinetic stages exists.

We can now compare our results with those of Bogoliubov. He assumed that the s-body distributions became functionals of the one-body distribution after long times and in addition assumed the somewhat unphysical "streaming" boundary conditions. We see that the solution given here does not need the first assumption and replaces the second by a natural limitation on the initial correlations. In fact the first assumption need not necessarily be true in the presence of irregular initial correlations. Indeed, the method of solution used here corresponds so completely to Bogoliubov's philosophy that it is somewhat surprising that he did not use it.

Comparing our results with those of Prigogine and Balescu, we remark that they only sum the most divergent diagrams or those which lead to secular behavior. We see from above, that in general it is true that isolating the secular terms leads to the kinetic equation.

Finally, it should be mentioned that the method has been applied to the derivation of the Boltzmann equation, the Balescu–Lenard equation[10,11], to the master equation, and to systems with large spatial inhomogeneities. Papers embodying these results are in the course of preparation.

APPENDIX

We here present the calculations to next order in ϵ for the case where the initial correlations vanish. From Section III we have

$$\frac{\partial f_1^{(0)}}{\partial t} = \frac{\partial f_1^{(0)}(\epsilon\tau)}{\partial(\epsilon\tau)} = \frac{\partial f_1^{(1)}}{\partial t} = \frac{\partial f_1^{(1)}(\epsilon\tau)}{\partial(\epsilon\tau)} = g^{(0)} = h^{(0)} = 0. \quad (A1)$$

In addition, we have

$$\frac{\partial f_1^{(2)}}{\partial t} + \frac{\partial f_1^{(0)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)} = \frac{n}{m}\int d\mathbf{x}_2\, d\mathbf{v}_2\, \frac{\partial\phi}{\partial\mathbf{x}_1} \cdot \frac{\partial g^{(1)}}{\partial\mathbf{v}_1}, \quad (A2)$$

$$\frac{\partial g^{(1)}}{\partial t} + (\mathbf{v}_1 - \mathbf{v}_2) \cdot \frac{\partial g^{(1)}}{\partial\mathbf{x}} - \frac{1}{m}\frac{\partial\phi}{\partial\mathbf{x}} \cdot \left(\frac{\partial}{\partial\mathbf{v}_1} - \frac{\partial}{\partial\mathbf{v}_2}\right) f_1^{(0)} f_1^{(0)} = 0. \quad (A3)$$

In the next order we get

$$\frac{\partial f_1^{(3)}}{\partial t} + \frac{\partial f_1^{(2)}(\epsilon\tau)}{\partial(\epsilon\tau)} + \frac{\partial f_1^{(1)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)} + \frac{\partial f_1^{(0)}(\epsilon^3\sigma)}{\partial(\epsilon^3\sigma)} = \frac{n}{m}\int d\mathbf{x}_2\, d\mathbf{v}_2\, \frac{\partial\phi}{\partial\mathbf{x}_1} \cdot \frac{\partial g^{(2)}}{\partial\mathbf{v}_1}. \quad (A4)$$

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[10] R. Balescu, Phys. Fluids **3**, 52, (1960).
[11] A. Lenard, Ann. Phys. **10**, 390 (1960).

Further,

$$\frac{\partial g^{(2)}}{\partial t} + (\mathbf{v}_1 - \mathbf{v}_2)\cdot\frac{\partial g^{(2)}}{\partial \mathbf{x}} - \frac{1}{m}\frac{\partial \phi}{\partial \mathbf{x}}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)g^{(1)}$$

$$- \frac{1}{m}\frac{\partial \phi}{\partial \mathbf{x}}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)[f_1^{(1)}(1)f_1^{(0)}(2) + f_1^{(0)}(1)f_1^{(1)}(2)]$$

$$= \frac{n}{m}\int d\mathbf{x}_3\, d\mathbf{v}_3 \left[\frac{\partial \phi}{\partial \mathbf{x}_1}\cdot\frac{\partial f_1^{(0)}(1)}{\partial \mathbf{v}_1}\, g^{(1)}(2, 3) + \frac{\partial \phi}{\partial \mathbf{x}_2}\cdot\frac{\partial f_1^{(0)}(2)}{\partial \mathbf{v}_2}\, g^{(1)}(1, 3)\right]. \tag{A5}$$

It is easy to see that $h^{(1)}$ satisfies a free-streaming equation like Eq. (20), and therefore $h^{(1)}$ remains zero if initially zero. The solution of Eq. (A5) is

$$g^{(2)}(\mathbf{k}, \mathbf{v}_1, \mathbf{v}_2, p) = \frac{1}{p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_2)}\left\{\frac{1}{m}\frac{\phi(k)i\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)[f_1^{(1)}(1)f_1^{(0)}(2) + f_1^{(0)}(1)f_1^{(1)}(2)]}{p}\right.$$

$$+ \frac{1}{m}\int d\mathbf{k}'\, \phi(k')i\mathbf{k}'\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)\frac{1}{m}\frac{\phi(k - k')i(\mathbf{k} - \mathbf{k}')\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)f_1^{(0)}f_1^{(0)}}{p[p + i(\mathbf{k} - \mathbf{k}')\cdot(\mathbf{v}_1 - \mathbf{v}_2)]}$$

$$- (2\pi)^3\frac{n\phi(k)}{m^2}\left[i\mathbf{k}\cdot\frac{\partial f_1^{(0)}}{\partial \mathbf{v}_1}\int d\mathbf{v}_3\, \frac{\phi(k)i\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_2} - \frac{\partial}{\partial \mathbf{v}_3}\right)f_1^{(0)}(2)f_1^{(0)}(3)}{p[p - i\mathbf{k}\cdot(\mathbf{v}_2 - \mathbf{v}_3)]}\right.$$

$$\left.\left. + i\mathbf{k}\cdot\frac{\partial f_1^{(0)}}{\partial \mathbf{v}_2}\int d\mathbf{v}_3\, \frac{\phi(k)i\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_3}\right)f_1^{(0)}(1)f_1^{(0)}(3)}{p[p + i\mathbf{k}\cdot(\mathbf{v}_1 - \mathbf{v}_3)]}\right]\right\}. \tag{A6}$$

When Eq. (A6) is substituted in (A4), secular terms again arise. We eliminate them in the way prescribed above which yields

$$\partial f_1^{(2)}(\epsilon\tau)/\partial(\epsilon\tau) = 0. \tag{A7}$$

In addition we find

$$\frac{\partial f_1^{(1)}(\epsilon^2\theta)}{\partial(\epsilon^2\theta)} + \frac{\partial f_1^{(0)}(\epsilon^3\sigma)}{\partial(\epsilon^3\sigma)} = (2\pi)^3\frac{n\pi}{m^2}\int d\mathbf{v}_2\int d\mathbf{k}\, |\phi(k)|^2 k\cdot\frac{\partial}{\partial \mathbf{v}_1}$$

$$\times\left\{\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)[f_1^{(1)}(1)f_1^{(0)}(2) + f_1^{(0)}(1)f_1^{(1)}(2)]\delta(\mathbf{k}\cdot\mathbf{v}_1 - \mathbf{k}\cdot\mathbf{v}_2)\right\}$$

$$+ (2\pi)^3\pi\frac{n}{m^3}\int d\mathbf{v}_2\int d\mathbf{k}\, \phi(k)\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{v}_1}\left\{\frac{P}{\mathbf{k}\cdot\mathbf{v}_1 - \mathbf{k}\cdot\mathbf{v}_2}\int d\mathbf{k}'\, \phi(k')\phi(k - k')\right.$$

$$\left.\times\mathbf{k}'\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)\right](\mathbf{k} - \mathbf{k}')\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)f_1^{(0)}f_1^{(0)}\Big]\delta[(\mathbf{k} - \mathbf{k}')\cdot(\mathbf{v}_1 - \mathbf{v}_2)]$$

$$+ \delta(\mathbf{k}\cdot\mathbf{v}_1 - \mathbf{k}\cdot\mathbf{v}_2)\int d\mathbf{k}'\, \phi(k')\phi(k - k')\mathbf{k}'\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)\left[(\mathbf{k} - \mathbf{k})\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)f_1^{(0)}f_1^{(0)}\right]\frac{P}{(\mathbf{k} - \mathbf{k}')\cdot(\mathbf{v}_1 - \mathbf{v}_2)}\Big\}$$

$$- (2\pi)^6\pi\frac{n^2}{m^3}\int d\mathbf{v}_2\int d\mathbf{k}\, |\phi(k)|^3\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{v}_1}$$

$$\times\left[\frac{P}{k\cdot\mathbf{v}_1 - \mathbf{k}\cdot\mathbf{v}_2}\left\{\mathbf{k}\cdot\frac{\partial f_1^{(0)}}{\partial \mathbf{v}_1}\int d\mathbf{v}_3\left[\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_2} - \frac{\partial}{\partial \mathbf{v}_3}\right)f_1^{(0)}(3)f_1^{(0)}(2)\right]\delta(\mathbf{k}\cdot\mathbf{v}_2 - \mathbf{k}\cdot\mathbf{v}_3)\right.\right.$$

$$\left.+ \mathbf{k}\cdot\frac{\partial f_1^{(0)}}{\partial \mathbf{v}_2}\int d\mathbf{v}_3\left[\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_3}\right)f_1^{(0)}(1)f_1^{(0)}(3)\right]\delta(\mathbf{k}\cdot\mathbf{v}_1 - \mathbf{k}\cdot\mathbf{v}_3)\right\}$$

$$+ \delta(\mathbf{k}\cdot\mathbf{v}_1 - \mathbf{k}\cdot\mathbf{v}_2)\left\{-\mathbf{k}\cdot\frac{\partial f_1^{(0)}}{\partial \mathbf{v}_1}\int d\mathbf{v}_3\left[\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_2} - \frac{\partial}{\partial \mathbf{v}_3}\right)f_1^{(0)}(2)f_1^{(0)}(3)\right]\frac{P}{\mathbf{k}\cdot\mathbf{v}_2 - \mathbf{k}\cdot\mathbf{v}_3}\right.$$

$$\left.+ \mathbf{k}\cdot\frac{\partial f_1^{(0)}}{\partial \mathbf{v}_2}\int d\mathbf{v}_3\left[\mathbf{k}\cdot\left(\frac{\partial}{\partial \mathbf{v}_1} - \frac{\partial}{\partial \mathbf{v}_2}\right)f_1^{(0)}(1)f_1^{(0)}(3)\right]\frac{P}{\mathbf{k}\cdot\mathbf{v}_1 - \mathbf{k}\cdot\mathbf{v}_3}\right\}. \tag{A8}$$

It is clear that the first term on the right-hand side of Eq. (A8) is the Fokker–Planck operator again. Thus we may choose to lump $f_1^{(1)}$ in with $f_1^{(0)}$ and regard the rest of (A8) as yielding an equation for $f_1^{(0)}$ which holds on an even longer time scale. Since an H theorem exists for the Fokker–Planck equation without the correction terms, it is clear that (A8) can only modify the rate of approach to equilibrium by an amount of order ϵ.

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Some Properties of the Reduced Density Matrix

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(Received 18 October 1962)

Two conjectures made in a previous paper are proved. A further remark is made concerning the largest eigenvalue of the reduced density matrices.

SOME properties of the reduced density matrix of an N-particle system of fermions or bosons were discussed in a recent paper.[1] Two conjectures were made in that paper concerning the largest eigenvalue of the reduced-density matrices. One of these conjectures has now been proved by Bell.[2] The purpose of this note is to supply a proof of the other conjecture and to make a further remark. For completeness, we repeat here Bell's proof. Both conjectures are restated here as theorems. All notations follow that of reference 1.

Theorem: In a mixture of particles, consider

$$\langle a', b', c' \cdots |\rho_n| a, b, c, \cdots\rangle, \tag{1}$$

where a, b, c are states of bosons or fermions. If the collection of particles in $a, b, c, \cdots >$ contain an odd number or fermions, then the largest eigenvalue of (1) is $\leqq$ a function, independent of N, of the largest eigenvalues of the reduced density matrices

$$\langle a''', b''', \cdots |\rho_m| a'', b'', c'', \cdots\rangle,$$

where a'', b'', c'', $\cdots$ is a subgroup of the particles in (1).

Proof: The following proof is due to Bell. We consider the case of a collection of fermions and take the case $n = 3$. The proof can easily be generalized to more complicated cases involving any value of n and involving a mixture of bosons and fermions.

Let ξ_{123} be the eigenfunction of ρ_3 with the largest eigenvalue λ_3. Clearly ξ_{123} is antisymmetrical in 1, 2 and 3.
Write

$$F = \sum_{123} \xi^*_{123} a_1 a_2 a_3.$$

Then,

$$\lambda_3 = \mathrm{Sp}\, F^\dagger F \rho \leqq \mathrm{Sp}\, (F^\dagger F + F F^\dagger)\rho.$$

Now the anticommutator $F^\dagger F + F F^\dagger$ can be easily computed in terms of products of four or less $a^\dagger$ and a's. It then follows that

$$\lambda_3 \leq 9 \sum_1 \sum_{232'3'} \xi^*_{123}\langle 23 |\rho_2| 2'3'\rangle \xi_{12'3'} - 18 \sum_{12} \sum_{33'} \xi^*_{123}\langle 3 |\rho_1| 3'\rangle \xi_{123'} + 6 \sum_{123} \xi^*_{123}\xi_{123}. \tag{2}$$

Thus,

$$\lambda_3 \leq 9\lambda_2 + 6. \tag{3}$$

Q.E.D.

As stated in reference 1, it follows from this theorem that the basic group must contain a collection of particles forming a boson when taken together as a single unit.

Theorem: There exists numerical constants β_3,

[1] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).
[2] J. S. Bell, Phys. Letters **2**, 116 (1962).

It is clear that the first term on the right-hand side of Eq. (A8) is the Fokker–Planck operator again. Thus we may choose to lump $f_1^{(1)}$ in with $f_1^{(0)}$ and regard the rest of (A8) as yielding an equation for $f_1^{(0)}$ which holds on an even longer time scale. Since an H theorem exists for the Fokker–Planck equation without the correction terms, it is clear that (A8) can only modify the rate of approach to equilibrium by an amount of order ϵ.

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Thus,

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Q.E.D.

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Theorem: There exists numerical constants β_3,

[1] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).
[2] J. S. Bell, Phys. Letters **2**, 116 (1962).

$\beta_4, \cdots$ so that

$$\lambda_n \leq (N)^{\frac{1}{2}n}\beta_n \qquad \text{for} \quad n = \text{even},$$
$$\lambda_n \leq (N)^{\frac{1}{2}(n-1)}\beta_n \quad \text{for} \quad n = \text{odd},$$

for a system of identical fermions.

Proof: (a) From (3) above and[3] theorem 6 of reference 1, we obtain

$$\lambda_3 \leq 9N + 6. \tag{4}$$

(b) Let ξ_{1234} be the eigenfunction of ρ_4 with the largest eigenvalue λ_4. A spectral separation can be made:

$$\langle 1234\ |\rho_4|\ 1'2'3'4'\rangle = \lambda_4\xi_{1234}\xi^*_{1'2'3'4'} + \text{positive semidefinite matrix.} \tag{5}$$

Let $4 = 4' =$ fixed, and regard (5) as a matrix equation with the initial and final states $1'2'3' >$ and <123. The largest eigenvalue of the right-hand side is

$$\geq \lambda_4 \sum_{123} |\xi_{1234}|^2. \tag{6}$$

The left-hand side is

$$A = \text{Sp}\ a_3^\dagger a_2^\dagger a_1^\dagger a_1 a_2 a_3 (a_4 \rho a_4^\dagger).$$

Now $a_4\rho a_4^\dagger$ is a positive definite Hermitian matrix. It is therefore equal to $\rho'\ \text{Sp}\ (a_4\rho a_4^\dagger)$ where ρ' is a density matrix for $N - 1$ particles. Thus,

$$A = [\text{Sp}\ (a_4\rho a_4^\dagger)]\rho_3',$$

where ρ_3' is a reduced density matrix constructed from ρ'. Thus the largest eigenvalue of A [using (4)] is

$$\leq [\text{Sp}\ a_4\rho a_4^\dagger][9(N-1) + 6].$$

Using (6), one obtains

$$\lambda_4 \sum_{123} |\xi_{1234}|^2 \leq 9N[\text{Sp}\ a_4\rho a_4^\dagger].$$

Summation over 4 gives

$$\lambda_4 \leq 9N^2. \tag{7}$$

(c) To find an upper bound for λ_5 we proceed as in step (a) above. Then we find an upper bound for λ_6 by steps similar to (b) above. It is obvious that the theorem follows by induction.

Q.E.D.

[3] Theorem 6 of reference 1 can be generalized to read

$$\lambda_2 \leq [(N')(L' + 2)/(L' + N')] \tag{A}$$

for a system of N fermions in M possible states where $N' = N$ or $(N - 1)$ whichever is even, and $L' = M - N$ or $M - N - 1$, whichever is even. Furthermore, the limit (A) for λ_2 is realizable. It follows that $\lambda_2 \leq [N(M - N + 2)/M] \leq N$.

One may ask, what is the kinematically *attainable* upper bound of the largest eigenvalue of ρ_3, ρ_4, etc. for fixed M and N? This problem has not yet been solved. However, the following speculation seems to be very reasonable. We have seen in reference 1 that to obtain the largest eigenvalue of ρ_2, one constructs a density matrix ρ which describes a pure state with the BCS pairing, i.e. with single-particle states grouped into pairs, each pair never singly occupied. It seems that the largest eigenvalue of ρ_4 is also attained with such a density matrix. Its value is then given by

$$3N(N-2)(M-N+4) \times (M-N+2)M^{-1}(M-2)^{-1}, \tag{8}$$

where we assume both M and N to be even.

More generally, it seems that for a system of N fermions in M states, the largest attainable eigenvalue of ρ_{2l} is

$$\frac{(2l)!}{l!2^l}[N(N-2)\cdots(N-2l+2)] \times [(M-N+2)(M-N+4)\cdots(M-N+2l)] \times [M(M-2)\cdots(M-2l+2)]^{-1}, \tag{9}$$

where M and N are assumed to be even. These large eigenvalues are obtained with the same pure-state density matrix for all values of l, (i.e. the pure-state N-particle wavefunction discussed in reference 1 for the largest eigenvalue of ρ_2; it is a state with BCS pairing).

For the largest *attainable* eigenvalue of ρ_{2l+1}, take a system of N fermions in M states where M and N are both even. Construct a pure N-particle wavefunction with single-particle states 1 and 2 always occupied, and the other M-2 states occupied by N-2 particles in the same manner as that described in reference 1 for maximizing the eigenvalue of ρ_2. The largest eigenvalue of ρ_{2l+1} is then

$$\frac{(2l+1)!}{l!2^l}[(N-2)(N-4)\cdots(N-2l)] \times [(M-N+2)(M-N+4)\cdots(M-N+2l)] \times [(M-2)(M-4)\cdots(M-2l)]^{-1}. \tag{10}$$

It thus seems that for all M, N,

$$\lambda_{2l} \leq \frac{(2l)!}{l!2^l} N^l \left(\frac{M-N+2l}{M}\right)^l, \tag{11}$$

$$\lambda_{2l+1} \leq \frac{(2l+1)!}{l!2^l} N^l \left(\frac{M-N+2l}{M}\right)^l. \tag{12}$$

Equivalence and Antiequivalence of Irreducible Sets of Operators. I. Finite Dimensional Spaces*

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A fundamental problem which arises in determining whether two quantum mechanical systems are essentially identical is whether a unitary or antiunitary transformation exists which maps one set of dynamical variables into another. Since an elementary dynamical system is specified by giving an irreducible set of dynamical variables, we are led to investigate the following problem: Given two irreducible sets of operators with a one-to-one correspondence between them, find the algebraic properties of the two sets which make it possible to infer the existence of a unitary or antiunitary operator relating them. A series of theorems is obtained from such considerations for finite dimensional spaces. It is shown that if the second set of operators contains some of the algebraic properties of the first set, the two sets are related by a similarity transformation. By altering the requirements, this transformation is a unitary transformation. Indications are also given to show how the theorems can be extended to Hilbert spaces. The rigorous statements of the theorems and the proofs will be given in a second paper. Finally, in the Appendix there is given a definition of invariance of elementary quantum-mechanical systems based on the above theorems, giving the same results as Wigner's definition in terms of transition probabilities.

1. INTRODUCTION

IN quantum mechanics one is frequently confronted with the problem of determining whether two dynamical systems are identical. Such a situation occurs when one wishes to determine whether a quantum mechanical system is invariant under a change in frame of reference. If one has a set of dynamical variables referring to the original frame, one can introduce an analogous set associated with the second frame. The two sets of dynamical variables can be interpreted as describing two dynamical systems as viewed from the original frame. If the two dynamical systems are identical, one says that the original dynamical system is invariant under the change of frame of reference.

Whether two dynamical systems are identical or not is basically a matter of proper definition. The definition most frequently used is due to Wigner.[1] He requires transition probabilities given in terms of the first set of dynamical variables equal those given by the second set. His definition leads to the requirement that the second set of dynamical variables must either be unitarily equivalent to the first set, or unitarily equivalent to the set of operators formed by taking the complex conjugates of the operators of the first set.

The present theorems arose out of an attempt to see whether one could infer the existence of such unitary operators by examining the algebraic structure of the sets of dynamical variables. One might think, for example, that if the commutation rules of the second set of dynamical variables were the same as the first set, a unitary operator would exist. It is well known, however, that there are numerous counter-examples. Hence such an algebraic property is not adequate. We will present a set of adequate properties.

We shall now state the basic algebraic theorems, after introducing some notation.

We shall be concerned with two irreducible sets of $n \times n$ matrices. By an irreducible set of $n \times n$ matrices we mean a set for which there is no nontrivial invariant subspace in the n-dimensional carrier space (see reference 2, page 19). We shall denote the two sets by $\{A_\alpha\}$ and $\{B_\alpha\}$, where α goes through a range of values which is the same for both set of matrices. We permit the range of α to be either finite or infinite or even nondenumerable. We regard the matrices of the two sets as having a one-to-one correspondence as indicated by the same subscript.

A finite polynomial in the set of matrices $\{A_\alpha\}$

* This work was done while H. E. Moses was at Geophysics Corporation of America.

[1] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), p. 325 ff.

is defined as a finite sum of ordered products of matrices selected from the set with complex numbers as coefficients, i.e. a polynomial will have the form

$$cI + \sum_i c_i A_i + \sum_{ij} c_{ij} A_i A_j + \cdots ,$$

where c, c_i, c_{ij} $\cdots$ are complex numbers and A_i, A_j $\cdots$ are matrices selected from the set.

We shall denote by $p(A)$, $q(A)$, etc., finite polynomials in the matrices A_α. The matrices $p(B)$, $q(B)$ etc. will be polynomials in the matrices B_α obtained from $p(A)$, $q(A)$, $\cdots$ by replacing the matrices A_α by the corresponding matrices B_α. By $\bar{p}(B)$, $\bar{q}(B)$ $\cdots$ we denote matrices obtained by replacing the scalars in $p(A)$, $q(A)$ by their complex conjugates and the matrices A_α by the corresponding matrices B_α.

By $\bar{B}_\alpha$ we mean the matrix whose elements are the complex conjugates of B_α. A Hermitian adjoint is denoted by a dagger.

Theorem I. Let $\{A_\alpha\}$ and $\{B_\alpha\}$ be two irreducible sets of $n \times n$ matrices which are labeled by the index set $\{\alpha\}$. Then a necessary and sufficient condition for the existence of a nonsingular matrix S such that

$$A_\alpha = SB_\alpha S^{-1},$$

is that $p(A) = 0$ implies $p(B) = 0$ (all p).

Theorem I.* A necessary and sufficient condition that a nonsingular matrix S exists such that

$$A_\alpha = S\bar{B}_\alpha S^{-1},$$

is that $p(A) = 0$, implies $\bar{p}(B) = 0$ (all p).

Theorem II. Let the matrices of the irreducible sets $\{A_\alpha\}$ and $\{B_\alpha\}$ be Hermitian. Then a necessary and sufficient condition for the existence of a unitary matrix U such that

$$A_\alpha = UB_\alpha U^{-1},$$

is that $p(A) = 0$ implies $p(B) = 0$ (all p).

Theorem II.* Let the matrices of the irreducible sets $\{A_\alpha\}$ and $\{B_\alpha\}$ be Hermitian. Then a necessary and sufficient condition for the existence of a unitary matrix U such that

$$A_\alpha = U\bar{B}_\alpha U^{-1},$$

is that $p(A) = 0$ implies $\bar{p}(B) = 0$ (all p).

Let us discuss Theorem I which is the most important of the theorems. Surprisingly, the condition is not symmetric with respect to the irreducible sets of matrices. But a consequence of the theorem is that the condition is indeed symmetric.

For applications, Theorems II and II* are the most interesting. The sets of matrices correspond to the sets of dynamical variables. One can then test to see whether a unitary or antiunitary operator exists which transforms one set into another.

A definition of invariance based on these theorems is given in the Appendix.

2. PROOFS OF THE THEOREMS

We shall now prove Theorem I. Since the necessity is obvious, we shall prove only the sufficiency. The proof depends very heavily on the properties of the irreducible representations of the rotation group.[3] Consider three $n \times n$ matrices s_1, s_2, s_3 which form an irreducible set and which satisfy the following commutation rules.

$$[s_1, s_2] = is_3, \quad [s_3, s_2] = is_1, \quad [s_1, s_2] = is_3. \tag{1}$$

Consider a second set of $n \times n$ matrices which we call t_1, t_2, t_3 which also form an irreducible set and also satisfy (1). Then by the theory of representations of the rotation group, a nonsingular matrix S exists such that

$$s_i = St_iS^{-1}$$

for all i.

The matrices s_i and t_i are spin matrices. We shall use them as a sort of basis in which to express our matrices A_α and B_α. The spin matrices are in a sense the simplest irreducible set of matrices which can be found in an n-dimensional vector space.

Let us take a particular irreducible set of $n \times n$ spin matrices $\{s_i\}$. Since the set $\{A_\alpha\}$ is an irreducible set, each spin matrix can be expressed as a finite polynomial in terms of the set.

$$s_1 = p(A), \qquad s_2 = q(A), \qquad s_3 = r(A). \tag{2}$$

Let us define t_1, t_2, and t_3 by

$$t_1 = p(B), \qquad t_2 = q(B), \qquad t_3 = r(B). \tag{3}$$

We shall now show that the set of matrices $\{t_i\}$ satisfies the spin commutation rules (1). Since the set $\{s_i\}$ were chosen to be the spin matrices we can write

$$\begin{aligned} s_3 &= -i[s_1, s_2] \\ &= v(A), \end{aligned} \tag{4}$$

where $v(A)$ is the polynomial obtained by using (2) for s_1 and s_2. But also from (2),

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[2] H. Weyl, *Classical Groups* (Princeton University Press, Princeton, New Jersey, 1946).

[3] J. S. Lomont, *Applications of Finite Groups* (Academic Press Inc., New York, 1959), p. 149 ff.

$$r(A) = v(A). \tag{5}$$

Now using (3),

$$-i[t_1, t_2] = v(B). \tag{6}$$

By the condition of the theorem,

$$v(B) = r(B). \tag{7}$$

Hence,

$$-i[t_1, t_2] = t_3. \tag{8}$$

That $\{t_i\}$ satisfies the remaining commutation rules is proved similarly. We shall now show that the set $\{t_i\}$ is an irreducible set.

Since the matrices $\{s_i\}$ form an irreducible set, we can express each of the matrices A_α as a polynomial in these matrices:

$$A_\alpha = u_\alpha(s). \tag{9}$$

If we now substitute for s_i the expressions (2) into (9), we obtain

$$A_\alpha = w_\alpha(A). \tag{10}$$

That is, A_α is expressed as a polynomial in $\{A_\alpha\}$.

Let us define

$$M_\alpha = u_\alpha(t), \tag{11}$$

where $u_\alpha(t)$ is obtained from $u_\alpha(s)$ by replacing each s_i by the corresponding t_i.

On using (3), we obtain

$$M_\alpha = w_\alpha(B). \tag{12}$$

But from (11) and the conditions of the theorem, $M_\alpha = B_\alpha$ and hence,

$$B_\alpha = u_\alpha(t). \tag{13}$$

Now if the matrices $\{t_i\}$ are reducible, the matrix which reduced the set $\{t_i\}$ would also reduce the set $\{B_\alpha\}$. But the set $\{B_\alpha\}$ is irreducible. Hence the set $\{t_i\}$ is irreducible. Thus, a nonsingular matrix S exists which transforms the set $\{t_i\}$ into $\{s_i\}$. On using (9) and (13) it is seen that the same matrix S transforms the set $\{B_\alpha\}$ into $\{A_\alpha\}$, which proves the theorem.

Theorem I* follows directly from Theorem I.

Theorem II is proved as follows:

Since the matrices $\{A_\alpha\}$ and $\{B_\alpha\}$ are now assumed to be Hermitian, the equations

$$A_\alpha = SB_\alpha S^{-1}$$

lead to

$$A_\alpha = S^{-1\dagger} B_\alpha S^\dagger$$

on taking Hermitian adjoints. From this it follows

$$B_\alpha S^\dagger S = S^\dagger S B_\alpha.$$

But from Schur's lemma,

$$S^\dagger S = \lambda I,$$

where λ is a scalar. On taking adjoints,

$$S^\dagger S = \bar{\lambda} I.$$

Hence, λ is real. Also, since S is nonsingular, λ is not zero.

Finally, using the fact that the trace of the matrix $S^\dagger S$ is positive definite, it follows that λ is positive. Then the operator U defined by

$$U = S/\lambda^{\frac{1}{2}}$$

satisfies the requirements of the theorem.

Theorem II* is proved easily from Theorem II.

It should be mentioned that the theorems can be proved by more conventional algebraic means. For example, by the conditions of Theorem I, it can be shown that the enveloping matrix algebras of $\{A_\alpha\}$ and $\{B_\alpha\}$ are simple and that one is obtained by an automorphism from the other. Then the existence of S follows from lemma 9.1 A.[2]

3. EXTENSION TO HILBERT SPACES

For applications to quantum mechanics, one would naturally want to extend the results to Hilbert space. It seems possible to proceed in a formal way and get similar results if one ignores the real difficulties of domains of definition and problems of convergence of infinite series. The operators which take the place of the spin operators are the irreducible set P and Q which satisfy

$$[P, Q] = i.$$

In accordance with Von Neumann's theorems, these operators are essentially unique if they are hypermaximal.

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We are grateful to Professor W. Magnus for his criticisms of the theorems.

APPENDIX. RELATED THEOREMS AND A PROPOSED DEFINITION OF INVARIANCE

The Theorems which were given in the previous sections are some of a class of related theorems all of which are proved in the same way. A theorem which is useful for a proposed definition of invariance is the following:

Theorem III. Let $\{A_\alpha\}$ and $\{B_\alpha\}$ be two ir-

reducible sets of Hermitian matrices. Let $p(A)$, $q(A)$, etc. be all the polynomials in $\{A_\alpha\}$ which are Hermitian. Then, necessary and sufficient conditions for the existence of a unitary matrix U such that

$$A_\alpha = UB_\alpha U^{-1},$$

is that (1) $p(B)$, $q(B)$, $\cdots$ also be Hermitian, and (2) if $p(A) = q(A)$, then $p(B) = q(B)$, etc.

*Theorem III**. A necessary and sufficient condition that a unitary operator U exist such that

$$A_\alpha = U\bar{B}_\alpha U^{-1},$$

is that (1) $\bar{p}(B)$, $\bar{q}(B)$, etc. be Hermitian and (2) that $p(A) = q(A)$ implies $\bar{p}(B) = \bar{q}(B)$.

On the basis of these theorems which we also assume to hold in Hilbert space (where polynomials are replaced by more general functions), we give a definition of invariance in terms of operators, which will have the same consequences as Wigner's definition in terms of transition probabilities. We are concerned with the way dynamical variables can be constructed from a given set of dynamical variables. (Incidently, we take the attitude that all hypermaximal operators are dynamical variables for elementary systems which have no superselection rules). We state that one dynamical variable is constructed from a set of dynamical variables in the same way as a second dynamical variable is constructed from the second set of dynamical variables, if the first and second dynamical variables are the same functions of the first and second set, respectively.

We further state that a dynamical variable is constructed in a complex-conjugate manner if the scalars which are involved are replaced by complex conjugates.

Now to our definition: Let us consider two dynamical systems (1) and (2) which are elementary in the sense that there are no superselection rules (for example, systems in which there is no particle creation or destruction). Such dynamical systems are always specified by giving an irreducible set of dynamical variables which we denote by $\{A_\alpha\}$ and $\{B_\alpha\}$ for systems 1 and 2, respectively. We shall say that systems 1 and 2 are identical if the following three requirements are met:

(1) It is possible to select the set $\{B_\alpha\}$ such that there is a one-to-one correspondence with the set $\{A_\alpha\}$.

(2) Let C be any dynamical variable in system (1). Then C can be constructed from the set $\{A_\alpha\}$. Let C' be the operator constructed from the set $\{B_\alpha\}$ in the same way as C is from the set $\{A_\alpha\}$. Let C'' be constructed from $\{B_\alpha\}$ in the complex-conjugate way. Then either the entire set $\{C'\}$ *or* $\{C''\}$ must consist of hypermaximal operators.

(3) For operators C which can be constructed in a second way from $\{A_\alpha\}$, the corresponding operator of the set of hypermaximal operators C' or C'' must be constructed in an analogous second way from $\{B_\alpha\}$.

From *Theorem III and III** (actually the Hilbert-space extensions of these theorems), there is either a unitary or antiunitary operator which transforms all dynamical variables of system 1 into those of system 2.

It might be mentioned that in classical mechanics where we deal only with real functions of scalar dynamical variables, the dynamical variables C' and C'' would be identical and real. Furthermore, there would be only one way to construct C from $\{A_\alpha\}$. Hence, requirements (2) and (3) are quantum mechanical in nature. It is rather interesting to note that we need not make any requirements relative to the spectra of the dynamical variables.

On Strain Energy Functions for Isotropic Elastic Materials*

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This article deals with isotropic elastic materials which possess a strain energy function. For such materials the strain energy of a material point is given, of course, by a symmetric function $\bar{\sigma}$ of the principal stretches v_1, v_2, v_3 at that point. It is known that a *necessary* condition to have an isotropic material compatible with the axioms for thermostatics proposed by Coleman and Noll is that the function $\bar{\sigma}$ be jointly and strictly convex in its three variables v_1, v_2, v_3. Here we show that this condition is *not sufficient* for compatibility with the thermostatic axioms.

INTRODUCTION

IT is the purpose of this note to settle a point in finite elasticity theory. We consider the theory of materials which are perfectly elastic in the sense of Green, i.e. materials for which the strain energy σ is given by a smooth function $\hat{\sigma}$ over the set of all deformation gradients (i.e., all invertible tensors) F.[1] We deliberately ignore the possible dependence of σ on thermodynamic variables, such as the temperature or entropy, and thus σ may be interpreted as either the internal energy or the Helmholtz free energy, per unit mass. We assume, of course, that the function $\hat{\sigma}$ is compatible with the principle of material objectivity, i.e. that

$$\hat{\sigma}(QF) = \hat{\sigma}(F) \tag{1}$$

for all tensors F and all orthogonal tensors Q.

In a recent axiomatization[2] of the thermostatics of continuous media, postulates are made which in our present context are equivalent to the assumption that every stored energy function $\hat{\sigma}$ should obey the following

Fundamental Thermostatic Inequality (FTI): For all pairs of deformation gradients F'', F' such that $F'' \neq F'$ and $F''F'^{-1}$ is positive-definite and symmetric, we have

$$\hat{\sigma}(F'') - \hat{\sigma}(F') - \text{tr}\,[(F'' - F')\hat{\sigma}_F(F')] > 0, \tag{2}$$

where $\hat{\sigma}_F$ is the (tensor-valued) gradient of the (scalar-valued) function $\hat{\sigma}$.

We say that $\hat{\sigma}$ is a strain energy function (relative to an undistorted configuration) of an *isotropic material* if

$$\hat{\sigma}(F) = \hat{\sigma}(FQ) \tag{3}$$

for all invertible tensors F and all orthogonal tensors Q.

Let $F = VR$ be the (unique) left polar decomposition of a deformation gradient tensor F. Here R is an orthogonal tensor, called the *rotation tensor* for F, and V is a symmetric positive-definite tensor called the *left stretch tensor* for F. The proper numbers v_i of V are called the *principal stretches* corresponding to F.

It is a well known result in elasticity theory that a necessary and sufficient condition that $\hat{\sigma}$ be a strain energy function of an isotropic material is that there exist a symmetric function $\bar{\sigma}$ of three positive scalar variables, such that for each deformation gradient F,

$$\hat{\sigma}(F) = \bar{\sigma}(v_1, v_2, v_3). \tag{4}$$

Here v_1, v_2, v_3 are the principal stretches corresponding to F, and $\bar{\sigma}$ is symmetric in the sense that

$$\bar{\sigma}(v_1, v_2, v_3) = \bar{\sigma}(v_{\pi_1}, v_{\pi_2}, v_{\pi_3}), \tag{5}$$

where π_i is any permutation operator over 1, 2, 3.

On page 115 in reference 1, it was pointed out that for an isotropic material, a *necessary* condition that $\hat{\sigma}$ obey the FTI is that the function $\bar{\sigma}(v_1, v_2, v_3)$ of (4) be strictly and jointly convex in the v_1, v_2, v_3, i.e. that

$$\bar{\sigma}(v_1'', v_2'', v_3'') - \bar{\sigma}(v_1', v_2', v_3') - \sum_{i=1}^{3} (v_i'' - v_i') \frac{\partial \bar{\sigma}}{\partial v_i}(v_1', v_2', v_3') > 0, \tag{6}$$

whenever $v_i'' \neq v_i'$ for at least one i. When this result was obtained, it was remarked that it was not known whether or not strict and joint convexity of $\bar{\sigma}$ be a

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[1] We denote scalars by Latin and Greek minuscules and tensors by Latin majuscules. Superimposed hats, $\hat{\sigma}$, and bars, $\bar{\sigma}$, are used to distinguish different functions whose values are the same physical quantity, σ.

[2] B. D. Coleman and W. Noll, Arch. Rational Mech. Anal. 4, 97–128 (1959).

sufficient condition for an isotropic material to obey the FTI. It is this point which we wish to settle here.

SOLUTION BY COUNTER EXAMPLE

We now produce a simple counter example to show that strict and joint convexity of $\bar{\sigma}$ is *not sufficient* for the FTI to hold for isotropic materials.

Continuing to let v_1, v_2, v_3 be the principal stretches corresponding to F, we consider the following particular strain energy function:

$$\hat{\sigma}^*(F) = \bar{\sigma}^*(v_1, v_2, v_3) = \tfrac{1}{2}(v_1^2 + v_2^2 + v_3^2) - \kappa(v_1 + v_2 + v_3); \quad (7)$$

$\hat{\sigma}^*$ obviously defines an isotropic material. Here κ is a real number to be determined later. We note that for any choice of κ, $\bar{\sigma}^*$ is strictly and jointly convex in the v_i for all values of the v_i. (Indeed, independently of κ, the Hessian matrix of the second partial derivatives of $\bar{\sigma}^*$ has, for all v_i, the form

$$\left|\frac{\partial^2 \bar{\sigma}^*}{\partial v_i\, \partial v_j}\right| = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}, \quad (8)$$

and hence is always positive-definite.) We shall now show that there exist values of κ such that $\bar{\sigma}^*$ does not obey the FTI for particular F' and F''.

Let F' be such that the matrix of its components relative to some fixed orthonormal basis $\mathbf{h}^i$, $i = 1, 2, 3$, is given by

$$|F'_{ij}| = \begin{vmatrix} v'_1 & 0 & 0 \\ 0 & v'_2 & 0 \\ 0 & 0 & v'_3 \end{vmatrix}. \quad (9)$$

Let G be such that relative to $\mathbf{h}^i$,

$$|G_{ij}| = \begin{vmatrix} 1 & \lambda & 0 \\ \lambda & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}. \quad (10)$$

The symmetric tensor G is positive-definite and not equal to I whenever $0 < |\lambda| < 1$. We now put

$$F'' = GF', \quad \text{i.e.} \quad F''F'^{-1} = G, \quad (11)$$

and evaluate

$$g(F'', F') = \hat{\sigma}^*(F'') - \hat{\sigma}^*(F') - \operatorname{tr}[(F'' - F')\hat{\sigma}^*_F(F')]. \quad (12)$$

It follows from (1) and (3) that if $\hat{\sigma}$ determines an isotropic material, then for all F and all orthogonal Q,

$$\hat{\sigma}(F) = \hat{\sigma}(QFQ^T); \quad (13)$$

i.e., $\hat{\sigma}$ is an isotropic function. The gradient of an isotropic function is also an isotropic function (albeit of higher tensorial rank). Thus, whenever F is symmetric, $\hat{\sigma}^*_F(F)$ and F have the same proper vectors. We make use of this fact, and Eqs. (7) and (9), to calculate the matrix of the components of $\hat{\sigma}^*_F(F')$ relative to $\mathbf{h}^i$ and find

$$|\hat{\sigma}^*_F(F')_{ij}| = \begin{vmatrix} \dfrac{\partial \bar{\sigma}^*}{\partial v_1} & 0 & 0 \\ 0 & \dfrac{\partial \bar{\sigma}^*}{\partial v_2} & 0 \\ 0 & 0 & \dfrac{\partial \bar{\sigma}^*}{\partial v_3} \end{vmatrix} = \begin{vmatrix} v'_1 - \kappa & 0 & 0 \\ 0 & v'_2 - \kappa & 0 \\ 0 & 0 & v'_3 - \kappa \end{vmatrix}. \quad (14)$$

Equations (9)–(11), and (14) yield, after a direct calculation,

$$\operatorname{tr}[(F'' - F')\hat{\sigma}^*_F(F')] = 0. \quad (15)$$

From Eqs. (12), (15), and (7), we have

$$g(F'', F') = \bar{\sigma}^*(v''_1, v''_2, v''_3) - \bar{\sigma}^*(v'_1, v'_2, v'_3), \quad (16)$$

where the v''_1, v''_2, v''_3, are the principal stretches corresponding to F'', i.e., the proper numbers of V'' in the left polar decomposition

$$V''R'' = F'' = GF'. \quad (17)$$

We now calculate the v''_i. It is evident from (9) and (10) that the rotation R'' in (17) must be such that relative to $\mathbf{h}^i$,

$$|R^T_{ij}| = \begin{vmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{vmatrix}. \quad (18)$$

Hence, since $V'' = GF'R''^T$,

$$|V''_{ij}| = \begin{vmatrix} 1 & \lambda & 0 \\ \lambda & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \begin{vmatrix} v'_1 & 0 & 0 \\ 0 & v'_2 & 0 \\ 0 & 0 & v'_3 \end{vmatrix} \begin{vmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

$$= \begin{vmatrix} v'_1\cos\theta - v'_2\lambda\sin\theta & v'_1\sin\theta + v'_2\lambda\cos\theta & 0 \\ v'_1\lambda\cos\theta - v'_2\sin\theta & v'_1\lambda\sin\theta + v'_2\cos\theta & 0 \\ 0 & 0 & v'_3 \end{vmatrix}. \quad (19)$$

Since $|V''_{ij}|$ is symmetric by definition, it follows

from (19) that

$$\tan \theta = \frac{v_1' - v_2'}{v_1' + v_2'} \lambda. \tag{20}$$

We now consider the characteristic equation

$$\det (V'' - uI) = 0. \tag{21}$$

It follows from (19) and (20) that (21) has the form

$$(u - v_3)[u^2 - 2ua(1 + \lambda^2 b^2)^{\frac{1}{2}} + v_1' v_2' (1 - \lambda^2)] = 0, \tag{22a}$$

where

$$a = \frac{v_1' + v_2'}{2}, \qquad b = \frac{v_1' - v_2'}{v_1' + v_2'}. \tag{22b}$$

Identifying the v_i'' with the roots of (21), we find that

$$v_i'' = a[(1 + \lambda^2 b^2)^{\frac{1}{2}} \pm (b^2 + \lambda^2)^{\frac{1}{2}}], \quad i = 1, 2 \tag{23a}$$

$$v_3'' = v_3', \tag{23b}$$

and

$$g(F'', F') = a\{a\lambda^2(1 + b^2) - 2\kappa[(1 + \lambda^2 b^2)^{\frac{1}{2}} - 1]\}. \tag{24}$$

When $\kappa = 20$, the choice, $v_1' = 3$, $v_2' = 1$, $\lambda = \frac{1}{10}$, v_3' arbitrary, yields, through Eqs. (22b) and (24),

$$g(F'', F') = 0.05 - 80[(1.0025)^{\frac{1}{2}} - 1] < 0. \tag{25}$$

When $\kappa = 1$, which would make the reference state $v_1 = v_2 = v_3 = 1$ a stress-free state, the choice, $v_1' = \frac{3}{20}$, $v_2' = \frac{1}{20}$, $\lambda = \frac{5}{6}$, v_3' arbitrary, yields

$$g(F'', F') = -23/2880 < 0. \tag{26}$$

Thus we construct strain energy functions which do not obey the FTI although they are convex in the principal stretches.

The possibility of finding such a simple counter example was suggested to us by a theory of "convexity curves for the FTI," which one of us (LEB) is to publish soon in the Archive for Rational Mechanics and Analysis.

Note on the Riccati Equation

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A simple modification of a method introduced by R. Bellman is proposed, which under certain circumstances produces both upper and lower bounds for the solution of the Riccati equation. An application to scattering theory is suggested.

I. INTRODUCTION

IN this note we consider the generalized Riccati equation

$$y'(x) + a(x)y^2(x) + b(x)y(x) + c(x) = 0, \qquad y(0) = y, \tag{I.1}$$

for real positive values of the variable x. This equation is of interest *per se*, as it arises in many problems of physical relevance. Moreover, its solution $y(x)$ is connected to the solution $\varphi(x)$ of the linear second-order equation

$$\varphi''(x) + [b(x) - a'(x)/a(x)]\varphi'(x) + c(x)a(x)\varphi(x) = 0, \tag{I.2}$$

through

$$a(x)y(x) = \varphi'(x)/\varphi(x). \tag{I.3}$$

Note that the zeros and poles of $y(x)$ correspond to the zeros of $\varphi'(x)$ and $\varphi(x)$, respectively [assuming $a(x)$ to be nonzero, and $a(x)$, $\varphi'(x)$, and $\varphi(x)$ nonsingular].

An elegant representation for the solution $y(x)$ of Eq. (I.1) has been derived by R. Bellman.[1] In this representation, which holds in the interval from 0 to x provided in this interval $a(x)$ is positive semidefinite and $y(x)$ is continuous, the solution $y(x)$ appears as the *minimum* of an explicitly known functional, namely

$$y(x) = \min_u \left[y_0 \exp\left(-\int_0^x [b(x') + 2a(x')u(x')]\,dx' \right) + \int_0^x [a(x')u^2(x') - c(x')]\,dx' \times \exp\left(-\int_{x'}^x [b(x'') + 2a(x'')u(x'')]\,dx'' \right) \right] \tag{I.4}$$
$$= B[u; x].$$

The minimum is actually achieved for

$$u(x) = y(x). \tag{I.5}$$

This expression may be used to obtain approximate evaluations of $y(x)$, using trial functions $u(x)$ which "resemble" $y(x)$ as much as possible. Upper bounds for $y(x)$ are thus provided as long as one knows that in the interval from 0 to x, $y(x)$ is continuous. Note that the representation Eq. (I.4) implies that, if instead, a divergency occurs in that interval, it is one in which $y(x)$ goes to $-\infty$; or, in other words, any pole in that interval of the positive real axis must have a positive residue. This is also obvious from the differential equation (I.1), remembering the condition $a(x) \geq 0$.

The purpose of the present note is to point out that by means of an elementary modification of Bellman's method, a second representation for the solution $y(x)$ of the Riccati equation can be derived, in which $y(x)$ appears as the *maximum* of an explicitly known functional. This representation is valid in the interval from 0 to x, provided in that interval $c(x)$ is negative semidefinite and $y(x)$ never vanishes. It states

$$y(x) = \max_v \left[\frac{1}{y_0} \exp\left(\int_0^x [b(x') + 2c(x')v(x')]\,dx' \right) + \int_0^x [a(x') - c(x')v^2(x')]\,dx' \times \exp\left(\int_{x'}^x [b(x'') + 2c(x'')v(x'')]\,dx'' \right) \right]^{-1} \tag{I.6}$$
$$= \max C[v; x].$$

The maximum is now achieved for

$$v(x) = 1/y(x). \tag{I.7}$$

The validity of the representation (I.6) also requires that the bracket in the right-hand side (r.h.s.) of Eq. (I.6) does not vanish in the interval from 0 to x.

If $a(x)$ is positive semidefinite, $c(x)$ is negative semidefinite, and y_0 is finite and nonzero, there will

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[1] R. Bellman, Proc. Natl. Acad. Sci. U.S. **41**, 743 (1955).

certainly be an interval from 0 to x in which both representations [Eqs. (I.4) and (I.6)] hold. In fact, both representations hold for all positive x's if y_0 is positive, because they imply that $y(x)$ is positive definite and bounded.[2] They can therefore be used to evaluate $y(x)$ and lead to the statement that its value falls within a definite interval, and the smaller that interval, the better the trial functions approximate the solution $y(x)$. Such controlled approximations are obviously of great value to the physicist. Also, if y_0 is negative and $y(x)$ has a pole on the real axis, the functional $C[v; x]$ may be used to locate the position x_p of the pole, through the relation

$$x_p = \max_v X[v], \tag{I.8}$$

where the functional $X[v]$ is defined by

$$\begin{aligned} \{C[v; X]\}^{-1} &= 0 \\ C[v; x] &< 0 \quad \text{for} \quad 0 \leq x < X. \end{aligned} \tag{I.9}$$

The maximum in Eq. (I.8) above is achieved for $v(x) = 1/y(x)$. This method thus provides, through the transformation Eq. (I.3), a lower bound on the position of the zero, if any, of the solution of a second-order linear differential equation, whose coefficients satisfy the previously stated conditions.

In the next section, Bellman's derivation of the representation (I.4) is recalled, and the modification necessary to derive the representation (I.6) is introduced. In the last section, an application to scattering theory is proposed.

In the following we will generally assume that $a(x)$ and $c(x)$ are semidefinite, positive and negative respectively. This limitation, however, is less restrictive than it might appear, due to the possibility of transforming the coefficients of the Riccati equation. In fact, the function $Y(x)$, connected to the original function $y(x)$ through

$$\begin{aligned} Y(x) &= (p(x) + q(x)y(x))(r(x) + s(x)y(x))^{-1} \\ y(x) &= -(p(x) - r(x)Y(x))(q(x) - s(x)Y(x))^{-1}, \end{aligned} \tag{I.10}$$

also satisfies a Riccati equation

$$\begin{aligned} Y'(x) + A(x)Y^2(x) + B(x)Y(x) + C(x) &= 0, \\ Y(0) &= (p(0) + q(0)y_0)(r(0) + s(0)y_0)^{-1}. \end{aligned} \tag{I.11}$$

The new coefficients are connected to the old ones through

$$\begin{aligned} A &= Q(cs^2 - brs + ar^2 + rs' - r's), \\ B &= Q(-2cqs + b(ps + qr) - 2apr \\ &\qquad + p's - ps' + qr' - q'r), \\ C &= Q(cq^2 - bpq + ap^2 + pq' - p'q), \\ Q &= (qr - ps)^{-1}. \end{aligned} \tag{I.12}$$

It is thus often possible to choose the functions p, q, r and s in such a way, so as to ensure the correct semidefiniteness properties of $A(x)$ and $C(x)$.[3] One can then obtain a controlled approximation for $Y(x)$, which, through Eq. (I.10), produces a controlled approximation for $y(x)$. Of course, in the neighborhood of a pole of $y(x)$, a small indeterminacy in $Y(x)$ results in a large indeterminacy for $y(x)$. This method may also be used to locate the poles of $y(x)$ on the real axis.

In the following we will always consider nonnegative values of the variable x. All the results are trivially extended to the case of nonpositive x's introducing

$$z(x) = -y(-x), \tag{I.13}$$

which satisfies the equation

$$z'(x) + a(-x)z^2(x) - b(-x)z(x) + c(-x) = 0. \tag{I.14}$$

II. BELLMAN'S METHOD

Recalling the identity

$$-y^2(x) = \min_u [u^2(x) - 2y(x)u(x)], \tag{II.1}$$

and using the property that $a(x)$ is positive semidefinite, we may write Eq. (I.1) in the form

$$\begin{aligned} y'(x) = \min_u [&a(x)(u^2(x) - 2y(x)u(x)) \\ &- b(x)y(x) - c(x)]. \end{aligned} \tag{II.2}$$

We then introduce the functional $B[u; x]$ through

$$\begin{aligned} B'[u; x] &= a(x)\{u^2(x) - 2B[u; x]\} \\ &\qquad - b(x)B[u; x] - c(x), \\ B[u; 0] &= y_0. \end{aligned} \tag{II.3}$$

Note that $B[u; x]$ is a functional of $u(x)$ and a function of x, and $B'[u; x]$ indicates its derivative with respect to x.

Now as long as $y(x)$ is continuous in the interval

[2] That $y(x)$ is finite and nonzero if $y_0 > 0$, can be seen directly from the differential equation (I.1), because $a(x) \geq 0$ implies that $y(x)$ cannot diverge to $+\infty$, and $c(x) \leq 0$ implies that $y(x)$ can cross zero only from negative to positive values. It is similarly seen that if y_0 is negative, $y(x)$ either has one zero (and no pole), or is negative definite, or has one pole (and no zero).

[3] A trivial example is the case $a(x) \leq 0$, $c(x) \geq 0$, when $p = s = 0$, $r = 1$, $q = -1$ does the job.

from 0 to x, we certainly have

$$y(x) = \min_u B[u; x], \tag{II.4}$$

because $y(0)$ and $B[u; 0]$ coincide and $y'(x) \leq B'[u; x]$. The minimum is actually achieved for $u(x) = y(x)$, as is seen comparing Eqs. (II.2) and (I.1).

But Eq. (II.3) can be solved, and it yields

$$B[u; x] = y_0 \exp\left(-\int_0^x [b(x') + 2a(x')u(x')]\,dx'\right) + \int_0^x [a(x')u^2(x') - c(x')]\,dx' \times \exp\left(-\int_{x'}^x [b(x'') + 2a(x'')u(x'')]\,dx''\right). \tag{II.5}$$

Eq. (I.4) is thus proved.

Now, to prove Eq. (I.6), we introduce the function $w(x) = 1/y(x)$. It satisfies the equation

$$w'(x) - c(x)w^2(x) - b(x)w(x) - a(x) = 0, \qquad w(0) = 1/y_0. \tag{II.6}$$

Using the fact that $-c(x)$ is positive semidefinite, and proceeding as before, we obtain

$$w(x) = \min_v \left[y_0^{-1} \exp\left(\int_0^x [b(x') + 2c(x')v(x')]\,dx'\right) + \int_0^x [a(x') - c(x')v^2(x')]\,dx' \times \exp\left(\int_{x'}^x [b(x'') + 2c(x'')v(x'')]\,dx''\right)\right]. \tag{II.7}$$

This equation is valid as long as $w(x)$ is continuous, i.e. as long as $y(x)$ does not vanish.

Finally, using the fact that as long as the values of A are of the same sign;

$$\{\min [A]\}^{-1} = \max [A^{-1}], \tag{II.8}$$

we prove Eq. (I.6), which will thus hold as long as the bracket in the r.h.s. of Eq. (II.7) does not go through zero.

III. CONCLUSION

As previously mentioned, a Riccati equation occurs in a number of physical problems, so that the possibility of a controlled approximation to its solution should provide a useful tool to the physicist. We discuss here only one application, to elementary scattering theory.

Let $V(r)\theta(r_0 - r)$ be a spherically symmetric finite-range potential. The l-wave S-matrix element $S(l, k) = \exp(2i\,\delta(l, k))$ is then given by the relation[4]

$$S(l, k) = e^{2i\tau_l}(q_l - q_l^{(-)})(q_l - q_l^{(+)})^{-1}, \tag{III.1}$$

where τ_l and $q_l^{(\pm)}$ are known functions (defined in Reference 4), and

$$q_l = r_0\varphi'(r_0)/\varphi(r_0). \tag{III.2}$$

$\varphi(r)$ is that solution of the radial Schrödinger equation

$$\varphi''(r) + (k^2 - V(r) - l(l+1)r^{-2})\varphi(r) = 0, \tag{III.3}$$

which is regular in the origin, i.e. such that

$$\varphi(r) \underset{r\to 0}{\longrightarrow} \text{const} \times r^{l+1}. \tag{III.4}$$

Introducing the function

$$y(r) = (l+1)^{-1}r\varphi'(r)/\varphi(r), \tag{III.5}$$

which satisfies the Riccati equation

$$y'(r) + \frac{l+1}{r}y^2(r) - \frac{1}{r}y(r) + (k^2 - V(r))r(l+1)^{-1} - lr^{-1} = 0, \qquad y(0) = 1, \tag{III.6}$$

we have

$$q_l = (l+1)y(r_0). \tag{III.7}$$

Let us now consider the low-energy, high-angular momentum case,[5] so that

$$\theta(r_0 - r)[(k^2 - V(r))r - l(l+1)r^{-1}] \leq 0. \tag{III.8}$$

We may then conclude that

$$q_l = (l+1)r_0 \min_u \left\{\lim_{\epsilon\to 0}\left[\epsilon^{-1}\exp\left(-2(l+1)\int_\epsilon^{r_0} r^{-1}u(r)\,dr\right) + \int_\epsilon^{r_0} dr\,[(l+1)r^{-2}u^2(r) + (l+1)^{-1}(V(r) - k^2) + lr^{-2}]\exp\left(-2(l+1)\int_r^{r_0} t^{-1}u(t)\,dt\right)\right]\right\},$$

[4] A. Messiah, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, 1961), Vol. I, p. 391.
[5] It is of course well known that under these circumstances $S(l, k)$ will be very close to 1.

$$q_l = (l+1)r_0 \max_{\epsilon} \left\{ \lim_{\epsilon \to 0} \left[\epsilon \exp\left(2 \int_{\epsilon}^{r_0} [(l+1)^{-1} r (k^2 - V(r)) - l r^{-1}]\, dr\, v(r) \right) \right.\right.$$
$$+ \int_{\epsilon}^{r_0} dr\, [l + 1 + v^2(r)(l - r^2(k^2 - V(r))(l+1)^{-1})]$$
$$\left.\left. \times \exp\left(2 \int_{r}^{r_0} [(l+1)^{-1} t (k^2 - V(t)) - l t^{-1}] v(t)\, dt \right) \right]^{-1} \right\}. \quad \text{(III.8)}$$

With the simple choices

$$u(r) = m > [2(l+1)]^{-1}, \quad v(r) = n > -(2l)^{-1}, \quad \text{(III.9)}$$

m and n being constant, we have

$$q_l \leq (l+1)[l + m^2(l+1)][2(l+1)m - 1]^{-1} - [2(l+1)m + 1]^{-1}(kr_0)^2$$
$$+ r_0^{1-2(l+1)m} \int_0^{r_0} dr\, r^{2(l+1)m} V(r). \quad \text{(III.10)}$$

$$q_l \geq (l+1) r_0^{2nl+1} \exp[-(l+1)^{-1} n (kr_0)^2]$$
$$\times \left[\int_0^{r_0} dr\, [(l + 1 + ln^2) r^{2ln} + (l+1)^{-1} n^2 (V(r) - k^2) r^{2(ln+1)}] \right.$$
$$\left. \times \exp\left(-(l+1)^{-1} n \left[(kr)^2 + 2 \int_r^{r_0} r' V(r')\, dr' \right] \right) \right]^{-1}. \quad \text{(III.11)}$$

Finally, choosing $m = 1$, $n = 0$, one obtains the simple (but poor) bounds

$$1 \leq q_l \leq l + 1 - (2l+3)^{-1}(kr_0)^2$$
$$+ r_0^{1-2(l+1)} \int_0^{r_0} dr\, r^{2(l+1)} V(r). \quad \text{(III.12)}$$

In the case of a square-well potential, Eqs. (III.10) and (III.11) simplify to

$$q_l \leq (l+1)[l + m^2(l+1)][2(l+1)m - 1]^{-1}$$
$$- [2(l+1)m + 1]^{-1}(pr_0)^2, \quad \text{(III.13)}$$

$$q_l \geq (l+1) r_0^{2nl+1} \exp[-(l+1)^{-1} n (pr_0)^2]$$
$$\times \left\{ \int_0^{r_0} dr\, [(l + 1 + ln^2) r^{2ln} - (l+1)^{-1} n^2 p^2 r^{2(ln+1)}] \right.$$
$$\left. \times \exp[-(l+1)^{-1} n (pr)^2] \right\}^{-1}, \quad \text{(III.14)}$$

where

$$p^2 = k^2 - V. \quad \text{(III.15)}$$

To simplify even more, let us consider the S-wave case, also assuming the potential to be repulsive so that $p^2 < 0$. We then obtain

$$q_0 \leq m^2(2m-1)^{-1} - (2m+1)^{-1}(pr_0)^2, \quad \text{(III.16)}$$

$$q_0 \geq r_0 \exp[-n(pr_0)^2]$$
$$\times \left\{ \int_0^{r_0} dr\, [1 - n^2 p^2 r^2] \exp[-n(pr)^2] \right\}^{-1}. \quad \text{(III.17)}$$

Finally, let us assume $-(pr_0)^2 \ll 1$. With the choices $m = n = 1$, we then have

$$q_0 \leq 1 - \tfrac{1}{3}(pr_0)^2, \quad \text{(III.18)}$$

$$q_0 \geq 1 - \tfrac{1}{3}(pr_0)^2 + O[(pr_0)^4], \quad \text{(III.19)}$$

so that we may assert that

$$q_0 = 1 - \tfrac{1}{3}(pr_0)^2 + O[(pr_0)^4]. \quad \text{(III.20)}$$

The exact solution is

$$q_0 = pr_0 \cot(pr_0), \quad \text{(III.21)}$$

which is in agreement with what we have found.

Symmetry Functions of the Cube

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A simple method is presented for reducing the $2J + 1$ state vectors of good total angular momentum J to cubic symmetry types (basic vectors of the irreducible representations of the cubic rotation group). The cubic symmetry functions are written explicitly in terms of the eigenfunctions of J_z, J_x, and J_y, and formulas and tables which facilitate their use in obtaining eigenfunctions and energy splittings of ions in fields of cubic symmetry are presented and applied.

I. INTRODUCTION

IN the course of studying the mechanism of magnetic ordering of the rare-earth intermetallics[1] (the anion in the nitrogen column), it became necessary to obtain the energy eigenvalues and eigenfunctions of the rare-earth ion in a "crystal field" of cubic symmetry. Earlier work[2] neglected either the sixth-order potential (see below), which can be important,[1] or the eigenfunctions, which are needed for computing the effect of magnetic (or exchange) fields. Recently Ebena and Tsuya[3] have computed and tabulated the energy eigenvalues and eigenfunctions in the general cubic potential for atoms with $J \leq 8$. The availability of these tables make it unnecessary to give here our computations of the energy splittings of the second-half rare-earth ions; however, it is worthwhile to record a different method for finding and representing the eigenfunctions. The purpose of this note is to indicate how, from a manifold of states of given angular momentum, symmetry functions of the cube may be immediately constructed, and how these may be used expeditiously to obtain the eigenfunctions and eigenvalues (within a manifold of given J) in the crystalline potential.

According to Bethe,[4] the irreducible representations of the single-cubic group consists of two one-dimensional, one two-dimensional, and two three-dimensional representations called by him Γ_1 to Γ_5, respectively, whereas the double group has in addition two two-dimensional and one four-dimensional representation, Γ_6, Γ_7, and Γ_8. States of integral angular momentum transform according to the single group; those of half-odd integer angular momentum according to Γ_6, Γ_7, and Γ_8.

If the Hamiltonian transforms as Γ_1 under a group of transformations, i.e., is invariant under the group, then since $\Gamma_1 \times \Gamma_i = \Gamma_i$, where Γ_i is any of the irreducible representations of the group, the result of the Hamiltonian operating on a good symmetry function—a basis vector of one of the irreducible representations of the group—again gives a symmetry function of the same type. Hence, the eigenfunctions of the Hamiltonian are simultaneously good symmetry functions (with the degeneracy of the eigenvalue equal to the dimension of the irreducible representation to which the symmetry function belongs).

From the character tables,[4] the number of times a given irreducible representation appears in the reduction of the matrices representing the group operations on the $2J + 1$ states spanning the manifold of constant angular momentum may be obtained, and Bethe[4] gives these reductions for the various point groups. This immediately gives one the number and degeneracies of the levels into which an initially $(2J + 1)$ degenerate level is split when the symmetry of a spherically symmetrical Hamiltonian is lowered by the introduction of a potential invariant only under the operations of a lower symmetry group. The actual splittings must be found by solving secular determinants involving the matrix elements of the perturbing potential between the various $(2J + 1)$ zeroth-order degenerate states. The dimension of the secular determinant of the levels of symmetry type Γ_i is equal to the number of times Γ_i appears in the reduction of the original $(2J + 1)$-dimensional matrices. Thus for the lowest level of Ho^{3+}, which, according to Hund's rule, has $J = 8$, no cubic symmetry type will appear more than twice in the

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[1] A preliminary account of this work was reported at the Conference on Magnetism and Magnetic Materials, Detroit, Michigan, November, 1959, [G. T. Trammell, J. Appl. Phys. **31**, 362S (1960)].

[2] G. J. Kynch, Trans. Faraday Soc. **33**, 1402 (1937); S. Odiot and D. Saint-James, J. Phys. Chem. Solids **17**, 117 (1960); R. L. White and J. P. Andeline, Phys. Rev. **115**, 1435 (1959).

[3] Y. Ebina and N. Tsuya, Sci. Repts. Research Insts, Tohoku University **B12**, Nos. 1 and 3-4 (1960).

[4] H. A. Bethe, Ann. Physik **3**, 133 (1929).

TABLE I. Cubic symmetry types corresponding to integral total angular momentum. Following the symbol for the irreducible representation, the prototype function(s) and then the symmetry functions in terms of even m states, m_i (Eq. 1), are given, it being understood that instead of 2 or 4 for m, any multiple of 4 may be added (or subtracted).

Γ_1: $x^4 + y^4 + z^4$: $4_z + 4_{-z} + 4_x + 4_{-x} + 4_y + 4_{-y}$
Γ_2: $x\cdot y\cdot z$: $2_z + 2_{-z} - (2_x + 2_{-x}) + 2_y + 2_{-y}$
Γ_3: $z^2 - \frac{1}{2}(x^2 + y^2)$, $x^2 - \frac{1}{2}(z^2 + y^2)$:
$2_x + 2_{-x} + 2_y + 2_{-y}$, $2_z + 2_{-z} - (2_y + 2_{-y})$
or $4_z + 4_{-z} - \frac{1}{2}(4_x + 4_{-x} + 4_y + 4_{-y})$, $(4_x + 4_{-x}) - \frac{1}{2}(4_z + 4_{-z} + 4_y + 4_{-y})$
Γ_4: z, x, y: $4_z - 4_{-z}$, $4_x - 4_{-x}$, $4_y - 4_{-y}$
Γ_5: XY, YZ, ZX: $2_z - 2_{-z}$, $-(2_x - 2_{-x})$, $2_y - 2_{-y}$

17-dimensional space spanned by the eigenfunctions of J. If, rather than first choosing 17 functions of good symmetry types, one sets up the secular determinant on the basis of states of good J_z, one will be faced with the solution of four- and five-dimensional secular determinants.

II. SYMMETRY FUNCTIONS OF THE CUBE

One cannot hope to find simple descriptions of cubic symmetry functions in terms of the eigenfunctions of J_z.

Let it be understood that throughout this note we refer to states of good total J, and that we seek to construct states of good cubic symmetry types from these states. Let m_z stand for an eigenfunction of J_z with eigenvalue m; then

$$J_z m_z = m\cdot m_z, \tag{1}$$

and similarly m_x, m_{-y}, etc. stand for eigenfunctions of J_x, J_{-y}, etc. In order to fix the phases, we take $m_x = R_y m_z$, $m_y = R_x m_x$, $m_{-x} = R_z m_y$, $m_{-y} = R_z m_{-x}$, and $m_{-z} = R_y^2 m_z$, where R_y and R_z are $\frac{1}{2}\pi$ "rotators" about the y and z axes:

$$\begin{aligned} R_y f(xyz) &= f(-z, y, x), \\ R_z f(xyz) &= f(y, -x, z). \end{aligned} \tag{2}$$

The six states m_i, where i ranges over the plus and minus cartesian coordinates, transform among themselves under the group of operations which carry a cube into itself; hence they span each of the cubic symmetry function spaces an integral (including zero) number of times.

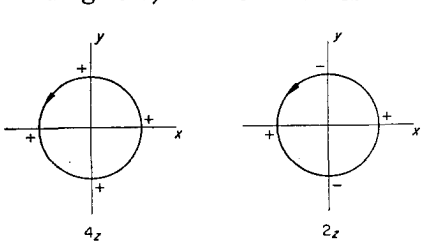

FIG. 1. The relevant properties of 4_z and 2_z entering into the construction of Table I.

TABLE II. Cubic symmetry types for odd m, m_i's.

Γ_4: z, x, y: $1_x + 1_{-x} + 1_y + 1_{-y}$,
$1_{-z} - 1_z - i1_y + i1_{-y}$, $i1_{-z} + i1_z - i1_{-x} + i1_x$
$3_x + 3_{-x} + 3_y + 3_{-y}$, $3_{-z} - 3_z + i3_y - i3_{-y}$,
$i3_{-z} - i3_z + i3_{-x} - i3_x$
Γ_5: xy, yz, zx: $1_x + 1_{-x} - (1_y + 1_{-y})$,
$1_z - 1_{-z} - i(1_y - 1_{-y})$, $i(1_z + 1_{-z} + 1_{-x} - 1_x)$
$3_x + 3_{-x} - (3_y + 3_{-y})$, $3_z - 3_{-z} + i(3_y - 3_{-y})$,
$-i(3_z + 3_{-z} + 3_{-x} - 3_x)$

Integral J

One easily finds that for integral J, the character of the six states belonging to a given m is [6, 2 cos $(m\pi)$, 2 cos $(m\frac{1}{2}\pi)$, 0, 0] corresponding to the five classes C_1 to C_5 of Bethe.[4] From Bethe's character tables we then know that the six states belong to $\Gamma_4 + \Gamma_5$ if m is odd; $\Gamma_2 + \Gamma_3 + \Gamma_5$, if $m = 2$ (mod 4); $\Gamma_1 + \Gamma_3 + \Gamma_4$, if $m = 4$ (mod 4). In some cases the six states m_i will not all be linearly independent and some of the symmetry types constructed from them will be identically zero. For example, if $m = 0$, only three of the states are linearly independent (since $0_z = 0_{-z}$ if J is even; $0_z = -0_{-z}$ if J is odd). From Table I, discussed below, it is seen that if J is odd, 0_z, 0_x, 0_y, are of symmetry type Γ_4, while if J is even, $0_x + 0_y + 0_z$ is of symmetry type Γ_1 and $0_z - \frac{1}{2}(0_x + 0_y)$, $0_x - \frac{1}{2}(0_z + 0_y)$, are of symmetry type Γ_3.

We show in the appendix that for integral J any eigenfunction of J_z may be expressed in terms of the *even* eigenvalued eigenfunctions of J_z, J_x, and J_y. In Table I we present symmetry types constructed from the functions m_z, m_x, etc. where m is even, it being understood that instead of 2 and 4 in the table, we may add or substract any multiple of 4. In Table I, following the symmetry type symbol, we give prototype function (s) which transforms according to the symmetry type; then we give the linear combination of the m_i which transform properly (that they do transform like the prototypes is easily verified for R_z and R_y which generate the cubic group).

The functions given which transform like Γ_3 are not orthogonal (they are more symmetrical in appearance than the orthogonal functions). If we call these two functions γ_1^3 and γ_2^3, then we may obtain the orthogonal functions (which are a basis for Γ_3) $\gamma_\alpha^3 = \gamma_1^3$, and $\gamma_\beta^3 = 3^{-\frac{1}{2}}(\gamma_1^3 + 2\gamma_2^3)$; for the prototypes this gives $\gamma_\alpha^3 = \frac{1}{2}(3z^2 - r^2)$, $\gamma_\beta^3 = (\frac{3}{2})^{\frac{1}{2}}(x^2 - y^2)$. It is easier to exploit the symmetry to obtain relations among matrix elements in the γ_1^3, γ_2^3, basis than in the γ_α^3, γ_β^3 basis, which is why we prefer to work

TABLE III. Half-odd integral angular momentum cubic symmetry types. After the symbol for the irreducible representation, we give the prototype spinors after which the cubic symmetry types in terms of the m_i's (Eq. 1) are given.

	$m = \pm\frac{1}{2} \bmod (4)$	$m = \pm\frac{3}{2} \bmod (4)$
Γ_6: $\left\vert \frac{1}{2}, \frac{1}{2}\right)$:	$m_{\pm z} + 2^{-\frac{1}{2}}F(\frac{1}{4}\pi, m)$	
$\left\vert \frac{1}{2}, -\frac{1}{2}\right)$:	$\pm[m_{\mp z} + 2^{-\frac{1}{2}}F(-\frac{1}{4}\pi, m)]$	
Γ_7: $xyz \left\vert \frac{1}{2}, \frac{1}{2}\right)$:		$m_{\mp z} - 2^{-\frac{1}{2}}F(-\frac{3}{4}\pi, m)$
$xyx \left\vert \frac{1}{2}, -\frac{1}{2}\right)$:		$\mp[m_{\pm z} - 2^{-\frac{1}{2}}F(\frac{3}{4}\pi, m)]$
Γ_8: $\left\vert \frac{3}{2}, \frac{3}{2}\right)$:	$F(\frac{3}{4}\pi, m)$	$m_{\pm z} + 2^{-\frac{1}{2}}F(\frac{3}{4}\pi, m)$
$\left\vert \frac{3}{2}, \frac{1}{2}\right)$:	$\mp 3^{-\frac{1}{2}}[2^{\frac{1}{2}}m_{\pm z} - F(\frac{1}{4}\pi, m)]$	$\pm 3^{\frac{1}{2}}2^{-\frac{1}{2}}F(\pi\frac{1}{4}, m)$
$\left\vert \frac{3}{2}, -\frac{1}{2}\right)$:	$3^{-\frac{1}{2}}[2^{\frac{1}{2}}m_{\mp z} - F(-\frac{1}{4}\pi, m)]$	$3^{\frac{1}{2}}2^{-\frac{1}{2}}F(-\pi\frac{1}{4}, m)$
$\left\vert \frac{3}{2}, -\frac{3}{2}\right)$:	$\mp F(-\frac{3}{4}\pi, m)$	$\pm[m_{\mp z} + 2^{-\frac{1}{2}}F(-\frac{3}{4}\pi, m)]$

$$F(p, m) = m_x + e^{ip}m_y + e^{2ip}m_{-x} + e^{3ip}m_{-y}$$

with the nonorthogonal basis, leaving the transformation to the orthogonal basis to the last step in a given calculation.

The only properties of 4_z and 2_z that have been utilized in the construction of the functions is that 4_z is invariant under $\frac{1}{2}\pi$ rotations about the z axis, and that 2_z changes sign under rotation by $\frac{1}{2}\pi$ round the z axis (Fig. 1). Any functions which transform thusly under $\frac{1}{2}\pi$ notations about the z axis could be substituted for the functions in Table I to provide good cubic symmetry functions. The results in Table I could be obtained from the idempotent reduction method,[5] but they are most easily obtained from inspection of Fig. 1 and the prototype functions of Table I.

Now if for m_z in Table I we substitute $Y_l^m(\theta, \phi) \propto (x + iy)^m P_l^m(z)$ and similarly for m_x, etc. remembering that $m_x = R_y m_z$ and $R_y f(xyz) = f(-z, y, x)$ then we shall obtain VonderLage and Bethe's[6] "Kubic Harmonics." Since the P_l^m's are tabulated, with the aid of Table I, we may write the Kubic Harmonics immediately. This, however, is not useful; for practical calculations, the cubic symmetry functions as given in Table I in terms of the symmetry, functions of the sphere are in the best form.

It may sometimes be useful to write the cubic symmetry types in terms of the odd m, m_i's. The reduction is given in Table II.

[5] Generally the reduction of a function or a set of functions to symmetry functions of a group may be carried out by the idempotent or projection operator technique [see, e.g., D. E. Littlewood, *The Theory of Group Characters* (Oxford University Press, New York, 1940) Chap. IV, or a more modern work, M. Hammermesh, *Group Theory* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1962), p. 111]. It was brought to the author's attention by the referee that P. H. E. Meijer, Phys. Rev. 95, 1443 (1954), has given an exposition of how the method is used, together with formulas and tables to facilitate its use in obtaining the symmetry functions for various point groups, including the cubic group. The method given here for obtaining and representing the cubic symmetry functions is different and perhaps easier to use than the previous method.

[6] F. C. VonderLage and H. A. Bethe, Phys. Rev. 71, 612 (1947).

Half-Odd Integral J

These cases are somewhat more complicated than the integral J case. The prototypes are spinors rather than simple polynomials as in the case of integral J, and the cubic symmetry types cannot be written so immediately as was possible in Table I. The character of the six functions m_i corresponding to the eight classes[4] E, R, C_2, C_3', C_3'', C_4, C_5', C_5'' of the double group are $(6, -6, 0, 2\cos(m\frac{1}{2}\pi), -2\cos(m\frac{1}{2}\pi), 0, 0, 0)$. Then from the characters of Γ_6, Γ_7, and Γ_8,[4] we find that the six functions m_i transform as $\Gamma_6 + \Gamma_8$ if $m = \pm\frac{1}{2} \pmod 4$, and as $\Gamma_7 + \Gamma_8$, if $m = \pm\frac{3}{2} \pmod 4$. Only Γ_6 appears (once) in the reduction of the two $J = \frac{1}{2}$ states, and only Γ_8 appears (once) in the reduction of the four $J = \frac{3}{2}$ states, and we may take the two functions $|J, J_z) = |\frac{1}{2}, \pm\frac{1}{2})$, and the four functions $|J, J_z) = |\frac{3}{2}, \pm\frac{3}{2})$, $|\frac{3}{2}, \pm\frac{1}{2})$ as prototypes for these two symmetry types. $\Gamma_7 = \Gamma_2 \times \Gamma_6$ and thus we may take $x \cdot y \cdot z\ |\frac{1}{2}, \pm\frac{1}{2})$ as prototypes of Γ_7. We now take the phases of the functions $|J, m)$ in the standard way such that

$$(J_x \pm iJ_y)\ |J, m) = [J(J+1) - m(m \pm 1)]^{\frac{1}{2}}\ |J, m \pm 1). \quad (3)$$

Then, according to Wigner,[7]

$$R_y q_z = q_x = \sum_m d^j_{mq}(\tfrac{1}{2}\pi)m_z, \quad (4)$$

where

$$d^j_{mq}(\tfrac{1}{2}\pi) = \sum_t 2^{-j}[j+m!\ j-m!\ j+q!\ j-q!]^{\frac{1}{2}}(-)^t \times [(j-q-t)!\,(j+m-t)!\,t-m+q!\,t!]^{-1}, \quad (5)$$

where the sum is over integral (plus and minus) t's.

Table III gives the spinor cubic symmetry func-

[7] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), p. 167.

TABLE IV(a). The number of times a given irreducible representation of the cubic rotation group appears in the reduction of the $(2J + 1)$-dimensional matrices belonging to integral J.

J	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
0	1	0	0	0	0
1	0	0	0	1	0
2	0	0	1	0	1
3	0	1	0	1	1
4	1	0	1	1	1
5	0	0	1	2	1
6	1	1	1	1	2
7	0	1	1	2	2
8	1	0	2	2	2

tions. That they do transform properly (like the prototype spinors) under R_y and R_z may be verified by using Eq. (5), Eq. (2) and the definitions preceding it, and the relations $R_y m_z = m_x$, $R_y m_x = m_{-z}$, $R_y m_y = \exp[-im\tfrac{1}{2}\pi]m_y$, $R_y m_{-y} = \exp[+im\tfrac{1}{2}\pi]m_{-y}$, $R_y m_{-x} = \exp[-im\pi]m_z$, $R_y m_{-z} = -\exp[im\pi]m_{-x}$, $R_z m_{-y} = -m_x$ (for spinors), which come from the group multiplication table and Eq. (1).

III. DISCUSSION AND APPLICATIONS

In Table IV we give the number of times a given irreducible representation of the cubic-rotational group appears in the reduction of the $2J + 1$-dimensional matrices belonging to a given J.[4] By means of Tables I and II, or III, and Tables IV, one may immediately reduce the $2J + 1$ states belonging to a given J to cubic-symmetry types. One may express these functions in terms of the eigenstates of J_z by means of the expression for $d^j_{mq}(\tfrac{1}{2}\pi)$ given in Eq. (5), but this is not generally useful except for small J values.[8]

If now V is an operator which is invariant under the cubic-rotation group, its matrix elements be-

TABLE IV(b). The number of times a given irreducible representation of the cubic rotation group appears in the reduction of the $(2J + 1)$-dimensional matrices belonging to half-odd integral J.

J	Γ_6	Γ_7	Γ_8
1/2	1	0	0
3/2	0	0	1
5/2	0	1	1
7/2	1	1	1
9/2	1	0	2
11/2	1	1	2
13/2	1	2	2
15/2	1	1	3

[8] The expressions obtained from Table III for γ^6 and γ^8 (bases for Γ_6 and Γ_8) are obviously clumsy expressions of these functions in the cases of $J = \frac{1}{2}$ and $J = \frac{3}{2}$, respectively.

TABLE V. Integral J coefficients for Eq. (6).

	n (mod 4)	m (mod 4)	α_{zz}	$\alpha_{z\bar{z}}$	α_{zx}
Γ_1	0	0	6	6	24
Γ_2	2	2	6	6	−24
Γ_3	0	0	3	3	−6
	2	2	4	4	+8
	0	2	−2	−2	12
Γ_4	0	0	2	−2	0
Γ_5	2	2	2	−2	0

tween symmetry function (Tables I and III) are given by

$$(\gamma^i(n), V\gamma^i(m)) = \alpha_{zz}(n_z, Vm_z) + \alpha_{z\bar{z}}(n_z, Vm_{-z}) + \alpha_{zx}(n_z, Vm_x), \quad (6)$$

where $\gamma^{(i)}(n)$ and $\gamma^i(m)$ are two functions of the same symmetry type (unnormalized) selected from Table I or III. The α's and relevant n and m's are given in Table V. The corresponding table for the spinor symmetry functions would be unnecessarily large; we merely note the following relations which may serve to reduce the matrix elements of V between spinors of the same symmetry type to the form of Eq. (6):

$$(F(p,n), VF(p,m)) = 4\{(n_z, Vm_z) - \exp[i(n\pi + 2p)](n_z, Vm_{-z}) + 2\cos[p + (m-n)\tfrac{1}{2}\pi](n_z, Vm_z)\}, \quad (7)$$

$$(n_{\pm z}, VF(p,m)) = 4(n_{\pm z}, Vm_x), \quad (8)$$

$$(F(p,n), Vm_{\pm z}) = 4(n_x, Vm_{\pm z}), \quad (9)$$

$$(n_x, Vm_{-z}) = (n_z, Vm_x), \quad (10)$$

$$(n_{-z}, Vm_x) = (n_x, Vm_z) = \exp[i(m-n)\pi](n_z, Vm_x), \quad (11)$$

where $F(p, n)$ is defined in Table IV(a).

As an example, we consider the splitting of the ground state of Tb^{3+} or Tm^{3+}, each of which, according to Hund's rule, have $J = 6$ when the ions are placed in a crystal field of cubic symmetry. According to Table IV(a), Γ_1 to Γ_4 are each represented once, and Γ_5 twice. For the eigenfunctions we may take (Table I):

$$\begin{aligned}
\gamma^1 &= 2\sqrt{2}/3\,(0_z + 0_y + 0_z),\\
\gamma_1^2 &= (\tfrac{4}{3}\sqrt{10})(6_z + 6_{-z} - 6_z - 6_{-z} + 6_y + 6_{-y}),\\
\gamma_1^3 &= (4/\sqrt{66})(6_z + 6_{-z} - 6_y - 6_{-y}),\\
\gamma_1^4 &= (4_z - 4_{-z})/\sqrt{2},\\
\gamma_1^5(6) &= (6_z - 6_{-z})/\sqrt{2},
\end{aligned} \quad (12)$$

$\gamma_1^5(2) = (2_z - 2_{-z})/\sqrt{2}$.

The normalization follows from Eq. (6) and Table V with $V = 1$. For example,

$$(0_x + 0_y + 0_z, 0_x + 0_y + 0_z) = 3[1 + 2(0_z, 0_z)] = 9/8.$$

Where we have used the fact that

$$d^j_{m0} = (-)^{\frac{1}{2}(j+m)}2^{-j}\left[\begin{pmatrix} j+m \\ \frac{j+m}{2} \end{pmatrix}\begin{pmatrix} j-m \\ \frac{j-m}{2} \end{pmatrix}\right]^{\frac{1}{2}},$$

which may be derived from Eq. (5). The two γ^5 functions given are not yet the eigenfunctions; the cubic potential will have matrix elements between them.

For the cubic potential, we have from Tables IV(a) and I:

$$V = V_0 + V_4 + V_6 + \cdots,$$

$$\begin{aligned} V_4 &= \sum_i f_4(r_i)[P_4(x_i/r_i) + P_4(y_i/r_i) + P_4(z_i/r_i)] \\ &\to B[J_x^4 + J_y^4 + J_z^4 - \tfrac{1}{5}J(J+1)(3J^2 + 3J - 1)] \\ &\to B\{\tfrac{1}{2^0}[35J_z^4 - 30J(J+1)J_z^2 + \cdots] \\ &\quad + \tfrac{1}{8}(J_+^4 + J_-^4)\}, \end{aligned} \tag{13}$$

$$\begin{aligned} V_6 &= \sum_i f_6(r_i)[P_6(x_i/r_i) + P_6(y_i/r_i) + P_6(z_i/r_i)] \\ &\to D[231(J_z^6 + J_x^6 + J_y^6) \\ &\quad - 315\,J(J+1)(J_z^4 + J_x^4 + J_y^4) + \cdots] \\ &\to D\{[231J_z^6 - 315J(J+1)J_z^4 + \cdots] \\ &\quad - \frac{21}{2}\,J_+^4[11\,J_z(J_z+4) + 50 - J(J+1)] \\ &\quad - \frac{21}{2}\,[11J_z(J_z+4) + 50 - J(J+1)]J_-^4\}. \end{aligned} \tag{14}$$

Where the sums in (13) and (14) refer to the sum over the coordinates of the $4f$ electrons, and the arrows indicate the "operator equivalents" of Stevens,[9] V_0 does not split the level, and V_8 and higher have zero expectation value for f electrons. Making use of the operator equivalents and Table V, we have

$$\begin{aligned} &(\gamma^5(6),\ V\gamma^5(6)) = (6_z,\ V6_z), \\ &(\gamma^3(6),\ V\gamma^3(6)) = (6_z,\ V6_z) \\ &\qquad + 2[1 + 2(6_z,\ 6_z)]^{-1}(6_z,\ V_+6_z), \\ &(\gamma^2(6),\ V\gamma^2(6)) = (6_z,\ V6_z) \\ &\qquad - 3[1 - 4(6_z,\ 6_z)]^{-1}(6_z,\ V_+6_z), \end{aligned} \tag{15}$$

where V_+ refers to the part of $V_4 + V_6$ containing J_+^4. Making use of the tabulated matrix elements of the operator equivalents,[9] we obtain

$$\begin{aligned} (6_z,\ V6_z) &= 3 \times 99B + 22 \times 7560\ D, \\ (6_z,\ V_+6_z) &= 2^{-6}\left[\binom{12}{8}\right]^{\frac{1}{2}}(6_z,\ V_+2_z) \\ &= (27 \times 55/64)[B + 16 \times 21 \times 35\ D], \end{aligned} \tag{16}$$

which together with $(6_z,\ 6_z) = 2^{-6}$ serves to evaluate the quantities in Eq. (15). The other four matrix elements required to obtain the splitting for this case ($J = 6$) may be obtained in the same manner, but we forego their computation.

IV. CONCLUSION

We have shown how, from the manifold of states of given J, $(2J + 1)$ symmetry functions of the cube may be immediately obtained in terms of eigenfunctions of J_z, J_y, etc. We have shown how these functions may be used to compute matrix elements of invariants of the cubic group most expeditiously (usually), without expressing these functions in terms of the eigenfunctions of J_z. The matrix elements of $\mathbf{J}(\Gamma_4)$ and higher-order operators are also conveniently evaluated in this representation, but they will be dealt with in a succeeding paper on the theory of the magnetic ordering of some rare-earth compounds.

APPENDIX

We prove here that the even-valued eigenfunctions of J_x, J_y, and J_z are sufficient to represent the $(2J + 1)$ eigenfunctions of J_z for a given integer J.

With the conventions of Eqs. (1) and (2) of the text,

$$p_x = R_y p_z = \sum_m d_{mp} m_z. \tag{A1}$$

With the standard phases of Eq. (3), the d's are real and are given by Eq. (5). From the unitarity of the d matrix,

$$m_z = \sum_p d_{mp} p_x. \tag{A2}$$

Applying R_z (Eq. 2) to (A2),

$$m_z = e^{im\frac{1}{2}\pi} \sum_q d_{mq} q_y, \tag{A3}$$

and applying R_y to (A3),

$$p_x = \sum_q d_{pq} e^{i(p-q)\frac{1}{2}\pi} q_y. \tag{A4}$$

[9] K. H. W. Stevens, Proc. Phys. Soc. (London) 65, 210 (1952). In this reference are given the remainder of the expressions for the operator equivalents of P_4 and P_6 which we indicate by dots in Eqs. (13) and (14).

Substituting (A4) into (A2),

$$m_x = \sum_{p,q} d_{mp}\, d_{pq} e^{i(p-q)\frac{1}{2}\pi} q_y. \qquad \text{(A5)}$$

We now see, on comparing Eqs. (A3) and (A5), that if m is odd, an odd q term of the sum in Eq. (A5) is contributed to only by the even p terms in that sum, and furthermore the even p terms do not contribute to the even q terms; therefore,

$$m_x = \sum_{\text{even } p} d_{mp}(p_x + e^{im\frac{1}{2}\pi} p_y), \quad (\text{odd } m). \qquad \text{(A6)}$$

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On the Representations of the Semisimple Lie Groups.* I. The Explicit Construction of Invariants for the Unimodular Unitary Group in N Dimensions

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(Received 7 August 1962)

It is intended in the present series of papers to discuss explicit constructive determinations of the representations of the semisimple Lie groups SU_n by an extension of the Racah-Wigner techniques developed for the two-dimensional unimodular unitary group (SU_2). The present paper defines, and explicitly determines, a *symmetric* vector-coupling coefficient for the group SU_n. These coefficients are utilized to construct a series of canonical invariants for SU_n, of which the first I_2 is the familiar Casimir invariant, and it is proved (by construction) that these invariants form a complete system of independent invariants suitable for uniquely labeling the irreducible inequivalent representations of SU_n.

1. INTRODUCTION

THE fundamental importance of group theoretical methods in applications to physics has been clear since the pioneer researches of Weyl[1] and Wigner.[2] Of the important groups, the continuous compact groups (the semisimple Lie groups in particular) play a predominant role, as is clear from current applications in fields as disparate as elementary particle physics[3] and the rotational model for nuclear structure[4] (Elliott's application of SU_3).

Despite the fundamental importance of the semisimple Lie groups, not too much has been done for these groups as a whole, regarding an explicit discussion of their representations, let alone any general treatment of the properties of these representations.

This neglect has been largely due to a difference in emphasis between a mathematician's approach to the subject and a physicist's approach, this difference being manifested most clearly in the great importance the latter attaches to the representations *per se*. The outstanding researches on the representations of the semisimple Lie groups, beginning with Frobenius, Schur, Cartan, and Weyl, have by and large been concerned primarily with the *characters* of the representations, rather than the representations themselves. Where the representations *per se* have been considered, the general procedure—following Schur and Weyl—has been to exploit the close connection that exists with the symmetric group, thus utilizing the theory of the symmetric group as a technique for studying the Lie groups.[5]

Such a procedure is of great elegance and leads to a canonical procedure for discussing the characters of the semisimple Lie groups. The most complete treatment for the representations along these lines appears to be Littlewood's explicit construction of the representations by an extension of Frobenius's methods for defining invariant matrices.[6]

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† Summer Lecturer at the University of Colorado Summer Institute for Theoretical Physics, (Fifth Annual Series, 1962).

[1] H. Weyl, *The Theory of Groups and Quantum Mechanics*, translated by H. P. Robertson (Methuen and Company, Ltd., London, 1931).

[2] E. P. Wigner, *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra*, translated by J. J. Griffin (Academic Press Inc., New York, 1959).

[3] R. E. Behrends, J. Dreitlein, C. Fronsdal, and W. Lee, Rev. Mod. Phys. **34**, 1 (1962).

[4] J. P. Elliott, Proc. Roy. Soc. (London) **A245**, 128 (1958); *ibid*, 562 (1958).

[5] H. Weyl, *The Classical Groups* (Princeton University Press, Princeton, New Jersey, 1946).

[6] D. E. Littlewood, *The Theory of Group Characters* (Clarendon Press, Oxford, England, 1950).

Substituting (A4) into (A2),

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We now see, on comparing Eqs. (A3) and (A5), that if m is odd, an odd q term of the sum in Eq. (A5) is contributed to only by the even p terms in that sum, and furthermore the even p terms do not contribute to the even q terms; therefore,

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Such a procedure is of great elegance and leads to a canonical procedure for discussing the characters of the semisimple Lie groups. The most complete treatment for the representations along these lines appears to be Littlewood's explicit construction of the representations by an extension of Frobenius's methods for defining invariant matrices.[6]

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It is clear from these preliminary remarks that the subject under discussion is not only important, but has already received several classic treatments. Why then further discussion? The question is not frivolous, and there is a genuine reason. It is this: the methods used for the classic discussions of the Lie groups employ techniques quite foreign to those utilized by (mathematical) physicists. Global techniques, which employ properties of the whole group have predominated, while the purely infinitesimal methods, which are the natural tools of the physicist (local interactions, complete set of commuting constants of the motion), have not been employed nearly as systematically.

There is a very good reason for this neglect; namely, that the appropriate techniques had to be developed (by Wigner and by Racah) in their fundamental researches on the representations of the rotation group (including spin representations, i.e., SU_2). It is the intention of the present series of papers to extend to the general unimodular unitary group, SU_n, the explicit constructive, predominantly algebraic, methods of Racah and Wigner, with particular emphasis on SU_3 and SU_4. As we shall see, the *direct* extension of the procedures to be developed here for SU_n is not possible for the general semisimple Lie group. For this important remark, I am indebted to Professor Racah. [*Note added in proof:* Professor A. P. Stone has independently made the same observation (private communication).] Nonetheless, the present methods afford an *indirect* treatment of the general case, since an arbitrary but fixed semisimple Lie group may always be embedded in a suitable SU_n. (A good example is the group G_2 which may be embedded in SU_7.)

As Wigner has emphasized—and Racah also in his Princeton lectures[7]—that there are three problems standing in the way of this program.

The first of these problems is the explicit construction of all the invariants of the group in question. (The well-known Casimir invariant, the only invariant for SU_2, furnishes one general invariant; the task is to find the remaining $l - 1$ invariants for a Lie group of rank l.)

Although the *dominant weights* furnish a unique designation of the irreducible inequivalent representations, it is well known that the weights themselves do not afford a unique characterization of the *states* belonging to a given irreducible inequivalent representation. This is the second problem posed by Wigner and by Racah: to determine suitable operators whose eigenvalues will uniquely characterize the states of a given (irreducible inequivalent) representation.

The third problem, which has been especially emphasized by Wigner, is the construction of matrices to reduce the (inner) Kronecker product. The major difficulty lies in the occurrence of groups which are not *simply reducible*.[8] Expressed differently, the difficulty is that a given representation may occur more than once in the reduction, so that the reducing matrices are not uniquely determined by the group itself.

It is the purpose of the present paper to give an explicit solution, for all SU_n, to the first of these problems. A second paper will detail an equally explicit solution to the "state-labeling" problem (again for SU_n). [*Note added in proof:* A brief summary of the main results of papers I and II has been presented in Phys. Letters, **3**, 69 (1962). A proposed solution to the 'simple reducibility' problem for SU_3 based upon these results has been given in Phys. Letters, **3**, 254 (1963).] With these two ancillary tasks accounted for, the proposed treatment of the representations of SU_n now becomes possible; application to SU_3 and SU_4 in particular is carried out.

In order to set the present discussion in the proper perspective, let us note that the emphasis here is strongly on the words "explicit" and "constructive". Were it not for this emphasis, the subject of the group invariants would otherwise have to be considered as solved implicitly by the researches of Killing, Cartan, and particularly Weyl, as long ago as 1894–1925.

2. THE CASIMIR INVARIANT AND GENERALIZATIONS

The infinitesimal generators $\{X_A\}$ of a semisimple Lie group obey the commutation rules:

$$[X_A, X_B] \equiv X_A X_B - X_B X_A = \sum_C (AB^C) X_C. \tag{1}$$

The three-index symbols (AB^C) are the *structure constants* of the group. Cartan's criterion for a semisimple Lie group is that the two-index symbols

$$g_{AB} = \sum_{B\bar{C}} (A\bar{B}^{\bar{C}})(B\bar{C}^{\bar{B}}) \tag{2}$$

have a nonvanishing determinant. The g_{AB} has the

[7] G. Racah, lecture notes, Institute for Advanced Study, Princeton, New Jersey, 1951 (unpublished).

[8] E. P. Wigner, Am. J. Math. **63**, 57 (1941); G. W. Mackey, Pac. J. Math. **51**, 730 (1950); W. T. Sharp, CRT-935 (AECL 1098) Sept. (1960); E. P. Wigner, lecture notes, Princeton University, Princeton, New Jersey, 1955 (unpublished).

property that it may be used to define metric tensors $\sum_B g_{AB}g^{BC} = \delta_A^{\ C}$ suitable for raising and lowering indices. Using this, Casimir constructed a general invariant

$$I_2 \equiv \sum_{A,B} g^{AB}X_AX_B, \tag{3}$$

which may be easily shown to satisfy the defining equation for an invariant

$$[X_A, I_n] = 0, \quad \text{all} \quad X_A. \tag{4}$$

A generalization of the Casimir invariant immediately suggests itself, namely

$$I_n^{\#} \equiv \sum_{\substack{\text{all}\\ \text{indices}}} (A_1\bar{B}_1^{\bar{C}_1})(A_2\bar{C}_1^{\bar{C}_2}) \cdots \times (A_n\bar{C}_n^{\bar{B}_1})X^{A_1}X^{A_2} \cdots X^{A_n}. \tag{5}$$

The $I_n^{\#}$ are seen to obey Eq. (4). As pointed out by Racah,[7] this explicit construction of invariants ($I_2^{\#} = I_2, I_3^{\#}, \cdots I_n^{\#}$) is not satisfactory since there exist inequivalent irreducible representations that have the *same* values for all $I_n^{\#}$. Going further, Racah[9] discussed a method whereby the desired l invariants (for a semisimple group of rank l) could be obtained from the invariants of the *adjoint group*.[10]

Racah's method consisted in noting that Eq. (4) is equivalent to the definition of the characteristic differential equation of the invariants of the adjoint group. Since Killing and Cartan had shown how to obtain invariants of the adjoint group, and since the number of independent invariants of the adjoint group is equal to the rank l of the original group, the first problem may be considered solved. Since Racah's paper is relatively inaccessible,[11] and is, moreover, so brief as to be difficult to understand fully, it might be useful to discuss Racah's contribution in some detail here.

Let us first consider Killing's method.[12] Killing's procedure utilized the characteristic equation defined by the adjoint representation. That is,

$$\det\left(\sum_A X^A(AB^C) - \rho\,\delta_B^C\right) = 0. \tag{6}$$

[The determinant is defined in the form

$$\det A_{ij} = \sum_{\substack{\text{permutations}\\ (i_1\cdots i_n)}} (-)^p(A_{i_11}A_{i_22}\cdots A_{i_nn}),$$

so that the fact that the X^A do not commute is properly considered.] Eq. (6) can be shown to be invariant under all X_A. Since ρ is arbitrary, this implies that each power of ρ is separately an invariant.

To discuss the invariants defined by (6) let us employ the theorem[13] that the coefficient of ρ^i in the characteristic polynomial $\det(D - \rho 1) = 0$ is $(-)^i$ tr $(D_{[d-i]})$, where d is the dimension of D and tr (D_m) is defined as

$$\text{tr}\,(D_{[m]}) \equiv (m!)^{-1}\begin{vmatrix} T_1 & 1 & 0 & \cdots & 0 \\ T_2 & T_1 & 2 & 0\cdots & 0 \\ T_{m-1} & T_{m-2} & & \cdots & m-1 \\ T_m & T_{m-1} & & \cdots & T_1 \end{vmatrix},$$

with the further definition, that T_n is the trace of the nth power of D, i.e., $T_n \equiv \text{tr}\,(D^n)$.

The trace of the powers of D are in the present case none other than the invariants previously denoted by $I_n^{\#}$. We have shown therefore,[14] that the invariants defined by the adjoint representation are algebraic (polynomial) combinations of the invariants $I_n^{\#}$, and are consequently not satisfactory for distinguishing the inequivalent irreducible representations.[15]

In his paper, Racah noted that, besides Killing's determination, one might use Cartan's generalization which employs in place of the *adjoint representation*, the representation of the infinitesimal group induced by an *arbitrary* representation of Racah's essential contribution in his paper[16] was an enumera-

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[9] G. Racah, Rend. Atti. Accad. Naz. Lincei **8**, 108 (1950).

[10] For convenience, let us note that the adjoint group is defined in terms of the mapping of the group into itself, induced by conjugation with the group element x. That is, x: $g \to g' = x^{-1}gx$. For infinitesimal elements of the group, the above transformation induced by x, defines a transformation in the space of the parameters, that is, for $g = E + \sum_A p_AX_A + 0(p^2)$, the mapping x: $g \to g'$ induces $p_A \to p_A'$. The transformations $p \to p'$ constitute the *adjoint group*, A.

The transformation x also provides a representation of the original group G, the *adjoint representation*. For infinitesimal elements, this gives a representation of the 'infinitesimal group' whose elements are the $\{X_A\}$. That is,

$$x\text{: } \{X_A\} \to \{X_A\}' \equiv \{[X_x, X_A]\}.$$

[11] I am indebted to Professor B. Bayman for an English translation of this paper, and to Professor U. Fano for a discussion on both the original and translated papers. My thanks are due also to Professor Racah for the favor of further interpretive remarks as to the meanings intended.

[12] G. Killing, Math. Ann. **31**, **33**, **34**, **36** (1888–1890). This reference is quoted in Weyl, reference 5, and Racah, reference 9.

[13] D. E. Littlewood, reference 6, Chap. X; J. S. Lomont, *Applications of Finite Groups* (Academic Press Inc., New York, 1959).

[14] Questions concerning the proper ordering of the noncommuting operators X_A can be avoided by a lengthier treatment, or can by avoided completely by dealing with numerical quantities and symmetrizing the invariants, with respect to the X_A, after they are determined (Racah's procedure, in fact).

[15] The recent paper of Stone (see ref. 17) may be interpreted as establishing this result also.

[16] I am indebted to Professor Racah for a discussion of this point.

tion of suitable representations which will suffice to define (by the Killing–Cartan procedure), acceptable invariants for all the semisimple Lie groups.

Since, however, we are interested in an *explicit* construction of the invariants, Racah's paper needs to be supplemented by further calculation. The ultimate goal is, of course, to utilize these invariants to construct all the inequivalent, irreducible, representations.

Fortunately, as is shown in the next section, there is a wholly different procedure available for the SU_n group which leads quite immediately to the desired goal.

Before turning to this demonstration, let us remark that the reason why the Killing invariants fail to be acceptable is in some ways more interesting than the problem of the invariants itself. Since this point is not directly of concern in the next sections, further discussion has been relegated to Appendix B.

3. THE CONSTRUCTION OF INVARIANTS FOR SU_n

Before proceeding with this construction, it is useful first to introduce a very convenient canonical basis for the generators $\{X_A\}$ of the group SU_n. This basis is a sort of hybrid, and combines both the basis e_{ij} used by Weyl, and the basis (introduced by Racah) using the Wigner coefficients.

Every $n \times n$ unitary matrix may be written in the form $U = \exp(iH)$, where H is Hermitian. In the vicinity of the identity, U becomes $U \cong 1 + iH$. Parametrizing H in terms of the parameters p_{ij} with $p_{ij}^* = p_{ji}$, we have

$$H = \sum_i p_{ii}e_{ii} + \sum_{i \neq j} p_{ij}e_{ij}, \tag{7}$$

where e_{ij} is the matrix consisting of unity in the (ij)th position and zeros elsewhere.

The unimodular restriction is the requirement that $\det U = 1$; this is equivalent to requiring $\operatorname{tr} H \equiv 0$, mod (2π), and we shall identify 0 and 2π as the same point in parameter space. The unimodular restriction on Eq. (7) is a requirement that $\sum_i p_{ii} = 0$, so that the number of independent parameters is $n^2 - 1$. Rather than introducing a redundant parameter (as is conventional), let us define a new basis h_i for the diagonal elements

$$h_i \equiv (2n)^{-\frac{1}{2}} \sum_{l=1}^{n} \lambda_l^{(i)} e_{ll}, \tag{8a}$$

with

$$\lambda_l^{(i)} \equiv \left[\left(\frac{2i+1}{n}\right)^{\frac{1}{2}} \times \left(\frac{n-1}{2}\ l - \frac{n+1}{2}\ i\ 0 \middle| \frac{n-1}{2}\ l - \frac{n-1}{2}\right)\right], \tag{8b}$$

where $(\cdots \mid \cdots)$ is a Wigner coefficient. The λ's have the useful properties expressed by the equations

$$\begin{aligned} \sum_{i=0}^{n-1} \lambda_l^{(i)} \lambda_m^{(i)} &= \delta_{lm}, \\ \sum_{l=1}^{n} \lambda_l^{(i)} \lambda_l^{(i)} &= \delta_{ij}, \end{aligned} \tag{8c}$$

which are a consequence of the properties of the Wigner coefficients.

[It should be noted that the particular element h_0 is a multiple of the identity ($h_0 = 2^{-\frac{1}{2}} n^{-1} E$). In order to obtain the orthonormality properties expressed by Eq. (8c), it is necessary that the index i run over 0 to $n - 1$; that is, h_0 is considered a member of the algebra. This is always possible, since the identity always occurs in the group; however, h_0 is not a generator for SU_n (This is just the unimodular restriction.) This logical distinction is important, but should not cause confusion if not stated explicitly in all cases below.]

Let us further introduce the customary designation, $e_\alpha \equiv (2n)^{-\frac{1}{2}} e_{ij}$ where α denotes now the index pair (i, j). The index pair (j, i) then denotes $e_{-\alpha}$.

The structure constants are determined by the commutation relations of the generators h_i and e_α, collectively denoted as x_A. Thus one finds

$$[h_i, h_j] = 0, \tag{9a}$$

$$[h_k, e_\alpha] = (2n)^{-\frac{1}{2}} (\lambda_i^{(k)} - \lambda_j^{(k)}) e_\alpha \equiv \alpha_k e_\alpha, \tag{9b}$$

$$\begin{aligned} &[e_\alpha, e_\beta] = (2n)^{-\frac{1}{2}} e_\gamma, \text{ if } \alpha = (kl), \beta = (lm), \gamma = (km), \\ &[e_\alpha, e_\beta] = -(2n)^{-\frac{1}{2}} e_\gamma, \\ &\qquad \text{if} \quad \alpha = (kl), \quad \beta = (mk), \quad \gamma = (ml), \\ &[e_\alpha, e_\beta] = 0 \quad \text{otherwise (and } \beta \neq -\alpha), \end{aligned} \tag{9c}$$

$$[e_\alpha, e_{-\alpha}] = \sum_i \alpha_i h_i. \tag{9d}$$

These equations determine the canonical form of the structure constants, (AB^C). (The notation is that lower-case Latin letters denote h's (and where a numerical designation is used, a Roman numeral) while the lower-case Greek letters (and European numerals) denote e's. A capital Latin index is used to denote the h's and e's collectively, i.e., x_A.) The metric, Eq. (2), has the canonical form, $g_{AB} = \delta_A^{-B}$, with the usual convention that $h_{-i} = h_i$. (It was to obtain this form that the irritating normalization $(2n)^{-\frac{1}{2}}$ had to be introduced.) Under Hermitian conjugation, the generators behave as

$$e_\alpha^\dagger = e_{-\alpha}, \; h_i^\dagger = h_i. \tag{10}$$

A representation of the infinitesimal group is then given by the correspondence

$$e_\alpha \to E_\alpha, \; h_i \to H_i, \text{ (collectively } x_A \to X_A), \tag{11a}$$

which implies that the correspondence extends to the commutators

$$[X_A, X_B] = \sum_C (AB^C) X_C. \tag{11b}$$

The finite elements of a representation G are then the matrices

$$D(g) = \exp\left(i \sum_A p_A X_A\right). \tag{12}$$

It is customary to associate with the structure constants $(i\alpha^a) \equiv \alpha_i$, the vector $\boldsymbol{\alpha}$, whose "space" is labeled by the h_i (or H_i). This leads to the *vector diagram* of Cartan. It is useful to note that $\sum_D (AB^D) g_{DC} = (ABC)$ is antisymmetric in all indices, and $A + B + C = 0$, with the convention $i \sim 0$.

Let us return now to the task of constructing invariants for SU_n. We may regard Casimir's construction [Eq. (3)], not so much as furnishing *an* invariant, but rather as a prescription for obtaining an invariant if given two "vectors," $\{X_A\}$ and $\{X_B\}$. This suggests that we agree to call a "vector with respect to SU_n", any set of operators $\{Y_A\}$ which obey the commutation relations

$$[X_A, Y_B] = \sum_C (AB^C) Y_C, \tag{13}$$

where $\{X_A\}$ are the generators of SU_n. [Naturally, for a particular representation, the matrices must all have appropriate dimension, but we would prefer to regard Eq. (13) abstractly.]

It is immediately obvious that Eq. (13), (and its evident generalization to tensors in SU_n) is simply an extension of those ideas that stem originally from the work of Pauli and Güttinger, from the Wigner–Eckart theorem, and from Racah's definition of tensor operators.

Given two such vectors, $\{Y_A\}$ and $\{Z_A\}$, Casimir's construction guarantees that the combination $\sum_{AB} g^{AB} Y_A Z_B$ is an invariant under the generators $\{X_A\}$ of SU_n. The next step is equally clear: Given two such vectors, how can one construct a third vector? In other words, what are the vector-coupling coefficients, denoted by $[AB^C]$, such that $\{W_A\}$, defined by

$$W_C \equiv \sum_{A,B} [AB^C] Y_A Z_B, \tag{14}$$

shall be a vector, if $\{Y_A\}$ and $\{Z_A\}$ are vectors.

One solution to Eq. (14) is immediate—namely, the structure constants themselves.[17] It is precisely this property that underlies the generalized Casimir invariants I_n^*.

The content of the present paper is the assertion that there exists a second, *symmetric*, solution to Eq. (14), which is defined, in analogy to the structure constants themselves, directly from the representation given by the $\{e_\alpha, h_i\}$. In particular, the explicit definition of the symmetric coupling coefficients, $[AB^C]$, is given by the *anticommutator*:

$$[x_A, x_B]_{(+)} \equiv x_A x_B + x_B x_A \equiv \sum_C [AB^C] x_C. \tag{15}$$

[Note that in Eq. (15), the sum includes h_0, i.e., the index C includes $i = 0$. Confer also the remarks after Eq. (8c).]

For the SU_n group, the coupling constants $[ABC] \equiv \sum_D [AB^D] g_{DC}$ are given by the following equations:

$$[ijk] = \left[\frac{2(2i+1)(2j+1)}{n}\right]^{\frac{1}{2}} (i0j0 \mid k0) \times W\left(\frac{n-1}{2}\, i\, \frac{n-1}{2}\, j; \frac{n-1}{2}\, k\right), \tag{16a}$$

$$[i\alpha - \alpha] = (2n)^{-\frac{1}{2}} (\lambda_l^{(i)} + \lambda_m^{(i)}), \quad \alpha = (lm), \quad l \neq m, \tag{16b}$$

$$= (2n)^{-\frac{1}{2}}, \quad \alpha + \beta + \gamma = 0, \quad \gamma \neq 0. \tag{16c}$$

[$W(\cdots)$ here denotes the Racah coefficient].

The coefficients $[ABC]$ have a number of general properties:

(a) $[ABC] = 0$ unless $A + B + C = 0$,

(b) $[ABC]$ is totally symmetric.

The proof that for SU_n, the symmetric coupling coefficients given in Eqs. (16) do indeed define a coupled vector according to Eq. (15), which satisfies the definition of a vector given by Eq. (13), is carried out in an appendix. The method is by straightforward substitution, and no doubt a more economical proof could be devised.

It is now a straightforward matter to construct a series of invariants, I_n. Such a series begins with Casimir's invariant

$$I_2 = \sum_{AB} g^{AB} X_A X_B, \tag{17a}$$

[17] A. P. Stone [Proc. Cambridge Phil. Soc. **57**, Part 3, 46ff (1961); *ibid*, 469 (1961).] has independently defined tensor operators under general semisimple Lie groups. His work is rather closely related to the antisymmetric solution to Eq. (14) discussed in the text.

proceeds to a third-order invariant

$$I_3 \equiv \sum_{AB} g^{AB} X_A X_B^{(d)} = \sum_{ABC} [ABC] X_A X_B X_C, \tag{17b}$$

and a fourth-order invariant

$$I_4 = \sum_{ABCDE} [ABC][DE - C] X_A X_B X_D X_E, \text{ etc.} \tag{17c}$$

For the SU_n group there exists only $(n - 1)$ independent invariants, whose order is $2, 3, \cdots, n$. Thus the series of invariants given in Eq. (17) necessarily must become redundant after the invariant I_n is reached. In order to prove that the series of invariants given in Eq. (17) is a suitable basis for the $(n - 1)$ invariants of the SU_n group, we must demonstrate that the invariants $I_2 \cdots I_n$ exist, and are independent. This is done in the following section.

4. PROOF OF THE SUITABILITY OF THE INVARIANTS I_n

The researches of Weyl,[18] of Coxeter,[19] and of Racah[7] have demonstrated some remarkable properties that must be possessed by the invariants of semisimple Lie groups, of their connection with the symmetry properties of the vector diagram, and of the invariants of the symmetry groups of the fundamental region of the reflection groups that define these vector diagrams.

The symmetry group (Weyl's S) of the fundamental region of the SU_n group is a group of order $n!$, the complete symmetry group of the Euclidean simplex, P_n.[20] This group [15] is defined by the abstract generator and relations

$$R_i^2 = (R_i R_j)^3 = E \qquad (i \neq j; i = 1, 2, \cdots, n - 1), \tag{18}$$

or by Coxeter's graph with $n - 1$ nodes:

•—•—• ⋯ •—• .

The characteristic roots of this group have the exponents $m_i = 1, 2, \cdots n$, which obey the general properties: (1) The product $\prod_i (1 + m_i)$ = order of the group, and (2) $\sum_i m_i$ = number of reflections that generate the group. Moreover, the degrees of the basic invariants[19] of S are $m_i + 1$.

If we note one further general property[7] of the invariants of a semisimple Lie group, the connection between the invariants of S and of G becomes clear. This is the property that the nth-order invariant of the group G when evaluated in terms of the highest weight Λ, becomes, under the substitution $\Lambda \to \Lambda - \frac{1}{2} \sum_{+ve} \alpha \equiv M$, an invariant[21] of the group S. Since, however, this substitution is equivalent to considering only the highest-order terms in the invariant—that is, only the terms in the H's alone—we need only show that the I_n when restricted to H_i define the nth-order invariants of S. This is still a sizeable task.

Upon restricting the invariants I_n to the terms involving the H_i alone—that is, the generation of the corresponding invariants of the group S—one finds that the commutability of the H's allows the replacement: $H_i \to \Lambda_i$ (the ith term of the dominant weight), and the following forms result:

$$I_2 \to J_2 = \sum_i \Lambda_i^2, \tag{19a}$$

$$I_3 \to J_3 = \sum_{ijk} [ijk] \Lambda_i \Lambda_j \Lambda_k, \tag{19b}$$

$$I_4 \to J_4 = \sum_{ijklm} [ijk][klm] \Lambda_i \Lambda_j \Lambda_l \Lambda_m, \cdots, \tag{19c}$$

$$I_n \to J_n = \sum_{\substack{\text{all} \\ \text{indices}}} [i_1 i_2 j_1][j_1 i_3 j_2][j_2 i_4 j_3] \cdots \times [j_{n-2} i_{n-1} i_n] \Lambda_{i_1} \Lambda_{i_2} \cdots \Lambda_{i_n}. \tag{19d}$$

These invariants are quite complicated to discuss in the form in which they appear in Eqs. (19). We may, however, avail ourselves of the definition of the $[ijk]$ to put these results in a more tractable form. That is, we utilize Eq. (15), and the commutability of the h_i, to write first

$$2 h_i h_j = \sum_k [ijk] h_k, \tag{15'}$$

and then, using Eqs. (8),

$$[ijk] = 2 \text{ tr } (h_i h_j h_k). \tag{20}$$

Introducing this result into Eq. (19b) for J_3, we find that this invariant may be written in a very suggestive form:

$$J_3 = 2 \text{ tr } (\sum_{ijk} h_i h_j h_k \Lambda_i \Lambda_j \Lambda_k). \tag{21}$$

It is apparent that one should introduce a notation

[18] H. Weyl, lecture notes, The Institute for Advanced Study, Princeton, New Jersey, 1935 (unpublished); E. Cartan, Bull. Sci. Math. 2, 49 (1925). (This reference is quoted in Weyl, reference 18a)

[19] The researches of Coxeter referred to, span a number of years. A complete referencing (and discussion) is contained in the Ergebnisse series [H. S. M. Coxeter and W. O. J. Moser, *Generators and Relations for Discrete Groups* (Springer-Verlag, Berlin, 1957), Vol. 14, Chap. 9]. See also the paper by H. S. M. Coxeter, Can. J. Math. 9, 243 (1957) and the recent paper by H. S. M. Coxeter, Arch. Math. **XIII**, Fasc. 1, p. 86, (1962).

[20] H. S. M. Coxeter, *Regular Polytopes* (Pitman Publishing Corporation, New York, 1947).

[21] The validity of this property in the form stated is not, in fact, essential to the present proofs.

for the sum $\Lambda_i h_i$: we let

$$A \equiv \sum_i \Lambda_i h_i, \tag{22}$$

and then J_3 assumes the form

$$J_3 = 2 \text{ tr } (A^3). \tag{21'}$$

It is quickly seen that $J_2 = \text{tr } (A^2)$, using the properties expressed in Eqs. (8). The remaining invariants are, however, *not* in this simple form. For example, one finds that

$$J_4 = 4 \text{ tr } (A^4) - 4(J_2)^2. \tag{19c'}$$

The difficulty this poses is easily remedied, since the introduction of lower invariants does not affect the suitability of the J_n as a basis. Similarly, the numerical factors are not essential. We therefore replace the J_n by the equivalent set K_n, defined as

$$K_n = \text{tr } (A^n). \tag{23}$$

The proof of the suitability of the K_n will be demonstrated if we show that the Jacobian of the invariants, K_n, with respect to the weights, Λ_i, does not vanish. One may, however, prove a much more interesting result which explicitly illustrates a theorem of Coxeter.[19] Coxeter has shown that the Jacobian of the invariants of the general irreducible finite groups of the form of Eq. (18) *factorizes* into $\sum m_i$ [$=\frac{1}{2}n(n-1)$ for SU_n] linear forms, which when equated to zero, give the reflecting hyperplanes that generate S. It is sufficient to demonstrate then that the Jacobian of the set K_n possesses this remarkable property.

The (diagonal) matrix A has for its elements n linear forms in the components of the weight vector Λ. Only $n-1$ of these linear forms are independent, however. Rather than deal with the components Λ_i directly, it is expedient to use the multiplicative property of the Jacobian to deal directly with these linear forms. Defining the linear form that appears in the ith diagonal of A as $f_i(\Lambda)$, one has

$$A_{ii} \equiv f_i(\Lambda) = \sum_j \Lambda_j \lambda_i^{(j)}, \quad i = 1 \cdots n-1, \tag{24a}$$

$$A_{nn} = -\sum_{i=1}^{n-1} f_i, \tag{24b}$$

using Eqs. (8a) and discarding the factor $(2n)^{-\frac{1}{2}}$ as irrelevant. The desired Jacobian is then

$$\frac{\partial(K_2 K_3 \cdots K_n)}{\partial(\Lambda_1 \Lambda_2 \cdots \Lambda_{n-1})} = \frac{\partial(K_2 \cdots K_n)}{\partial(f_1 \cdots f_{n-1})} \cdot \frac{\partial(f_1 \cdots f_{n-1})}{\partial(\Lambda_1 \cdots \Lambda_{n-1})}. \tag{25}$$

The last Jacobian in Eq. (25) is just the $i = 0$, $j = 0$ cofactor of the complete matrix of the $\lambda_j^{(i)}$, and using the fact that this $n \times n$ matrix is real and orthogonal, with $\lambda_j^{(0)} = (n)^{-\frac{1}{2}}$, it follows that this Jacobian never vanishes.

The Jacobian $\partial K/\partial f$ has the form ($\sum$ denotes the sum $\sum_{i=1}^{n-1} f_i$)

$$\bar{J} \equiv \frac{1}{n!} \frac{\partial(K_2 K_3 \cdots K_n)}{\partial(f_1 f_2 \cdots f_{n-1})} = \begin{vmatrix} f_1 + \sum, & f_1^2 - \sum^2, & f_1 + \sum^3, \cdots f_1^{n-1} + (-)^n \sum^{n-1} \\ f_2 + \sum, & f_2^2 - \sum^2, & \\ \vdots & \vdots & \\ f_{n-1} + \sum, & f_{n-1}^2 - \sum^2, & \cdots f_{n-1}^{n-1} + (-)^n \sum^{n-1} \end{vmatrix}. \tag{26}$$

By multiplying the first column by powers of $\sum$, and adding to the other columns, this determinant assumes the form

$$\bar{J} = \begin{vmatrix} f_1 + \sum & (f_1 + \sum) f_1 & f_1^3 - f_1 \sum^2 \cdots f_1 (f_1^{n-2} + (-)^{n-1} \sum^{n-2}) \\ f_{n-1} + \sum & (f_{n-1} + \sum) f_{n-1} & \cdots \end{vmatrix}. \tag{27}$$

It is clear that each row has a factor of the form $(f_i + \sum)$. Thus $\bar{J}$ now becomes

$$\bar{J} = \left(\prod_{i=1}^{n-1} (f_i + \sum) \right) \times \begin{vmatrix} 1 & f_1 & f_1(f_1 - \sum) & \cdots \\ 1 & f_{n-1} & f_{n-1}(f_{n-1} - \sum) & \cdots \end{vmatrix} \tag{28}$$

[To be quite complete, it should be noted that the general term in the determinant in Eq. (28) has the form: $f_i(f_i^k + (-)^{k-1} \sum^k)/(f_i + \sum)$, which, of course, is a polynomial.] With obvious manipulations, the determinant in (28) may be put in the form of Vandermonde's determinant, that is

$$\det \text{ in Eq. (28)} = \prod_{i<j} (f_i - f_j), \quad i, j = 1, \cdots, n-1. \tag{29}$$

The final result is that the Jacobian assumes a completely factored form. In order to express this most simply, we observe that the h_i are traceless, so that the linear forms, $f_i + \sum_{i=1}^{n-1} f_i$, in Eq. (28), are simply $f_i - f_n$. Hence the Jacobian is finally

$$\frac{\partial(K_2 \cdots K_n)}{\partial(f_1 \cdots f_{n-1})} = n! \prod_{i>j} (f_i - f_j)$$
$$i, j = 1, \cdots n. \qquad (30)$$

This is a product of $\frac{1}{2}n(n-1)$ linear forms in the components of the weight vector Λ, and noting the definition of the root vectors $\{\alpha_i\}$ in Eq. (9b), one sees that each linear form in Eq. (30), when set to zero, is precisely the hyperplane perpendicular to the root vector $\alpha = (ji)$.

This demonstrates that the invariants defined by the J_n are a suitable basis for *all* the invariants of S, and it then follows that the I_n defined by Eqs. (17) are similarly a suitable basis for all the invariants of the group SU_n.

5. ACKNOWLEDGMENTS

It probably needs little emphasis that the present work is heavily indebted to the classic researches of Weyl, Wigner, and Racah, and especially to their (unpublished) lectures, which have been the direct source for the results obtained above.

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APPENDIX A

Let $\{W_A\}$ be defined by the equation

$$W_C = \sum_{AB} [AB^C] Y_A Z_B, \qquad (A1)$$

where $[AB^C]$ are the symmetric coupling coefficients given in Eq. (16). It is the object of this appendix to show that $\{W_A\}$ is a vector, i.e.,

$$[X_A, W_B] = \sum_C (AB^C) W_C, \qquad (A2)$$

if $\{Y_A\}$ and $\{Z_A\}$ are vectors. We must show therefore that

$$\sum_{A,B,E} [AB^C]((DA^E) Y_E Z_B + (DB^E) Y_A Z_E)$$
$$= \sum_{A,B,E} (DC^E)[AB^E] Y_A Z_B. \qquad (A3)$$

To demonstrate (A3), it is sufficient to show that the coefficients of the independent terms in YZ vanish. Using the metric tensor to lower indices, and the symmetry of the various coefficients, this is equivalent to showing that the expression

$$\sum_E \{(DEC)[ABE] + (DE - A)[B - CE]$$
$$+ (DE - B)[A - CE]\} = 0 \qquad (A4)$$

vanishes for all values of A, B, C, D. The proof will consist of examining the various possible cases separately.

(a) Consider $[X_j, W_{nm}]$, i.e., $D = j$ and $c = nm$ in (A4).

This is the simplest case, since it corresponds to the generalization of the "magnetic quantum-number rule" that applies to the Wigner coefficients. In the case of (A4), this takes the form

$$\sum_E (\cdots) = \sum_E \{(j\,E\,nm)[ABE] + (j\,E\,-A)$$
$$\times [B\,mn\,E] + (j\,E\,-B)[A\,mn\,E]\}$$
$$= (j\,mn\,nm)[AB\,mn] + (j\,A\,-A)$$
$$\times [B\,mn\,A] + (j\,B\,-B)[A\,mn\,B]$$
$$= [AB\,mn]\{(j\,mn\,nm)$$
$$+ (j\,A\,-A) + (j\,B\,-B)\}, \qquad (A5)$$

and the term in brackets is now seen to vanish, whenever the coefficient $[AB\ nm]$ is nonzero, i.e., whenever $A + B + (mn) = 0$.

Although the notation implies that $n \neq m$ (that is, $c = \gamma$), the result is clearly valid for $n = m$ (that is, $c = k$). Thus $[X_j, W_k]$ and $[X_j, W_\alpha]$ have been shown to be correct.

(b) Consider next the case $[X_\alpha, W_{-\alpha}]$, i.e., $C = nm$ and $D = mn$, $m \neq n$.

In this case, (A4) becomes

$$\sum_E (\cdots) = \sum_i \left(\frac{\lambda_n^{(i)} - \lambda_m^{(i)}}{(2N)^{\frac{1}{2}}}\right)[ABi]$$
$$+ \sum_E (mn\,E\,-A)[B\,mn\,E]$$
$$+ \sum_E (mn\,E\,-B)[A\,mn\,E]. \qquad (A6)$$

There are only two cases to examine: (1) $A = j$, $B = k$; and (2) $A = -B \neq i, j$.

For the first case, (A6) becomes (discarding $(2N)^{-\frac{1}{2}}$)

$$\sum_i (\lambda_n^{(i)} - \lambda_m^{(i)})[jki] + (\lambda_m^{(j)} - \lambda_n^{(j)})[k\ mn\ nm] + (\lambda_m^{(k)} - \lambda_n^{(k)})[j\ mn\ nm] = \sum_i (\lambda_n^{(i)} - \lambda_m^{(i)})[jki] + \frac{(\lambda_m^{(j)} - \lambda_n^{(j)})(\lambda_m^{(k)} + \lambda_n^{(k)})}{(2N)^{\frac{1}{2}}} + \frac{(\lambda_m^{(k)} - \lambda_n^{(k)})(\lambda_m^{(j)} + \lambda_n^{(j)})}{(2N)^{\frac{1}{2}}}. \quad \text{(A7)}$$

Using the identity

$$\lambda_m^{(j)}\lambda_m^{(k)} = \sum_r (N/2)^{\frac{1}{2}}\lambda_m^{(r)}[jkr], \quad \text{(A8)}$$

the latter two groups of terms in (A7) are seen to cancel the first summation.

For the second case $A = -B = (rs)$, $r \neq s$, the summation over i in (A6) is seen to have the form

$$\sum_i (\cdots) = \sum_i \left(\frac{\lambda_n^{(i)} - \lambda_m^{(i)}}{(2N)^{\frac{1}{2}}}\right)\left(\frac{\lambda_r^{(i)} + \lambda_s^{(i)}}{(2N)^{\frac{1}{2}}}\right) = \frac{1}{2N}(\delta_r^n + \delta_s^n - \delta_r^m - \delta_s^m), \quad \text{(A9)}$$

using the properties of the λ's expressed by Eqs. (8).

Consider now the first of the sums over E in (A6), that is,

$$\sum_E (mn\ E - A)[B\ mn\ E] = \frac{1}{2N}(\delta_r^m - \delta_s^n). \quad \text{(A10)}$$

This result, and a similar result for the second sum over E shows that (A6) again vanishes.

These results show that $[X_\alpha, W_{-\alpha}]$ is correctly given.

(c) Consider now the case $[X_\alpha, W_i]$, i.e., $C = i$ and $D = mn$, $m \neq n$. For this case, (A6) assumes the form

$$(i\ mn\ nm)[AB\ nm] + \sum_E (mn\ E - A)[B\ i\ E] + \sum_E (mn\ E - B)[A\ i\ E]. \quad \text{(A11)}$$

There are four instances to verify: (1) $A = j$, $B = k$; (2) $A = (ab)$, $B = j$; (3) $A = j$, $B = ab$; and (4) $A = ab$, $B = cd$. Of these, the second and third are equivalent. The first is easily eliminated since it requires $m = n$, contrary to hypothesis. For the second case, (A11) becomes

$$(i\ mn\ nm)[ab\ j\ nm] + \delta_{ab}^{mn}\sum_k (k\ nm\ mn)[jik] + (j\ mn\ nm)[ab\ i\ nm]. \quad \text{(A12)}$$

Using the identity in (A8) once again, one finds

$$(i\ mn\ nm)[ab\ j\ nm] + (j\ mn\ nm)[ab\ i\ nm] = \delta_{ab}^{mn}\cdot\frac{1}{N}\cdot(\lambda_m^{(i)}\lambda_m^{(j)} - \lambda_n^{(i)}\lambda_n^{(j)}) = (2N)^{-\frac{1}{2}}\sum_k (\lambda_m^{(k)} - \lambda_n^{(k)})[ijk] = \sum_k (k\ mn\ nm)[ijk]. \quad \text{(A13)}$$

This latter result is seen to cancel with the remaining sum in (A12).

For the fourth instance, $A = ab$, $B = cd$, and (A11) becomes

$$(i\ mn\ nm)[ab\ cd\ nm] + (2N)^{-\frac{1}{2}}\{\delta_a^m[cd\ i\ nb] - \delta_b^n[cd\ i\ am]\} + (2N)^{-\frac{1}{2}}\{\delta_c^m[ab\ i\ nd] - \delta_d^n[ab\ i\ cm]\}.$$

Using the definitions of the coefficients, these terms are all seen to cancel out.

(d) The final case to be treated involves $[X_\beta, W_\alpha]$, $\beta + \alpha \neq 0$, i.e., $D = rs$, $C = mn$. Just as in case (c) above, there are four instances to examine, of exactly the same type as in case (c). The method of proof is just the same also, and no new relations are required. It is of little value to repeat this substitution and evaluation, except for the assertion that it is found that (A6) once again vanishes.

The form of these results makes one suspect there is a simple underlying reason which could lead to a more economical and satisfying proof. The fact that a totally symmetric and a totally antisymmetric form are being combined is presumably the basic cause for (A6) vanishing identically. On the other hand, this explicit proof has the advantage of illustrating several nice properties of the canonical form of the $\{h_i, e_\alpha\}$.

APPENDIX B

It is interesting to consider a little further the question as to why the invariants defined by the adjoint representation were unsuitable. For the SU_3 group, one can show (by direct calculation) that Eq. (6) defines only *even*-order invariants, and that only the second and sixth-order invariants are independent, the fourth-order invariant of Eq. (6) being exactly the square of the second order (Casimir) invariant. Since (as given in Sec. 4 above), the canonical invariants for SU_3 are of the second and third order, the lack of odd-order invariants in Eq. (6) is suggestive. It suggests, loosely speaking, that the invariants of the adjoint group are some-

how invariant under a reflection not in the original group G.

This vague statement may be replaced by the more precise considerations[18] of *the group of automorphisms of the group G*. It is readily seen that an automorphism of the group G defines an automorphism of the infinitesimal group, $\mathfrak{G}$, (whose elements are $\{X_A\}$). One distinguishes the *inner* automorphisms—those produced by conjugation—from the *outer* automorphisms (all others). Moreover, one may consider automorphisms in the neighborhood of the identical automorphism; these are called the infinitesimal automorphisms of $\mathfrak{G}$. Cartan[18] has proved: The infinitesimal automorphisms of semisimple infinitesimal group are all inner-infinitesimal automorphisms, $x \to [a, x]$ of $\mathfrak{G}$.

This is relevant to the problem of constructing invariants in that there may exist *outer* automorphisms with the property that the elements $\{X_A\}$ are carried into their negatives. (For example, "time reversal" in R_3, $\mathbf{J} \to -\mathbf{J}$; in SU_3 there exists an outer automorphism cyclically interchanging the E_α's is into their negatives.) The precise statement of the relevance of outer automorphisms is contained in a result given by Weyl,[18] to the effect that the invariants of the characteristic polynomial of the adjoint representation [Eq. (6)] are also invariant under *outer* automorphisms of G.[22]

Weyl went on to show that the adjoint group, A, is a subgroup of the automorphism group of G, namely the subgroup of those elements which can be connected with the unit element (the identical automorphism).

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[22] To be quite precise, Weyl stated this result only for the quadratic invariant, but it is clear that it is more general.

Moments of the Neutron Time–Energy Distribution and the Use of Random Functionals

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The time moments of the neutron time–energy distribution are derived under the following conditions: infinite homogeneous moderator with no absorption, elastic scattering, and distribution of scattering angle independent of energy in center-of-mass frame. However, no assumption is made on the variation of the scattering cross section with energy. This is in contrast to previous papers in which a scattering cross section proportional to v^δ (δ any real number) is assumed. The moments are derived in two ways: first, by means of Laplace transforms, and then through the use of random functionals. Random functionals have not been previously employed in neutron moderation theory and they offer certain advantages which are discussed.

INTRODUCTION

A number of recent papers have been devoted to the analysis of the time-dependent slowing down of neutrons. Common to all these papers (and to ours) is the assumption of an infinite homogeneous moderator consisting of free neutrons at rest. For the case of no absorption, isotropic scattering in the center-of-mass (c.m.) frame, and a scattering cross section varying like v^δ (δ any real number). Waller[1] obtained an exact expression for the distribution function. Eriksson,[2] using this expression, considered both the positive and negative time moments. Their method was based on the use of Laplace transforms. Guth and Inönü[3] have recently applied the group-theoretical methods of Wigner[4] to various problems in neutron moderation. They obtain (among others) results similar to those of Eriksson; however, somewhat weaker conditions are imposed on the distribution of the scattering angle (it need only be energy independent).

The present paper is divided essentially into two parts. In Section I retaining the assumptions of Guth and Inönü (cf. below), but now allowing the scattering cross section to vary in an *arbitrary* way, expressions for the time moments are obtained. These formulas lend themselves rather readily to numerical calculation and also to *asymptotic evaluation* in the limit of large lethargies (low energy). The approach here is fairly standard, involving the judicious application of Laplace transforms to a transport equation.

In Section II, we consider the use of stochastic methods. We prove that finding the neutron time–energy distribution function is equivalent to finding the distribution of a certain *random functional.* The formulation of problems in terms of random functionals represents a prominent trend in recent mathematical physics.[5] This trend, however, has not previously appeared in neutron moderation theory even though—at least in the present context—the use of random functionals has at least two important advantages: (1) The moments may be calculated in a very transparent way and the physical meaning of the results becomes very clear; (2) Side conditions on the energy (e.g. requiring the neutron to have a given energy after a specific collision) can be readily taken into account.

I. THE TIME MOMENTS

Consider an infinite, homogeneous moderator consisting of free atoms at rest, and suppose that at time $t = 0$, Q neutrons with the definite velocity v_0 enter this medium. Through collisions with the atomic nuclei, these neutrons will slow down. Let v be the neutron velocity, and $u = \ln(v_0/v)$ its *lethargy*, so that for any neutron, u is a non-decreasing function of time.

The distribution of neutron lethargies at any time $t \geq 0$ is most conveniently described by means of $F(u, t)$: the average number of neutron collisions per unit lethargy interval and time interval. Supposing that absorption can be neglected, and that all collisions are elastic with scattering isotropic in the c.m. frame, the *collision density* $F(u, t)$ satisfies the following equation[6]:

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[1] I. Waller (unpublished).
[2] K. E. Eriksson, Arkiv Fysik **16**, 1 (1959).
[3] E. Guth and E. Inönü, J. Math. Phys. **2**, 451 (1961).
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[5] I. M. Gelfand and A. M. Yaglom, J. Math. Phys. **1**, 48 (1960).
[6] R. E. Marshak, Rev. Mod. Phys. **19**, 185 (1947).

$$F(u, t) = Q\delta(u)\delta(t) + \int_0^t dt' \int_0^u f(u - u')e^{-\Sigma(u)v(t-t')}F(u', t')\, du'. \quad (1)$$

$\Sigma(u)$ is the macroscopic scattering cross section, and $f(\Delta u) = f(u - u')$ is the probability density of the neutron lethargy increase Δu at a collision:

$$f(\Delta u) = \begin{cases} \dfrac{(M+1)^2}{4M} e^{-\Delta u} & 0 \le \Delta u \le \ln\left(\dfrac{M+1}{M-1}\right)^2 \\ 0 & \text{otherwise,} \end{cases} \quad (2)$$

M being the atomic weight of the nuclei.

Though (2) represents the physically most important case, it is not at all necessary that $f(\Delta u)$ have this form. All that we need is that $f(\Delta u)$ in fact depends only on Δu and not on the lethargy of the neutron u' before collision (i.e. u' and Δu should be independent random variables). For this to be true, it is enough that the distribution of the scattering angle in the c.m. frame be independent of energy.

It will be of use to introduce a function $W(u, t)$ such that $W(u, t)\, du$ is the average number of neutrons per unit time interval which have just acquired a lethargy in the range $(u, u + du)$. Since it is these neutrons which at their next collision contribute to $F(u, t)$, we have the relations

$$F(u, t) = \int_0^t e^{-\Sigma(u)v(t-t')}\Sigma(u)vW(u, t')\, dt', \quad (3)$$

$$W(u, t) = Qf(u)e^{-\Sigma_0 v_0 t}\Sigma_0 v_0 + \int_0^t dt' \int_0^u f(u - u')e^{-\Sigma(u')v'(t-t')} \times \Sigma(u')v'W(u', t')\, du'. \quad (4)$$

In Eq. (4), v' is the velocity corresponding to lethargy u' ($v' = v_0 e^{\frac{1}{2}u'}$), and we are considering only those neutrons which have made at least one collision.

We proceed to calculate the time moments $\langle t^i(u)\rangle$ given by

$$\langle t^i(u)\rangle = \frac{\int_0^\infty t^i F(u, t)\, dt}{\int_0^\infty F(u, t)\, dt}. \quad (5)$$

To this end, we define functions $W^{(i)}(u)$ by

$$W^{(i)}(u) = \int_0^\infty t^i W(u, t)\, dt \quad (j = 0, 1, 2 \cdots). \quad (6)$$

In particular, we denote $W^{(0)}(u)$ by simply $W(u)$. This function gives the number of neutron collisions per unit lethargy interval and it enters in a crucial way in our analysis. It was first studied by Placzek[7] for the case of isotropic scattering in the c.m. frame.

Let $\Psi(u, r)$ be the Laplace transform with respect to r:

$$\Psi(u, r) = \int_0^\infty e^{-rt}W(u, t)\, dt. \quad (7)$$

An integral equation for $\Psi(u, r)$ can be obtained by the transform of Eq. (4), using the convolution theorem[8] and noting that

$$\int_0^\infty \exp\,[\Sigma(u)vt]e^{-rt}\, dt = \frac{1}{r + \Sigma(u)v}.$$

Thus,

$$\Psi(u, r) = Qf(u)\Sigma_0 v_0/(r + \Sigma_0 v_0) + \int_0^u f(u - u')\frac{\Sigma(u')v'}{r + \Sigma(u')v'}\Psi(u', r)\, du'. \quad (8)$$

It follows from (7) that the $W^{(i)}(u)$ and the derivatives of $\Psi(u, r)$ are related by

$$W^{(i)}(u) = (-1)^i[\partial^i\Psi(u, r)/\partial r^i]_{r=0}. \quad (9)$$

Let us denote, below, the Laplace transform of any function, say $g(u)$, by $\mathfrak{L}[g(u)]$. Setting $r = 0$ in (8) and using (9) for $j = 0$, one finds that

$$W(u) = Qf(u) + \int_0^u f(u - u')W(u')\, du'. \quad (10)$$

Hence, if $\varphi = \mathfrak{L}[f(u)]$, we have, again using the convolution theorem in Eq. (10),

$$\mathfrak{L}[W(u)] = Q\varphi + \varphi\mathfrak{L}[W(u)]$$
$$\mathfrak{L}[W(u)] = Q\varphi/(1 - \varphi), \quad (11)$$

a well known result.[6] $W^{(1)}(u)$ may be found by differentiating Eq. (9) with respect to r, setting $r = 0$ and replacing Ψ, $-\partial\Psi/\partial r$ by $W(u)$, $W^{(1)}(u)$, respectively. Thus,

$$W^{(1)}(u) = \frac{f(u)Q}{\Sigma_0 v_0} + \int_0^u f(u - u')W^{(1)}(u')\, du' + \int_0^u f(u - u')\frac{W(u')}{\Sigma(u')v'}\, du', \quad (12)$$

or

$$\mathfrak{L}[W^{(1)}(u)] = \frac{\varphi Q}{\Sigma_0 v_0} + \varphi\mathfrak{L}[W^{(1)}(u)] + \varphi\mathfrak{L}\left[\frac{W(u)}{\Sigma(u)v}\right].$$

[7] G. Placzek, Phys. Rev. **69**, 423 (1946).
[8] I. Sneddon, *Fourier Transforms* (McGraw-Hill Book Company, Inc., New York, 1951.), p. 3.

Hence,

$$\mathfrak{L}[W^{(1)}(u)] = \frac{\varphi}{1-\varphi}\frac{Q}{\Sigma_0 v_0} + \frac{\varphi}{1-\varphi}\mathfrak{L}\left[\frac{W(u)}{\Sigma(u)v}\right]. \quad (13)$$

Recalling Eq. (11), we can invert (13) to obtain

$$W^{(1)}(u) = \frac{W(u)}{\Sigma_0 v_0} + \int_0^u \frac{W(u-u')W(u')}{\Sigma(u')v'}\,du'. \quad (14)$$

In exactly the same way we can obtain an expression for $W^{(i)}(u)$ in terms of $W(u)$, $W^{(1)}(u)$, $\cdots$, $W^{(i-1)}(u)$. Differentiating (9) j times, using Leibniz's rule to evaluate

$$\frac{\partial^n}{\partial r^n}\left[\frac{\Psi(r,u)}{\Sigma(u)v + r}\right],$$

making use of (8), and then taking Laplace transforms, we have

$$\mathfrak{L}[W^{(j)}(u)] = \frac{j!\varphi Q}{1-\varphi}\left(\frac{1}{\Sigma_0 v_0}\right)^j + \sum_{i=0}^{j-1}\frac{j!}{i!}\frac{\varphi}{1-\varphi}\mathfrak{L}\left[\left(\frac{1}{\Sigma(u')v'}\right)^{j-i}W^{(i)}(u')\right]. \quad (15)$$

Finally,

$$W^{(j)}(u) = \frac{j!W(u)}{(\Sigma_0 v_0)^j} + \sum_{i=0}^{j-1}\frac{j!}{i!}\int_0^u \frac{W(u-u')W^{(i)}(u')}{[\Sigma(u')v']^{j-i}}\,du'. \quad (16)$$

Returning to Eq. (3), we can find by means of (16), the moments $\langle t^i(u)\rangle$. Let us first note that if $\Theta(u, r)$ is the Laplace transform of $F(u, t)$ with respect to t; then

$$\Theta(u,r) = \frac{\Sigma(u)v}{\Sigma(u)v + r}\Psi(r,u). \quad (17)$$

It follows at once from (17), on setting $r = 0$, that

$$\int_0^\infty F(u,t)\,dt = \int_0^\infty W(u,t)\,dt = W(u). \quad (18)$$

From (5), (8), and (18) we obtain the following expression for the moments $\langle t^i(u)\rangle$:

$$\langle t^i(u)\rangle W(u) = \sum_{i=0}^{j}\frac{j!}{i!}\frac{W^{(i)}(u)}{[\Sigma(u)v]^{j-i}} \quad (19)$$

Equations (16) and (19) give a set of recurrence relations from which the moments $\langle t^i(u)\rangle$ may be calculated. If the cross section has certain functional forms, it is possible to express the moments as inverse Laplace transforms of known quantities. Such is the case if $\Sigma(u)v \sim e^{-\lambda u}$ (λ any real number), for then

$\mathfrak{L}[(\Sigma(u'(v')^{i-j}W^{(i)}(u)]$ is simply related to $\mathfrak{L}[W^{(1)}(u')]$, and the recurrence relations (15) may be solved to obtain $\mathfrak{L}[W^{(i)}(u)]$ explicitly, and also $\mathfrak{L}[\langle t^i(u)\rangle W(u)]$. If this is done, Eriksson's result is obtained.

However, there does not seem to us to be any particular advantage in having such a representation even when it is possible. For numerical purposes, (19) is more convenient, unless one wanted to find a given moment without first obtaining the preceding ones. Furthermore, a rather complete treatment of the asymptotic behavior of $\langle t^i(u)\rangle$ for large u (low energy) can be given on the basis of Eq. (15). Since we intend to do this elsewhere, the details are not given here.

II. THE USE OF RANDOM FUNCTIONALS

The preceding analysis was based on the transport equation (1). We will now use directly the fact that neutron moderation is a stochastic process by regarding the time required by the neutron to slow down to a given lethargy as the sum of a number of elementary random events.

First, we will need to reinterpret the functions $F(u, t)$, $W(u)$. This is because their definitions involved the phrase "number of neutrons" while here the quantities of interest are probability distributions over the ensemble of all possible ways a given neutron may slow down.

Consider an interval of positive numbers I, of length $L(I)$, and let $P(I)$ be the probability that a neutron will, during its history, have a lethargy lying in I. If $L(I)$ exceeds the maximum possible neutron lethargy gain at a collision, then obviously $P(I) = 1$; otherwise $P(I) < 1$. Now let the interval I contract to a point u, so that $L(I) \to 0$ and let

$$W(u) = \lim_{L(I)\to 0}\frac{P(I)}{L(I)}.$$

It is not difficult to see from this definition that $W(u)$ coincides with the function $W(u)$ (with $Q = 1$) above. But, this can also be shown by noting that if $L(I)$ is sufficiently small, the probability of a neutron having a lethargy in I after more than one collision is $O[L(I)^2]$ i.e., it is negligible. Hence, letting $W_n(u)$ be the probability density of the neutron lethargy at the nth collision,

$$P(I) = L(I)\sum_{n=1}^{\infty} W_n(u) = L(I)W(u).$$

Since $W_1(u) = f(u)$, one easily verifies that

$$W(u) = \sum_{n=1}^{\infty} W_n(u)$$

satisfies Eq. (10).

$F(u, t)$ is not a probability density since it is not normalized [$\int_0^\infty F(u, t)\, dt = W(u)$]. But

$$F(t \mid u) = F(u, t)/W(u)$$

is, and it has the following meaning: $F(t \mid u)$ is the probability density of the time that a neutron with lethargy u makes a collision, *given* that the neutron does, at some moment, have the lethargy u. The moments $\langle t^j(u)\rangle$ of Sec. I are, of course, identical to those of $F(t \mid u)$ and these we proceed to find.

Let t_j be the time of the neutron's jth collision so that

$$t_j = \Delta t_1 + \Delta t_2 + \cdots + \Delta t_j, \tag{20}$$

where $\Delta t_i = t_i - t_{i-1}$.

The Δt_i are random variables with probability density $\exp\,[-v_{i-1}\ \Sigma\ (u_{i-1})t]v_{i-1}\ \Sigma\ (u_{i-1})$; $u_i(v_i)$ is the lethargy (velocity) just after the ith collision. Because of this dependence of the distribution of Δt_i on u_{i-1}, t_j is a function not only of $\Delta t_i (i = 1, \cdots, j)$ but also implicitly of $u_i (i = 1, \cdots j - 1)$. It will be convenient to make this latter dependence explicit in the following way. We introduce random variables $\Delta\tau_i$ related to Δt_i by

$$\Delta t_i = \frac{\Delta\tau_i}{\Sigma(u_{i-1})v_{i-1}}. \tag{21}$$

The $\Delta\tau_i$ then have identical distributions with densities $e^{-\Delta\tau_i}$ independent of u_i, and (20) becomes

$$t_j = \frac{\Delta\tau_1}{\Sigma(u_0)v_0} + \frac{\Delta\tau_2}{\Sigma(u_1)v_1} + \cdots + \frac{\Delta\tau_j}{\Sigma(u_{j-1})v_{j-1}}. \tag{22}$$

The variable $\Delta\tau_i$ has a simple physical meaning: By (21), it would be the time between the $(i - 1)$st and ith collision in a fictitious medium with a cross section $\Sigma(u) \sim 1/v$ (and with units chosen so that the proportionality constant is unity). In a similar way

$$\tau_j = \sum_{i=1}^{j} \Delta\tau_i$$

corresponds to t_j.

Writing $\Delta\tau_i = \tau_i - \tau_{i-1}$, substituting in (22) and transforming slightly, we obtain

$$t_j = \frac{\tau_j}{\Sigma(u_{j-1})v_{j-1}} - \sum_{i=1}^{j-1}\left[\frac{1}{\Sigma(u_i)v_i} - \frac{1}{\Sigma(u_{i-1})v_{i-1}}\right]\tau_i. \tag{23}$$

Now, let us impose the requirement that u_{j-1} has some given value, say u, and introduce the function $\tau_s(u')(0 \le u' \le u)$ defined by $\tau_s(u') = \tau_i$ if $u_{i-1} \le u' < u_i$. $\tau_s(u')$ would therefore be in a medium with cross section $1/v$, the time at which a neutron first slows down to a lethargy u' or greater.

The expression

$$\sum_{i=1}^{j-1}\left[\frac{1}{\Sigma(u_i)v_i} - \frac{1}{\Sigma(u_{i-1})v_{i-1}}\right]\tau_i$$

can be written as

$$\int_0^u \frac{d}{du'}\left[\frac{1}{\Sigma(u')v'}\right]\tau_s(u')\, du',$$

where we have used the fact that $u_{j-1} = u$.

Finally, denote t_j by $t(u)$ to indicate that this is the time at which a neutron with lethargy u makes a collision; and similarly denote τ_j by $\tau_j(u)$. Then (23) becomes

$$t(u) = \frac{\tau(u)}{\Sigma(u)v} - \int_0^u \frac{d}{du'}\left[\frac{1}{\Sigma(u')v'}\right]\tau_s(u')\, du'. \tag{24}$$

Note that in Eq. (24), the variable giving the number of collisions made by the neutron no longer appears. Let us then drop the requirement that the lethargy u be attained at the jth collision, and merely demand that there be *some* collision just after which the neutron has the lethargy u. Then $t(u)$ is the time at which such a neutron makes its next collision. Therefore, $t(u)$ has the probability density $F(t \mid u)$; $\tau(u)$ is the analogous quantity for a medium with cross section $1/v$, [i.e., its distribution coincides with that of $t(u)$ if $\Sigma(u) = 1/v$].

Let us find $\langle t(u)\rangle$. From (24) we have

$$\begin{aligned}\langle t(u)\rangle &= \frac{\langle\tau(u)\rangle}{\Sigma(u)v} - \int_0^u \frac{d}{du'}\left[\frac{1}{\Sigma(u')v'}\right]\langle\tau_s(u')\rangle\, du' \\ &= \frac{\langle\tau(u)\rangle - \langle\tau_s(u)\rangle}{\Sigma(u)v} - \frac{\langle\tau_s(0)\rangle}{\Sigma_0 v_0} \\ &\quad + \int_0^u \frac{1}{\Sigma(u')v'}\frac{d}{du'}\langle\tau_s(u')\rangle\, du'. \end{aligned}\tag{25}$$

But $\tau(u) - \tau_s(u)$ would be, if $\Sigma(u) = 1/v$, just the time inteval between the collision at which the lethargy u is attained and the next collision, so that $\langle\tau(u) - \tau_s(u)\rangle = 1$. Similarly $\langle\tau_s(0)\rangle = 1$. To obtain $\frac{d}{du'}\langle\tau_s(u')\rangle$, observe that

$$\frac{d}{du'}\langle\tau_s(u')\rangle = \lim_{h\to 0}\langle\tau_s(u' + h) - \tau_s(u')\rangle/h.$$

But $\tau_s(u' + h) - \tau_s(u')$ vanishes unless the neutron slows down past u' and past $u' + h$ at different collisions; or equivalently, unless the neutron has after some collision, a lethargy in the interval $(u', u' + h)$. Let us denote the probability of this last event for sufficiently small h by $P(u' \mid u)h$. Now, by the definition of $W(u')$ it might appear that $P(u' \mid u) = W(u')$. However, this is not so since the

condition that the neutron later have lethargy u must be imposed. Since the probability that a neutron with lethargy in the interval $(u', u' + h)$ later has lethargy u is $W(u - u')h$, we see that

$$P(u' \mid u) = \frac{W(u' - u)W(u')}{W(u)}. \tag{26}$$

Noting that, if $\Sigma(u) = 1/v$, the mean time between collisions is unity, it follows that

$$\frac{d}{du'} \langle \tau_s(u') \rangle = \frac{W(u' - u)W(u')}{W(u)}. \tag{27}$$

Substituting this in Eq. (25) and comparing with (14), we see that our previous expression (19) for $\langle t(u) \rangle$ is once again obtained.

The higher moments of $t(u)$ may be found similarly from (24). The calculations are simplified considerably if (24) is integrated by parts and the relations

$$\langle [\tau(u) - \tau_s(u)]^n \rangle = 1/n!,$$

$$\langle d\tau(u'') \, d\tau(u') \rangle = P(u'' \mid u')P(u' \mid u) \qquad (u'' < u')$$

are used.

This last result generalizes immediately to products of n differentials $d\tau(u)$.

III. GENERALIZATIONS

The preceding results may be generalized immediately to the case where an absorption cross section $\Sigma_A(u)$ proportional to the scattering cross section $\Sigma(u)$ is assumed. We need only replace the quantity $W(u)$ throughout by $W_A(u)$ where $W_A(u)$ satisfies the equation

$$W_A(u) = \lambda f(u) + \lambda \int_0^u f(u - u')W(u') \, du',$$

with

$$\lambda = \Sigma(u)/[\Sigma(u) + \Sigma_A(u)].$$

It is also easy to find $\langle t(u) \rangle$, say, if we assume that the lethargy u is attained at a specific collision, e.g., the nth. The argument runs exactly the same as before except that the expression (26) for $P(u' \mid u)$ must be changed to

$$\sum_{k=1}^{n-1} W_k(u')W_{n-k}(u - u')/W_n(u).$$

Finally, consider the case where the probability density of the lethargy increase Δu, depends on the lethargy u' before collision. Denote this function by $f(\Delta u \mid u')$. Then we can still find $\langle t(u) \rangle$. To show this, the above method may be employed again, but the probability of a neutron with lethargy in $(u', u' + h)$ to later have lethargy u, no longer depends solely on the difference $u - u'$. If we call this probability $W(u \mid u')h$, then $W(u \mid u')$ satisfies the following equation (generalizing Eq. 10):

$$W(u \mid u') = f(u \mid u') + \int_{u'}^{u} f(u - u'' \mid u'')W(u \mid u'') \, du'';$$

$P(u' \mid u)$ is now

$$W(u' \mid 0)W(u \mid u')/W(u \mid 0).$$

The extension to higher moments is straightforward, though somewhat complicated.

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