JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Invariants of $\pi N \to \pi B_s$

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(Received 12 June 1970)

The kinematic singularities and threshold relations of helicity amplitudes for inelastic pion-nucleon scattering involving higher baryons in the final state are discussed. A recipe for writing the s- and t-channel helicity amplitudes is obtained using Wigner-Bargmann formalism. Explicit expressions for helicity amplitudes are worked out for the processes where the final state baryon has spin $\frac{3}{2}$ or $\frac{5}{2}$.

INTRODUCTION

The problem of kinematic singularities and threshold relations for helicity amplitudes of the process $\pi N \to \pi\Delta$ has recently been dealt with by Jackson and Hite.[1] They have used the concepts of nonrelativistic quantum mechanics to combine the spins of the particles into channel spins S and Russel-Saunders coupling of $L + S = J$. They have shown the kinematic singularities to follow from a mismatch between J and L for each term in the partial wave series and the threshold relations to result from the presence of fewer Russel-Saunder amplitudes than the independent helicity amplitudes at thresholds. They have used the method of invariant amplitudes as an alternative to give directly the kinematic singularities and threshold relations among the helicity amplitudes.

In the present work, we have used Wigner-Bargmann[2] formalism to calculate invariant amplitudes in s and t channels for the general process

$$(0^-) + (\tfrac{1}{2}^+) \to (0^-) + (S^+),$$

where (S^+) is some higher-spin baryon. In t channel, because of zero-spin particles of same intrinsic parity in initial state, the allowed angular-momentum parity states belong to the natural parity sequence ($\eta = +1$). Therefore, in this case, the parity conserving amplitudes are the same as Jacob-Wick helicity amplitudes. For the $S = \frac{3}{2}$ case, our results for the s channel are the same as those of Jackson and Hite, but the t-channel amplitudes differ in some signs from their amplitudes. However, the kinematic singularity structure is the same. Helicity amplitudes for $S = \frac{5}{2}$ have been worked out both in s and t channels.

We will be using the following results.

(i) The normal (T_N, T_N') and pseudo (T_P, T_P') threshold factors defined for the t-channel process $1 + 2 \to 3 + 4$ as

$$T_N = [t - (m_1 + m_2)^2]^{\frac{1}{2}}, \quad T_P = [t - (m_1 - m_2)^2]^{\frac{1}{2}}, \tag{1}$$
$$T_N' = [t - (m_3 + m_4)^2]^{\frac{1}{2}}, \quad T_P' = [t - (m_3 - m_4)^2]^{\frac{1}{2}},$$

such that $T_N T_P = 2(t)^{\frac{1}{2}} p$, $T_N' T_P' = 2(t)^{\frac{1}{2}} p'$, where p and p' are initial and final c.m. momenta and the prime corresponds to the final state. Following Jackson and Hite,[1] pseudothresholds are treated on an equal footing as normal thresholds with two modifications: (a) Pseudo-amplitudes $f_{\lambda_3\lambda_4;\lambda_1\lambda_2}^{p}$

$$(f_{\lambda_3\lambda_4;\lambda_1\lambda_2}^{p} = (-1)^{S_1-\lambda_1} f_{\lambda_3\lambda_4;\lambda_1\lambda_2})$$

are considered rather than normal amplitudes $f_{\lambda_3\lambda_4;\lambda_1\lambda_2}$. (b) The parity η_l of the lighter particles is replaced by $(-1)^{2sl}\eta l$.

(ii) The Kibble[3] boundary functions,

$$\phi = 4tp^2p'^2 \sin^2\theta. \tag{2}$$

(iii) Wigner-Bargmann[2,4] momentum space particle and antiparticle wavefunctions $U^{(\lambda)}(p)$ and $V^{(\lambda)}(p)$, respectively, given by

$$U^{(\lambda)}(p) = L(p) \times L(p) \times \cdots \times L(p)U^{(\lambda)}(0),$$
$$V^{(\lambda)}(p) = L(p) \times L(p) \times \cdots \times L(p)C^{-1} \times C^{-1} \times \cdots \times C^{-1}U^{(-\lambda)}.$$

$L(p)$ is the boost matrix for the Dirac spinors

$$L(p) = \exp[\tfrac{1}{2}\gamma_5 \boldsymbol{\sigma}\cdot\hat{\mathbf{p}} \tanh^{-1}(p/p_0)] = \frac{p_0 + m + \gamma_5\boldsymbol{\sigma}\cdot\mathbf{p}}{[2m(p_0+m)]^{\frac{1}{2}}}. \tag{3}$$

$U^{(\lambda)}(0)$ is formed from the symmetrized n-fold Kronecker products of the Dirac spinors for particles of spin $\frac{1}{2}$ at rest:

$$U^{(+)} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \qquad U^{(-)} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix},$$

$$U^{(\lambda)}(0) = \sum_P U^{(+)} \times U^{(-)} \times U^{(+)} \times \cdots \times U^{(-)} \cdot ({}^{2S}C_{n^-})^{-\frac{1}{2}}. \tag{4}$$

P stands for all distinguishable permutations of $U^{(+)}$ and $U^{(-)}$ and n^- is the number of U^-.

(iv) The representations for γ matrices are

$$\gamma_4 = \rho_3 \times 1, \quad \boldsymbol{\gamma} = -\rho_2 \times \boldsymbol{\sigma}, \quad \gamma_5 = -\rho_1 \times 1, \tag{5}$$

with γ_4 diagonal and $\gamma_1, \gamma_2, \gamma_3$, and γ_4 all Hermitian. The charge conjugation matrix C^{-1} has the form

$$C^{-1} = \gamma_5 i\sigma_2 = -\rho_1 \times i\sigma_2. \tag{6}$$

(v) The parity conserving amplitudes as defined by Gell-Mann *et al.*[5]:

$$F_{\lambda_3\lambda_4;\lambda_1\lambda_2}^{\eta} = (\sqrt{2}\cos\tfrac{1}{2}\theta)^{-|\lambda+\mu|}(\sqrt{2}\sin\tfrac{1}{2}\theta)^{-|\lambda-\mu|}f_{\lambda_3\lambda_4;\lambda_1\lambda_2} + \eta(-1)^{m-\mu}\eta_1\eta_2(-1)^{S_1+S_2-v} \times (\sqrt{2}\sin\tfrac{1}{2}\theta)^{-|\lambda+\mu|} \times (\sqrt{2}\cos\tfrac{1}{2}\theta)^{-|\lambda-\mu|}f_{\lambda_3\lambda_4;-\lambda_1-\lambda_2}, \tag{7}$$

$f_{\lambda_3\lambda_4;\lambda_1\lambda_2}$ are Jacob-Wick[6] helicity amplitudes, v is zero for integral values of $S_1 + S_2$ and $\frac{1}{2}$ for half-integral values, $u = \lambda_3 - \lambda_4$, $\lambda = \lambda_1 + \lambda_2$, and m is the larger of the two.

S-CHANNEL INVARIANT AMPLITUDES AND THRESHOLD RELATIONS

The most general form of amplitudes for the process $(0^-) + (\frac{1}{2}^+) \to (0^-) + (S^+)$ is

$$\langle p'\lambda', q|\,T\,|p\lambda, k\rangle = \sum_{n_2=0}^{n_1+n_2=N} \bar{U}^{(\lambda')}(p')^{u_1u_2\cdots u_N} \times X_{u_1}X_{u_2}\cdots X_{u_{n_1}}Y_{u_{n_1+1}}Y_{u_{n_1+2}}\cdots Y_{u_N} \times \gamma_5(-A_{n_2} - \tfrac{1}{2}i\gamma\cdot XB_{n_2})U^{(\lambda)}(p),$$

where $U^{(\lambda')}(p')^{u_1u_2\cdots u_N}$ is Rarita–Schwinger[7] wavefunction for the final-state baryon (S^+), $U(p)$ is a Dirac spinor for nucleon $(\frac{1}{2}^+)$, k and q are the 4-momenta of pions in the initial and final states, respectively, X and Y are linear combinations of k and q $(X = k + q,\ Y = k - q)$, and $N = S - \frac{1}{2}$.

Changing[4] Rarita–Schwinger wavefunction to the Wigner–Bargmann wavefunction, we write

$$\langle p'\lambda', q|\,T\,|p\lambda, k\rangle = \sum_{n_2=0}^{n_1+n_2=N} \frac{1}{(2N)^{\frac{1}{2}}}\bar{U}^{(\lambda')}_{\beta_1\beta_2\cdots\beta_N\alpha}(p') \times (\gamma\cdot XC)_{\beta_1\beta_2}(\gamma\cdot XC)_{\beta_3\beta_4}\cdots(\gamma\cdot XC)_{\beta_{2n_1-1}\beta_{2n_1}} \times (\gamma\cdot YC)_{\beta_{2n_1+1}\beta_{2n_1+2}}\cdots(\gamma\cdot YC)_{\beta_{2N-1}\beta_{2N}} - \{(\gamma_5A_{n_2} - \tfrac{1}{2}i\gamma_5\gamma\cdot XB_{n_2})_{\alpha\alpha''}\}U^{(\lambda)}_{\alpha''}(p).$$

Now

$$\bar{U}^{(\lambda')}_{\beta_1\beta_2\cdots\beta_N\alpha}(p') = [U^\dagger(0)R^\dagger L^{-1}(p') \times R^\dagger L^{-1}(p') \times \cdots]_{\beta_1\beta_2\cdots\beta_N\alpha} = U_{\beta_1'\beta_2'\cdots\beta_N'\alpha'}(0)[R^\dagger L^{-1}(p')]_{\beta_1'\beta_1}\cdots \times [R^\dagger L^{-1}(p')]_{\beta_N'\beta_N}[R^\dagger L^{-1}(p')]_{\alpha'\alpha},$$

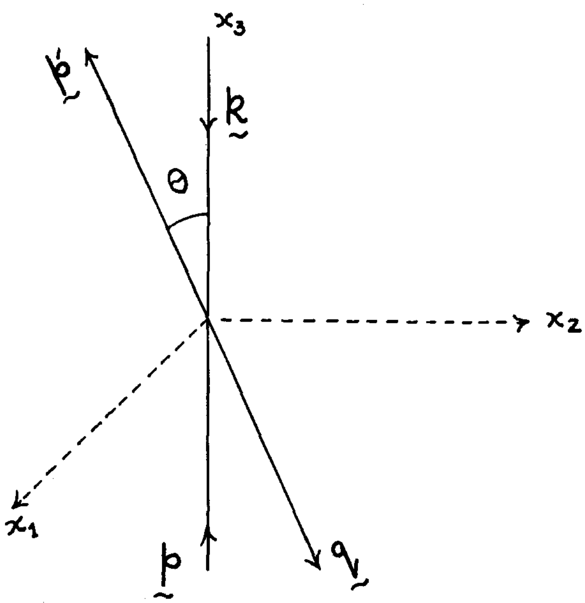

FIG. 1. The process $\pi + N \to \pi + B_s$. k, p, and q, p' represent the momenta of the initial pion, initial nucleon, final pion, and final baryon (of spin S), respectively

where $R = e^{-\frac{1}{2}i\sigma_2\theta}$ is the rotation required to bring p' in the direction of the x_3 axis (*see Fig. 1*).

This gives factors like

$$\{R^\dagger L^{-1}(p')\gamma\cdot XC[R^\dagger L^{-1}(p')]^T\}_{\beta_1'\beta_2'} = [R^\dagger L^{-1}(p')\gamma\cdot XCL(p')RC]_{\beta_1'\beta_2'} \equiv x_{\beta_1'\beta_2'}$$

and

$$[R^\dagger L^{-1}(p')\gamma\cdot YCL(p')RC]_{\beta_{2n_1+1}\beta_{2n_1+2}} \equiv y_{\beta_{2n_1+1}\beta_{2n_1+2}};$$

$$\therefore\ \langle p'\lambda', q|\,T\,|p\lambda, k\rangle = \frac{1}{(2N)^{\frac{1}{2}}}\sum_{n_2=0}^{n_1+n_2=N}\bar{U}^{(\lambda')}_{\beta_1'\beta_2'\cdots\beta_N'\alpha}(0)x_{\beta_1'\beta_2'}x_{\beta_3'\beta_4'}\cdots x_{\beta_{2n_1-1}\beta_{2n_1}} \times y_{\beta_{2n_1+1}'\beta_{2n_1+2}}\cdots y_{\beta_{2N-1}'\beta_{2N}'}[R^\dagger L^{-1}(p') \times \{-\gamma_5A_{n_2} - \tfrac{1}{2}i\gamma_5\gamma\cdot XB_{n_2}\}L(p)]_{\alpha\alpha'}U^{(\lambda)}_{\alpha'}(0).$$

We find

$$x = -i\left(p\sin\theta\sigma_1C - \sigma_3C\,\frac{p'W + p'k_0 + p_0'p\cos\theta}{m'}\right)$$

and

$$y = -i\left(p\sin\theta\sigma_1C - \sigma_3C \times \frac{-p'W + p'k_0 + p_0'p\cos\theta}{m'}\right), \quad C = -i\sigma_2.$$

Let

$$p\sin\theta = a,$$

$$\frac{1}{m'}(p'k_0 + p_0'p\cos\theta + p'W) = \tfrac{1}{2}d_1,$$

$$\frac{1}{m'}(p'k_0 + p_0'p\cos\theta - p'W) = \tfrac{1}{2}d_2,$$

and

$$R^{\dagger}L^{-1}(p')(-\gamma_5 A_{n_2} - \tfrac{1}{2}i\gamma_5\gamma\cdot X B_{n_2})L(p) = \sigma_3 \cos\tfrac{1}{2}\theta D_1^{(n_2)} + \sigma_1 \sin\tfrac{1}{2}\theta D_2^{(n_2)},$$

with

$$D_1^{(n_2)} = \frac{1}{(NN')^{\frac{1}{2}}}\{WB^{(n_2)}[p(p_0' + m') + p'(p_0 + m)] + [A^{(n_2)} + \tfrac{1}{2}(m' - m)B^{(n_2)}] \times [p'(p_0 + m) - p(p_0' + m')]\},$$

$$D_2^{(n_2)} = \frac{1}{(NN')^{\frac{1}{2}}}\{WB^{(n_2)}[p'(p_0 + m) - p(p_0' + m')] + [A^{(n_2)} + \tfrac{1}{2}(m' - m)B^{(n_2)}] \times [p'(p_0 + m) + p(p_0' + m')]\},$$

where

$$W = k_0 + q_0 = (s)^{\frac{1}{2}}$$

and

$$N = 2m(p_0 + m), \quad N' = 2m'(p_0' + m')$$

and where m' and m are the masses of (S^+) and $(\frac{1}{2}^+)$, respectively.

We will require the following linear combinations of $D_1^{(n_2)}$ and $D_2^{(n_2)}$:

$$D_1^{(n_2)} + D_2^{(n_2)} = \frac{2p'(p_0 + m)}{(NN')^{\frac{1}{2}}}\{A^{(n_2)} + [\tfrac{1}{2}(m' - m) + W]B^{(n_2)}\}$$

and

$$-D_1^{(n_2)} + D_2^{(n_2)} = \frac{2p(p_0' + m')}{(NN')^{\frac{1}{2}}}\{A^{(n_2)} + [\tfrac{1}{2}(m' - m) - W]B^{(n_2)}\}.$$

Now

$$\langle p'\lambda', q|\, T\, |p\lambda, k\rangle = \sum_{n_2=0}^{n_1+n_2=N} \frac{(-i)^N}{(2N)^{\frac{1}{2}}} \bar{U}^{(\lambda')}_{\beta_1\beta_2\cdots\beta_N\alpha} \times [a(\phi^1 - \phi^{-1}) + \phi^0 d_1]^{n_1} \times [a(\phi^1 - \phi^{-1}) + \phi^0 d_2]^{n_2} \times [\sigma_3 \cos\tfrac{1}{2}\theta D_1^{(n_2)} + \sigma_1 \sin\tfrac{1}{2}\theta D_2^{(n_2)}]U^{(\lambda)}.$$

Choosing $\lambda = \frac{1}{2}$,

$$(\sigma_3 \cos\tfrac{1}{2}\theta D_1^{(n_2)} + \sigma_1 \sin\tfrac{1}{2}\theta D_2^{(n_2)})U^+ = (\cos\tfrac{1}{2}\theta D_1^{(n_2)}U^+ + \sin\tfrac{1}{2}\theta D_2^{(n_2)}U^-),$$

choosing $\lambda = -\frac{1}{2}$,

$$(\sigma_3 \cos\tfrac{1}{2}\theta D_1^{(n_2)} + \sigma_1 \sin\tfrac{1}{2}\theta D_2^{(n_2)})U^- = (-\cos\tfrac{1}{2}\theta D_1^{(n_2)}U^- + \sin\tfrac{1}{2}\theta D_2^{(n_2)}U^+),$$

we now show how $\sigma_1 C = (\phi^1 - \phi^{-1})$ and $\sigma_3 C = -\sqrt{2}\,\phi^0$:

$$\sigma_1 C = (\sigma^+ + \sigma^-)C,$$

$$\sigma^+ C = \tfrac{1}{2}(\sigma_1 + i\sigma_2)C = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix},$$

$$\sigma^- C = \tfrac{1}{2}(\sigma_1 - i\sigma_2)C = -\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},$$

$$U^+ = \begin{pmatrix}1\\0\end{pmatrix}, \quad U^- = \begin{pmatrix}0\\1\end{pmatrix},$$

$$\phi^1_{\alpha\beta} = U^+_\alpha U^+_\beta = (U^+ \times U^+)_{\alpha\beta} = \begin{pmatrix}U_1^+U_1^+ & U_1^+U_2^+\\ U_2^+U_1^+ & U_2^+U_2^+\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix},$$

$$\phi^{-1}_{\alpha\beta} = U^-_\alpha U^-_\beta = (U^- \times U^-)_{\alpha\beta} = \begin{pmatrix}U_1^-U_1^- & U_1^-U_2^-\\ U_2^-U_1^- & U_2^-U_2^-\end{pmatrix} = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},$$

$$\therefore \quad \sigma_1 C = (\phi^1 - \phi^{-1});$$

similarly

$$\phi^0_{\alpha\beta} = \frac{1}{\sqrt{2}}(U^+_\alpha U^-_\beta + U^-_\alpha U^+_\beta) = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = -\frac{1}{\sqrt{2}}\sigma_3 C,$$

$$\therefore \quad \sigma_3 C = -\sqrt{2}\,\phi^0.$$

Since

$$U^{(\lambda')}(0) = ({}^{2S}C_{n^-})^{-\frac{1}{2}} \sum_P U^+ \times U^- \times U^+ \times \cdots \times U^+$$

is completely symmetric,

$$\therefore \quad \frac{\sqrt{2}}{2}\phi^0 = \frac{\sqrt{2}}{2}\frac{U^+U^- + U^-U^+}{\sqrt{2}} \to U^+U^- \equiv \phi^0.$$

Expanding binomially,

$$[a(\phi^1 - \phi^{-1}) + \phi^0 d_1]^{n_1}[a(\phi^1 - \phi^{-1}) + \phi^0 d_2]^{n_2} = \sum_{l_1=0}^{n_1}\sum_{l_2=0}^{n_2}[a(\phi^1 - \phi^{-1})]^{N-l_1-l_2} \times (\phi^0)^{l_1+l_2} d_1^{l_1} d_2^{l_2}\cdot\frac{n_1!\,n_2!}{(n_1 - l_1)!\,(n_2 - l_2)!\,l_1!\,l_2!}$$

$$= \sum_{l_1=0}^{n_1}\sum_{l_2=0}^{n_2} a^{N-l_1-l_2}\sum_{l=0}^{N-l_1-l_2}(\phi^1)^{N-l_1-l_2-l} \times (\phi^{-1})^l \frac{(N - l_1 - l_2)!\,(-1)^l}{(N - l_1 - l_2 - l)!\,l!} \times (\phi^0)^{l_1+l_2} d_1^{l_1} d_2^{l_2}\cdot\frac{n_1!\,n_2!}{(n_1 - l_1)!\,(n_2 - l_2)!\,l_1!\,l_2!}.$$

Powers of U^+ and U^- are

$$(U^+)^{2N-l_1-l_2-2l} \quad \text{and} \quad (U^-)^{2l+l_1+l_2},$$

denoting

$$2N - l_1 - l_2 - 2l = n^+ \quad \text{and} \quad 2l + l_1 + l_2 = n^-$$

such that

$$n^+ + n^- = 2S, \quad n^+ - n^- = 2\lambda'.$$

The contribution of the $\cos\theta/2 D_1^{(n_2)} U^+$ term gives

$$2N - l_1 - l_2 - 2l = n^+ - 1$$

and

$$2l + l_1 + l_2 = n^-,$$

while that of the $\sin\theta/2 D_2^{(n_2)} U^-$ term gives

$$2N - l_1 - l_2 - 2l = n^+$$

and

$$2l + l_1 + l_2 = n^- - 1;$$

l, l_1, and l_2 are positive integers and constraints on them in the $2l + l_1 + l_2 = n^-$ case are $l_1 \leq n^-$, $l_2 \leq n^-$, $l_1 + l_2 \leq n^-$, $l \leq n^-/2$. Therefore the explicit expression for Jacob–Wick helicity amplitudes in s channel is

$$f_{\lambda',+\frac{1}{2}} = \frac{(-i)^N}{(2N)^{\frac{1}{2}}}({}^{2S}C_{n^-})^{-\frac{1}{2}} \times \Bigg[\sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^-/2} a^{N-n^-+2l} C_l^{N-n^-+2l}(-1)^l \times P_{n_1n_2}^{n^--2l}(d_1d_2)\cos\tfrac{1}{2}\theta D_2^{(n_2)} + \sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^--1/2} a^{N-n^-+2l+1} C_l^{N-n^-+2l+1}(-1)^l \times P_{n_1n_2}^{n^--1-2l}(d_1d_2)\sin\tfrac{1}{2}\theta D_2^{(n_2)}\Bigg] \tag{8}$$

and

$$f_{\lambda',-\frac{1}{2}} = \frac{(-i)^N}{(2N)^{\frac{1}{2}}}\cdot({}^{2S}C_{n^-})^{-\frac{1}{2}} \times \Bigg[\sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^-/2} a^{N-n^-+2l} C_l^{N-n^-+2l}(-1)^l \times P_{n_1n_2}^{n^--2l}(d_1d_2)\sin\tfrac{1}{2}\theta D_2^{(n_2)} + \sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^--1/2} a^{N-n^-+2l+1} C_l^{N-n^-+2l+1}(-1)^l \times P_{n_1n_2}^{n^--2l-1}(d_1d_2)\cos\tfrac{1}{2}\theta(-D_1^{(n_2)})\Bigg], \tag{9}$$

where

$$P_{n_1n_2}^{n^--2l}(d_1d_2) = \sum_{l_1,l_2}^{l_1+l_2=n^--2l} d_1^{l_1}d_2^{l_2}\frac{n_1!\,n_2!}{(n_1-l_1)!\,(n_2-l_2)!\,l_1!\,l_2!}$$

is a polynomial in d_1d_2. Now parity conserving amplitudes using Eq. (7) are

$$F_{\lambda',\frac{1}{2}}^{-} = \frac{(-i)^N}{2^{N/2}}({}^{2S}C_{n^-})^{-\frac{1}{2}} \times \Bigg(\sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^-/2}\frac{p^{N-n^-+2l}}{\sqrt{2}}(\sin^2\theta)^l \times C_l^{N-n^-+2l}(-1)^l P_{n_1n_2}^{n^--2l}(d_1d_2)(D_1^{(n_2)} + D_2^{(n_2)}) + \sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^--1/2}\sqrt{2}\,p^{N-n^-+2l+1}(\sin^2\theta)^l \times C_l^{N-n^-+1+2l}(-1)^l P_{n_1n_2}^{n^--1-2l}(d_1d_2) \times \tfrac{1}{2}\{(D_2^{(n_2)} - D_1^{(n_2)}) - z(D_2^{(n_2)} + D_1^{(n_2)})\}\Bigg),$$

$$z = \cos\theta. \tag{10}$$

$$F_{\lambda',\frac{1}{2}}^{+} = \frac{(-i)^N}{2^{N/2}}\cdot({}^{2S}C_{n^-})^{-\frac{1}{2}} \times \Bigg(\sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^-/2}\frac{p^{N-n^-+2l}}{\sqrt{2}}(\sin^2\theta)^l \times C_l^{N-n^-+2l}(-1)^l P_{n_1n_2}^{n^--2l}(d_1d_2)(D_1^{(n_2)} - D_2^{(n_2)}) + \sum_{n_2=0}^{n_1+n_2=N}\sum_{l=0}^{n^--1/2}\sqrt{2}\,p^{N-n^-+2l+1}(\sin^2\theta)^l \times C_l^{N-n^-+1+2l}(-1)^l P_{n_1n_2}^{n^--1-2l}(d_1d_2) \times \tfrac{1}{2}[(D_2^{(n_2)} + D_1^{(n_2)}) + z(D_1^{(n_2)} - D_2^{(n_2)})]\Bigg). \tag{11}$$

For the $S = \frac{3}{2}$ case where $N = 1$, we have the following values of λ', n^-, and n^+.

λ'	n^-	n^+
$\frac{3}{2}$	0	3
$\frac{1}{2}$	1	2

The invariant amplitudes for this case are easily calculated to be

$$F_{\frac{3}{2},\frac{1}{2}}^{+} = -p^2\left(\frac{p_0' + m'}{p_0 + m}\right)^{\frac{1}{2}} \times \left[A_1 + A_2 + (B_1 + B_2)\left(\sqrt{s} - \frac{m' - m}{2}\right)\right],$$

$$F_{\frac{3}{2},\frac{1}{2}}^{-} = pp'\left(\frac{p_0 + m}{p_0' + m'}\right)^{\frac{1}{2}} \times \left[A_1 + A_2 - (B_1 + B_2)\left(\sqrt{s} + \frac{m' - m}{2}\right)\right],$$

$$F_{\frac{1}{2},\frac{1}{2}}^{+} = \frac{1}{\sqrt{3}}F_{\frac{3}{2},\frac{1}{2}}^{-} + \frac{1}{\sqrt{3}}F_{\frac{3}{2},\frac{1}{2}}^{+}\left[\left(\frac{2p_0'}{m'} + 1\right)z - \frac{2p'p_0}{m'p}\right] - \frac{4}{\sqrt{3}}\left(\frac{p_0' + m'}{p_0 + m}\right)^{\frac{1}{2}}\frac{pp'\sqrt{s}}{m'} \times \left[A_1 + B_1\left(\sqrt{s} - \frac{m' - m}{2}\right)\right],$$

$$F^-_{\frac{1}{2},\frac{1}{2}} = -\frac{1}{\sqrt{3}} F^+_{\frac{3}{2},\frac{1}{2}} + \frac{1}{\sqrt{3}} F^-_{\frac{3}{2},\frac{1}{2}}\left[\left(\frac{2p_0'}{m'} - 1\right)z - \frac{2p'p_0}{m'p}\right] + \frac{4}{\sqrt{3}}\frac{p'^2\sqrt{s}}{m'}\left(\frac{p_0 + m}{p_0' + m'}\right)^{\frac{1}{2}} \times \left[A_1 - B_1\left(\sqrt{s} + \frac{m' - m}{2}\right)\right], \tag{12}$$

where we have defined the new constants as

$$\frac{-iA^0}{(4mm')^{\frac{1}{2}}} = A_1, \quad \frac{-iA^1}{(4mm')^{\frac{1}{2}}} = A_2,$$
$$\frac{iB^0}{(4mm')^{\frac{1}{2}}} = B_1, \quad \frac{iB^1}{(4mm')^{\frac{1}{2}}} = B_2.$$

For the $S = \frac{5}{2}$ case where $n = 2$ we have the following values of λ', n^-, and n^+.

λ'	n^-	n^+
$\frac{5}{2}$	0	5
$\frac{3}{2}$	1	4
$\frac{1}{2}$	2	3

The invariant amplitudes in this case are

$$F^+_{\frac{5}{2},\frac{1}{2}} = \frac{-p^2}{\sqrt{2}}\left(\frac{p_0' + m'}{p_0 + m}\right)^{\frac{1}{2}} \times \left[A_1 + A_2 + A_3 + (B_1 + B_2 + B_3) \times \left(\sqrt{s} - \frac{m' - m}{2}\right)\right],$$

$$F^-_{\frac{5}{2},\frac{1}{2}} = \frac{p^2p'}{\sqrt{2}}\left(\frac{p_0 + m}{p_0' + m'}\right)^{\frac{1}{2}} \times \left[A_1 + A_2 + A_3 + (B_1 + B_2 + B_3) \times \left(\sqrt{s} + \frac{m' - m}{2}\right)\right],$$

$$F^+_{\frac{3}{2},\frac{1}{2}} = \frac{1}{2\sqrt{5}}\left\{\frac{8}{m'}\left(-\frac{p'p_0}{p} + p_0'z\right)F^+_{\frac{5}{2},\frac{1}{2}} + 2(F^-_{\frac{5}{2},\frac{1}{2}} + zF^+_{\frac{5}{2},\frac{1}{2}}) + \frac{4\sqrt{2}\,p^2p'\sqrt{s}}{m'}\left(\frac{p_0' + m'}{p_0 + m}\right)^{\frac{1}{2}} \times \left[2A_1 + A_2 + (2B_1 + B_2) \times \left(\sqrt{s} - \frac{m' - m}{2}\right)\right]\right\},$$

$$F^-_{\frac{3}{2},\frac{1}{2}} = \frac{1}{2\sqrt{5}}\left\{\frac{8}{m'}\left(-\frac{p'p_0}{p} + p_0'z\right)F^-_{\frac{5}{2},\frac{1}{2}} + 2(-F^+_{\frac{5}{2},\frac{1}{2}} - zF^-_{\frac{5}{2},\frac{1}{2}}) + \frac{4\sqrt{2}\,pp'^2\sqrt{s}}{m'} \times \left[2A_1 + A_2 - (2B_1 + B_2) \times \left(\sqrt{s} + \frac{m' - m}{2}\right)\right]\right\},$$

$$F^+_{\frac{1}{2},\frac{1}{2}} = \frac{1}{2\sqrt{10}}\left(\frac{1}{\sqrt{2}}\frac{4}{m'^2}2p\left(\frac{p_0' + m'}{p_0 + m}\right)^{\frac{1}{2}}\left\{(-p'p_0 + p_0'pz)^2 \times \left[A_1 + A_3 + (B_1 + B_3)\left(\sqrt{s} - \frac{m' - m}{2}\right)\right] + 4p'^2s\left[A_1 + B_1\left(\sqrt{s} - \frac{m' - m}{2}\right)\right] + 4p'\sqrt{s}(-p'p_0 + p_0'pz) \times \left[A_1 + B_1\left(\sqrt{s} - \frac{m' - m}{2}\right)\right]\right\}\right.$$
$$- 4\sin^2\theta F^+_{\frac{5}{2},\frac{1}{2}} + \frac{8}{m'}\left(-\frac{p'p_0}{p} + p_0'z\right) \times (F^-_{\frac{3}{2},\frac{1}{2}} + zF^+_{\frac{3}{2},\frac{1}{2}}) + \frac{4\sqrt{2}\,pp'\sqrt{s}}{m'} \times \left\{p'\left(\frac{p_0 + m}{p_0' + m'}\right)^{\frac{1}{2}}\left[A_1 + 2A_2 - (B_1 + 2B_2) \times \left(\sqrt{s} + \frac{m' - m}{2}\right)\right]\right.$$
$$\left.\left. + zp\left(\frac{p_0' + m'}{p_0 + m}\right)^{\frac{1}{2}}\left[2A_1 + A_2 + (2B_1 + B_2) \times \left(\sqrt{s} - \frac{m' - m}{2}\right)\right]\right\}\right),$$

$$F^-_{\frac{1}{2},\frac{1}{2}} = \frac{1}{2\sqrt{10}}\left(\frac{4\sqrt{2}\,p'}{m'^2}\left(\frac{p_0 + m}{p_0' + m'}\right)^{\frac{1}{2}}\left\{(-p'p_0 + p_0'pz)^2 \times \left[A_1 + A_3 - (B_1 + B_3)\left(\sqrt{s} + \frac{m' - m}{2}\right)\right] + 4p^{2'}s\left[A_1 - B_1\left(\sqrt{s} + \frac{m' - m}{2}\right)\right] + 4p'\sqrt{s}(-p'p + p_0'pz) \times \left[A_1 - B_1\left(\sqrt{s} + \frac{m' - m}{2}\right)\right]\right\}\right.$$
$$- 4\sin^2\theta F^-_{\frac{5}{2},\frac{1}{2}} + \frac{8}{m'}\left(-\frac{p'p_0}{p} + p_0'z\right) \times (-F^+_{\frac{3}{2},\frac{1}{2}} - zF^-_{\frac{3}{2},\frac{1}{2}}) + \frac{4\sqrt{2}\,pp'\sqrt{s}}{m'} \times \left\{p\left(\frac{p_0' + m'}{p_0 + m}\right)^{\frac{1}{2}}\left[2A_1 + A_2 + (2B_1 + B_2) \times \left(\sqrt{s} - \frac{m' - m}{2}\right)\right]\right.$$
$$\left.\left. - zp'\left(\frac{p_0 + m}{p_0' + m'}\right)^{\frac{1}{2}}\left[2A_1 - A_2 - (2B_1 - B_2) \times \left(\sqrt{s} + \frac{m' - m}{2}\right)\right]\right\}\right). \tag{13}$$

Again the constants are redefined as

$$\frac{-A^0}{(4mm')^{\frac{1}{2}}} = A_1, \quad \frac{-A^1}{(4mm')^{\frac{1}{2}}} = A_2, \quad \frac{-A^2}{(4mm')^{\frac{1}{2}}} = A_3,$$
$$\frac{B^0}{(4mm')^{\frac{1}{2}}} = B_1, \quad \frac{B^1}{(4mm')^{\frac{1}{2}}} = B_2, \quad \frac{B^2}{(4mm')^{\frac{1}{2}}} = B_3.$$

In both these cases, threshold relations are easily seen as $p' \to 0$.

t-channel amplitudes: Following exactly similar lines as in *s* channel we can write for *t*-channel amplitude

$$\langle p'\lambda', p\lambda|\, T\, |q, k\rangle = \sum_{n_2=0}^{N=n_1+n_2} \frac{(+1)}{(2N)^{\frac{1}{2}}} \bar{U}^{(\lambda')}_{\beta_1\beta_2\cdots\beta_N\alpha} x_{\beta_1\beta_2} x_{\beta_3\beta_4} \cdots x_{\beta_{2n_1-1}\beta_{2n_1}}$$
$$\times\, y_{\beta_{2n_1+1}\beta_{2n_1+2}} y_{\beta_{2n_1+3}\beta_{2n_1+4}} \cdots y_{\beta_{2N-1}\beta_{2N}}$$
$$\times\, [R^\dagger L^{-1}(p')(-A_{n_2} + \tfrac{1}{2} i\gamma\cdot XB_{n_2})\gamma_5 V(p)]_\alpha,$$

where

$$X = q - k, \quad Y = q + k,$$
$$V(p) = L(p)RC^{-1}U^{(-\lambda)}(0)(-1)^{\lambda-\frac{1}{2}},$$
$$x = R^\dagger L^{-1}(p')\gamma\cdot XCL(p')RC = -i\frac{2q}{m'}[m'\sin\theta(\phi^{-1} - \phi^1) - 2p_0'\cos\theta\phi^0],$$
$$y = R^\dagger L^{-1}(p')\gamma\cdot YCL(p')RC = -i\frac{4q_0 p}{m'}\phi^0,$$

and

$$R^\dagger L^{-1}(p')(-A_{n_2} + \tfrac{1}{2}i\gamma\cdot XB_{n_2})\gamma_5 L(p)RC^{-1} = (NN')^{-\frac{1}{2}}\{-A_{n_2}(p_0 + m)(W + m' - m)$$
$$+ B_{n_2}pq[\cos\theta(p_0 - p_0' + m - m') - i\sigma_2\sin\theta(W + m' + m)]\}i\sigma_2,$$

or

$$\langle p'\lambda', p\lambda|\, T\, |q, k\rangle = \sum_{n_2=0}^{n_1+n_2=N} \frac{(-i)^N}{(2N)^{\frac{1}{2}}} \bar{U}^{(\lambda')}_{\beta_1\beta_2\cdots\beta_N\alpha}$$
$$\times \left(2q\sin\theta(\phi^{-1} - \phi^1) - \frac{4qp_0'}{m'}\cos\theta\phi^0\right)^{n_1}$$
$$\times \left(\frac{4q_0 p}{m'}\phi^0\right)^{n_2}(NN')^{-\frac{1}{2}}$$
$$\times \{-A_{n_2}(p_0 + m)(W + m' - m) + B_{n_2}pq[\cos\theta(p_0 - p_0' + m - m') - i\sigma_2\sin\theta(W + m' + m)]\}i\sigma_2 U^{-\lambda}(-1)^{\lambda-\frac{1}{2}},$$

where

$$W = q_0 + k_0 = \sqrt{t};$$

because of equal mass particles in the initial state, $W = 2q_0$. We can write it in a more convenient form by introducing

$$a = (2q\sin\theta), \quad b = \frac{4qp_0'\cos\theta}{m'}, \quad \text{and} \quad d = \frac{4q_0 p}{m'}.$$

Then

$$\langle p'\lambda', p\lambda|\, T\, |q, k\rangle = \sum_{n_2=0}^{n_1+n_2=N} \frac{(-i)^N}{(2N)^{\frac{1}{2}}} \bar{U}^{(\lambda')}_{\beta_1\beta_2\cdots\beta_N\alpha}$$
$$\times [a(\phi^{-1} - \phi^1) - b\phi^0]^{n_1}[d\phi^0]^{n_2}(NN')^{-\frac{1}{2}}$$
$$\times \{-A_{n_2}(p_0 + m)(W + m' - m) + B_{n_2}pq[\cos\theta(p_0 - p_0' + m - m') - i\sigma_2\sin\theta(W + m' + m)]\}i\sigma_2 U^{-\lambda}(-1)^{\lambda-\frac{1}{2}},$$
$$\lambda = \pm\tfrac{1}{2}.$$

Following almost the same lines as in case of *s* channel, we get finally for Jacob–Wick amplitudes in *t* channel

$$f_{\lambda',\frac{1}{2};00} = ({}^{2S}C_{n^-})^{-\frac{1}{2}} \times \Bigg(\sum_{n_2=0}^{n^-} \frac{(-i)^N}{(2N)^{\frac{1}{2}}} a^{n_1} \sum_{l_1=0}^{n^-} \frac{(b/a)^{l_1}}{l_1!\,(n_1 - l_1 - l)!} \times \sum_{l=0}^{n^-/2} (-1)^{n_1+l}\frac{n_1!}{l!} d^{n_2}(NN')^{-\frac{1}{2}}$$
$$\times [-A_{n_2}(p_0 + m)(W + m' - m) + B_{n_2}pq\cos\theta(p_0 - p_0' + m - m')]$$
$$+ \sum_{n_2=0}^{n^- -1} \frac{(-i)^N}{(2N)^{\frac{1}{2}}} a^{n_1} \sum_{l_1=0}^{n^- -1} \frac{(b/a)^{l_1}}{l_1!\,(n_1 - l_1 - l)!} \times \sum_{l=0}^{n^- -1/2} (-1)^{n_1+l}\frac{n_1!}{l!} d^{n_2}(NN')^{-\frac{1}{2}}$$
$$\times B_{n_2}pq\sin\theta(W + m' + m)\Bigg), \tag{14}$$

$$f_{\lambda',-\frac{1}{2};00} = ({}^{2S}C_{n^-})^{-\frac{1}{2}} \times \Bigg(\sum_{n_2=0}^{n^- -1} \frac{(-i)^N}{(2N)^{\frac{1}{2}}} a^{n_1} \sum_{l_1=0}^{n^- -1} \frac{(b/a)^{l_1}}{l_1!\,(n_1 - l_1 - l)!} \times \sum_{l=0}^{n^- -1/2} (-1)^{n_1+l}\frac{n_1!}{l!} d^{n_2}(NN')^{-\frac{1}{2}}$$
$$\times [-A_{n_2}(p_0 + m)(W + m' - m) + B_{n_2}pq\cos\theta(p_0 - p_0' + m - m')]$$
$$+ \sum_{n_2=0}^{n^-} \frac{(-i)^N}{(2N)^{\frac{1}{2}}} a^{n_1} \sum_{l_1=0}^{n^-} \frac{(b/a)^{l_1}}{l_1!\,(n_1 - l_1 - l)!} \times \sum_{l=0}^{n^-/2} (-1)^{n_1+l}\frac{n_1!}{l!} d^{n_2}(NN')^{-\frac{1}{2}}$$
$$\times [-B_{n_2}pq\sin\theta(W + m' + m)]\Bigg);$$

l, l_1, and n^- are positive integers with the restriction

$$2l + l_1 + n_2 = n^- \quad \text{or} \quad n^- - 1$$

when

$$2l + l_1 + l_2 = n^-$$

and

$$l \leq n^-/2, \quad l_1 \leq n^-, \quad n_2 \leq n^-.$$

The explicit form of t-channel amplitudes for $s = \frac{3}{2}$ case is, with $z = \cos\theta$,

$$f_{\frac{3}{2},\frac{1}{2};00} = \frac{\sqrt{2}\sqrt{\phi}}{T_{N'}}[-A_1 - (m' - m)(2pqZ)B_1],$$

$$f_{\frac{3}{2},-\frac{1}{2};00} = -\frac{\sqrt{2}\,\phi}{T_{N'}T_{P'}^2} B_1,$$

$$\begin{aligned} f_{\frac{1}{2},\frac{1}{2};00} = {} & -\left(\frac{2}{3}\right)^{\frac{1}{2}} \frac{t + m'^2 - m^2}{m'T_{N'}}(2pqZ)A_1 \\ & + \frac{1}{\sqrt{6}}\frac{T_{N'}T_{P'}^2}{m'}A_2 + \left(\frac{2}{3}\right)^{\frac{1}{2}}\frac{1}{T_{N'}^2T_{P'}^2} \\ & \times \left[\left(\frac{m' + m}{m'}\right)T_{P'}^2(2pqZ)^2 \right. \\ & \left. - 12t(pqZ)^2 + 4tp^2q^2\right]B_1 \\ & + \left(\frac{2}{3}\right)^{\frac{1}{2}}\left(\frac{m' - m}{m'}\right)T_{N'}(pqZ)B_2, \end{aligned}$$

$$\begin{aligned} f_{\frac{1}{2},-\frac{1}{2};00} = {} & \frac{\sqrt{\phi}}{T_{N'}}\left(-\left(\frac{2}{3}\right)^{\frac{1}{2}}A_1 - \left(\frac{2}{3}\right)^{\frac{1}{2}}\frac{3m'(m' - m) + T_{P'}^2}{m'T_{P'}^2}\right. \\ & \left. \times (2pqZ)B_1 + \frac{1}{\sqrt{6}}\frac{T_{N'}^2}{m'}B_2\right). \end{aligned}$$

For the $s = \frac{5}{2}$ case, we have

$$f_{\frac{5}{2},\frac{1}{2};00} = (2\phi/T_{N'}^2T_{P'})[A_1 + (m' - m)/T_{P'}^2(2pqZ)B_1],$$

$$f_{\frac{5}{2},-\frac{1}{2};00} = (2\phi\sqrt{\phi}/T_{N'}^2T_{P'}^3)B_1,$$

$$\begin{aligned} f_{\frac{3}{2},\frac{1}{2};00} = {} & \frac{\sqrt{\phi}}{\sqrt{5}\,T_{N'}^2T_{P'}} \\ & \times \left\{2\frac{t + m'^2 - m^2}{m'}(2pqZ)A_1 - \frac{T_{N'}^2T_{P'}^2}{m'}A_2\right. \\ & + \left[2\frac{m' - m}{T_{P'}^2}(2pqZ)^2\right. \\ & \left.\times \frac{t + m'^2 - m^2}{m'} - \frac{4\phi}{T_{P'}^2}\right]B_1 \\ & \left. - \left(\frac{m' - m}{m'}\right)T_{N'}^2(2pqZ)B_2\right\}, \end{aligned}$$

$$\begin{aligned} f_{\frac{3}{2},-\frac{1}{2};00} = {} & \frac{\phi}{\sqrt{5}\,T_{N'}^2T_{P'}} \\ & \times \left[4A_1 + \frac{4}{T_{P'}^2}\frac{3m'(m' - m) + T_{P'}^2}{m'T_{P'}^2}\right. \\ & \left.\times (2pqZ)B_1 - \frac{1}{m'}B_2\right], \end{aligned}$$

$$\begin{aligned} f_{\frac{1}{2},\frac{1}{2};00} = {} & \left[2(2pqZ)^2\frac{(t + m'^2 - m^2)^2}{m'^2} - 4\phi\right] \\ & \times \frac{A_1}{T_{N'}^2T_{P'}}\frac{1}{\sqrt{10}} - \frac{t + m'^2 - m^2}{\sqrt{10}\,m'^2} \\ & \times (2pqZ)T_{P'}A_2 + \frac{1}{2}\frac{T_{N'}T_{P'}^2}{m'}\frac{A_3}{\sqrt{10}} \\ & - \frac{4\phi}{T_{N'}^2T_{P'}^3}(2pqZ)\frac{3m'(m' - m) + T_{P'}^2}{\sqrt{10}\,m'}B_1 \\ & - (2pqZ)^3\frac{(t + m'^2 - m^2)^2}{\sqrt{10}\,m'^2T_{N'}^2T_{P'}^3}(m - m')B_1 \\ & + \left[\frac{t + m'^2 - m^2}{\sqrt{10}\,m'^2}(2pqZ)^2\frac{(m - m')}{T_{P'}^2}\right. \\ & \left. - \frac{\phi}{m'T_{P'}\sqrt{10}}\right]B_2 \\ & - \frac{1}{2}\frac{T_{N'}}{\sqrt{10}}\left(\frac{m - m'}{m'}\right)(2pqZ)B_3, \end{aligned}$$

$$\begin{aligned} f_{\frac{1}{2},-\frac{1}{2};00} = {} & \frac{2\sqrt{\phi}}{\sqrt{10}\,T_{N'}^2T_{P'}}\frac{t + m'^2 - m^2}{m'} \\ & \times (2pqZ)A_1 - \frac{\sqrt{\phi}\,T_{P'}}{\sqrt{10}\,m'}A_2 \\ & + \left[2\frac{(2pqZ)^2}{T_{N'}^2T_{P'}^3}\frac{(t + m'^2 - m^2)^2}{m'^2}\right. \\ & - \frac{2}{T_{N'}^2T_{P'}^3}\frac{t + m'^2 - m^2}{m'}(m - m')(2pqZ)^2 \\ & \left. - \frac{4\phi}{T_{N'}^2T_{P'}^3}\right]\frac{\sqrt{\phi}}{\sqrt{10}}B_1 \\ & - \frac{\sqrt{\phi}}{m'T_{P'}}(2pqZ)\frac{3m'(m' - m) + T_{P'}^2}{m'\sqrt{10}}B_2 \\ & + \frac{1}{2}\frac{T_{N'}^2T_{P'}}{m'^2}\frac{\sqrt{\phi}}{\sqrt{10}}B_3, \end{aligned} \qquad (15)$$

with a proper redefinition of coefficients in each case.

These t-channel amplitudes have a general singularity structure

$$f_{\lambda',\lambda;00} = \frac{(\sqrt{\phi})^{|u|} A_{\lambda'\lambda}(s,t)}{T_{N'}^{\lambda'-\lambda} T_{P'}^{\lambda'-\lambda+1}}, \quad u = \lambda' - \lambda, \quad \lambda = \pm\tfrac{1}{2},$$

where $A_{\lambda'\lambda}(s,t)$ is free of singularities at the kinematic thresholds. This can easily be seen in both of the cases ($\lambda = \pm\frac{1}{2}$). For example, in the first term of $f_{\lambda',\frac{1}{2};00}$, the rest is free of singularities at the kinematic thresholds except the portion

$$\begin{aligned}
&\sum_{n_2=0}^{n^-} a^{n_1-l_1}\frac{1}{T_{P'}} \\
&= \sum_{n_2=0}^{n^-} (2q\sin\theta)^{n_1-l_1}\frac{1}{T_{P'}} \\
&= \frac{1}{T_{P'}}[(2q\sin\theta)^{s-\frac{1}{2}-l_1} + (2q\sin\theta)^{(s-\frac{1}{2})-1-l_1} \\
&\quad + (2q\sin\theta)^{(s-\frac{1}{2})-2-l_1} + \cdots + (2q\sin\theta)^{(s-\frac{1}{2})-n^--l_1}] \\
&= \frac{1}{T_{P'}}(2q\sin\theta)^{s-n^--\frac{1}{2}} \\
&\quad \times [(2q\sin\theta)^{-l_1} + (2q\sin\theta)^{1-l_1} \\
&\qquad + \cdots + (2q\sin\theta)^{n^--l_1}] \\
&= \frac{1}{T_{P'}}(2q\sin\theta)^{\lambda'-\frac{1}{2}} \\
&\quad \times [(2q\sin\theta)^{-l_1} + (2q\sin\theta)^{1-l_1} \\
&\qquad + \cdots + (2q\sin\theta)^{n^--l_1}],
\end{aligned}$$

since $2l + l_1 + n_2 = n^-$,

$$\begin{aligned}
-l_1 &= 2l, & n_2 &= n^-, \\
1 - l_1 &= 2l, & n_2 &= n^- - 1, \\
&\vdots & &\vdots \\
n^- - l_1 &= 2l, & n_2 &= 0.
\end{aligned}$$

Inside the bracket, only even powers of $\sin\theta$ occur; therefore, it is free of kinematic singularities. Hence the singularity structure is

$$\begin{aligned}
f_{\lambda',\lambda;00} &= \frac{(2pq\sqrt{t}\sin\theta)^{|\lambda'-\lambda|}}{(2p\sqrt{t})^{\lambda'-\lambda}T_{P'}} A_{\lambda'\lambda}(s,t) \\
&= \frac{(\sqrt{\phi})^{|u|}}{T_{N'}^{\lambda'-\lambda}T_{P'}^{\lambda'-\lambda+1}} A_{\lambda'\lambda}(s,t). \qquad (16)
\end{aligned}$$

ACKNOWLEDGMENT

The authors would like to thank Professor Fayyazuddin for discussion.

[1] J. D. Jackson and G. E. Hite, Phys. Rev. **169**, 1248 (1968).
[2] V. Bargmann and E. P. Wigner, Proc. Natl. Acad. Sci. (U.S.) **34**, 212 (1948).
[3] T. Kibble, Phys. Rev. **117**, 1159 (1959).
[4] Arif-Uz-Zaman, Nuovo Cimento, Ser. X, **56A**, 493 (1968).
[5] M. Gell-Mann, M. L. Golberger, F. E. Low, E. Marx, and F. Zachariasen, Phys. Rev. **133**, B145 (1964).
[6] M. Jacob and G.-C. Wick, Ann. Phys. (N.Y.) **7**, 404 (1959).
[7] W. Rarita and J. Schwinger, Phys. Rev. **60**, 61 (1941).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Static Gravitational Field of Multipoles in the Second Approximation*

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(Received 19 November 1970)

A method of obtaining the explicit form of the gravitational field of multipoles in the second approximation is furnished here. The generalization of this method to any superposition of multipoles is straightforward. We obtain as an example the second-order metric for the superposition of a monopole and a quadrupole.

I. INTRODUCTION

The experimental tests of general relativity are unfortunately very few in number, but ever increasing use of satellites and improvements in satellite observations will in the not too distant future provide further tests of general relativity. It is, in this connection, important to study the motion of particles in the gravitational field of a body at rest. This in turn requires knowledge of the metric satisfying the static gravitational equations. A method of obtaining an exact static metric for cylindrically symmetric mass distributions is already known.[1] We also have methods of obtaining a second-order approximation for the metric in the case of a single body of arbitrary shape.[2,3]

Those methods give the components of the metric tensor in the form of integrals, which are shown to exist but not given in the explicit form.

The present work shows how, starting from the multipole expansion of the Newtonian potential, we can obtain a second approximation in the explicit form.

II. THE FIELD OF A STATIC MULTIPOLE IN THE SECOND ORDER

Greek suffixes take the values 1, 2, 3, capital Latin suffixes 1, 2, $\cdots$, n, and lower case Latin suffixes

These t-channel amplitudes have a general singularity structure

$$f_{\lambda',\lambda;00} = \frac{(\sqrt{\phi})^{|u|} A_{\lambda'\lambda}(s,t)}{T_{N'}^{\lambda'-\lambda} T_{P'}^{\lambda'-\lambda+1}}, \quad u = \lambda' - \lambda, \quad \lambda = \pm\tfrac{1}{2},$$

where $A_{\lambda'\lambda}(s,t)$ is free of singularities at the kinematic thresholds. This can easily be seen in both of the cases $(\lambda = \pm\frac{1}{2})$. For example, in the first term of $f_{\lambda',\frac{1}{2};00}$, the rest is free of singularities at the kinematic thresholds except the portion

$$\sum_{n_2=0}^{n^-} a^{n_1-l_1} \frac{1}{T_{P'}}$$
$$= \sum_{n_2=0}^{n^-} (2q \sin\theta)^{n_1-l_1} \frac{1}{T_{P'}}$$
$$= \frac{1}{T_{P'}} [(2q\sin\theta)^{s-\frac{1}{2}-l_1} + (2q\sin\theta)^{(s-\frac{1}{2})-1-l_1} + (2q\sin\theta)^{(s-\frac{1}{2})-2-l_1} + \cdots + (2q\sin\theta)^{(s-\frac{1}{2})-n^--l_1}]$$
$$= \frac{1}{T_{P'}} (2q\sin\theta)^{s-n^--\frac{1}{2}} \times [(2q\sin\theta)^{-l_1} + (2q\sin\theta)^{1-l_1} + \cdots + (2q\sin\theta)^{n^--l_1}]$$
$$= \frac{1}{T_{P'}} (2q\sin\theta)^{\lambda'-\frac{1}{2}} \times [(2q\sin\theta)^{-l_1} + (2q\sin\theta)^{1-l_1} + \cdots + (2q\sin\theta)^{n^--l_1}],$$

since $2l + l_1 + n_2 = n^-$,

$$-l_1 = 2l, \quad n_2 = n^-,$$
$$1 - l_1 = 2l, \quad n_2 = n^- - 1,$$
$$\vdots$$
$$n^- - l_1 = 2l, \quad n_2 = 0.$$

Inside the bracket, only even powers of $\sin\theta$ occur; therefore, it is free of kinematic singularities. Hence the singularity structure is

$$f_{\lambda',\lambda;00} = \frac{(2pq\sqrt{t}\sin\theta)^{|\lambda'-\lambda|}}{(2p\sqrt{t})^{\lambda'-\lambda} T_{P'}} A_{\lambda'\lambda}(s,t) = \frac{(\sqrt{\phi})^{|u|}}{T_{N'}^{\lambda'-\lambda} T_{P'}^{\lambda'-\lambda+1}} A_{\lambda'\lambda}(s,t). \tag{16}$$

ACKNOWLEDGMENT

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A method of obtaining the explicit form of the gravitational field of multipoles in the second approximation is furnished here. The generalization of this method to any superposition of multipoles is straightforward. We obtain as an example the second-order metric for the superposition of a monopole and a quadrupole.

I. INTRODUCTION

The experimental tests of general relativity are unfortunately very few in number, but ever increasing use of satellites and improvements in satellite observations will in the not too distant future provide further tests of general relativity. It is, in this connection, important to study the motion of particles in the gravitational field of a body at rest. This in turn requires knowledge of the metric satisfying the static gravitational equations. A method of obtaining an exact static metric for cylindrically symmetric mass distributions is already known.[1] We also have methods of obtaining a second-order approximation for the metric in the case of a single body of arbitrary shape.[2,3]

Those methods give the components of the metric tensor in the form of integrals, which are shown to exist but not given in the explicit form.

The present work shows how, starting from the multipole expansion of the Newtonian potential, we can obtain a second approximation in the explicit form.

II. THE FIELD OF A STATIC MULTIPOLE IN THE SECOND ORDER

Greek suffixes take the values 1, 2, 3, capital Latin suffixes $1, 2, \cdots, n$, and lower case Latin suffixes

1, 2, 3, 4 with the summation convention in each case. Partial derivatives w.r.t. the coordinates are indicated by commas (e.g., $w_{,r} = \partial w/\partial x^r$).

Theorem 1[4]: Let $L_{ABCD}(x)$ be the linearized Riemann tensor for a n-dimensional Riemannian manifold, i.e.,

$$L_{ABCD} = \tfrac{1}{2}(g_{AD,BC} + g_{BC,AD} - g_{AC,BD} - g_{BD,AC}). \tag{1}$$

The metric tensor g_{AB} in terms of L_{ABCD} is then given by

$$g_{AB} = \eta_{AB} + 2x^C x^D \int_b^1 L_{ACDB}(x)\lambda(1-\lambda)\,d\lambda, \tag{2}$$

where

$$b = \begin{cases} 0 & \text{if} \quad L_{ABCD}(0) \quad \text{is finite} \\ \infty & \text{for} \quad \lim_{\lambda\to\infty} \lambda^3 L_{ABCD}(\lambda x) = 0 \end{cases} \tag{2'}$$

and $\eta_{AB} = \operatorname{diag}(\pm 1, \pm 1, \cdots, \pm 1)$.

Proof: Let us try to find a g_{AB} satisfying Eq. (1), having the form

$$g_{AB} = \eta_{AB} + x^C x^D S_{ACDB}, \tag{3}$$

where we assume that S_{ACDB} has all the symmetries of the linearized Riemann tensor, viz.,

$$S_{ABCD} = -S_{ABDC} = -S_{BACD} = S_{CDAB},$$
$$S_{A[BCD]} = S_{AB[CD,E]} = 0. \tag{4}$$

Plugging Eq. (3) into Eq. (1) gives, by use of Eq. (4),

$$L_{ABCD} = 3S_{ABCD} + \tfrac{5}{2}x^E S_{ABCD,E} + \tfrac{1}{2}x^F(x^E S_{ABCD,E})_{,F}. \tag{5}$$

We try to find a solution of the form

$$S_{ABCD}(x) = c\int_u^v L_{ABCD}(\lambda x) f(\lambda)\,d\lambda. \tag{5'}$$

Equation (5′) into Eq. (5) gives (after several integrations by parts)

$$\begin{aligned} L_{ABCD}(x) = {} & c\int_u^v L_{ABCD}(\lambda x) \\ & \times [3f - \tfrac{5}{2}(\lambda f)' + \tfrac{1}{2}(\lambda(\lambda f)')']\,d\lambda \\ & + c\{\tfrac{5}{2}L_{ABCD}(\lambda x)\lambda f - \tfrac{1}{2}L_{ABCD}(\lambda x)\lambda(\lambda f)' \\ & + \tfrac{1}{2}x^E(L_{ABCD}(\lambda x)\lambda f)_{,E}\}_u^v. \end{aligned} \tag{5''}$$

We now have to choose c, u, v, and $f(\lambda)$ in such a way that the rhs of Eq. (5″) is L_{ABCD}. We first choose

$$f(\lambda) = \lambda(1-\lambda). \tag{6}$$

This makes the term in the square brackets (and thus the integral) in Eq. (5″) equal to zero. With this $f(\lambda)$, we find that the term in the curly brackets becomes $\tfrac{1}{2}L_{ABCD}(x)$ if

(i) either $L_{ABCD}(0)$ is finite and $u = 0$, $v = 1$,
(ii) or $\lim_{\lambda\to\infty} \lambda^3 L_{ABCD}(\lambda x) = 0$ and $u = \infty$, $v = 1$;

we thus have to take $c = 2$ in either case.

From (i), (ii), (6), (5′), and (3) the theorem follows.

Corollary: If L_{ABCD} is homogeneous of degree d, i.e., if

$$L_{ABCD}(\lambda x) = \lambda^d L_{ABCD}(x), \tag{7}$$

then it follows immediately from Eqs. (2) and (2′) that for $d < -3$

$$g_{AB} = \eta_{AB} + 2x^C x^D L_{ACDB}(x)[(d+2)(d+3)]^{-1}. \tag{8}$$

Theorem 2: Let $W(x^1, x^2, x^3)$ be a Newtonian harmonic function which is homogeneous in x^α of degree $n \le -1$. Let the metric of a static V_4 be given by

$$g_{\alpha\beta} = e^{-kW}(\delta_{\alpha\beta} + \gamma_{\alpha\beta}), \quad g_{\alpha 4} = 0, \quad g_{44} = -e^{kW}, \tag{9}$$

where $k > 0$ is a dimensionless constant and[5]

$$\gamma_{\alpha\delta} = -k^2[2n(2n+1)]^{-1}x^\beta x^\gamma \cdot [\delta_{\beta[\gamma}W_{,\delta]}W_{,\alpha} + \delta_{\alpha[\delta}W_{,\gamma]}W_{,\beta} - \tfrac{1}{2}\delta_{\alpha[\delta}\delta_{\gamma]\beta}W_{,\sigma}W_{,\sigma}]. \tag{10}$$

Then the Ricci tensor R_{ij} of V_4 satisfies[6]

$$R_{ij} \equiv \sum_{m=0}^{\infty} k^m \underset{(m)}{R_{ij}} = O(k^3). \tag{11}$$

Proof: Consider a static V_4 with the metric

$$g_{\alpha\beta} = e^{-kW}\bar{g}_{\alpha\beta} = e^{-kW}(\delta_{\alpha\beta} + \gamma_{\alpha\beta}),$$
$$g_{\alpha 4} = 0, \quad g_{44} = -e^{kW}, \tag{12}$$

where W satisfies the harmonic equation

$$W_{,\alpha\alpha} = 0. \tag{13}$$

Straightforward calculation of the Ricci tensor R_{ij} by Eqs. (12) and (13) yields

$$R_{\alpha\beta} = \bar{R}_{\alpha\beta} + \tfrac{1}{2}k^2 W_{,\alpha}W_{,\beta} + O(k^3),$$
$$R_{\alpha 4} = 0, \quad R_{44} = O(k^3), \tag{14}$$

where $\bar{R}_{\alpha\beta}$ is the Ricci subtensor of the $\bar{V}_3$ with the metric $\bar{g}_{\alpha\beta}$.

Now the linearized part $\bar{L}_{\alpha\beta}$ of $\bar{R}_{\alpha\beta}$ is made to satisfy[7]

$$\bar{L}_{\alpha\beta} \equiv \tfrac{1}{2}(\bar{g}_{\alpha\beta,\sigma\sigma} + \bar{g}_{\sigma\sigma,\alpha\beta} - \bar{g}_{\alpha\sigma,\sigma\beta} - \bar{g}_{\beta\sigma,\sigma\alpha}) = -\tfrac{1}{2}k^2 W_{,\alpha}W_{,\beta}. \tag{15}$$

If solutions $\bar{g}_{\alpha\beta} = \delta_{\alpha\beta} + \gamma_{\alpha\beta}$ are found to satisfy the above equations, then

$$\bar{R}_{\alpha\beta} = \bar{L}_{\alpha\beta} + O(k^4), \tag{16}$$

and plugging Eqs. (15) and (16) into (14) would establish the theorem. Therefore, the proof hinges on the solubility of Eq. (15) to obtain $\gamma_{\alpha\beta}$. So we shall sketch the solution procedure in the following. Recalling that the Riemann tensor $\bar{R}_{\alpha\beta\gamma\delta}$ of a $\bar{V}_3$ is the linear combination of $\bar{R}_{\alpha\beta}$, we can state the corresponding linearized version as

$$\bar{L}_{\alpha\beta\gamma\delta} = \delta_{\beta[\gamma}\bar{L}_{\delta]\alpha} + \delta_{\alpha[\delta}\bar{L}_{\gamma]\beta} - \tfrac{1}{2}\delta_{\alpha[\delta}\delta_{\gamma]\beta}\bar{L}_{\sigma\sigma} \tag{17}$$

$$= \tfrac{1}{2}k^2\delta_{\beta[\delta}W_{,\gamma]}W_{,\alpha} + \delta_{\alpha[\gamma}W_{,\delta]}W_{,\beta} - \tfrac{1}{2}\delta_{\alpha[\gamma}\delta_{\delta]\beta}W_{,\sigma}W_{,\sigma}. \tag{17'}$$

Equations (15) and (17′) are equivalent. Under the assumption that W is homogeneous of degree n, which implies via Eq. (17′) that $\bar{L}_{\alpha\beta\gamma\delta}$ is homogeneous of degree $2n-2$, we have the setting of the previous corollary. Therefore, by Eqs. (8) and (17′) the solutions $\gamma_{\alpha\beta}$ as cited in Eq. (10) are constructed. This completes the proof. On the underlying question of convergence of power series as in Eq. (11), we might make the following comment.

If we have considered a domain D of V_4 in the background Euclidean topology, then the convergence is assured by choosing k such that

$$|k| < \liminf_{n\to\infty} \rho_n^{-1/n},$$

where $\rho_n = \max \left|\underset{(n)}{R_{ij}}(x)\right|$, $x \in D$, $i, j = 1, 2, 3, 4$.

III. THE FIELD FOR SUPERPOSITIONS OF MULTIPOLES

The previous considerations will now be generalized to find a second approximation for the metric in the case where W is a sum of homogeneous harmonic functions. Suppose W is a superposition of the first p multipoles. Then the expression $\frac{1}{2}W_{,\alpha}W_{,\beta}$ is no longer homogeneous but can be written as the sum of $(2p-1)$ homogeneous terms. We, therefore, can generalize the arguments which proved Theorem 2 to each one of the $2p-1$ terms, because of the linearity of the basic differential equations (15).

Physical importance of this stems from the fact that the Newtonian potential for any of the usual mass distributions has a multipole expansion.

Now we shall consider a concrete example of constructing the second-order metric where the corresponding Newtonian potential kW is the sum of a monopole ($kW_{\rm I}$) and a quadrupole ($kW_{\rm II}$), i.e.,

$$kW = kW_{\rm I} + kW_{\rm II}. \tag{18}$$

We take for simplicity a spherical body of unit radius, $r \equiv (x^{1^2} + x^{2^2} + x^{3^2})^{\frac{1}{2}} = 1$. Subscripts e and i denote the exterior and interior of the body, respectively.

For $kW_{\rm I}$ we choose the potential of the homogeneous unit sphere; thus

$$kW_{\rm Ie} = kr^{-1}, \tag{19}$$

and

$$kW_{\rm Ii} = \tfrac{3}{2}k - \tfrac{1}{2}kr^2. \tag{20}$$

The corresponding mass density is

$$\rho_{\rm I} \equiv -(4\pi)^{-1}(kW_{\rm Ii})_{,\alpha\alpha} = (4\pi)^{-1}3k. \tag{21}$$

For $kW_{\rm II}$ we choose the following expression:

$$kW_{\rm IIe} = k[-r^{-3}(a+b+c) + 3r^{-5}(ax^{1^2} + bx^{2^2} + cx^{3^2})], \tag{22}$$

$$kW_{\rm IIi} = kW_{\rm IIe}(2r^5 - r^{10}), \tag{23}$$

where a, b, and c are arbitrary constants. This expression for $kW_{\rm II}$ is indeed continuous across the boundary, has continuous normal derivative, and is harmonic in the exterior. The mass density corresponding to $kW_{\rm II}$ is

$$\rho_{\rm II} \equiv -(4\pi)^{-1}(kW_{\rm IIi})_{,\alpha\alpha} = -(4\pi)^{-1}50k[r^5(a+b+c) - 3r^3(ax^{1^2} + bx^{2^2} + cx^{3^2})]. \tag{24}$$

To secure a positive total mass density ρ, where

$$\rho \equiv \rho_{\rm I} + \rho_{\rm II}, \tag{25}$$

it is sufficient to demand

$$|a| + |b| + |c| < \tfrac{3}{200}. \tag{26}$$

Let us now find the exterior metric of the body in second approximation. To simplify our notation, we now omit the suffix e. We have by Eq. (18) that

$$\tfrac{1}{2}k^2W_{,\alpha}W_{,\beta} = \tfrac{1}{2}k^2(W_{{\rm I},\alpha}W_{{\rm I},\beta}) + \tfrac{1}{2}k^2(W_{{\rm II},\alpha}W_{{\rm II},\beta}) + \tfrac{1}{2}k^2(W_{{\rm I},\alpha}W_{{\rm II},\beta} + W_{{\rm II},\alpha}W_{{\rm I},\beta}). \tag{27}$$

Let us introduce the following abbreviations:

$$\begin{aligned} \bar{L}^{(1)}_{\alpha\beta} &\equiv -\tfrac{1}{2}k^2W_{{\rm I},\alpha}W_{{\rm I},\beta}, \\ \bar{L}^{(2)}_{\alpha\beta} &\equiv -\tfrac{1}{2}k^2W_{{\rm II},\alpha}W_{{\rm II},\beta}, \\ \bar{L}^{(3)}_{\alpha\beta} &\equiv -\tfrac{1}{2}k^2(W_{{\rm I},\alpha}W_{{\rm II},\beta} + W_{{\rm II},\alpha}W_{{\rm I},\beta}). \end{aligned} \tag{28}$$

Each one of these three terms is homogeneous of degree -4, -8, and -6, respectively. The corresponding linearized Riemann tensors

$$L^{(\nu)}{}_{\alpha\beta\gamma\delta} = \delta_{\beta[\gamma}L^{(\nu)}{}_{\delta]\alpha} + \delta_{\alpha[\delta}L^{(\nu)}{}_{\gamma]\beta} - \tfrac{1}{2}\delta_{\alpha[\delta}\delta_{\gamma]\beta}L^{(\nu)}_{\sigma\sigma}, \quad \nu = 1, 2, 3, \tag{29}$$

are again homogeneous of degree -4, -8, and -6, respectively. We therefore get by Eqs. (7) and (8) that

$$\begin{aligned} \gamma^{(1)}_{\alpha\delta} &= x^\beta x^\gamma L^{(1)}{}_{\alpha\beta\gamma\delta}, \\ \gamma^{(2)}_{\alpha\delta} &= \tfrac{1}{15}x^\beta x^\gamma L^{(2)}{}_{\alpha\beta\gamma\delta}, \\ \gamma^{(3)}_{\alpha\delta} &= \tfrac{1}{6}x^\beta x^\gamma L^{(3)}{}_{\alpha\beta\gamma\delta}. \end{aligned} \tag{30}$$

The exterior metric up to the second order is finally given by

$$ds^2 = e^{-kW}(\delta_{\alpha\beta} + \gamma^{(1)}_{\alpha\beta} + \gamma^{(2)}_{\alpha\beta} + \gamma^{(3)}_{\alpha\beta})\,dx^\alpha\,dx^\beta - e^{kW}(dx^4)^2. \tag{31}$$

* This work has been supported by NRC Grants Nos. A-5205 and A-3993.

[1] J. H. Young and C. A. Coulter, Phys. Rev. **184**, 1313 (1969).

[2] A. Das, P. S. Florides, and J. L. Synge, Proc. Roy. Soc. **A263**, 451 (1961).

[3] J. L. Synge, Proc. Roy. Irish Acad. **A67**, 47 (1969).

[4] Private communications with J. L. Synge and I. Robinson; see also J. L. Synge, *Relativity: The General Theory* (North-Holland, Amsterdam, 1960), p. 80, Eq. (166).

[5] Square brackets in the indices denote antisymmetrization.

[6] That is, in the power series expansion of R_{ij} in terms of k the first three terms will vanish; cf. Ref. 2.

[7] Note that $\bar{L}_{\alpha\beta} = \bar{L}_{\beta\alpha}$ and $(\bar{L}_{\alpha\beta} - \frac{1}{2}\delta_{\alpha\beta}\bar{L})_{,\beta} = 0$ are compatible with Eq. (15).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Resonant Oscillations: A Regular Perturbation Approach

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(Received 9 November 1970)

The resonant oscillations of a gas in a closed-end tube are treated. The time-periodic motion is given by a regular perturbation method in which the expansion parameter is the Mach number of the resulting flow. The solution at the first order exhibits a shock traveling in the tube, but, to this order, the waves do not interact. The interaction of the waves is calculated at the second order. The perturbation procedure proceeds systematically by an application of the Fredholm alternative at each stage.

1. INTRODUCTION

Most of the work which has been done on nonlinear wave propagation has been directed to cases when only one component of the motion is excited. Reflections are then excluded, and consequently the problems associated with the interaction of the waves are bypassed. Recently,[1] Mortell and Varley investigated the nonlinear initial-value, boundary-value problem associated with small amplitude free vibrations of an elastic panel of finite width rigidly bonded at both ends. The key result of that paper was that in the limit when the amplitude of the motion remained small, but the acceleration was unrestricted, then the motion, uniformly to first order, could be represented as the superposition of two noninteracting simple waves traveling in opposite directions. This representation is uniformly valid in time and was used in Ref. 1 to study the evolution of prescribed initial conditions up until shock formation. Subsequently, Mortell[2] used the simple wave representation to study the time-periodic oscillations of a gas, in a tube of finite length, under periodic excitation. In particular, the resonant time-periodic motion was treated. One disadvantage of the method used in Ref. 2 is that one was confined to the first-order solution and corrections could not be calculated. This meant that one could not assess the effect of the interaction of the waves. The object of the present paper is to give a perturbation scheme which allows the systematic calculation, to any desired order, of the resonant time-periodic motion.

The experimental observations on the resonant motion of a column of gas confined to a tube with a closed end have been given by Saenger and Hudson.[3] The theoretical explanation seems to have been first given by Betchov.[4] Subsequently, the problem was treated by Chu,[5] Chester,[6,7] and Mortell.[2] All used entirely different approaches. The method used here is essentially the systematic exploitation of an idea implicit in the work of Chester.[6] It is recognized that the resonant motion may be viewed as lying in the neighborhood of a linear standing wave, and this is the basis of the perturbation procedure used.

The procedure is also closely related to that used by Keller and his co-workers[8–10] in dealing with nonlinear periodic vibrations. Their basic assumption is that linear theory gives the first term in an expansion in powers of the amplitude, and subsequent terms yield information on how the frequency and form of the vibration depend on the amplitude, whereas in linear theory they are independent of it. A direct application of this method is not feasible here, since there is no resonant solution within linear, inviscid theory. The key to the problem lies in taking the linear standing wave as the first term in the asymptotic expansion. This idea is formalized by taking as expansion parameter the Mach number of the resulting motion which is the square root of the Mach number of the applied velocity.

The bulk of the paper is concerned with calculating the main flow and the first correction to it. The final section is devoted to pointing out the different roles of various terms which "formally" occur at the same order in a representation for the characteristics derived using a method of Lin.[11]

2. FORCED MOTION OF A POLYTROPIC GAS: FORMULATION

A column of gas, which has length L in some reference state, is contained in a tube. At one end the tube is closed, while at the other end a piston imparts a periodic motion, with zero mean velocity, to the gas. The gas is polytropic, and the motion is assumed to be one dimensional, inviscid, and isentropic.

Lagrangian coordinates are used throughout, since then the boundaries of the gas are fixed. Let a_0 and ρ_0 be the sound speed and density in the reference state, and let $a_0u(t, x)$ and $\rho_0\rho$ be the fluid velocity and density at time $(L/a_0)t$ at the particle x, which in the reference state was at a distance Lx from the closed end. The equations expressing the conservation of mass and momentum then are

$$\frac{\partial \rho}{\partial t} + \rho^2 \frac{\partial u}{\partial x} = 0 \tag{2.1}$$

and

$$\frac{\partial u}{\partial t} + a^2 \frac{\partial \rho}{\partial x} = 0, \tag{2.2}$$

where the sound speed a is given in terms of the density by the constitutive equation for a polytropic gas

$$a^2 = \rho^{\gamma-1}. \tag{2.3}$$

Via the method of Riemann,[12] Eqs. (2.1)–(2.3) may be reformulated as

$$\left(\frac{\partial}{\partial t} + a^{(\gamma+1)/(\gamma-1)} \frac{\partial}{\partial x}\right)\left(u + \frac{2}{\gamma-1} a\right) = 0 \tag{2.4}$$

and

$$\left(\frac{\partial}{\partial t} - a^{(\gamma+1)/(\gamma-1)} \frac{\partial}{\partial x}\right)\left(u - \frac{2}{\gamma-1} a\right) = 0. \tag{2.5}$$

To Eqs. (2.4) and (2.5) are adjoined the boundary conditions that

$$\text{on} \quad x = 0, \quad u = 0, \tag{2.6}$$

and

$$\text{on} \quad x = 1, \quad u = \epsilon \sin \omega t, \tag{2.7}$$

where ϵ ($\ll 1$) is the Mach number of the piston motion.

Conditions (2.4)–(2.7) are usually supplemented by initial conditions. However, as for linear theory where one restricts the class of initial conditions, these are replaced by the requirement that the flow is to be periodic with period $2\pi/\omega$. That is, we seek a velocity field with the property

$$u(x, t + 2\pi/\omega) = u(x, t). \tag{2.8}$$

In the Appendix, it is shown quite generally that, for time-periodic motions of an elastic material, the mean stress and mean velocity do not vary from particle to particle. Therefore,

$$\int_0^{2\pi/\omega} u(x, t)\, dt = 0, \tag{2.9}$$

since the mean of the velocity is zero at $x = 0$ and $x = 1$. It is emphasized that (2.9) is not a further assumption, but is a consequence of the governing equations, the boundary conditions, and the assumed periodicity of the solution.

The natural reference configuration is thus the state corresponding to the constant mean pressure p_m and mean velocity $u_m = 0$. Then, for isentropic motions in the limit of vanishingly small amplitudes, the sound speed and density in the mean configuration are independent of x. [For isentropic motions and in the limit of vanishingly small amplitudes, the temperature of the mean state (which determines the sound speed) is independent of x when the pressure is. The temperature of the mean state is determined by the previous history of the motion.]

3. FIRST-ORDER SOLUTION

It is well known[2,5,6] that acoustic theory fails to predict the motion of the gas when the piston frequency is a resonant one. The analysis here will concentrate on calculating the time-periodic response of the gas when the piston is driven at the fundamental resonant frequency $\omega = \pi$. The existence of the resonant time-periodic motion has been confirmed experimentally in Ref. 3. The main features of the observations are the noticeable increase in amplitude at the resonant frequency and the appearance of shocks in the flow.

The evolution of the motion from its initial state until the periodic state has been set up is not the concern of this paper. Rather, a perturbation procedure is given which has the specific object of picking out the final periodic state, without any reference to how the motion evolved to that state.

We shall assume an asymptotic expansion for the dependent variables $u(t, x; \epsilon)$ and $a(t, x; \epsilon)$ of the form

$$a(t, x; \epsilon) = 1 + \epsilon^{\frac{1}{2}} a_1(t, x) + \epsilon a_2(t, x) + \cdots \tag{3.1}$$

and

$$u(t, x; \epsilon) = \epsilon^{\frac{1}{2}} u_1(t, x) + \epsilon u_2(t, x) + \cdots. \tag{3.2}$$

The boundary conditions (2.6) and (2.7) are

$$u(t, 0; \epsilon) = 0 \tag{3.3}$$

and

$$u(t, 1; \epsilon) = \epsilon \sin \pi t. \tag{3.4}$$

The expansion parameter in (3.1) and (3.2) is the square root of the Mach number of the imposed piston velocity. It will emerge that it is also the Mach number of the resulting flow.

The insertion of (3.1) and (3.2) into (2.4) and (2.5), and noting (3.3) and (3.4), lead to the first-order problem

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right)\left(u_1 + \frac{2}{\gamma-1} a_1\right) = 0 \tag{3.5}$$

and

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right)\left(u_1 - \frac{2}{\gamma-1} a_1\right) = 0, \tag{3.6}$$

with the homogeneous boundary conditions

$$u_1(t, 0) = u_1(t, 1) = 0. \tag{3.7}$$

The solution is

$$u_1(t, x) = f(t - x) - f(t + x), \qquad (3.8)$$

where f is an arbitrary periodic function with period 2. At this stage, the basic solution is a standing wave with an arbitrary signal f.

The nonhomogeneous equations to determine the second-order terms, $u_2(t, x)$ and $a_2(t, x)$, now have the form

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right) U_1 = F_1(t, x), \qquad (3.9)$$

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right) U_2 = F_2(t, x), \qquad (3.10)$$

where

$$U_1 = u_2 + [2/(\gamma - 1)]a_2, \quad U_2 = u_2 - [2/(\gamma - 1)]a_2, \qquad (3.11)$$

$$F_1 = (\gamma + 1)f'(t - x)[f(t - x) + f(t + x)], \qquad (3.12)$$

and

$$F_2 = -(\gamma + 1)f'(t + x)[f(t - x) + f(t + x)]. \qquad (3.13)$$

The boundary conditions at this order, $O(\epsilon)$, are

$$u_2(t, 0) = 0, \quad u_2(t, 1) = \sin \pi t, \qquad (3.14)$$

and these are also nonhomogeneous.

It is well known that a necessary condition for the existence of a solution U_1 to (3.9) is that $F_1(t, x)$ should be orthogonal to the solutions of the homogeneous adjoint of Eq. (3.9). A similar remark holds for Eq. (3.10). Thus there is a restriction on the functions F_1 and F_2 and hence on the function f. When one fully utilizes the periodicity requirement on f, then the restriction on f may be stated in the form of a differential equation which f must satisfy. The conclusion then is that while, at order $\epsilon^{\frac{1}{2}}$, f is an arbitrary periodic function of period 2, in order to be able to calculate the correction at order ϵ, f must be restricted to be the solution of a differential equation. The derivation of this differential equation for f is now given. Equation (3.9) is multiplied through by $f(t - x)$ and integrated over $0 \le t \le 2$, $0 \le x \le 1$. Equation (3.10) is multiplied through by $-f(t + x)$ and integrated over $0 \le t \le 2$, $0 \le x \le 1$. The resulting equations are added and, when use is made of integration by parts, the fact that f has period 2, and the boundary conditions (3.14), the result is that f must satisfy

$$2\int_0^2 f(\eta) \sin \pi(\eta + 1)\, d\eta = \int_0^2 \int_0^1 [f(t - x)F_1 - f(t + x)F_2]\, dx\, dt. \qquad (3.15)$$

The right-hand side of (3.15) takes the form

$$\int_0^2 f(\eta)\left(\int_0^2 (F_1 + F_2)\, d\xi\right) d\eta \qquad (3.16)$$

when a lemma due to Keller and Ting[8] is used, where $\xi = t + x$ and $\eta = t - x$. It is worth noting that the periodicity requirement on f is crucial for the result (3.16) and hence for the ensuing results. Equation (3.15) now reads

$$\int_0^2 (F_1 + F_2)\, d\xi = 2 \sin \pi(\eta + 1). \qquad (3.17)$$

When the condition that f have zero mean value over one cycle is imposed and the definitions of F_1 and F_2 are used, (3.17) yields

$$(\gamma + 1)f(\eta)f'(\eta) = -\sin \pi\eta, \quad 0 < \eta < 2, \qquad (3.18)$$

as the further condition which f must satisfy in order to be able to calculate $u_2(t, x)$ and $a_2(t, x)$ at order ϵ. Since periodicity has been used throughout the derivation, (3.18) is valid only over a period of the motion. Equation (3.18), which determines the signal f carried by a wave at first order $[O(\epsilon^{\frac{1}{2}})]$, is the necessary condition for the existence of a correction [i.e., terms at $O(\epsilon)$] to the first order. It is closely related to the "secular" equation of Betchov.[4] In Eq. (3.18), the term $(\gamma + 1)$ is twice the second-order elastic constant for a polytropic gas and the product term ff' is a result of the "amplitude dispersion" or nonlinear convection in the original partial differential equations. On examining the representation (3.8) for $u(t, x)$, where the signal f is given by (3.18), we notice the interesting dichotomy that whereas the signal f carried by a wave is determined by a nonlinear equation which reflects the presence of amplitude dispersion, the wave itself progresses like a linear wave. Hence there is no interaction, at this order, between the forward and backward components of the motion.

The nonlinear differential equation (3.18) was derived in Ref. 2 when the motion was predicated to be the superposition of two simple waves, traveling in opposite directions, whose only interaction occurred at the boundaries. This hypothesis could not yield the interaction terms which will be calculated in the next section.

The solution to (3.18) which satisfies the periodicity and zero mean-value conditions is given by

$$f(t) = \pm\{2/[\pi(\gamma + 1)]^{\frac{1}{2}}\} \cos \tfrac{1}{2}\pi t, \quad 0 < t < 2,$$
$$f(t + 2) = f(t). \qquad (3.19)$$

On noting (3.2) and (3.8), it is clear that the particle velocity in the gas is $O(\epsilon^{\frac{1}{2}})$, while that of the piston velocity is $O(\epsilon)$. Furthermore, the signal f, defined by (3.19), is periodic and discontinuous. Thus there is a traveling discontinuity in the solution which is easily checked to satisfy the shock relations. These conclusions are in agreement with experiment.[3]

The derivative of f is defined by

$$f'(t) = \mp[\pi/(\gamma+1)]^{\frac{1}{2}} \sin \tfrac{1}{2}\pi t, \quad 0 < t < 2,$$
$$f'(t+2) = f'(t). \tag{3.20}$$

If the piston frequency is $\omega = N\pi$, N an integer, then solutions of the form (3.19) with the appropriate amplitude factor and periodicity property can be patched together to yield a solution with N shocks in the tube.

4. SECOND-ORDER SOLUTION

In the previous section it has been shown that even though the phenomenon is nonlinear, the waves, to first order, do not interact. By this is meant that the path of a wave is unaffected by the oppositely traveling waves through which it passes. In this section we shall calculate the solution at order ϵ and we shall see that interaction terms arise.

When (3.18) is invoked, (3.9) and (3.10) become

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right)\left(u_2 + \frac{2}{\gamma-1} a_2\right) = -\sin \pi(t-x) + (\gamma+1) f(t+x) f'(t-x) \tag{4.1}$$

and

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right)\left(u_2 - \frac{2}{\gamma-1} a_2\right) = \sin \pi(t+x) - (\gamma+1) f(t-x) f'(t+x), \tag{4.2}$$

where f is given by (3.19). The boundary conditions associated with (4.1) and (4.2) are given by (3.14), and then the boundary value problem defined by (4.1), (4.2), and (3.14) is non-self-adjoint. The most direct way to solve the problem is to observe $-x \sin \pi \times (t-x)$ is a particular integral of (4.1) which accounts for the term $-\sin \pi(t-x)$. Similarly, $-x \sin \pi(t+x)$ is a particular integral of (4.2) which takes care of the term $\sin \pi(t+x)$. Furthermore, the combination of these two particular integrals satisfies the boundary conditions (3.14), and so the remainder of the solution satisfies homogeneous boundary conditions. The solution then is

$$u_2 + [2/(\gamma-1)]a_2 = -x \sin \pi(t-x) + \tfrac{1}{2}(\gamma+1) f'(t-x) \times \int^{t+x} f(s)\, ds + f_2(t-x), \tag{4.3}$$

$$u_2 - [2/(\gamma-1)]a_2 = -x \sin \pi(t+x) - \tfrac{1}{2}(\gamma+1) f'(t+x) \times \int^{t-x} f(s)\, ds - f_2(t+x), \tag{4.4}$$

where f_2 is an arbitrary periodic function with period 2. One cycle of the calculation has now been completed.

It is clear that the contribution of the interaction of the waves to the solution is given by the terms involving integrals in (4.3) and (4.4). This contribution may be explicitly calculated in terms of the solution at the first order, since f is given by (3.19).

The determination of the function f_2 is straightforward, but tedious. The boundary conditions at the next order, $O(\epsilon^{\frac{3}{2}})$, are homogeneous, and so the problem is self-adjoint and a direct orthogonality condition may be applied.

The equations to determine $u_3(t,x)$ and $a_3(t,x)$ are

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right)\left(u_3 + \frac{2}{\gamma-1} a_3\right) = -\frac{\gamma+1}{\gamma-1} a_1 \frac{\partial}{\partial x}\left(u_2 + \frac{2}{\gamma-1} a_2\right) - \frac{\gamma+1}{\gamma-1}\left(a_2 + \frac{1}{\gamma-1} a_1^2\right)\frac{\partial}{\partial x}\left(u_1 + \frac{2}{\gamma-1} a_1\right), \tag{4.5}$$

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right)\left(u_3 - \frac{2}{\gamma-1} a_3\right) = \frac{\gamma+1}{\gamma-1} a_1 \frac{\partial}{\partial x}\left(u_2 - \frac{2}{\gamma-1} a_2\right) + \frac{\gamma+1}{\gamma-1}\left(a_2 + \frac{1}{\gamma-1} a_1^2\right)\frac{\partial}{\partial x}\left(u_1 - \frac{2}{\gamma-1} a_1\right), \tag{4.6}$$

subject to the boundary conditions

$$u_3(t,0) = u_3(t,1) = 0. \tag{4.7}$$

A solution to (4.5)–(4.7) exists if

$$\int_0^2 \frac{\partial}{\partial x}\left(a_1 a_2 + \frac{1}{3(\gamma-1)} a_1^3\right) d\xi = 0. \tag{4.8}$$

This condition determines f_2 in terms of the known function f, but we will pursue it no further.

The dominant flow occurs at $O(\epsilon^{\frac{1}{2}})$. The boundary condition on $x = 1$ and the interaction of the waves occur at $O(\epsilon)$ and thus appear as corrections to the main flow, which is a standing wave.

It is noted that u_2 as defined by (4.3) and (4.4) has zero mean when f_2 has zero mean, whereas a_2 has not. This is consistent with the remarks made in the Appendix. The presence of the derivative term in (4.3) and (4.4) shows that the expansion is valid under the restriction

$$\epsilon^{\frac{1}{2}}\omega \ll 1,$$

where ω is the piston frequency.

5. A REMARK ON THE USE OF LIN'S TECHNIQUE

In the Appendix of Ref. 2, it was shown how at technique due to Lin[11] provides the following representation for the characteristics of (2.4) and (2.5) when the assumption of small amplitudes is made and the condition that the velocity is zero at $x = 0$ has been enforced:

$$\alpha(t, x; \epsilon) = t - x + \tfrac{1}{2}(\gamma + 1)\epsilon x\phi(\alpha) + \tfrac{1}{4}(\gamma + 1)\epsilon \times \int_\alpha^\beta \phi(s)\, ds + o(\epsilon\phi), \quad (5.1)$$

$$\beta(t, x; \epsilon) = t + x - \tfrac{1}{2}(\gamma + 1)\epsilon x\phi(\beta) - \tfrac{1}{4}(\gamma + 1)\epsilon \times \int_\alpha^\beta \phi(s)\, ds + o(\epsilon\phi), \quad (5.2)$$

where

$$u(t, x; \epsilon) = \epsilon[\phi(\alpha) - \phi(\beta)]. \quad (5.3)$$

It is noted that $\alpha = \beta = t$ on $x = 0$ and, by the representation (5.3) for u, the boundary condition $u(t, 0; \epsilon) = 0$ is automatically satisfied. We further note that ϕ is the exact Riemann invariant.

We wish to consider how an α wavelet propagates, and so α and x are taken as independent variables, while the dependent variables are $t = t(\alpha, x)$ and $\beta = \beta(\alpha, x)$. On using (5.1), the speed $c(\alpha, x)$ at which a wavelet α travels is given by

$$c^{-1}(\alpha, x) = \left.\frac{\partial t}{\partial x}\right|_\alpha = 1 - \frac{\gamma + 1}{2}\epsilon\phi(\alpha) - \frac{\gamma + 1}{4}\epsilon\phi(\beta)\left.\frac{\partial \beta}{\partial x}\right|_\alpha. \quad (5.4)$$

Thus the speed of an α wavelet depends on the β wavelets through which it passes, and the representation (5.1) implies there is an interaction of the waves.

The results of Sec. 3 and 4 are that to order $\epsilon^{\frac{1}{2}}$ there is no interaction of the waves, but to order ϵ there is. In order to reconcile the consequences of the representations (5.1) and (5.2) with this result, it is clear that a distinction must be drawn between the two terms which are coefficients of ϵ. At $x = 1$, (5.1) and (5.2) reduce to

$$\alpha = t - 1 + \tfrac{1}{2}(\gamma + 1)\epsilon\phi(\alpha), \quad (5.5)$$

$$\beta = t + 1 - \tfrac{1}{2}(\gamma + 1)\epsilon\phi(\beta), \quad (5.6)$$

where *the interaction term has been lost*, because the governing equations and boundary conditions *demand* that the solution have zero mean to this order. We shall now solve the resonant problem, using (5.5) and (5.6). The boundary condition

$$u(t, 1; \epsilon) = \epsilon \sin \pi t,$$

together with (5.3), (5.5), and (5.6), yields the nonlinear difference equation

$$\phi[t - 1 + \tfrac{1}{2}(\gamma + 1)\epsilon\phi(\alpha)] - \phi[t + 1 - \tfrac{1}{2}(\gamma + 1)\epsilon\phi(\beta)] = \sin \pi t \quad (5.7)$$

for the determination of the signal ϕ. Using the condition that ϕ has period 2 and the small amplitude restriction $|\epsilon\phi| \ll 1$, one finds easily from (5.7)

$$(\gamma + 1)\epsilon\phi(t)\phi'(t) = -\sin \pi t + \text{higher order terms}.$$

We make the identification

$$f = \epsilon^{\frac{1}{2}}\phi,$$

and then f has period 2 and satisfies

$$(\gamma + 1)f(t)f'(t) = -\sin \pi t,$$

which is exactly (3.18).

We now conclude that to first order the progress of the waves and the signals carried by them can be determined *independently of the interaction of the waves*. Thus the integral terms in (5.1) and (5.2) do not properly belong to the first order. The other terms involving ϵ in (5.1) and (5.2) represent amplitude dispersion, and the role of these terms is to determine the signal carried at the first order. To properly describe, to first order, the progress of waves and the signals carried by them, we may truncate (5.1) and (5.2) by omitting the integral terms. The resulting representation for α and β, together with (5.3), is nothing more than the assertion that the motion is the superposition of two simple waves traveling in opposite directions.

6. DISCUSSION

The method used in solving the problem posed here is essentially different to that used by Kruskal and Zabusky[13] when they considered the free vibration problem for a nonlinear string. For this latter problem it was shown first by Zabusky,[14] and later in Refs. 8 and 15, that the solution was not time periodic. As a result, one has no option but to follow the evolution of the motion, and hence a uniform perturbation expansion, such as the "stroboscopic" procedure of Ref. 13, must be used to examine the problem. For the resonant problem treated here, the situation is entirely different. Experiments show that there is a time-periodic resonant motion, and, using the results derived in the Appendix, we have shown how to define a reference state about which the periodic motion takes place. The essential unknown in the reference state is the temperature, and this is the element in the problem which is determined by the history of the motion. The perturbation procedure given here has been devised specifically to pick out the periodic motion about the mean state. There is close agreement between the theoretical predictions and the experimental observations.

The results of the investigation[13] agree with those given here on some important points. In Ref. 13 the perturbation solution exhibited a discontinuity or "breakdown" in the first order. There is a shock in our first-order solution. With regard to the results of Ref. 13, it is noted by Zabusky in Ref. 16 that, "although the phenomena are nonlinear, signals propagating (or functions evolving) along the different characteristics did not interact with each other to lowest order." It was found here that the periodic signal functions, which to first order do not interact, are determined by a nonlinear equation. Furthermore, to the order that the signals do not interact, they are effectively moving into a constant state, and hence must be simple waves. This is the conclusion of Sec. 5. The same result was found by an entirely different method in Ref. 17; it has been exploited to treat resonant motions in Ref. 2.

A glance at Refs. 13 and 14 will reveal that an approach to the resonant problem via the hodograph space will not simplify either the analysis or the understanding of the problem.

The main contribution of the paper is to give a perturbation technique for dealing with the time-periodic solutions to a class of nonlinear wave propagation problems in which the reflected waves are as significant are the primary waves. The key factor is that to first order the waves travel as linear waves and do not interact, even though the signal carried is determined by a nonlinear equation. Consequently, the nonlinear interaction of the waves is then calculated at the second order.

The perturbation method given here may be applied to the thermal-acoustic oscillations treated in Refs. 5 and 18, and also to the magnetohydrodynamic problems treated in Refs. 19 and 20.

Note: The author has learned by private communication that Professor W. D. Collins of the University of Strathclyde has been working along similar lines.

ACKNOWLEDGMENT

The results presented in this paper were obtained in the course of research sponsored by Department of Defense Project THEMIS and monitored by the Ballistics Research Laboratories, Aberdeen Proving Ground, Aberdeen, Maryland.

APPENDIX

It is shown here that, for an elastic material undergoing a time-periodic deformation, the mean values of the stress and velocity fields do not vary from particle to particle.

Let $\sigma(t, x)$, $\lambda(t, x)$, and $u(t, x)$ be measures of the normal traction, strain, and material velocity at time t at the particle x, which in some reference configuration was at a distance x from a reference particle. The equations expressing the principles of conservation of mass and linear momentum are

$$\frac{\partial \lambda}{\partial t} - \frac{\partial u}{\partial x} = 0 \tag{A1}$$

and

$$\rho \frac{\partial u}{\partial t} - \frac{\partial \sigma}{\partial x} = 0, \tag{A2}$$

where ρ is the constant density of the material in the reference configuration. Conditions (A1) and (A2) are supplemented by the equation of state for an elastic material

$$\sigma = \sigma(\lambda). \tag{A3}$$

Let the period of the motion be normalized to unity, and integrate (A1) with respect to time over one period. We assume, for convenience, there is at most one shock, and then

$$\frac{\partial}{\partial x} u_m(x) = \lambda(x, 0) - \lambda(x, 1) + [\lambda] - U^{-1}[u], \tag{A4}$$

where $[\lambda]$ and $[u]$ denote the jumps in λ and u across the shock which has speed U and where

$$u_m(x) = \int_0^1 u(x, t)\, dt \tag{A5}$$

is the mean of u. If λ and u are continuous, then

$$\frac{\partial}{\partial x} u_m(x) = 0, \tag{A6}$$

by the periodicity of λ. If λ and u are not continuous, then (A6) again follows from the periodicity of λ and the shock relation

$$U = -[u]/[\lambda].$$

Thus, in any event, u_m is independent of x. For similar reasons

$$\sigma_m = \int_0^1 \sigma(x, t)\, dt \tag{A7}$$

is independent of x.

It is further noted that if one uses a *linear* approximation for (A3), then λ_m and the corresponding sound speed are independent of x. For higher approximations this is not so, in general. Finally we note an interesting consequence of the shock relations: They allow the possibility of time-periodic motions about a state of *constant stress* and *constant velocity*.

1 M. P. Mortell and E. Varley, Proc. Roy. Soc. (London) **A318**, 169 (1970).
2 M. P. Mortell, Intern. J. Eng. Sci. **9**, 175 (1971).
3 R. A. Saenger and G. E. Hudson, J. Acoust. Soc. Am. **32**, 961 (1960).
4 R. Betchov, Phys. Fluids **1**, 205 (1958).
5 B. T. Chu and S. J. Ying, Phys. Fluids **6**, 1625 (1963).
6 W. Chester, J. Fluid Mech. **18**, 44 (1964).
7 W. Chester, Proc. Roy. Soc. (London) **A306**, 5 (1968).
8 J. B. Keller and L. Ting, Commun. Pure Appl. Math. **19**, 371 (1966).
9 M. H. Millman and J. B. Keller, J. Math. Phys. **10**, 342 (1969).
10 J. B. Keller and M. H. Millman, Phys. Rev. **181**, 1730 (1969).
11 C. C. Lin, J. Math. & Phys. **33**, 117 (1954).
12 R. Courant and K. O. Friedrichs, *Supersonic Flow and Shock Waves* (Interscience, New York, 1948).
13 M. D. Kruskal and N. J. Zabusky, J. Math. Phys. **5**, 231 (1964).
14 N. J. Zabusky, J. Math. Phys. **3**, 1028 (1962).
15 P. D. Lax, J. Math. Phys. **5**, 611 (1964).
16 N. J. Zabusky, in *Nonlinear Partial Differential Equations*, W. F. Ames, Ed. (Academic, New York, 1967).
17 E. Varley, M. P. Mortell, and A. Trowbridge, in *Wave Propagation in Solids*, J. Miklowitz, Ed. (American Society of Mechanical Engineers, New York, 1969).
18 B. T. Chu, Phys. Fluids **6**, 1638 (1963).
19 R. M. Gundersen, Intern. J. Eng. Sci. **4**, 563 (1966).
20 R. M. Gundersen, Intern. J. Eng. Sci. **5**, 205 (1967).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Particles with Spin in a Gravitational Field*

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(Received 7 October 1970)

Papapetrou's covariant equations of motion for a spinning particle in a gravitational field are discussed. The equations of motion for the spin of a particle at rest outside a rotating mass are derived using the Kerr metric. It is shown that Schiff's formula for the mass-current effect follows from these equations in the lowest approximation.

I. INTRODUCTION

Preparations under way by Fairbank and collaborators to measure the precession of a gyroscope caused by the rotation of the earth give incentive to see the physical effects at work in as many ways as possible. Schiff has derived the precession in question from the Schwarzschild line element and the Lense–Thirring effect. Here we derive it by considering the motion of a spinning object in the Kerr geometry associated with a rotating black hole endowed with the same mass and angular momentum as the earth possesses.

Papapetrou[1] has derived the covariant equations of motion for a pole–dipole particle using the method of Fock.[2] In this method one starts from the "dynamical equation" $T^{\mu\nu}{}_{;\nu} = 0$ ($T^{\mu\nu}$ is the energy–momentum tensor), rather than the gravitational field equations (as in the EIH[3] method). Let us consider a test particle whose dimensions are very small compared with the characteristic length of the basic gravitational field, so the particle will describe a narrow tube in the four-dimensional space-time. Let us choose a line in this tube, whose coordinates will be denoted by X^α,[4] and this will "represent" the motion of the particle. Let X^α be functions of $X^4 = t$, or the proper time along the representative line. To characterize the particle, we shall assume that $T^{\mu\nu}$ will vanish for all t outside a sphere centered at X^i and having a small radius R. The results that follow will then be rigorous in the case $R \to 0$. Let $\delta x^\alpha = x^\alpha - X^\alpha$, and consider

$$\int T^{\mu\nu}\, dV,\ \int \delta x^\alpha T^{\mu\nu}\, dV,\ \int \delta x^\alpha \delta x^\beta T^{\mu\nu}\, dV, \cdots;$$

the integration is carried over the three-dimensional volume at a constant time t. A *single-pole* particle is defined as one which has at least one of the $\int T^{\mu\nu}\, dV \neq 0$, while all the other integrals are zero. A *pole–dipole* particle has at least some of the integrals $\int T^{\mu\nu}\, dV$ and $\int \delta x^\alpha T^{\mu\nu}\, dV$ not equal to zero, while all the others are zero. It can be shown[1] that the order of the highest nonvanishing multipole of a particle is invariant under coordinate transformations. In the following we shall refer to a pole–dipole particle as a "spinning particle."

The spin is defined to be

$$S^{\alpha\beta} \equiv \int (\delta x^\alpha T^{\beta 4} - \delta x^\beta T^{\alpha 4})\, dV.$$

It is further noted that if one uses a *linear* approximation for (A3), then λ_m and the corresponding sound speed are independent of x. For higher approximations this is not so, in general. Finally we note an interesting consequence of the shock relations: They allow the possibility of time-periodic motions about a state of *constant stress* and *constant velocity*.

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[2] M. P. Mortell, Intern. J. Eng. Sci. **9**, 175 (1971).
[3] R. A. Saenger and G. E. Hudson, J. Acoust. Soc. Am. **32**, 961 (1960).
[4] R. Betchov, Phys. Fluids **1**, 205 (1958).
[5] B. T. Chu and S. J. Ying, Phys. Fluids **6**, 1625 (1963).
[6] W. Chester, J. Fluid Mech. **18**, 44 (1964).
[7] W. Chester, Proc. Roy. Soc. (London) **A306**, 5 (1968).
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[9] M. H. Millman and J. B. Keller, J. Math. Phys. **10**, 342 (1969).
[10] J. B. Keller and M. H. Millman, Phys. Rev. **181**, 1730 (1969).
[11] C. C. Lin, J. Math. & Phys. **33**, 117 (1954).
[12] R. Courant and K. O. Friedrichs, *Supersonic Flow and Shock Waves* (Interscience, New York, 1948).
[13] M. D. Kruskal and N. J. Zabusky, J. Math. Phys. **5**, 231 (1964).
[14] N. J. Zabusky, J. Math. Phys. **3**, 1028 (1962).
[15] P. D. Lax, J. Math. Phys. **5**, 611 (1964).
[16] N. J. Zabusky, in *Nonlinear Partial Differential Equations*, W. F. Ames, Ed. (Academic, New York, 1967).
[17] E. Varley, M. P. Mortell, and A. Trowbridge, in *Wave Propagation in Solids*, J. Miklowitz, Ed. (American Society of Mechanical Engineers, New York, 1969).
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The spin is defined to be

$$S^{\alpha\beta} \equiv \int (\delta x^\alpha T^{\beta 4} - \delta x^\beta T^{\alpha 4})\, dV.$$

Let $DS^{\alpha\beta}/Ds$ be defined as

$$\frac{DS^{\alpha\beta}}{Ds} \equiv \frac{dS^{\alpha\beta}}{ds} + \Gamma^{\alpha}_{\mu\nu}S^{\mu\beta}u^{\nu} + \Gamma^{\beta}_{\mu\nu}S^{\alpha\mu}u^{\nu},$$

where

$$u^{\alpha} = \frac{dX^{\alpha}}{ds} \quad \text{and} \quad ds^2 = g_{\mu\nu}\, dX^{\mu}\, dX^{\nu}.$$

Then it can be shown that[1]

$$\frac{DS^{\alpha\beta}}{Ds} = u^{\beta}u_{\rho}\frac{DS^{\alpha\rho}}{Ds} - u^{\alpha}u_{\rho}\frac{DS^{\beta\rho}}{Ds}, \qquad (1)$$

$$\frac{D}{Ds}\left(m'u^{\alpha} + u_{\beta}\frac{DS^{\alpha\beta}}{Ds}\right) = \tfrac{1}{2}R^{\alpha}_{\mu\sigma\nu}u^{\sigma}S^{\mu\nu}, \qquad (2)$$

where

$$m' = u_{\alpha}\int T^{\alpha 4}\, dV + \frac{1}{u^4}\Gamma^{\alpha}_{\mu\nu}S^{\mu 4}u^{\nu}u_{\alpha}$$

is a scalar. Thus the spinning particle will not follow a geodesic. The equations (1) for the motion of the spin determine only three of the six unknown $S^{\alpha\beta} = -S^{\beta\alpha}$. Therefore, it is necessary to impose supplementary conditions on $S^{\alpha\beta}$. A natural choice is to put $S^{i4} = 0$ or $S_{i4} = 0$ in some convenient coordinate system.[5,6] We shall see in the following section that different supplementary conditions on the spin tensor lead to quite different physical phenomena as seen by an observer at rest with respect to the representative point of the spinning particle.

II. EQUATIONS OF MOTION

We have seen that Papapetrou's equations are rigorous only in the limiting case of a point particle. However, these equations are accurate even for extended objects if the dimensions of the spinning particle is very small compared with the characteristic length of the gravitational field under consideration.

Let us consider an observer, moving with the spinning particle, with respect to which the representative point is at rest. We shall assume that the observer refers space–time events to a set of orthogonal tetrads $\lambda^{\mu}_{(\alpha)}$, where $\lambda^{\mu}_{(4)} = u^{\mu}$, and $\lambda^{\mu}_{(i)}$ are spacelike 4-vectors, such that $\lambda^{\mu}_{(\alpha)}g_{\mu\nu}\lambda^{\nu}_{(\beta)} = \eta_{(\alpha)(\beta)}$. The flat-space metric is denoted by $\eta_{(\alpha)(\beta)}$ here. The spin tensor is $S^{\alpha\beta} = \int (\delta x^{\alpha}T^{\beta\sigma} - \delta x^{\beta}T^{\alpha\sigma})\, d\mathcal{S}_{\sigma}$, where $\mathcal{S}$ denotes a spacelike hypersurface. Then according to the observer, the spin tensor is

$$S_{(\alpha)(\beta)} = \lambda^{\mu}_{(\alpha)}\lambda^{\nu}_{(\beta)}S_{\mu\nu} = \int (\delta x_{(\alpha)}T^{\sigma}_{(\beta)} - \delta x_{(\beta)}T^{\sigma}_{(\alpha)})\, d\mathcal{S}_{\sigma}.$$

The velocity of the representative point is $u^{\mu} = dX^{\mu}/ds$, so that $u^{(\alpha)} = \lambda^{(\alpha)}_{\mu}u^{\mu} = \delta_{(\alpha),(4)}$. Let us now find the conditions that $S^{\mu\nu}$ should satisfy in order that the fixed representative point is just the center of mass of the spinning particle as measured by the observer. It is well known that the center of mass is a frame-dependent concept.[7] Therefore, what the observer measures as the center of mass is

$$x^{(\alpha)}_{\rm CM} = \frac{\int x^{(\alpha)}T^{\sigma}_{(4)}\, d\mathcal{S}_{\sigma}}{\int T^{\sigma}_{(4)}\, d\mathcal{S}_{\sigma}}.$$

Now, the choice of the spacelike hypersurface $\mathcal{S}$ for the observer is such that $\delta x_{\mu}u^{\mu} = 0$. Therefore, $\delta x_{(4)} = \lambda^{\mu}_{(4)}\delta x_{\mu} = 0$. Hence

$$\begin{aligned} S^{(\alpha)}_{(4)} &= \int \delta x^{(\alpha)}T^{\sigma}_{(4)}\, d\mathcal{S}_{\sigma} \\ &= \int x^{(\alpha)}T^{\sigma}_{(4)}\, d\mathcal{S}_{\sigma} - X^{(\alpha)}\int T^{\sigma}_{(4)}\, d\mathcal{S}_{\sigma} \\ &= (x^{(\alpha)}_{\rm CM} - X^{(\alpha)})\int T^{\sigma}_{(4)}\, d\mathcal{S}_{\sigma}. \end{aligned}$$

Thus in order that $x^{(\alpha)}_{\rm CM}$ and $X^{(\alpha)}$ coincide, we must have $S^{(\alpha)}_{(4)} = 0$. Therefore, $S^{\mu\nu}u_{\nu} = \lambda^{\mu}_{(\alpha)}S^{(\alpha)}_{(4)} = 0$.

The combination of $S^{\mu\nu}u_{\nu} = 0$ and Eqs. (1) and (2) easily leads to $dm'/ds = 0$, and $d(S_{\alpha\beta}S^{\alpha\beta})/ds = 0$.[5] If we define the spin 4-vector as

$$S_{\mu} = \tfrac{1}{2}(-g)^{\frac{1}{2}}\epsilon_{\mu\nu\rho\sigma}u^{\nu}S^{\rho\sigma},$$

where $(-g)^{\frac{1}{2}}\epsilon_{\mu\nu\rho\sigma}$ is the alternating tensor and $g = \det(g_{\alpha\beta})$, then, using $S^{\mu\nu}u_{\nu} = 0$, one obtains $S_{\mu}S^{\mu} = \frac{1}{2}S_{\alpha\beta}S^{\alpha\beta}$. Since $S^{\mu}u_{\mu} = 0$, $S_{(4)} = 0$, and $S_{(i)}S^{(i)} = S_{\mu}S^{\mu}$, so that the length of the spin does not change as measured by the observer. Thus, if the observer fixes any point of the spinning particle (the representative point) other than its center of mass, the magnitude of the spin will change.

It is interesting to note that in the limiting case of a vanishing gravitational field, the force equation (2) reduces to the expression of the constancy of the total momentum of the particle $P^{\alpha} = m'u^{\alpha} + u_{\beta}(dS^{\alpha\beta}/ds)$. This equation is formally identical with the result of Weyssenhoff and Raabe[8] for the free motion of a classical (nonquantum) particle endowed with intrinsic spin $S^{\alpha\beta}$ which is coupled to the orbital motion through $S^{\alpha\beta}u_{\beta} = 0$.

III. EQUATIONS OF MOTION OF A SPINNING PARTICLE, AT REST, OUTSIDE A ROTATING STAR

In the coordinate system under consideration in this section, the particle is at rest, therefore $u^i = 0$ and, assuming $S^{\mu\nu}u_{\nu} = 0$, $S_{i4} = 0$. It follows from (2) that $DS^{ij}/Ds = 0$ if $u^i = 0$. This can be written as

$$\frac{\partial S^{ij}}{\partial t} = \Gamma^j_{\mu 4} S^{\mu i} - \Gamma^i_{\mu 4} S^{\mu j}, \quad S_{i4} = 0.$$

In the following we shall assume that the gravitational field is produced by a rotating spherical body at the origin of the "rest system" of the test particle. This will constitute a physically realizable situation if there exist, besides the gravitational force and the force due to the coupling of spin and gravity, other nongravitational constraining forces acting on the particle which keep it at rest. Owing to the special coordinate system under consideration, further specification of such forces will not be necessary in what follows, except that they should be nonzero only in a small region around the test particle. It is assumed, however, that these forces exert no net torque on the particle. Let us assume that the gravitational field can be described by the Kerr metric[9]

$$-ds^2 = g_{\mu\nu}\, dX^\mu\, dX^\nu = \Sigma\left(\frac{dr^2}{\Delta} + d\theta^2\right) + (r^2 + a^2)\sin^2\theta\, d\phi^2 + \frac{2mr}{\Sigma}(a\sin^2\theta\, d\phi - dt)^2 - dt^2,$$

$$\Sigma \equiv r^2 + a^2\cos^2\theta,$$

$$\Delta \equiv r^2 + a^2 - 2mr,$$

where a spherical system of coordinates has been used. The source of the field is assumed to be a spherical object of mass m and angular momentum ma about the z direction. It is easy to see that in the (r, θ, φ, t) coordinate system

$$\lambda^\mu_{(1)}: \frac{1}{(g_{11})^{\frac{1}{2}}}(1, 0, 0, 0),$$

$$\lambda^\mu_{(2)}: (g_{22})^{-\frac{1}{2}}(0, 1, 0, 0),$$

$$\lambda^\mu_{(3)}: \left(g_{33} - \frac{g_{34}^2}{g_{44}}\right)^{-\frac{1}{2}}\left(0, 0, 1, -\frac{g_{34}}{g_{44}}\right)$$

are appropriate tetrads together with

$$\lambda^\mu_{(4)} = u^\mu : (-g_{44})^{-\frac{1}{2}}(0, 0, 0, 1).$$

One can then convert the equations obtained for $S^{\mu\nu}$ to those for S^μ, and then using $S_{(\alpha)} = \lambda^\mu_{(\alpha)} S_\mu$, to equations involving $S_{(\alpha)}$, which are directly measurable by the observer. The vector $\mathbf{S}$ (according to the observer) is then $\mathbf{S} = S_{(1)}\hat{r} + S_{(2)}\hat{\theta} + S_{(3)}\hat{\varphi}$, since $S_{(4)} = 0$. In the following we shall put $\varphi = 0$, without any loss in generality.

It is found that $d\mathbf{S}/dt = \mathbf{\Omega} \times \mathbf{S}$, where $\mathbf{\Omega}$ is a vector given in terms of r and θ. In the case $m/r \ll 1$ and $a/r \ll 1$, $\mathbf{\Omega}$ is given by

$$\mathbf{\Omega} = (ma/r^3)\{[3(\hat{z}\cdot\mathbf{r})\mathbf{r}/r^2 - \hat{z}] + (m/r)(\hat{z}\times\mathbf{r})\times\mathbf{r}/r^2 + \cdots\},$$

where $\hat{z}$ is a unit vector in the z direction. In the lowest order of approximation one obtains

$$\mathbf{\Omega} = \mathbf{\Omega}_s = \frac{ma}{r^3}\left[\frac{3(\hat{z}\cdot\mathbf{r})\mathbf{r}}{r^2} - \hat{z}\right]$$

This is Schiff's mass-current effect.[10] We emphasize that for any choice of supplementary conditions other than $S^{\mu\nu}u_\nu = 0$, $d\mathbf{S}/dt \neq \mathbf{\Omega}\times\mathbf{S}$, and consequently the magnitude of the spin, is not a constant of the motion.

If the spinning particle is outside the Earth, $r \geq R_{\text{Earth}}$, then $m/r < 7 \times 10^{-10}$, $a/r < 6 \times 10^{-7}$, and $\mathbf{\Omega}_s = I/r^3[(3\mathbf{r}/r^2)(\boldsymbol{\omega}\cdot\mathbf{r}) - \boldsymbol{\omega}]$, where $\boldsymbol{\omega} = \omega_0\hat{z}$. I is the Earth's moment of inertia, and $\omega_0 \simeq 7.29 \times 10^{-5}\ \text{sec}^{-1}$ is the frequency of the rotation of the Earth. The next-higher-order correction is smaller by a factor of $m/r < 7 \times 10^{-10}$.

ACKNOWLEDGMENTS

It is a pleasure to thank Dr. R. Ruffini, and Professor J. A. Wheeler and Professor J. W. York, Jr. for very helpful comments and encouragement. Thanks are also due to Professor L. I. Schiff for an interesting discussion.

* Work supported in part by NSF Grant GP7669 to Princeton University.

† Princeton National Fellow.

[1] A. Papapetrou, Proc. Roy. Soc. (London) **A209**, 248 (1951).

[2] V. A. Fock, J. Phys. USSR **1**, 81 (1939).

[3] A. Einstein, L. Infeld, and B. Hoffmann, Ann. Math. **39**, 65 (1938).

[4] Greek letters go from 1 to 4. Latin letters go from 1 to 3.

[5] F. A. E. Pirani, Acta Phys. Polonica **15**, 389 (1956).

[6] Another choice would be $S^{i4} = 0$ in a coordinate system related to the motion of the source of the gravitational field. See, e.g., E. Corinaldesi and A. Papapetrou, Proc. Roy. Soc. (London) **A209**, 259 (1951).

[7] C. Møller, Commun. Dublin Inst. Advan. Studies, Ser. A, No. 5 (1949).

[8] J. Weyssenhoff and A. Raabe, Acta Phys. Polonica **9**, 7 (1947).

[9] R. Kerr, Phys. Rev. Letters **11**, 237 (1963).

[10] L. I. Schiff, Phys. Rev. Letters **4**, 215 (1960). See also L. I. Schiff, Proc. Natl. Acad. Sci. (U.S.) **46**, 871 (1960).

Spatially Homogeneous Rotating World Models*

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(Received 16 December 1970)

We derive the Lagrangian function for four different rotating universes simultaneously. These models correspond in a certain sense to Gödel's "symmetric case."

1. INTRODUCTION

In a previous paper[1] we developed a formalism in order to treat the problem of spatially homogeneous universes: especially models allowing the most general motion of the "Weltsubstrat," that is, having nonvanishing shear, expansion, and rotation. This is an interesting basic question within Einstein's theory of gravitation and has some hopes for applications. This paper formulates the mathematical problem one is faced with by looking for the simplest expanding and rotating model without the compactness condition for the space sections. In order to save space, we only state some results obtained in Ref. 1. The reader might simply take these from us, or consult Ref. 1 for proofs. Suppose there is given a spatially homogeneous geometry by the line element

$$ds^2 = dt^2 + \gamma_{ab}(t)\omega^a\omega^b, \quad a, b = 1, 2, 3, \tag{1.1}$$

invariant under the left translations of the group G_3 given by

$$d\omega^a = -\tfrac{1}{2}C^a{}_{bc}\omega^b \wedge \omega^c. \tag{1.2}$$

It is shown in Ref. 1 that for Class I groups, that is, if

$$C^f{}_{fa} = 0 \tag{1.3}$$

is satisfied, Einstein's field equations with incoherent matter reduce to a mechanical problem characterized by the Lagrangian function

$$L = \gamma^{\frac{1}{2}}[K_f{}^gK_g{}^f - (K_f{}^f)^2 + R^*] - 2\kappa l(1 - u_fu^f)^{\frac{1}{2}}, \tag{1.4}$$

by the integrals

$$K_f{}^gC^f{}_{ga} = -(\kappa l/\gamma^{\frac{1}{2}})u_a, \quad a = 1, 2, 3, \tag{1.5}$$

and by the requirement that the constant of energy is zero, that is,

$$H = \gamma^{\frac{1}{2}}\{K_f{}^gK_g{}^f - (K_f{}^f)^2 - R^*\} + 2\kappa l(1 - u_fu^f)^{\frac{1}{2}} = h = 0. \tag{1.6}$$

(Solutions of the mechanical problem, for which the constant of energy is different from zero, have nothing to do with the cosmological problem at hand.)

As a consequence of the field equations, the u's satisfy the equations

$$\dot{u}_a = C^f{}_{ga}u^gu_f/(1 - u_fu^f)^{\frac{1}{2}}. \tag{1.7}$$

Explaining the notations, we mention that

$$\gamma = -\det(\gamma_{ab}), \tag{1.8}$$

$$K_a{}^b = \tfrac{1}{2}\dot{\gamma}_{af}\gamma^{fb}, \tag{1.9}$$

R^* is the Ricci scalar of the group space G_3, κ is the relativistic constant of gravitation, $l > 0$ is a constant connected with the density ρ of the matter through the equation $\rho = l/[\gamma(1 - u_fu^f)]^{\frac{1}{2}}$, and

$$\mu = (1 - u_fu^f)^{\frac{1}{2}}\,dt + u_a\omega^a \tag{1.10}$$

is the 1-form corresponding to the motion of the matter.

We apply the above formulas for the groups

$$\begin{aligned}
\mathrm{VI}_0&: \ d\omega^1 = \omega^2\wedge\omega^3, \quad d\omega^2 = -\omega^3\wedge\omega^1, \quad d\omega^3 = 0,\\
\mathrm{VII}_0&: \ d\omega^1 = -\omega^2\wedge\omega^3, \quad d\omega^2 = -\omega^3\wedge\omega^1, \quad d\omega^3 = 0,\\
\mathrm{VIII}&: \ d\omega^1 = \omega^2\wedge\omega^3, \quad d\omega^2 = -\omega^3\wedge\omega^1, \quad d\omega^3 = -\omega^1\wedge\omega^2,\\
\mathrm{IX}&: \ d\omega^1 = -\omega^2\wedge\omega^3, \quad d\omega^2 = -\omega^3\wedge\omega^1, \quad d\omega^3 = -\omega^1\wedge\omega^2,
\end{aligned} \tag{1.11}$$

and for the special case

$$u_1 \neq 0, \quad u_2 = u_3 = 0. \tag{1.12}$$

Most of the calculations can be carried out for the four cases simultaneously by observing that the structure constant tensors can be written as

$$C^1{}_{23} = a, \quad C^2{}_{31} = b, \quad C^3{}_{12} = c \tag{1.13}$$

with the values given in the following table.

	a	b	c
VI_0	-1	$+1$	0
VII_0	$+1$	$+1$	0
VIII	-1	$+1$	$+1$
IX	$+1$	$+1$	$+1$

(1.14)

We now specialize the above formulas for the case at hand.

2. EXPLICIT FORMULATION OF THE PROBLEM

Equations (1.7) read as

$$\dot u_1 = \frac{bu^3u_2 - cu^2u_3}{(1 - u_f u^f)^{\frac12}}, \quad \dot u_2 = \frac{cu^1u_3 - au^3u_1}{(1 - u_f u^f)^{\frac12}},$$
$$\dot u_3 = \frac{au^2u_1 - bu^1u_2}{(1 - u_f u^f)^{\frac12}}. \quad (2.1)$$

Using (1.12) and the fact that $a \neq 0$, we obtain

$$\dot u_1 = 0, \quad u^3 = 0, \quad u^2 = 0. \quad (2.2)$$

From this it follows that

$$u_1 = V \neq 0 \text{ const}, \quad \gamma^{31} = \gamma^{21} = 0$$

and further that

$$u_1 = V \neq 0 \text{ const} \quad (2.3)$$

and

$$\gamma_{12} = \gamma_{13} = 0. \quad (2.4)$$

Therefore,

$$\gamma_{ab}(t) = \begin{pmatrix} A & 0 & 0 \\ 0 & B & D \\ 0 & D & C \end{pmatrix},$$

$$\gamma^{ab}(t) = \begin{pmatrix} 1/A & 0 & 0 \\ 0 & C/(BC - D^2) & -D/(BC - D^2) \\ 0 & -D/(BC - D^2) & B/(BC - D^2) \end{pmatrix}, \quad (2.5)$$

and

$$K_a{}^b = \begin{pmatrix} \dot A/2A & 0 & 0 \\ 0 & (\dot BC - D\dot D)/2(BC - D^2) & (\dot BD - B\dot D)/2(BC - D^2) \\ 0 & (C\dot D - \dot CD)/2(BC - D^2) & (B\dot C - D\dot D)/2(BC - D^2) \end{pmatrix}, \quad (2.6)$$

where a is the row and b is the column index. One might mention that

$$u_\alpha = [(1 - V^2/A)^{\frac12}, V, 0, 0]$$

and $AV^2/4$ gives the length of the vector of rotation. The line element reads then as

$$ds^2 = dt^2 + A(\omega^1)^2 + B(\omega^2)^2 + C(\omega^3)^2 + 2D\omega^2\omega^3, \quad (2.7)$$

where

$$A, B, C, D \quad (2.8)$$

are the unknown functions of t only.

The three equations (1.5) reduce to

$$[(bB - cC)\dot D - (b\dot B - c\dot C)D]/2(BC - D^2) = -\kappa lV/\gamma^{\frac12} \quad (2.9)$$

and (1.4) reads as

$$L = \gamma^{\frac12}\left(-\frac{\dot A(BC - D^2)^{\cdot}}{2A(BC - D^2)} - \frac{A(\dot B\dot C - \dot D^2)}{2A(BC - D^2)} + R^*\right) - 2\kappa l\left(1 - \frac{V^2}{A}\right)^{\frac12}, \quad (2.10)$$

where

$$R^* = [2(a^2A^2 + b^2B^2 + c^2C^2) - (aA + bB + cC)^2 + 4bcD^2]/2A(BC - D^2), \quad (2.11)$$

which can readily be computed by using the corresponding formulas in Ref. 1. Therefore, our problem is reduced to a mechanical problem characterized by the Lagrangian function (2.10) and the first integral (2.9). We are interested only in those solutions for which the constant of energy is zero as we mentioned above.

We now reduce the mechanical problem by one degree of freedom with the help of the first integral.

3. GENERAL REMARKS TO THE REDUCTION OF THE PROBLEM

Since the integration theory is developed for mechanical systems written in Hamiltonian form, we introduce the conjugate momenta as usual by the equations

$$P = \frac{\partial L}{\partial \dot A}, \quad Q = \frac{\partial L}{\partial \dot B}, \quad R = \frac{\partial L}{\partial \dot C}, \quad S = \frac{\partial L}{\partial \dot D}. \quad (3.1)$$

As the first step we express the integral (2.9) with the momenta. A straightforward calculation shows that (2.9) takes the following remarkably simple form:

$$(bR - cQ)D + \tfrac12 S(bB - cC) = -\kappa lV. \quad (3.2)$$

The integral is linear and homogeneous in the momenta; consequently, the reduction problem is very simple.

For the convenience of the reader we quote the relevant remarks from the textbook literature.[2] Suppose that our mechanical system is described by

$$x^k \quad \text{and} \quad y_k$$

as coordinates and momenta, respectively. Our first remark: A point transformation

$$x^k = x^k(\xi^j), \quad (3.3)$$

where $x^k(\xi^j)$ are arbitrary functions subject to the only condition

$$\det\left(\frac{\partial x^k}{\partial \xi^j}\right) \neq 0, \tag{3.4}$$

can be extended to a conical transformation by

$$x^k = x^k(\xi^j), \quad \eta_j = \sum_k \frac{\partial x^k}{\partial \xi^j} y_k. \tag{3.5}$$

Our second remark: If the mechanical system has an integral of the form

$$\sum_k \alpha^k(x^j) y_k = \text{const}, \tag{3.6}$$

we can impose the following additional conditions on (3.3):

$$\frac{\partial x^k}{\partial \xi^n} = \alpha^k(x^j). \tag{3.7}$$

As a consequence of all that, the new momentum η^n is constant; therefore, the Hamiltonian function does not depend on ξ^n. The point transformation reduces naturally the Lagrangian function too.

In our case, (3.2) has the form (3.6) and the relevant system of ordinary equations corresponding to (3.7) has the form

$$\frac{\partial A}{\partial w} = 0, \quad \frac{\partial B}{\partial w} = -cD,$$
$$\frac{\partial C}{\partial w} = bD, \quad \frac{\partial D}{\partial w} = \tfrac{1}{2}(bB - cC), \tag{3.8}$$

with

$$x, y, z, w \tag{3.9}$$

as the new coordinates in the configuration space. Equations (3.8) and a glance at (1.14) suggest that we split the four systems into two pairs and treat them separately.

4. TYPE VI_0 AND VII_0

Using (1.14), we obtain in the case of Type VI_0 and VII_0, from (2.10) and (2.11), the Lagrangian function to be

$$L = \gamma^{\frac{1}{2}}\left(-\frac{\dot{A}(BC - D^2)^{\cdot}}{2A(BC - D^2)} - \frac{A(\dot{B}\dot{C} - \dot{D}^2)}{2A(BC - D^2)} + \frac{(A \pm B)^2}{2A(BC - D^2)}\right) - 2\kappa l\left(1 - \frac{V^2}{A}\right)^{\frac{1}{2}}. \tag{4.1}$$

The integral (2.9) takes the form

$$(B\dot{D} - \dot{B}D)/2(BC - D^2) = -\kappa l V/\gamma^{\frac{1}{2}} \tag{4.2}$$

and the system (3.8) gives the equations

$$\frac{dA}{dw} = 0, \quad \frac{dB}{dw} = 0, \quad \frac{dC}{dw} = D, \quad \frac{dD}{dw} = \tfrac{1}{2}B \tag{4.3}$$

to be integrated. The integration can be carried out trivially

$$A = \alpha, \quad B = \beta, \quad C = \tfrac{1}{4}\beta w^2 + \delta w + \gamma,$$
$$D = \tfrac{1}{2}\beta w + \delta, \tag{4.4}$$

where α, β, γ, and δ are arbitrary functions of x, y, and z subject to (3.4) only.

We pick

$$A = -x, \quad B = y, \quad C = \tfrac{1}{4}yw^2 + z, \quad D = \tfrac{1}{2}yw, \tag{4.5}$$

where naturally

$$z, y, z, \text{ and } w \tag{4.6}$$

are the new unknown functions of t. Substituting (4.5) into (4.2), we obtain

$$\dot{w} = -4\kappa l V/xy^2(xyz)^{\frac{1}{2}}, \tag{4.7}$$

and (4.1) reads as

$$L = -(xyz)^{\frac{1}{2}} \times \left(\frac{\dot{x}\dot{y}}{2xy} + \frac{\dot{y}\dot{z}}{2yz} + \frac{\dot{z}\dot{x}}{2zx} + \frac{(x \pm y)^2}{2xyz} - \frac{2\kappa^2 l^2 V^2}{xy^2}\right) - 2\kappa l\left(1 + \frac{V^2}{x}\right)^{\frac{1}{2}}. \tag{4.8}$$

This completes the reduction.

In order to obtain the world models with the symmetries in question, we have to find those solutions

$$x = x(t), \quad y = y(t), \quad \text{and} \quad z = z(t) \tag{4.9}$$

of the mechanical system (4.8), for which the constant of energy has the value zero, as mentioned already. We then compute

$$w = w(t), \tag{4.10}$$

using (4.7), and find the functions

$$A = A(t), \quad B = B(t), \quad C = C(t), \quad D = D(t) \tag{4.11}$$

by (4.5). The line element is given by (2.7), where in the case of Type VI_0

$$d\omega^1 = \omega^2 \wedge \omega^3, \quad d\omega^2 = -\omega^3 \wedge \omega^1, \quad d\omega^3 = 0. \tag{4.12}$$

The differential forms

$$\omega^1 = \tfrac{1}{2}e^{-x^3}\,dx^1 - \tfrac{1}{2}e^{+x^3}\,dx^2,$$
$$\omega^2 = \tfrac{1}{2}e^{-x^3}\,dx^1 + \tfrac{1}{2}e^{+x^3}\,dx^2, \tag{4.13}$$
$$\omega^3 = dx^3$$

satisfy (4.12). The finite transformations of the group are given by

$$y^1 = e^{z^3}x^1 + z^1, \quad y^2 = e^{-z^3}x^2 + z^3,$$
$$y^3 = x^3 + z^3, \tag{4.14}$$

meaning that we translate the group element (x^1, x^2, x^3) with the help of the group element (z^1, z^2, z^3) into the group element (y^1, y^2, y^3); we "multiply" (x^1, x^2, x^3) by (z^1, z^2, z^3). The corresponding formulas in case of Type VII_0 are given by

$$d\omega^1 = -\omega^2 \wedge \omega^3, \quad d\omega^2 = -\omega^3 \wedge \omega^1, \quad d\omega^3 = 0, \tag{4.15}$$

$$\begin{aligned} \omega^1 &= \sin x^3\, dx^1 - \cos x^3\, dx^2, \\ \omega^2 &= \cos x^3\, dx^1 + \sin x^3\, dx^2, \\ \omega^3 &= dx^3, \end{aligned} \tag{4.16}$$

and

$$\begin{aligned} y^1 &= x^1 \cos z^3 - x^2 \sin z^3 + z^1, \\ y^2 &= x^1 \sin z^3 + x^2 \cos z^3 + z^2, \\ y^3 &= x^3 + z^3, \end{aligned} \tag{4.17}$$

respectively.

One sees, therefore, that in both cases the underlying manifold is given by

$$R \times G_3, \tag{4.18}$$

where G_3 is homeomorphic to R^3 and geometrically a "distorted E^3," E^3 denoting the three-dimensional Euclidean space.

These models would allow, within the theory of gravitation, a study of the rotation of space sections extending into infinity.

5. TYPE VIII AND IX

Using (1.14), we find, from (2.10) and (2.11) in case of Type VIII and IX, that the Lagrangian function reads as

$$\begin{aligned} L = \gamma^{\frac{1}{2}}\biggl(&-\frac{\dot{A}(BC - D^2)^{\dot{}}}{2A(BC - D^2)} - \frac{A(\dot{B}\dot{C} - \dot{D}^2)}{2A(BC - D^2)} \\ &+ \frac{2(A^2 + B^2 + C^2) - (\pm A + B + C)^2 + 4D^2}{2A(BC - D^2)}\biggr) \\ &- 2\kappa l\left(1 - \frac{V^2}{A}\right)^{\frac{1}{2}}. \end{aligned} \tag{5.1}$$

The integral (2.9) takes the form

$$[(B - C)\dot{D} - (\dot{B} - \dot{C})D]/2(BC - D^2) = -\kappa l V/\gamma^{\frac{1}{2}}, \tag{5.2}$$

and the system (3.8) gives the equations

$$\frac{dA}{dw} = 0, \quad \frac{dB}{dw} = -D, \quad \frac{dC}{dw} = D, \quad \frac{dD}{dw} = \tfrac{1}{2}(B - C) \tag{5.3}$$

to be integrated. One integrates easily and obtains

$$\begin{aligned} A &= \alpha, \\ B &= -\gamma \sin w + \delta \cos w + \beta, \\ C &= \gamma \sin w - \delta \cos w + \beta, \\ D &= \gamma \cos w + \delta \sin w, \end{aligned} \tag{5.4}$$

where α, β, γ, and δ are arbitrary functions of x, y, and z subject to (3.4) only. We pick

$$\begin{aligned} A &= -x, \\ B &= -\tfrac{1}{2}(y + z) + \tfrac{1}{2}(y - z) \sin w, \\ C &= -\tfrac{1}{2}(y + z) - \tfrac{1}{2}(y - z) \sin w, \\ D &= -\tfrac{1}{2}(y - z) \cos w, \end{aligned} \tag{5.5}$$

where

$$x, y, z, w \tag{5.6}$$

are the new unknown functions of t. Substituting (5.5) into (5.2), we obtain

$$\dot{w} = -[4\kappa l V/x(y - z)^2](xyz)^{\frac{1}{2}}, \tag{5.7}$$

and (5.1) reads as

$$\begin{aligned} L = -(xyz)^{\frac{1}{2}}\biggl(&\frac{\dot{x}\dot{y}}{2xy} + \frac{\dot{y}\dot{x}}{2yx} + \frac{\dot{z}\dot{x}}{2zx} \\ &+ \frac{2(x^2 + y^2 + z^2) - (\pm x + y + z)^2}{2xyz} - \frac{2\kappa^2 l^2 V^2}{x(y - z)^2}\biggr) \\ &- 2\kappa l\left(1 + \frac{V^2}{x}\right)^{\frac{1}{2}}. \end{aligned} \tag{5.8}$$

This completes the reduction and we obtain Gödel's Lagrangian.[3]

In order to obtain the world models with the symmetries in question, we have to find those solutions

$$x = x(t), \quad y = y(t), \quad z = z(t) \tag{5.9}$$

of the mechanical system (5.8) for which the constant of energy is zero, as we mentioned already. We then compute

$$w = w(t), \tag{5.10}$$

using (5.7), and find the functions

$$A = A(t), \quad B = B(t), \quad C = C(t), \quad D = D(t) \tag{5.11}$$

with the help of (5.5). The line element is given by (2.7), where in the case of Type VIII

$$\begin{aligned} d\omega^1 &= \omega^2 \wedge \omega^3, \quad d\omega^2 = -\omega^3 \wedge \omega^1, \\ d\omega^3 &= -\omega^1 \wedge \omega^2. \end{aligned} \tag{5.12}$$

The differential forms

$$\omega^1 = dx^1 + e^{x^2}\, dx^3,$$
$$\omega^2 = \cos x^1\, dx^2 + e^{x^2} \sin x^1\, dx^3, \qquad (5.13)$$
$$\omega^3 = -\sin x^1\, dx^2 + e^{x^2} \cos x^1\, dx^3$$

satisfy (5.12). The group manifold is given by the hyperboloid

$$(a^1)^2 + (a^2)^2 - (a^3)^2 - (a^4)^2 = 1, \qquad (5.14)$$

where

$$a^1, a^2, a^3, a^4 \qquad (5.15)$$

are the Cartesian coordinates in a four-dimensional Euclidean space E^4 and the group operations are defined by the one-to-one correspondence

$$(a^1, a^2, a^3, a^4) \leftrightarrow \begin{pmatrix} a^1 + a^4 & a^2 + a^3 \\ -a^2 + a^3 & a^1 - a^4 \end{pmatrix} \qquad (5.16)$$

between the points of the hyperboloid (5.14) and the elements of the $SLG(2, R)$.[4]

The corresponding formulas in the case of Type IX are given by

$$d\omega^1 = -\omega^2 \wedge \omega^3, \quad d\omega^2 = -\omega^3 \wedge \omega^1,$$
$$d\omega^3 = -\omega^1 \wedge \omega^2. \qquad (5.17)$$

The differential forms

$$\omega^1 = dx^1 + \cos x^2\, dx^3,$$
$$\omega^2 = \cos x^1\, dx^2 + \sin x^2 \sin x^1\, dx^3, \qquad (5.18)$$
$$\omega^3 = -\sin x^1\, dx^2 + \sin x^2 \cos x^1\, dx^3$$

satisfy (5.17). The group manifold is given by the sphere

$$(a^1)^2 + (a^2)^2 + (a^3)^2 + (a^4)^2 = 1, \qquad (5.19)$$

and the group operations are defined by the one-to-one correspondence

$$(a^1, a^2, a^3, a^4) \leftrightarrow \begin{pmatrix} a^1 + ia^4 & a^2 + ia^3 \\ -a^2 + ia^3 & a^1 - ia^4 \end{pmatrix} \qquad (5.20)$$

between the point of the sphere (5.19) and the elements of the SU_2.[5]

6. MISCELLANEOUS REMARKS

Problem (4.8) is much simpler than (5.8). The singularities of the system are quite different, at first glance anyway.

Since the systems are conservative, one would reduce them by one further degree of freedom with the help of the energy integral.[2] I plan to investigate the properties of this system at some later time.

ACKNOWLEDGMENTS

I am indebted to G. F. R. Ellis for a remark and to H. Armstrong for typing the manuscript.

* This work was supported by the Air Force Office of Scientific Research and by the National Aeronautics and Space Administration.

[1] I. Ozsváth, J. Math. Phys. **11**, 2860 (1970).
[2] E. T. Whittaker, *A Treatise on the Analytical Dynamics* (Cambridge U.P., Cambridge, 1965).
[3] K. Gödel, Proc. Intern. Cong. Math. **1**, 175 (1950).
[4] I. Ozsváth, J. Math. Phys. **11**, 2871 (1970).
[5] I. Ozsváth and E. L. Schücking, Ann. Phys. (N.Y.) **55**, 166 (1969).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Equal-Time Commutation Relations between Components of a Current and the Energy-Momentum Tensor

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(Received 2 November 1970)

We consider an arbitrary physical system possessing a set of currents and an energy-momentum tensor. Without the use of canonical commutation rules we derive in a unified way equal-time commutation relations between the components of the currents and the energy-momentum tensor. The currents and energy-momentum tensor are defined by the response of the physical system to the variations of external fields. The formalism of infinite-dimensional continuous transformation groups is utilized.

INTRODUCTION

In this paper we derive in a unified manner the following equal-time commutation relations:

(i) ETCR's for the energy-momentum tensor,
(ii) ETCR's between the components of a current and the energy-momentum tensor,
(iii) ETCR's between the components of a current.

The ETCR's for the components of the energy-momentum tensor have been derived in a previous paper,[1] using a method outlined in Ref. 2. The result was, in flat space-time,

$$-i[\mathbf{T}_{0\mu}(x'), \tilde{\mathbf{T}}_{\nu0}(x'')]\delta(x_0', x_0'') = \partial^\rho \frac{\delta'\tilde{\mathbf{T}}_{\rho\mu}(x')}{\delta g^{\nu0}(x'')} - \int d^4x C^\rho_{\mu'\nu''}\mathbf{T}_{\rho0}(x). \quad (1)$$

The energy-momentum tensor is here defined using the response of the physical system to a change of an external gravitational field $g^{\mu\nu}(x)$:

$$\delta\mathbf{R} = \int \tilde{\mathbf{T}}_{\mu\nu}(x)\delta g^{\mu\nu}(x)d^4x \equiv \tilde{\mathbf{T}}_{\mu\nu}\delta g^{\mu\nu},$$

where

$$\tilde{\mathbf{T}}_{\mu\nu} = (-g)^{\frac{1}{2}}\mathbf{T}_{\mu\nu}.$$

The $C^\rho_{\mu'\nu''}$ are three-point functions given as follows:

$$C^\rho_{\mu'\nu''} = \delta^\rho_\mu\delta^{(4)}_{,\nu}(x, x')\delta^{(4)}(x, x'') - \delta^\rho_\nu\delta^{(4)}_{,\mu}(x, x'')\delta^{(4)}(x, x'). \quad (2)$$

The method used to derive Eq. (1) is a generalization of the procedure described by Schwinger in Ref. 3. In deriving Eq. (1), we have to study the infinite-dimensional general coordinate transformation group in four-dimensional Riemannian space-time.[4] The $C^\rho_{\mu'\nu''}$ can then be thought of as "structure constants" for this group.

We consider now an arbitrary physical system, and with this system we also associate the currents $\mathbf{J}_{k\mu}(x)$, where $\mu = 0, 1, 2, 3$ and $k = 1, 2, \cdots, N$ is an internal index. The currents are assumed to couple with the external parameters $A^{k\mu}(x)$. Thus the response in this case is

$$\delta\bar{\mathbf{R}} = -\mathbf{J}_{k\mu}\delta A^{k\mu}. \quad (3)$$

In Ref. 2 we used this response, here with negative sign, to derive the ETCR's between the components of the current operator $\mathbf{J}_{k\mu}(x)$:

$$-i[\mathbf{J}_{i0}(x'), \mathbf{J}_{k\rho}(x'')]\delta(x_0', x_0'') = -\partial^\sigma \frac{\delta'\mathbf{J}_{i\sigma}(x')}{\delta A^{k\rho}(x'')} - C^l_{ik}\mathbf{J}_{l\rho}(x')\delta^{(4)}(x', x''). \quad (4)$$

We remark that, in the derivation of the ETCR's expressed in Eqs. (1) and (4), one assumes that, to lowest order in the external fields, the divergencies $\mathbf{D}_\mu = \partial^\nu\tilde{T}_{\mu\nu}$ and $\mathbf{D}_i = \partial^\nu\mathbf{J}_{i\nu}$ respond linearly to the variation of the external fields, suggesting the divergence conditions

$$\delta'\mathbf{D}_\mu(x') = \int d^4x \int d^4x'' C^\rho_{\mu'\nu''}\tilde{\mathbf{T}}_{\sigma\rho}(x)\delta g^{\sigma\nu}(x'')$$

and

$$\delta'\mathbf{D}_i(x') = \int d^4x \int d^4x'' C^l_{ik}\delta^{(4)}(x, x') \times \delta^{(4)}(x, x'')\mathbf{J}_{l\rho}(x)\delta(-A^{k\rho}(x'')).$$

In this paper we shall construct the ETCR's between the current components and the energy-momentum tensor. These ETCR's must yield the correct transformation properties of the current under the Poincaré group. In order to achieve this, it is strongly suggested that the ETCR's (1) and (4) be put on equivalent forms in such a way that they can be looked upon as emerging from a common, unified set of relations. By introducing the generalized structure constants

$$C^l_{i'k''} = C^l_{ik}\delta^{(4)}(x, x')\delta^{(4)}(x, x''),$$

we can write Eq. (4) as

$$-i[\mathbf{J}_{i0}(x'), \mathbf{J}_{k\rho}(x'')]\delta(x_0', x_0'') = \partial^\sigma \frac{\delta'\mathbf{J}_{i\sigma}(x')}{\delta(-A^{k\rho}(x''))} - \int d^4x C^l_{i'k''}\mathbf{J}_{l\rho}(x). \quad (5)$$

The current algebra (5) and the energy–momentum algebra (1) would then be unified into one infinite-dimensional algebra if $\mathbf{T}_{\mu\nu}(x)$ and $\mathbf{J}_{k\nu}(x)$ could be considered as components of a symmetric quantity $\mathbf{T}_{ab}(x)$, and also if $g^{\mu\nu}(x)$ and $A^{k\nu}(x)$ were elements of a symmetric quantity $\bar{g}^{ab}(x)$. The indices a and b range over the space–time and the internal indices. $\mathbf{J}_{k\nu}(x)$ would be identified with $\mathbf{T}_{k\nu}$ and $-A^{k\nu}$ with $g^{k\nu}$. In such a manner Eqs. (1) and (4) would be contained in a single infinite-dimensional algebra.

This reasoning leads us then naturally to the study of the general ETCR's by using an infinite-dimensional group, which is obtained from a compact Lie group and the general coordinate transformation group in curved space–time. With the help of the Lie group we generate the corresponding Yang–Mills group and then combine this infinite-dimensional group with the coordinate transformation group.

We are thus led to consider an abstract space of $(4 + N)$ dimensions. The fields $A^{k\mu}(x)$ will now be identified with the universal field of the Yang–Mills group generated from the compact Lie group. The field $A^{k\mu}(x)$ gives the connection between space–time and the space of the Yang–Mills group, the internal space.

In Sec. 1 we state the results and show that the ETCR's between the currents $\mathbf{J}_{k\mu}(x)$ and $\mathbf{T}_{0\nu}(x)$ in flat space–time give the right transformation properties of $\mathbf{J}_{k\mu}(x)$ under the Poincaré group. In Sec. 2 we derive the commutation relations using the method of Ref. 2, generalized to the infinite-dimensional continuous group consisting of the combined Yang–Mills and coordinate transformation groups.

1. ETCR'S BETWEEN THE CURRENTS AND THE ENERGY-MOMENTUM TENSOR

The ETCR's between the components $\mathbf{T}_{\mu 0}(x)$ of the energy–momentum tensor derived in this paper are given by Eq. (1). Thus in flat space–time we have

$$-i[\mathbf{T}_{\mu 0}(x'), \mathbf{T}_{\nu 0}(x'')]\delta(x_0', x_0'') = \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{\mu\rho}(x')}{\delta g^{\nu 0}(x'')} - \int d^4x C^\rho_{\mu'\nu''}\mathbf{T}_{\rho 0}(x). \quad (1')$$

We construct the generators

$$\mathbf{P}_\mu(x_0) = \int d^3x\, \mathbf{T}_{\mu 0}(x) \quad (6)$$

and

$$\mathbf{M}_{\mu\nu}(x_0) = \int d^3x[x_\mu \mathbf{T}_{\nu 0}(x) - x_\nu \mathbf{T}_{\mu 0}(x)]. \quad (7)$$

It is shown in Ref. 1 that Eq. (1′) gives the Poincaré algebra for the momentum operators $\mathbf{P}_\mu(x_0)$ and the angular momentum operators $\mathbf{M}_{\mu\nu}(x_0)$. Using the fact that $\mathbf{T}_{\mu\nu}$ is conserved in flat space–time makes it possible to rewrite Eq. (1′) in the following way. We consider first the case $\mu = \nu = 0$. Then

$$\begin{aligned} -i[\mathbf{T}_{00}(x'), \mathbf{T}_{00}(x'')]\delta(x_0', x_0'') &= \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{0\rho}(x')}{\delta g^{00}(x'')} \\ &- [\mathbf{T}_{00}(x'')\delta^{(4)}_{,0}(x'', x') - \mathbf{T}_{00}(x')\delta^{(4)}_{,0}(x', x'')]. \quad (8) \end{aligned}$$

We eliminate the time derivatives of the delta functions, using the conservation law for $\mathbf{T}_{\mu\nu}$,

$$\partial^\mu \mathbf{T}_{\mu\nu}(x) = -\int d^4x' \delta^{(4)}_{,\mu}(x', x)\mathbf{T}^\mu{}_\nu(x') = 0, \quad (9)$$

and we obtain the expression

$$\begin{aligned} -i[\mathbf{T}_{00}(x'), \mathbf{T}_{00}(x'')]\delta(x_0', x_0'') &= \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{0\rho}(x')}{\delta g^{00}(x'')} \\ &- \delta(x_0', x_0'')[\mathbf{T}_0{}^m(x'') + \mathbf{T}_0{}^m(x')]\delta^{(3)}_{,m}(x'', x'). \quad (10) \end{aligned}$$

In the same way we have

$$\begin{aligned} -i[\mathbf{T}_{00}(x'), \mathbf{T}_{0m}(x'')]\delta(x_0', x_0'') &= \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{0\rho}(x')}{\delta g^{0m}(x'')} \\ &- [\mathbf{T}_{00}(x'')\delta^{(4)}_{,m}(x'', x') - \mathbf{T}_{0m}(x')\delta^{(4)}_{,0}(x', x'')] \\ &= \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{0\rho}(x')}{\delta g^{0m}(x'')} \\ &- \delta(x_0', x_0'')[\mathbf{T}_{00}(x'')\delta^{(3)}_{,m}(x'', x') - \mathbf{T}_m{}^n(x')\delta^{(3)}_{,n}(x', x'')], \\ & m, n = 1, 2, 3. \quad (11) \end{aligned}$$

We next consider the commutator

$$-i[\mathbf{T}_{00}(x'), \mathbf{T}_{mn}(x'')]\delta(x_0', x_0''), \quad m, n = 1, 2, 3.$$

In this case we must have an expression which is symmetrical in m and n. Thus the following expression is suggested:

$$\begin{aligned} -i[\mathbf{T}_{00}(x'), \mathbf{T}_{mn}(x'')]\delta(x_0', x_0'') &= \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{0\rho}(x')}{\delta g^{mn}(x'')} \\ &- [\delta^{(4)}_{,m}(x'', x')\mathbf{T}_{0n}(x'') + \delta^{(4)}_{,n}(x'', x')\mathbf{T}_{0m}(x'') \\ &- \delta^{(4)}_{,0}(x', x'')\mathbf{T}_{mn}(x')], \quad m, n = 1, 2, 3. \quad (12) \end{aligned}$$

In the same way

$$\begin{aligned} -i[\mathbf{T}_{k0}(x'), \mathbf{T}_{mn}(x'')]\delta(x_0', x_0'') &= \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{k\rho}(x')}{\delta g^{mn}(x'')} - \mathbf{T}_{kn}(x'')\delta^{(4)}_{,m}(x'', x') \\ &- \mathbf{T}_{km}(x'')\delta^{(4)}_{,n}(x'', x') + \mathbf{T}_{mn}(x')\delta^{(4)}_{,k}(x', x''), \\ & k, m, n = 1, 2, 3. \quad (13) \end{aligned}$$

Equation (13) has the consequence that

$$-i[\mathbf{M}_{kl}(x_0'), \mathbf{T}_{mn}(x)]_{x_0=x_0'} = (x_l\partial_k - x_k\partial_l)\mathbf{T}_{mn} + \mathbf{T}_{kn}g_{ml} - \mathbf{T}_{ln}g_{mk} + \mathbf{T}_{km}g_{ln} - \mathbf{T}_{lm}g_{nk}. \quad (14)$$

Compare with Ref. 5.

The ETCR's between the components $\mathbf{J}_{k\mu}(x)$ of the current and the energy-momentum tensor $\mathbf{T}_{\nu 0}(x)$ derived in Sec. 2 are, in the limit of flat space-time,

$$-i[\mathbf{T}_{\mu 0}(x'), \mathbf{J}_{k\nu}(x'')]\delta(x_0', x_0'') = \partial^\rho \frac{\delta' \tilde{\mathbf{T}}_{\mu\rho}(x')}{\delta(-A^{k\nu}(x''))} - \int d^4x C^{\rho}_{\mu'\nu''}\mathbf{J}_{k\rho}(x), \quad (15)$$

where $C^{\rho}_{\mu'\nu''}$ is given by Eq. (2).

We now check that these ETCR's give the right transformation properties of $\mathbf{J}_{k\mu}(x)$, i.e., that it transforms correctly as a vector under Lorentz transformations. For this purpose we compute the ETCR's between $\mathbf{M}_{\mu\nu}(x_0)$ and $\mathbf{J}_{k\mu}(x)$:

$$\begin{aligned}[\mathbf{M}_{\mu\nu}(x_0'), \mathbf{J}_{k\rho}(x'')]_{x_0'=x_0''} &= \int d^4x' x_\mu'[\mathbf{T}_{\nu 0}(x'), \mathbf{J}_{k\rho}(x'')]\delta(x_0', x_0'') \\ &\quad - \int d^4x' x_\nu'[\mathbf{T}_{\mu 0}(x'), \mathbf{J}_{k\rho}(x'')]\delta(x_0', x_0'') \\ &= + i(x_\nu''\partial_\mu - x_\mu''\partial_\nu)\mathbf{J}_{k\rho}(x'') \\ &\quad + i(g_{\nu\sigma}g_{\mu\rho} - g_{\mu\sigma}g_{\nu\rho})\mathbf{J}_k{}^\sigma(x''). \quad (16)\end{aligned}$$

We also get the following desired relation by integrating Eq. (15) over d^4x':

$$i\left(\int d^3x'\mathbf{T}_{\nu 0}(x'), \mathbf{J}_{k\mu}(x'')\right) = i[\mathbf{P}_\nu(x_0'), \mathbf{J}_{k\mu}(x'')] = \partial_\nu J_{k\mu}(x''). \quad (17)$$

2. DERIVATION OF THE EQUAL-TIME COMMUTATION RELATIONS

As mentioned in the Introduction, we shall use an infinite-dimensional continuous group to derive all the ETCR's in a unified way. We start with a compact Lie group with the structure constants C^i_{jk}. From this group we generate the corresponding infinite-dimensional Yang-Mills group with the "structure constants" $C^i_{j'k''}$ given by the relation

$$C^i_{j'k''} = C^i_{jk}\delta^{(4)}(x, x')\delta^{(4)}(x, x'') \quad i, j, k = 1, 2, \cdots, N. \quad (18)$$

Then we consider the general coordinate transformation group in a four-dimensional space with the metric tensor $g^{\mu\nu}(x)$. The corresponding "structure constants" are

$$C^{\rho}_{\nu'\sigma''} = \delta^\rho_\nu\delta^{(4)}_{,\sigma}(x, x')\delta^{(4)}(x, x'') - \delta^\rho_\sigma\delta^{(4)}_{,\nu}(x, x'')\delta^{(4)}(x, x'). \quad (19)$$

We now combine the two groups into a single infinite-dimensional continuous group. The Yang-Mills transformation is thought of as being performed first and then followed by a coordinate transformation. The new set of "structure constants" are denoted by $C^a_{b'c''}$, where the indices a, b', and c'' run over the internal indices i, j', k'' and the space-time indices μ, ν', σ''. The three-point functions $C^a_{b'c''}$ are given as follows:

$$C^i_{j'k''} = C^i_{jk}\delta^{(4)}(x, x')\delta^{(4)}(x, x''), \quad (20a)$$

$$C^i_{k'\sigma''} = -C^i_{\sigma''k'} = \delta^i_k\delta^{(4)}_{,\sigma}(x, x')\delta^{(4)}(x, x''), \quad (20b)$$

$$C^i_{\nu'\sigma''} = C^\mu_{k'l''} = C^\mu_{k'\sigma''} = 0, \quad (20c)$$

and

$$C^{\rho}_{\nu'\sigma''} = \delta^\rho_\nu\delta^{(4)}_{,\sigma}(x, x')\delta^{(4)}(x, x'') - \delta^\rho_\sigma\delta^{(4)}_{,\nu}(x, x'')\delta^{(4)}(x, x'). \quad (20d)$$

See Ref. 4, Problem 57.

As is seen from Eq. (20), the combined group is not the direct product of the two groups.

The adjoint representation is given by a vector field with $4 + N$ components denoted $\mathbf{X}^\mu$ and $\mathbf{X}^i$. $\mathbf{X}^a$ obeys the following transformation law:

$$\delta\mathbf{X}^a = C^a_{b'c''}\mathbf{X}^{c''}\delta\xi^{b'} \equiv \int d^4x' \int d^4x'' C^a_{b'c''}\mathbf{X}^{c''}\delta\xi^{b'}. \quad (21)$$

The parameters $\delta\xi^b$ are in component form,

$$\delta\xi^b = \begin{pmatrix}\delta\xi^\mu \\ \delta\xi^i\end{pmatrix}. \quad (22)$$

A general coordinate transformation is written as

$$\bar{x}^\mu = x^\mu + \delta\xi^\mu(x), \quad \mu = 0, 1, 2, 3. \quad (23)$$

The $\delta\xi^i$ are the parameters of the Yang-Mills group. They depend on the coordinates x^μ of space-time. The co-adjoint representation is a vector field with $4 + N$ components with the following transformation law:

$$\delta\mathbf{X}_a = -\int d^4x' \int d^4x'' C^{c'}_{b''a}\mathbf{X}_{c'}\delta\xi^{b''}. \quad (24)$$

We consider now the matrix $\bar{g}^{ab}$ defined as

$$\bar{g}^{ab} = \begin{pmatrix} g^{ij} + A^i{}_\sigma A^{j\sigma} & -A^{i\nu} \\ -A^{j\mu} & g^{\mu\nu}\end{pmatrix}, \quad (25)$$

where $A^{i\mu}(x)$ is the universal field of the Yang-Mills group. It is to be identified with the external field mentioned in the introduction that couples with the currents $\mathbf{J}_{k\mu}(x)$. g^{ij} is an internal metric and is used to raise and lower the indices i, j, and k. At the end of the calculations when we go to flat space-time and the external fields vanish, g^{ij} is to be identified with the group metric of the compact group.[2] The matrix $\bar{g}^{ab}$ transforms as the matrix with elements

$$\mathbf{X}^i\mathbf{X}^j,\quad \mathbf{X}^i\mathbf{X}^\nu,\quad \mathbf{X}^\mu\mathbf{X}^i,\quad \mathbf{X}^\mu\mathbf{X}^\nu. \tag{26}$$

The matrix

$$(-g)^{\frac{1}{2}}\bar{g}_{ab} = (-g)^{\frac{1}{2}}\begin{pmatrix} g_{ij} & A_{i\nu} \\ A_{j\mu} & g_{\mu\nu} + A_{k\mu}A^k{}_\nu \end{pmatrix} \tag{27}$$

transforms contragrediently to $\bar{g}^{ab}$. Further, $\bar{g}^{ab}$ satisfies the following relations:

$$\bar{g}^{ab}\bar{g}_{bc} = \delta^a{}_c$$

and

$$\bar{g}^{ab}\bar{g}_{ab} = g^{\mu\nu}g_{\mu\nu} + g^{ij}g_{ij} = 4 + N.$$

The matrix $\bar{g}^{ab}$ can then be used to raise and lower indices a and b. However, we do not necessarily interpret $\bar{g}^{ab}$ as a fundamental tensor in a $(4 + N)$-dimensional Riemannian space.

An infinitesimal variation of $\bar{g}^{ab}$ is written

$$\delta\bar{g}^{ab} = \begin{pmatrix} \delta(g^{ij} + A^i{}_\sigma A^{j\sigma}) & \delta(-A^{i\nu}) \\ \delta(-A^{j\mu}) & \delta g^{\mu\nu} \end{pmatrix}. \tag{28}$$

The response of the physical system to a change of the matrix $\bar{g}^{ab}$ is now assumed to be

$$\delta\mathbf{R} = \tilde{\mathbf{T}}_{ab}\delta\bar{g}^{ab}, \tag{29}$$

where

$$\tilde{T}_{ab} = (-g)^{\frac{1}{2}}\mathbf{T}_{ab} \tag{29'}$$

and it is assumed that $\delta\mathbf{R}$ is invariant under the combined group. The tensor $\mathbf{T}_{ab}$ is defined as follows:

$$\mathbf{T}_{ab} = \begin{pmatrix} \mathbf{T}_{ij} & \mathbf{J}_{i\nu} \\ \mathbf{J}_{j\mu} & \mathbf{T}_{\mu\nu} \end{pmatrix}. \tag{30}$$

The divergence of $\tilde{\mathbf{T}}_{ab}(x)$ is written

$$\partial^\mu\tilde{\mathbf{T}}_{a\mu} = \mathbf{D}_a, \tag{31}$$

where the index "a" ranges over the space–time indices and the internal indices. We now assume the following variational equation as a consequence of Schwinger's variational principle:

$$-i[\tilde{\mathbf{T}}_{a0}(x'), \tilde{\mathbf{T}}_{bc}(x'')]\delta(x_0', x_0'') = \partial^\mu\frac{\delta'\tilde{\mathbf{T}}_{a\mu}(x')}{\delta\bar{g}^{bc}(x'')} - \frac{\delta'\mathbf{D}_a(x')}{\delta\bar{g}^{bc}(x'')}, \tag{32}$$

where δ' gives the explicit dependence of the operators $\tilde{\mathbf{T}}_{a\mu}(x)$ and $\mathbf{D}_a(x)$ on the matrix $\bar{g}^{ab}(x)$. The following reciprocity condition must be satisfied under the variation[3]:

$$\delta'\tilde{\mathbf{T}}_{ab}(x')/\delta\bar{g}^{cd}(x'') = \delta'\tilde{\mathbf{T}}_{cd}(x'')/\delta\bar{g}^{ab}(x'). \tag{33}$$

When the external perturbation is turned off, Eq. (32) provides information about the closed physical system. In this limit, $g^{\mu\nu}$ equals the Minkowski metric tensor, g^{kl} tends to the metric tensor of the compact internal Lie group, and the fields $A^{k\mu}$ go to zero.

As a straightforward generalization of the results in Refs. 1 and 2, we assume that the explicit dependence of the operator $\mathbf{D}_a(x)$ on the external fields $\bar{g}^{ab}$ can be expressed in terms of the "generalized structure constants" $C^a_{b'c''}$ of the combined group. We can then write down the following six relations for $\delta'\mathbf{D}_a(x')/\delta\bar{g}^{bc}(x'')$, assumed to be valid to lowest order in the external fields:

$$\frac{\delta'\mathbf{D}_\mu(x')}{\delta g^{\sigma\nu}(x'')} = \int d^4x\, C^\rho_{\mu'\nu''}\tilde{\mathbf{T}}_{\rho\sigma}(x), \tag{34}$$

$$\frac{\delta'\mathbf{D}_\mu(x')}{\delta(-A^{k\nu}(x''))} = \int d^4x\, C^\rho_{\mu'\nu''}\tilde{\mathbf{T}}_{k\rho}(x), \tag{35}$$

$$\frac{\delta'\mathbf{D}_\mu(x')}{\delta\bar{g}^{kl}(x'')} = \int d^4x\, C^i_{\mu'k''}\tilde{\mathbf{T}}_{il}(x), \tag{36}$$

$$\frac{\delta'\mathbf{D}_i(x')}{\delta(-A^{k\rho}(x''))} = \int d^4x\, C^l_{i'k''}\tilde{\mathbf{T}}_{l\rho}(x), \tag{37}$$

$$\frac{\delta'\mathbf{D}_i(x')}{\delta\bar{g}^{kl}(x'')} = \int d^4x\, C^m_{i'k''}\tilde{\mathbf{T}}_{ml}(x), \tag{38}$$

$$\frac{\delta'\mathbf{D}_i(x')}{\delta g^{\rho\sigma}(x'')} = \int d^4x\, C^m_{i'\rho''}\tilde{\mathbf{T}}_{m\sigma}(x). \tag{39}$$

Because $\bar{g}^{ab}$ is a symmetric quantity, these expressions should be symmetrized when it is necessary. The six responses given above give rise to six equal-time commutation relations. From Eq. (32) there follows, in the limit of flat space–time and vanishing $A^{k\mu}$,

$$-i[\mathbf{T}_{\mu0}(x'), \mathbf{T}_{\nu0}(x'')]\delta(x_0', x_0'') = \partial^\rho\frac{\delta'\tilde{\mathbf{T}}_{\mu\rho}(x')}{\delta g^{0\nu}(x'')} - \int d^4x\, C^\rho_{\mu'\nu''}\mathbf{T}_{\rho0}(x), \tag{40}$$

$$-i[\mathbf{T}_{\mu0}(x'), \mathbf{J}_{k\nu}(x'')]\delta(x_0', x_0'') = \partial^\rho\frac{\delta'\tilde{\mathbf{T}}_{\mu\rho}(x')}{\delta(-A^{k\nu}(x''))} - \int d^4x\, C^\rho_{\mu'\nu''}\mathbf{J}_{k\rho}(x), \tag{41}$$

$$-i[\mathbf{T}_{\mu0}(x'), \mathbf{T}_{kl}(x'')]\delta(x_0', x_0'') = \partial^\rho\frac{\delta'\tilde{\mathbf{T}}_{\mu\rho}(x')}{\delta\bar{g}^{kl}(x'')} - \int d^4x\, C^i_{\mu'k''}\mathbf{T}_{il}(x), \tag{42}$$

$$-i[\mathbf{J}_{i0}(x'), \mathbf{J}_{k\rho}(x'')]\delta(x_0', x_0'') = \partial^\sigma\frac{\delta'\tilde{\mathbf{J}}_{i\sigma}(x')}{\delta(-A^{k\rho}(x''))} - \int d^4x\, C^l_{i'k''}\mathbf{J}_{l\rho}(x), \tag{43}$$

$$-i[\mathbf{J}_{i0}(x'), \mathbf{T}_{kl}(x'')]\delta(x_0', x_0'') = \partial^\sigma\frac{\delta'\tilde{\mathbf{J}}_{i\sigma}(x')}{\delta\bar{g}^{kl}(x'')} - \int d^4x\, C^m_{i'k''}\mathbf{T}_{ml}(x), \tag{44}$$

$$-i[\mathbf{J}_{i0}(x'), \mathbf{T}_{\epsilon\omega}(x'')]\delta(x_0', x_0'') = \partial^\sigma\frac{\delta'\tilde{\mathbf{J}}_{i\sigma}(x')}{\delta g^{\epsilon\omega}(x'')} - \int d^4x\, C^m_{i'\epsilon''}\mathbf{J}_{m\omega}(x). \tag{45}$$

Equations (40) are the previously derived ETCR's for the energy–momentum tensor. Equation (41) gives the right transformation properties of the current under the Poincaré group. Equation (42) means that $\mathbf{T}_{kl}$ transforms as a scalar under the Poincaré group. Equations (43) are the ETCR's for the currents, and Eq. (44) means that $\mathbf{T}_{kl}$ transforms as a tensor in the internal space.

We note that the symmetrized version of Eq. (45) is

$$-i[\mathbf{J}_{i0}(x'), \mathbf{T}_{\epsilon\omega}(x'')]\delta(x_0', x_0'') = \partial^\rho \frac{\delta'\tilde{\mathbf{J}}_{i\rho}(x')}{\delta g^{\epsilon\omega}(x'')} - \int d^4x\, C^m_{i'\epsilon''}\mathbf{J}_{m\omega}(x) + \int d^4x\, C^m_{i''\omega'}\mathbf{J}_{m\epsilon}(x) \qquad (45')$$

and that Eq. (45) is related to Eq. (41) through the reciprocity condition

$$\delta'\tilde{\mathbf{J}}_{i\rho}(x')/\delta g^{\epsilon\omega}(x'') = \delta'\tilde{\mathbf{T}}_{\epsilon\omega}(x'')/\delta(-A^{i\rho}(x')). \qquad (46)$$

Note added in proof: We remark that our ETCR's (40)–(45) are obtained by making a "minimal" assumption for the explicit dependence of $\mathbf{D}_a(x)$ on the external fields in Eq. (34)–(39). Clearly, one can add terms, which are total four-divergencies, on the right-hand sides of Eqs. (34)–(39), without spoiling the Poincaré invariance and the current algebra. These terms will then, together with the Schwinger terms, constitute the so-called model-dependent part of the ETCR's.[5–8]

3. DISCUSSION

In unifying the Poincaré group and a current algebra into the relations expressed by Eq. (32) and Eqs. (40)–(45), we introduced the symmetric quantity $\mathbf{T}_{kl}(x)$ that couples with the external perturbation

$$\delta\bar{g}^{kl} = \delta g^{kl} + \delta(A^k{}_\sigma A^{l\sigma}). \qquad (47)$$

Now the variations $\delta\bar{g}^{ab}$ are interpreted as changes in an external physical c-number field. A variation $\delta\langle\alpha \mid \beta\rangle$ of the transition amplitude $\langle\alpha \mid \beta\rangle$ is induced according to Schwinger's principle:

$$\delta\langle\alpha \mid \beta\rangle = i\,\langle\alpha|\, \tilde{\mathbf{T}}_{ab}\delta\bar{g}^{ab}\, |\beta\rangle. \qquad (48)$$

In principle $\delta\langle\alpha \mid \beta\rangle$ can be measured and, since $\delta\bar{g}^{ab}$ is externally controlled, one actually measures $\mathbf{T}_{ab}(x)$. [More strictly speaking, one measures space–time averages of $\mathbf{T}_{ab}(x)$ since $\tilde{\mathbf{T}}_{ab}\delta\bar{g}^{ab}$ is an integral over some space–time region.] Hence $\mathbf{T}_{ab}$ constitutes a set of observables for the system. So, if δg^{kl} in Eq. (47) is a variation of a set of external scalar fields, then $\mathbf{T}_{kl}$ is an observable for the system in addition to the observables $\mathbf{J}_{k\mu}$ and $\mathbf{T}_{\nu\mu}$.

If the variation δg^{kl} is nonphysical, one has, of course, $\mathbf{T}_{kl} = 0$ and Eqs. (42) and (44) disappear.

Possibly the situation is such that the complete Poincaré group observable set plus the invariants $\sum_{k'} \mathbf{Q}_{k'}\mathbf{Q}^{k'}$ ($Q_{k'} = \int \mathbf{J}_{k'0}d^3x$ constant of motion, generator of an invariant subgroup of the internal group) and mutually commuting conserved charges $\mathbf{Q}_{l'}$ do not suffice to specify the physical system completely. Then perhaps a complete set of observables could be constructed by bringing into consideration the internal tensor $\int \mathbf{T}_{kl}d^3x$.

Our observables belong to infinite-dimensional representations (if they exist) and the ETCR's we have put forward in this paper, loosely speaking, form an infinite-dimensional algebra. People have tried to combine the Poincaré group with an internal symmetry group of finite dimension with the result that only trivial direct sum combinations exist.[9]

We have tried to link the ETCR's to the geometrical structure of a fiber bundle. If this is correct, the current algebra dynamics has the same foundation as electromagnetic interaction theory and Einstein's gravitation theory expressed in the framework of gauge or "compensating field" theory. Our external perturbing fields are then connected to so-called Yang–Mills fields.[10] We have employed the general formalism of De Witt[4] for handling this type of theory.

ACKNOWLEDGMENT

The authors are indebted to Professor K. E. Eriksson for valuable discussions and encouraging interest in this work.

1 K. Bergström, J. Math. Phys. **11**, 2498 (1970).
2 K. Bergström, J. Math. Phys. **11**, 2489 (1970).
3 J. Schwinger, Phys. Rev. **130**, 406 (1963).
4 B. S. De Witt, *Dynamical Theory of Groups and Fields* (Gordon and Breach, New York, 1965).
5 D. G. Boulware and S. Deser, J. Math. Phys. **8**, 7 (1967).
6 S. Deser and L. K. Morrison, J. Math. Phys. **11**, 596 (1970).
7 J. C. Katzin and W. B. Rolnick, Phys. Rev. **182**, 5 (1969).
8 R. Jackniw, Phys. Rev. **175**, 5 (1968).
9 L. O'Raifeartaigh, Phys. Rev. **139**, 4B (1965).
10 C. N. Yang and R. L. Mills, Phys. Rev. **96**, 191 (1954).

Invariant Approach to a Space–Time Symmetry

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(Received 30 November 1970)

A study is made of Killing vector fields in vacuum Einstein spaces with a restriction primarily to those fields whose associated bivector is nonnull. However, a well-known theorem of Robinson is modified slightly to show that if such a space admits a null bivector associated with a Killing vector, the space must be algebraically special. Consequently, all algebraically general spaces admit a nonnull Killing bivector (KBV) if they admit a symmetry at all. Furthermore, it is shown that if a vacuum Einstein space admits a spacelike or timelike Killing vector field whose associated KBV is nonnull, the Killing trajectories are not geodesics. Computation of invariants from the curvature tensor and the KBV allows an approach which gives a general classification to such spaces which admit at least one hypersurface orthogonal Killing vector field. A few geometrical properties involving the principal null directions of the KBV are also derived for the hypersurface orthogonal cases. In addition, a topological result follows immediately from the behavior of the invariant $\mathfrak{J}$.

1. INTRODUCTION

This work is concerned with both algebraically special and algebraically general vacuum Einstein spaces. No attempt is made at this point to find new examples of gravitational fields with symmetry since so many are already known. The Robinsons[1] noted the existence of an algebraically special space[2] without symmetry, and the Weyl–Levi-Civita class (see Refs. 3 and 4) contains spaces which are algebraically general and yet possess two or three Killing vector fields. Consequently, there can be no obvious connection in general between the existence of a symmetry and the algebraic Petrov classification.[5]

The approach taken in this paper is to assume the existence of a Killing vector field $\mathbf{K}$ and examine the necessary conditions following the assumption that the bivector $K_{\mu;\nu}$ is nonnull. Theorem 2 says that no algebraically general space can have a Killing vector field whose bivector is null. Hence, to allow Petrov Type I spaces, we must examine the nonnull bivector case.[6] The invariants introduced in Sec. 6 give a way of describing the Petrov type without having the conformal scalars in some kind of canonical form. The Killing bivector represented in one of its canonical forms restricts the tetrad freedom so drastically that the conformal scalars cannot individually give much information.

The imposing of hypersurface orthogonality on $\mathbf{K}$ makes Sec. 7 a study of generalized Weyl–Levi-Civita spaces. Here the ordinarily independent set of invariants are not independent and, in fact, depend on one another in the manner indicated in Table I (Sec. 7).

A result obtained in Sec. 5 is given through Theorem 3. Here it is apparent that a space of Petrov Type I cannot have a geodesic Killing vector field. In fact, the only way a Killing vector (with $K_{\mu;\nu}$ nonnull) in any space can be geodesic is for it to be null itself; i.e., $K^\mu K_\mu = 0$. The latter case, however, is a geodesic and shear-free null vector field; hence, only algebraically special spaces admit this sort of geodesic Killing vector.

2. TETRAD FORMALISM

Let $\mathcal{E}$ be a C^∞ Lorentz 4-manifold with a metric tensor field g over $\mathcal{E}$ having signature $(+++-)$. The tangent space at any point $P \in \mathcal{E}$ is denoted by T_P and is the space of contravariant vectors. The space of covariant vectors at P, T_P^* is the vector-space dual of T_P. An orthonormal basis for T_P is any set of four linearly independent vectors $\{\mathbf{e}_a \mid a = 1, 2, 3, 4\}$ for which $g(\mathbf{e}_a, \mathbf{e}_a) = 1$ for $a = 1, 2, 3$ and $g(\mathbf{e}_4, \mathbf{e}_4) = -1$; all other inner products are zero. If we define[7] $g_{ab} \equiv g(\mathbf{e}_a, \mathbf{e}_b)$ at $P \in \mathcal{E}$, then, as a matrix, $(g_{ab}) = \mathrm{diag}\,(1, 1, 1, -1)$.

It is further possible to choose linearly independent vector *fields* $\{\mathbf{e}_a\}$ over a neighborhood of P so that the diagonal form of (g_{ab}) is preserved over the entire neighborhood.[8] The set $\{\mathbf{e}_a\}$ is then an *orthonormal tetrad* for $\mathcal{E}$. It is a basis for all contravariant vector and tensor fields over a neighborhood of $P \in \mathcal{E}$. The same argument may be applied to the tetrad $\{\epsilon^a \mid a = 1, 2, 3, 4\}$, dual to $\{\mathbf{e}_a\}$ and taken from T_P^*. Hence a basis for all tensor fields locally over $\mathcal{E}$ is established.

If $\{\partial_\mu \mid \mu = 1, 2, 3, 4\}$ is a coordinate basis with respect to a local coordinate system $\{x^\mu\}$, the basis dual to $\{\partial_\mu\}$ is $\{dx^\mu \mid \mu = 1, 2, 3, 4\}$; $\{\epsilon_a\}$ is defined to be dual to $\{\mathbf{e}_a\}$ and $\epsilon^a = \epsilon^a{}_\nu\, dx^\nu$. The fact that $\{\mathbf{e}_a\}$ and $\{\epsilon^a\}$ are dual implies

$$\epsilon^a{}_\mu e_b{}^\mu = \delta^a{}_b \quad \text{and} \quad e_a{}^\mu \epsilon^a{}_\nu = \delta^\mu{}_\nu . \tag{2.1}$$

Any contravariant vector field V may be expressed as

$$\mathbf{V} = V^a \mathbf{e}_a = V^\mu \partial_\mu , \tag{2.2}$$

where $V^a = \epsilon^a{}_\mu V^\mu$. Any covariant vector field W is given by

$$W = W_a \epsilon^a = W_\mu \, dx^\mu, \tag{2.3}$$

where $W^a = e_a{}^\mu W_\mu$. Similar multilinear relationships occur between coordinate components and tetrad components of higher-order tensor fields.

A complex null tetrad may be introduced in the following manner. Define

$$\mathbf{e}_1^* \equiv 2^{-\frac{1}{2}}(\mathbf{e}_1 + i\mathbf{e}_2), \quad \mathbf{e}_2^* \equiv 2^{-\frac{1}{2}}(\mathbf{e}_1 - i\mathbf{e}_2) = \bar{\mathbf{e}}_1^*,$$
$$\mathbf{e}_3^* \equiv 2^{-\frac{1}{2}}(\mathbf{e}_3 + \mathbf{e}_4), \quad \mathbf{e}_4^* \equiv 2^{-\frac{1}{2}}(\mathbf{e}_3 - \mathbf{e}_4), \tag{2.4}$$

where $i = \sqrt{-1}$ and "complex conjugation" is denoted by a bar.[9] An inner product (called g^*) on the set spanned by (2.4) over the complex numbers is defined by formal expansion of $\mathbf{e}_a^* \cdot \mathbf{e}_b^*$, using the values $\mathbf{e}_a \cdot \mathbf{e}_b$. Hence, define $g_{ab}^* = g^*(\mathbf{e}_a^*, \mathbf{e}_b^*) \equiv \mathbf{e}_a^* \cdot \mathbf{e}_b^*$. Then

$$(g_{ab}^*) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{2.5}$$

In view of the nullity of each $\mathbf{e}_a^*$, this tetrad (2.4) is called a *complex null* tetrad. The matrix (2.5) is its own inverse. The corresponding vectors dual to (2.4) are

$$\epsilon^{*1} = 2^{-\frac{1}{2}}(\epsilon^1 - i\epsilon^2), \qquad \epsilon^{*2} = 2^{-\frac{1}{2}}(\epsilon^1 + i\epsilon^2),$$
$$\epsilon^{*3} = 2^{-\frac{1}{2}}(\epsilon^3 - \epsilon^4), \qquad \epsilon^{*4} = 2^{-\frac{1}{2}}(\epsilon^3 + \epsilon^4). \tag{2.6}$$

For the work to follow, this complex null tetrad is used to express all geometric objects and fields over $\mathcal{E}$. The asterisk is then removed since no confusion should result, and all the algebraic properties before complexification go directly over into themselves.

The set of all nonsingular linear transformations on T_P (and T_P^*) preserving the constant form of the metric g_{ab} is called the set of Lorentz transformations of the complex null tetrad (2.4). The proper orthochronous subgroup of these is given by

$$\mathbf{e}_1' = \exp(-iB)\,|1 - \alpha\beta|^{-1}(\mathbf{e}_1 + \bar{\alpha}\beta\mathbf{e}_2 - \bar{\alpha}\mathbf{e}_3 + \beta\mathbf{e}_4),$$
$$\mathbf{e}_2' = \exp(iB)\,|1 - \alpha\beta|^{-1}(\alpha\bar{\beta}\mathbf{e}_1 + \mathbf{e}_2 - \alpha\mathbf{e}_3 + \bar{\beta}\mathbf{e}_4),$$
$$\mathbf{e}_3' = \exp(-A)\,|1 - \alpha\beta|^{-1}(-\bar{\beta}\mathbf{e}_1 - \beta\mathbf{e}_2 + \mathbf{e}_3 - \beta\bar{\beta}\mathbf{e}_4),$$
$$\mathbf{e}_4' = \exp(A)\,|1 - \alpha\beta|^{-1}(\alpha\mathbf{e}_1 + \bar{\alpha}\mathbf{e}_2 - \alpha\bar{\alpha}\mathbf{e}_3 + \mathbf{e}_4), \tag{2.7}$$

where A and B are real, α and β are complex parameters, and $\alpha\beta \neq 1$.

The formalism discussed here corresponds to that used by Kerr[10] and (modulo a transposition $1 \rightleftarrows 2$ and $3 \rightleftarrows 4$) Sachs.[11] In the former instance $\mathbf{e}_1 \sim t$, $\mathbf{e}_2 \sim \bar{t}$, $\mathbf{e}_3 \sim m$, and $\mathbf{e}_4 \sim k$. Similar formalisms have been developed by Newman and Penrose,[12] Cahen, Debever, and Defrise,[13] and others.

The connection coefficients (generalized Christoffel symbols) are most easily defined by means of the exterior derivative and the first structure equations of Cartan[14]

$$d\epsilon^a = \epsilon^b \wedge \Gamma^a{}_b = \Gamma^a{}_{bc}\epsilon^b \wedge \epsilon^c \tag{2.8}$$

or through the definition of the covariant derivative[15] ∇, where

$$\nabla_{\mathbf{e}_b}(\mathbf{e}_a) = \Gamma^m{}_{ab}\mathbf{e}_m \tag{2.9}$$

and where $\Gamma^a{}_b = \Gamma^a{}_{b\mu}\,dx^\mu = \Gamma^a{}_{bc}\epsilon^c$. The connection is chosen so that $\Gamma_{(ab)c} = 0$, where $\Gamma_{abc} \equiv g_{am}\Gamma^m{}_{bc}$. If between vector fields $\mathbf{e}_a$ and $\mathbf{e}_b$ we have $[\mathbf{e}_a, \mathbf{e}_b] = C^m{}_{ab}\mathbf{e}_m$ denoting the *Lie bracket* operation, we choose the connection to satisfy also $\Gamma^m{}_{ab} - \Gamma^m{}_{bc} = C^m{}_{ba}$.

The Riemannian curvature tensor components with respect to the connection above satisfy

$$\tfrac{1}{2}R^a{}_{bcd} = -\Gamma^a{}_{b[c,d]} + \Gamma^a{}_{bm}\Gamma^m{}_{[cd]} + \Gamma^a{}_{m[c}\Gamma^m{}_{b|d]}, \tag{2.10}$$

where ",d" denotes a directional derivative in the $\mathbf{e}_d$ direction. The Ricci tensor and Ricci scalar components are

$$R_{ab} \equiv R^m{}_{abm} \quad \text{and} \quad R \equiv R^m{}_m, \tag{2.11}$$

respectively. Weyl's conformal curvature tensor is expressed by

$$C_{abcd} = R_{abcd} + g_{a[c}R_{d]b} + g_{b[d}R_{c]a} - \tfrac{1}{6}(g_{ac}g_{bd} - g_{ad}g_{bc})R. \tag{2.12}$$

In view of (2.8) and the properties of the exterior derivative,

$$\begin{aligned} d(V_a\epsilon^a) &= V_{a,b}\epsilon^b \wedge \epsilon^a + V_a\, d\epsilon^a \\ &= V_{a,b}\epsilon^b \wedge \epsilon^a - V_m\Gamma^m{}_{ab}\epsilon^b \wedge \epsilon^a \\ &= V_{a;b}\epsilon^b \wedge \epsilon^a. \end{aligned}$$

The components $V_{a;b}$ are the components of the covariant derivative of V with respect to $\mathbf{e}_b$. Now

$$\begin{aligned} g^{ab}V_{b;c} &= g^{ab}V_{b,c} - g^{ab}\Gamma^m{}_{bc}V_m = V^a{}_{,c} - \Gamma_m{}^a{}_c V^m \\ &= V^a{}_{,c} + \Gamma^a{}_{mc}V^m = V^a{}_{;b}. \end{aligned}$$

Similarly, we can get all the familiar properties of covariant derivatives expressed in terms of tetrad components, directional derivatives, and connection coefficients.

3. CANONICAL REPRESENTATIONS AND INVARIANT CLASSIFICATION FOR BIVECTORS OVER $\mathcal{E}$

A bivector[16] may be represented in the system introduced in Sec. 2 by

$$F = F_{ab}\epsilon^a \wedge \epsilon^b. \tag{3.1}$$

Bivectors form a subspace $\bigwedge^2 (T_P^*)$ of the larger second-order covariant tensor space. The dimension of $\bigwedge^2 (T_P^*)$ is $\frac{1}{2} \times 4 \times 3 = 6$. An example of a basis for the space of bivectors is $\{\epsilon^a \wedge \epsilon^b \mid a < b\}$.

The following set of vectors is taken as a basis for the space of contravariant bivectors:

$$\begin{aligned} e_{\mathrm{I}} &\equiv \mathbf{e}_4 \wedge \mathbf{e}_2, \quad e_{\mathrm{II}} \equiv \tfrac{1}{2}(\mathbf{e}_1 \wedge \mathbf{e}_2 + \mathbf{e}_3 \wedge \mathbf{e}_4), \\ e_{\mathrm{III}} &\equiv \mathbf{e}_3 \wedge \mathbf{e}_1, \quad e_{\mathrm{IV}} \equiv \overline{e_{\mathrm{I}}} = \mathbf{e}_4 \wedge \mathbf{e}_1, \\ e_{\mathrm{V}} &\equiv \overline{e_{\mathrm{II}}} = \tfrac{1}{2}(\mathbf{e}_2 \wedge \mathbf{e}_1 + \mathbf{e}_3 \wedge \mathbf{e}_4), \\ e_{\mathrm{VI}} &\equiv \overline{e_{\mathrm{III}}} = \mathbf{e}_3 \wedge \mathbf{e}_2. \end{aligned} \tag{3.2}$$

A contravariant bivector $V = V^{ab}\mathbf{e}_a \wedge \mathbf{e}_b$ may also be expressed as $V^A e_A$, where $A = \mathrm{I}, \mathrm{II}, \cdots, \mathrm{VI}$. If ordinary double contraction of indices is allowed to form an inner product or "metric" (also called g) on bivectors, it is expressible as the linear extension of

$$g(\mathbf{e}_a \wedge \mathbf{e}_b, \mathbf{e}_c \wedge \mathbf{e}_d) \equiv g_{abcd} \equiv g_{ac}g_{bd} - g_{ad}g_{bc}$$

over any basis $\{\mathbf{e}_a \wedge \mathbf{e}_b\}$.[17] As a 6×6 matrix the metric of the above basis with $A = \mathrm{I}, \mathrm{II}, \cdots, \mathrm{VI}$ is

$$(g_{AB}) \equiv [g(e_A, e_B)] = \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix},$$

where

$$\Lambda = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -\frac{1}{2} & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

and 0 is the 3×3 zero matrix. Note that the inverse of (g_{AB}), (g^{AB}), is given by substitution of

$$\Lambda^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

in place of Λ above.

By ordinary methods of finding the basis dual to (3.2), we see that

$$\begin{aligned} \epsilon^{\mathrm{I}} &= 2\epsilon^4 \wedge \epsilon^2, & \epsilon^{\mathrm{IV}} &= 2\epsilon^4 \wedge \epsilon^1, \\ \epsilon^{\mathrm{II}} &= 2(\epsilon^1 \wedge \epsilon^2 + \epsilon^3 \wedge \epsilon^4), & \epsilon^{\mathrm{V}} &= 2(\epsilon^2 \wedge \epsilon^1 + \epsilon^3 \wedge \epsilon^4), \\ \epsilon^{\mathrm{III}} &= 2\epsilon^3 \wedge \epsilon^1, & \epsilon^{\mathrm{VI}} &= 2\epsilon^3 \wedge \epsilon^2, \end{aligned} \tag{3.3}$$

where $\epsilon^A(e_B) = \delta^A{}_B$.

Assuming that $\mathcal{E}$ admits an orientation, we can use any tensor T, skew-symmetric on two covariant indices $(\mu\nu)$, to form the (Hodge) adjoint

$$T^*_{\mu\nu\cdots} \equiv \tfrac{1}{2}\eta_{\mu\nu\rho\sigma}T^{\rho\sigma}\cdots, \tag{3.4}$$

where $\eta_{\mu\nu\rho\sigma} = [\det(g_{\mu\nu})]^{\frac{1}{2}} \cdot \epsilon_{\mu\nu\rho\sigma}$, with $\epsilon_{\mu\nu\rho\sigma}$ the completely skew-symmetric Levi-Civita permutation symbol. This goes over into

$$T^*_{ab\cdots} = \tfrac{1}{2}\eta_{abcd}T^{cd}\cdots \tag{3.5}$$

in terms of tetrads, where $\eta_{1234} = i = \sqrt{-1}$. Similarly one finds that

$$T^{*ab\cdots} = \tfrac{1}{2}\eta^{abcd}T_{cd\cdots} \tag{3.6}$$

on contravariant tensor indices. If V is any bivector, $*V$ denotes the adjoint bivector whose components are V^*_{ab}.

Let F be a (covariant) bivector and define

$$\mathcal{F}^{(+)} \equiv F - i\,{*F}, \quad \mathcal{F}^{(-)} \equiv F + i\,{*F}. \tag{3.7}$$

Then $F = \frac{1}{2}(\mathcal{F}^{(+)} + \mathcal{F}^{(-)})$. Furthermore, $*\mathcal{F}^{(+)} = i\mathcal{F}^{(+)}$ and $*\mathcal{F}^{(-)} = -i\mathcal{F}^{(-)}$. Writing F as a 6-vector, $F = F_A\epsilon^A = F_{\mathrm{I}}\epsilon^{\mathrm{I}} + \cdots + F_{\mathrm{VI}}\epsilon^{\mathrm{VI}}$, and insisting that F be real[18] implies

$$\begin{aligned} F = {} & F_{\mathrm{I}}\epsilon^{\mathrm{I}} + F_{\mathrm{II}}\epsilon^{\mathrm{II}} + F_{\mathrm{III}}\epsilon^{\mathrm{III}} \\ & + (\text{complex conjugate of first three terms}). \end{aligned} \tag{3.8}$$

The 6×6 matrix

$$E_A{}^B \equiv i\begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix}, \quad I = 3 \times 3 \text{ identity}, \tag{3.9}$$

acts as an operator taking components of a bivector to their respective adjoints; i.e., $*F_A = E_A{}^B F_B$. Hence,

$$\mathcal{F}^{(-)} = 2F_{\mathrm{I}}\epsilon^{\mathrm{I}} + 2F_{\mathrm{II}}\epsilon^{\mathrm{II}} + 2F_{\mathrm{III}}\epsilon^{\mathrm{III}}. \tag{3.10}$$

A proper orthochronous Lorentz transformation on the complex null tetrad induces a transformation on the space of bivectors indicated by the following change in components:

$$\begin{aligned} F_{\mathrm{I}'} &= (1 - \alpha\beta)^{-1}[\exp(A + iB)] \\ &\quad \times (F_{\mathrm{I}} + 2\alpha F_{\mathrm{II}} + \alpha^2 F_{\mathrm{III}}), \\ F_{\mathrm{II}'} &= (1 - \alpha\beta)^{-1}[\beta F_{\mathrm{I}} + (1 + \alpha\beta)F_{\mathrm{II}} + \alpha F_{\mathrm{III}}], \\ F_{\mathrm{III}'} &= (1 - \alpha\beta)^{-1}[\exp(-A - iB)] \\ &\quad \times (\beta^2 F_{\mathrm{I}} + 2\beta F_{\mathrm{II}} + F_{\mathrm{III}}). \end{aligned} \tag{3.11}$$

It is easy to see that

$$2\mathcal{K} \equiv g^{AB}\mathcal{F}^{(-)}_A F_B = 4(F_{\mathrm{I}}F_{\mathrm{III}} - F_{\mathrm{II}}) \tag{3.12}$$

is Lorentz invariant. Two invariant cases are then (a) $\mathcal{K} = 0$ and (b) $\mathcal{K} \neq 0$. The case $\mathcal{K} = 0$ is characterized by a repeated root α_r in $F_{\mathrm{I}'} = 0$ (or β_r in $F_{\mathrm{III}'} = 0$). Choosing α_r to be the α for a Lorentz transformation (2.7) gives *gratis* $F_{\mathrm{I}'} = F_{\mathrm{II}'} = 0$; $F_{\mathrm{III}} \neq 0$. Hence $\mathcal{F}^{(-)}$ has the canonical form

$$\mathcal{F}^{(-)} = 2F_{\mathrm{III}}\epsilon^{\mathrm{III}} = 4F_{\mathrm{III}}\epsilon^3 \wedge \epsilon^1 = 4F_{31}\epsilon^3 \wedge \epsilon^1 \tag{3.13a}$$

when F is a null bivector. The case $\mathcal{K} \neq 0$ has no repeated root in either $F_{\mathrm{I}'} = 0$ or $F_{\mathrm{III}'} = 0$. However, α and β can be fixed (fixing $\mathbf{e}_3$ and $\mathbf{e}_4$) so that $F_{\mathrm{I}'} = 0 = F_{\mathrm{III}'}$ and $F_{\mathrm{II}'} \neq 0$. Here we have the canonical form

$$\begin{aligned} \mathcal{F}^{(-)} &= 2F_{\mathrm{II}}\epsilon^{\mathrm{II}} = 4F_{\mathrm{II}}(\epsilon^1 \wedge \epsilon^2 + \epsilon^3 \wedge \epsilon^4) \\ &= 4(F_{12} + F_{34})(\epsilon^1 \wedge \epsilon^2 + \epsilon^3 \wedge \epsilon^4). \end{aligned} \tag{3.13b}$$

This classification goes back to the work of Ruse[19] and Synge[20] and their approach to the electromagnetic field. The Lorentz transformation group preserving (3.13a) allows β, A, and B to be free parameters holding $\alpha = 0$. However, (3.13b) is preserved by $\alpha = \beta = 0$ with A and B as free parameters.

It should be noted that in this formalism the equations $F_{[ab;c]} = 0$ and $F^{ab}{}_{;b} = 0$ may be stated concisely by

$$d\mathcal{F}^{(-)} = 0; \tag{3.14}$$

hence, (3.14) characterizes a source-free Maxwell field.

4. THE KILLING VECTOR FIELD IN A VACUUM EINSTEIN SPACE

A Killing vector field $K = K_a\epsilon^a = K_\mu\, dx^\mu$ is a vector field satisfying Killing's equations[21]

$$K_{(a;b)} \equiv \tfrac{1}{2}(K_{a;b} + K_{b;a}) = 0 \tag{4.1}$$

locally over the space. It induces a local symmetry in the sense that if t is a parameter for the integral curves defined by $dx^\mu/dt = K^\mu$, then there is a coordinate system with $t \in \{x^{\mu'}\}$ so that $\partial(g_{\mu'\nu'})/\partial t = 0$ for each $\mu', \nu' = 1, 2, 3, 4$.

Notice that Eq. (4.1) is equivalent to

$$K_{a;b} = K_{[a;b]}, \tag{4.2}$$

the components of the *Killing bivector* (KBV) for the Killing vector **K**. Furthermore, integrability conditions for (4.1) are[22]

$$K_{a;bc} = R_{abcm}K^m. \tag{4.3}$$

The first Bianchi identity for the curvature tensor implies with (4.3) that $K_{[a;bc]} = 0$. Hence, if $B \equiv K_{a;b}\epsilon^a \wedge \epsilon^b$, then $dB = 0$. Furthermore, $K^a{}_{;ba} = -R_{bm}K^m$. The field equations for the gravitational field in a vacuum are $R_{ab} = 0$, however, so that $K^a{}_{;ba} = 0$ in a vacuum Einstein space. If one defines $\mathcal{B}^{(-)} \equiv B + i\, {}^*B$, then it follows from the discussion above that $d\mathcal{B}^{(-)} = 0$. Consequently, B is a source-free Maxwell field.

Consider next the possibilities

$$\mathcal{B}^{(-)} = 0, \tag{4.4a}$$

$$\mathcal{B}^{(-)} \neq 0, \quad d\mathcal{B}^{(-)} = 0. \tag{4.4b}$$

Equation (4.4a) says that the Killing vector is a *parallel* field; i.e., $K_{\mu;\nu} = 0$. Furthermore, this gives

$$R_{abcm}K^m = 0. \tag{4.5}$$

An argument by Ehlers and Kundt[4] gives the result that **K** must be a null vector field, the space must be of Petrov type N, and the space represents a *pp wave* of gravitational radiation. Hence, the following theorem may be stated.

Theorem 1: Let $\mathcal{E}$ be a vacuum Einstein space with a Killing vector field K^μ so that $K_{\mu;\nu} = 0$. Then $\mathcal{E}$ represents a *pp wave*.

The case considered in the rest of this section is that of (4.4b). This further splits into (a) B is a null bivector or (b) B is a nonnull bivector (i.e., $K_{a;b}K^{a;b} = 0 = K^*_{a;b}K^{a;b}$ or its negation, respectively). Let $\{\epsilon^A\}$ be the basis (3.3) for the space of bivectors and let the KBV be written as

$$B = K_{a;b}\epsilon^a \wedge \epsilon^b = K_A\epsilon^A, \tag{4.6}$$

where $A = \mathrm{I}, \mathrm{II}, \cdots, \mathrm{VI}$. Then (3.10) implies

$$\mathcal{B}^{(-)} = 2(K_{\mathrm{I}}\epsilon^{\mathrm{I}} + K_{\mathrm{II}}\epsilon^{\mathrm{II}} + K_{\mathrm{III}}\epsilon^{\mathrm{III}}). \tag{4.7}$$

The null or nonnull cases are expressed by one of two canonical forms respectively,[23]

$$\mathcal{K} = 0 \Leftrightarrow K_{a;b}K^{a;b} = 0 = K^*_{a;b}K^{ab} \Leftrightarrow \mathcal{B}^{(-)} \to 2K_{\mathrm{III}}\epsilon^{\mathrm{III}}, \tag{4.8a}$$

$$\begin{aligned}\mathcal{K} \neq 0 \Leftrightarrow K_{a;b}K^{a;b} \neq 0 \ \text{ or}\\ K^*_{a;b}K^{a;b} \neq 0 \Leftrightarrow \mathcal{B}^{(-)} \to 2K_{\mathrm{II}}\epsilon^{\mathrm{II}},\end{aligned} \tag{4.8b}$$

where $\mathcal{K}$ is the complex invariant introduced in (3.12). These forms are always possible through an appropriate Lorentz transformation, as was shown in Sec. 3. Observation of the transformation freedom left on the tetrads gives us that (4.8a) is preserved by a null rotation about $\mathbf{e}_4$, whereas (4.8b) is preserved by scaling only. As was shown by Synge[20] and others in the context of the study of the electromagnetic field, the relation (4.8a) implies that $K_{a;b}$ admits *one* principal null eigendirection which coincides here with $\mathbf{e}_4$. [Alternatively, coincidence with $\mathbf{e}_3$ could have been arranged just as well.] The case of (4.8b) is that where $K_{a;b}$ admits *two* distinct principal null eigendirections, here coincident with $\mathbf{e}_3$ and $\mathbf{e}_4$.

Theorem 2: Let $\mathcal{E}$ be a nonflat vacuum Einstein space admitting a Killing vector whose associated bivector is null. Then $\mathcal{E}$ is algebraically special in the sense of Sachs[11]; i.e., $\mathcal{E}$ is not Petrov Type I.

Proof: This theorem is very similar to that of Robinson[24] in that the same basic mathematical situation exists as in Robinson's null electromagnetic case. We know that

$$B = K_{\mathrm{III}}\epsilon^{\mathrm{III}} + K_{\mathrm{VI}}\epsilon^{\mathrm{VI}} \equiv \alpha\epsilon^{\mathrm{III}} + \bar{\alpha}\epsilon^{\mathrm{VI}},$$
$$\mathcal{B}^{(-)} = 2\alpha\epsilon^{\mathrm{III}}, \tag{4.9}$$

where $\alpha \equiv K_{\mathrm{III}}$ for simplicity. Hence $d\mathcal{B}^{(-)} = 0$

(Maxwell's field equations) imply

$$\begin{aligned} 0 &= 2\,(d\alpha \wedge \epsilon^{\mathrm{III}} - \alpha\, d\epsilon^{\mathrm{III}}) \\ &= 4\,(d\alpha \wedge \epsilon^3 \wedge \epsilon^1 - \alpha\, d\epsilon^3 \wedge \epsilon^1 + \alpha\epsilon^3 \wedge d\epsilon^1) \\ &= 4\,(d\alpha \wedge \epsilon^3 \wedge \epsilon^1 - \alpha\Gamma_{4ab}\epsilon^a \wedge \epsilon^b \wedge \epsilon^1 \\ &\quad + \alpha\Gamma_{2ab}\epsilon^a \wedge \epsilon^b \wedge \epsilon^3). \end{aligned} \tag{4.10}$$

In particular (4.10) implies $4\alpha\Gamma_{424} = 4\alpha\Gamma_{242} = 0$, which leaves $\Gamma_{424} = \Gamma_{422} = 0$. This is one way of stating that $\mathbf{e}_4$ is a *geodesic* and *shear-free* vector field. Hence, by the Goldberg–Sachs theorem[25] $\mathbf{e}_4 = e_4{}^\mu\partial_\mu$ designates a *degenerate* principal null direction of the Weyl conformal curvature tensor (here, the Riemann tensor, since $R_{ab} = 0$); i.e., $\mathbf{e}_4$ is a multiple Debever vector of this nonflat space. Hence, the space is algebraically special, by the Goldberg–Sachs theorem.[26] QED

5. INTEGRABILITY CONDITIONS FOR THE NONNULL KBV

Sachs[11] and others who have written on Petrov types define a set of scalars $\{C^{(i)} \mid i = 1, \cdots, 5\}$ associated with canonical forms for the Weyl tensor (here, the Riemann tensor). The Weyl tensor may be expressed in terms of the basis bivectors of Sec. 3 by

$$\begin{aligned} C &= R_{\mu\nu\rho\sigma}\, dx^\mu \wedge dx^\nu \otimes dx^\rho \wedge dx^\sigma \\ &= R_{abcd}\epsilon^a \wedge \epsilon^b \otimes \epsilon^c \wedge \epsilon^d = R_{AB}\epsilon^A \otimes \epsilon^B. \end{aligned} \tag{5.1}$$

For any complex null tetrad of the type introduced earlier, the conformal scalars $C^{(i)}$ are expressible as the following tetrad components of the Riemann tensor[27]:

$$\begin{aligned} C^{(5)} &\equiv 2R_{\mathrm{I\,I}} = 2R_{4242}, \\ C^{(4)} &\equiv 2R_{\mathrm{I\,II}} = R_{4212} + R_{4234}, \\ C^{(3)} &\equiv 2R_{\mathrm{I\,III}} = 2R_{\mathrm{II\,II}} \\ &= \tfrac{1}{2}(R_{1212} + 2R_{1234} + R_{3434}) = 2R_{4231}, \\ C^{(2)} &\equiv 2R_{\mathrm{II\,III}} = R_{3112} + R_{3134}, \\ C^{(1)} &\equiv 2R_{\mathrm{III\,III}} = 2R_{3131}. \end{aligned} \tag{5.2}$$

The significance of these scalars is that there always exists a complex null tetrad for which $C^{(5)} = 0$ or $C^{(1)} = 0$. The space is algebraically special if and only if there exists a tetrad for which $C^{(5)} = C^{(4)} = 0$ or $C^{(1)} = C^{(2)} = 0$. The other canonical forms for algebraically special spaces are summarized thus:

Petrov Type II $\Leftrightarrow C^{(5)} = C^{(4)} = 0,\quad C^{(3)} \neq 0,\quad C^{(1)} \neq 0,$

Petrov Type D $\Leftrightarrow C^{(5)} = C^{(4)} = C^{(1)} = C^{(2)} = 0,\quad C^{(3)} \neq 0,$

Petrov Type III $\Leftrightarrow C^{(5)} = C^{(4)} = C^{(3)} = 0,\ C^{(2)} \neq 0,$

Petrov Type N $\Leftrightarrow C^{(1)} \neq 0,\quad$ all other $\ C^{(i)} = 0.$

The above forms are valid when one substitutes $C^{(1)}$ for $C^{(5)}$ concurrent with $C^{(2)}$ for $C^{(4)}$.

Type I (for a nonflat space), the algebraically general case, also may be broken down into more than one canonical form with a study of the invariants of $R_{\mu\nu\rho\sigma}$ (see, for example, Penrose's article,[23] from which the following is taken). The two main forms for Petrov Type I are: (1) $C^{(4)} = C^{(2)} = 0$, $C^{(5)}C^{(1)} \neq 0$, with $C^{(5)}C^{(1)} \neq 9C^{(3)^2}$; (2) $C^{(5)} = C^{(1)} = 0$, $C^{(4)}C^{(2)} \neq 0$, with $16C^{(4)}C^{(2)} \neq 9C^{(3)^2}$. The exceptions turn out to be an algebraically special case in disguise. Flat space ($R_{\mu\nu\rho\sigma} = 0$) is excluded from the rest of this work since it is well known that it admits *ten* Killing vector fields and that it is the space for special relativity.

The Ricci tensor components R_{ab} must all be zero in a vacuum Einstein space so that

$$\begin{aligned} &R_{22} = 2R_{4223}, \quad R_{24} = R_{4212} - R_{4234}, \quad R_{44} = 2R_{4214}, \\ &R_{12} = R_{1212} + R_{1234} - 2R_{4231}, \\ &R_{34} = R_{1234} + R_{3434} - 2R_{4231}, \quad R_{23} = R_{3212} + R_{3234}, \\ &R_{33} = 2R_{3123} \end{aligned} \tag{5.3}$$

are all zero.

Consider again Eq. (4.3) and the case where B is a nonnull bivector. We fix the tetrad directions so that B is in its canonical form: $K_{\mathrm{I}} = K_{\mathrm{III}} = 0$, $K_{\mathrm{II}} \neq 0$. In the formalism of bivector indices, (4.3) may be written

$$K_{A;c} = R_{Acm}K^m, \tag{5.4}$$

where $A = \mathrm{I}, \mathrm{II}, \cdots, \mathrm{VI}$ and Latin indices go from 1 to 4 as usual. In terms of the conformal scalars, (5.4) may be expanded to give

$$K_{\mathrm{II};c} = R_{\mathrm{II}cm}K^m = K_{\mathrm{II},c}, \tag{5.4'a}$$

$$K_{\mathrm{I};c} = R_{\mathrm{I}cm}K^m = K_{\mathrm{II}}\Gamma_{42c}, \tag{5.4'b}$$

$$K_{\mathrm{III};c} = R_{\mathrm{III}cm}K^m = -K_{\mathrm{II}}\Gamma_{31c}, \tag{5.4'c}$$

plus the complex conjugate equations. Further expansion yields

$$\begin{aligned} K_{\mathrm{II},1} &= 0 + C^{(3)}K^2 - C^{(2)}K^3 + 0, \\ K_{\mathrm{II},2} &= -C^{(3)}K^1 + 0 + 0 - C^{(4)}K^4, \\ K_{\mathrm{II},3} &= C^{(2)}K^1 + 0 + 0 + C^{(3)}K^4, \\ K_{\mathrm{II},4} &= 0 + C^{(4)}K^2 - C^{(3)}K^3 + 0 \end{aligned} \tag{5.5a}$$

from (5.4'a). The relations

$$\begin{aligned} K_{\mathrm{II}}\Gamma_{421} &= 0 + C^{(4)}K^2 - C^{(3)}K^3 + 0, \\ K_{\mathrm{II}}\Gamma_{422} &= -C^{(4)}K^1 + 0 + 0 - C^{(5)}K^4, \\ K_{\mathrm{II}}\Gamma_{423} &= C^{(3)}K^1 + 0 + 0 + C^{(4)}K^4, \\ K_{\mathrm{II}}\Gamma_{424} &= 0 + C^{(5)}K^2 - C^{(4)}K^3 + 0 \end{aligned} \tag{5.5b}$$

are the result of (5.4'b). Finally, (5.4'c) becomes

$$\begin{aligned} -K_{II}\Gamma_{311} &= 0 + C^{(2)}K^2 - C^{(1)}K^3 + 0, \\ -K_{II}\Gamma_{312} &= -C^{(2)}K^1 + 0 + 0 - C^{(3)}K^4, \\ -K_{II}\Gamma_{313} &= C^{(1)}K^1 + 0 + 0 + C^{(2)}K^4, \\ -K_{II}\Gamma_{314} &= 0 + C^{(3)}K^2 - C^{(2)}K^3 + 0. \end{aligned} \tag{5.5c}$$

Notice that $\Gamma_{42c}K^c = \Gamma_{31c}K^c = 0$ from the skew-symmetry in (5.4'b) and (5.4'c). Combining eight of these equations yields

$$\begin{aligned} K_{II,1} &= -K_{II}\Gamma_{314}, \quad K_{II,2} = -K_{II}\Gamma_{423}, \\ K_{II,3} &= K_{II}\Gamma_{312}, \quad K_{II,4} = K_{II}\Gamma_{421} \end{aligned} \tag{5.6}$$

and leaves

$$\begin{aligned} K_{II}\Gamma_{422} &= -C^{(4)}K^1 + 0 + 0 - C^{(5)}K^4, \\ K_{II}\Gamma_{424} &= 0 + C^{(5)}K^2 - C^{(4)}K^3 + 0, \\ K_{II}\Gamma_{311} &= 0 - C^{(2)}K^2 + C^{(1)}K^3 + 0, \\ K_{II}\Gamma_{313} &= -C^{(1)}K^1 + 0 + 0 - C^{(2)}K^4. \end{aligned} \tag{5.7}$$

If we define the 4×4 determinant of coefficients for each of the systems (5.5'a)–(5.5'c) and (5.7) to be $(\Delta_3)^2$, $(\Delta_1)^2$, $(\Delta_5)^2$, and $(\Delta_3')^2$ respectively, then

$$\begin{aligned} \Delta_3 &= C^{(4)}C^{(2)} - C^{(3)^2}, \quad \Delta_1 = C^{(5)}C^{(3)} - C^{(4)^2}, \\ \Delta_5 &= C^{(3)}C^{(1)} - C^{(2)^2}, \quad \Delta_3' = C^{(5)}C^{(1)} - C^{(4)}C^{(2)}, \end{aligned} \tag{5.8}$$

up to a $\pm$ sign.

Further integrability conditions on (5.4) are those which come from

$$K^m R_{abcd;m} = 2K_{m;[d}R^m{}_{c]ab} + 2K_{m;[b}R^m{}_{a]cd}. \tag{5.9}$$

With the nonnull KBV in its canonical form, Eq. (5.9) results in

$$\begin{aligned} \mathbf{K}C^{(5)} &= 2\kappa C^{(5)}, \quad \mathbf{K}C^{(1)} = -2\kappa C^{(1)}, \\ \mathbf{K}C^{(4)} &= \kappa C^{(4)}, \quad \mathbf{K}C^{(2)} = -\kappa C^{(2)}, \\ \mathbf{K}C^{(3)} &= 0, \quad \kappa \equiv \Gamma_{IIm}K^m - K_{II}, \end{aligned} \tag{5.10}$$

where $\Gamma_{IIm} = \Gamma_{12m} + \Gamma_{34m}$ and $\mathbf{K}C^{(i)} \equiv K^m C^{(i)}{}_{;m}$.

The following equations involve the Lie derivative $£_\mathbf{K}$ of some of the basic objects in the space:

$$£_\mathbf{K}(\epsilon^I) = \kappa\epsilon^I, \tag{5.11a}$$

$$£_\mathbf{K}(\epsilon^{II}) = 0, \tag{5.11b}$$

$$£_\mathbf{K}(\epsilon^{III}) = -\kappa\epsilon^{III}. \tag{5.11c}$$

Furthermore,

$$£_\mathbf{K}(\Gamma_I) = (\Gamma_{IIm}K^m)\Gamma_I - R_{Icm}K^m\epsilon^c, \tag{5.12a}$$

$$£_\mathbf{K}(\Gamma_{II}) = d(\Gamma_{IIm}K^m) - R_{IIcm}K^m\epsilon^c, \tag{5.12b}$$

$$£_\mathbf{K}(\Gamma_{III}) = (-\Gamma_{IIm}K^m)\Gamma_{III} - R_{IIIcm}K^m\epsilon^c. \tag{5.12c}$$

If one defines $\Gamma \equiv \Gamma_{Ac}\epsilon^c \otimes \epsilon^A$, Eqs. (5.5) are written equivalently as $£_\mathbf{K}(\Gamma) = 0$. Hence

$$\begin{aligned} 0 &= £_\mathbf{K}(\Gamma_I \otimes \epsilon^I + \Gamma_{II} \otimes \epsilon^{II} + \Gamma_{III} \otimes \epsilon^{III} \\ &\quad + \text{complex conjugate}) \\ &= (\Gamma_{IIm}K^m)\Gamma_I \otimes \epsilon^I - R_{Icm}K^m\epsilon^c \otimes \epsilon^I \\ &\quad + d(\Gamma_{IIm}K^m) \otimes \epsilon^{II} - R_{IIcm}K^m\epsilon^c \otimes \epsilon^{II} \\ &\quad + (-\Gamma_{IIm}K^m)\Gamma_{III} \otimes \epsilon^{III} - R_{IIIcm}K^m\epsilon^c \otimes \epsilon^{III} \\ &\quad + \kappa\Gamma_I \otimes \epsilon^I - \kappa\Gamma_{III} \otimes \epsilon^{III} + \text{complex conjugate}. \end{aligned}$$

Therefore,

$$(\Gamma_{IIm}K^m - \kappa)\Gamma_{Ic} = R_{Icm}K^m, \tag{5.13a}$$

$$-(\Gamma_{IIm}K^m - \kappa)\Gamma_{IIIc} = R_{IIIcm}K^m, \tag{5.13b}$$

$$(\Gamma_{IIm}K^m)_{,c} = R_{IIcm}K^m. \tag{5.13c}$$

The last equation says that $K_{II,c} = (\Gamma_{IIm}K^m)_{,c}$, which implies that $d\kappa = 0$. This suggests possible future approaches with regard to the cases (1) $\kappa = 0$, (2) $\mathrm{Re}\,(\kappa) = 0$, (3) $\mathrm{Im}\,(\kappa) = 0$, (4) $K_{II,c} = 0$, (5) $\mathrm{Re}\,(K_{II,c}) = 0$, and (6) $\mathrm{Im}\,(K_{II,c}) = 0$. The special case of (4) $\Gamma_{IIm}K^m = 0$ is the case where the tetrad $\{\mathbf{e}_a\}$ is parallel propagated along $\mathbf{K}$.

Theorem 3: Suppose a nonnull Killing vector field in a nonflat vacuum Einstein space defines a Killing bivector which is also nonnull. Then the Killing vector field is not geodesic.

Proof: Let $\mathbf{K} = K^a\mathbf{e}_a$ be geodesic. Then along the $\mathbf{K}$ trajectory

$$K_{a;b}K^b = \alpha K_a$$

for some scalar α. This means that $\mathbf{K}$ must be an eigenvector for its own bivector matrix $(K_{a;b})$. Considering a tetrad system $\{\mathbf{e}_a\}$ for which the canonical form (4.7) is a result, we obtain $\mathcal{B}^{(-)} = 2K_{II}\epsilon^{II}$. Next define $a \equiv \mathrm{Re}\,(K_{II})$ and $b \equiv \mathrm{Im}\,(K_{II})$. Then $(K^a{}_{;b})$ may be written as diag $(-ib, ib, -a, a)$. Hence, each of these four values is an eigenvalue; in fact, if $a \neq 0 \neq b$, the eigenvectors are, respectively, $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4$—the complex null tetrad itself. The remaining real cases (a or b is zero) are for zero eigenvalues resulting in $\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2$ for $b = 0$ and $\mathbf{K} = K^3\mathbf{e}_3 + K^4\mathbf{e}_4$ for $a = 0$. The following lemma is established.

Lemma: A necessary and sufficient condition that a real Killing vector field with nonnull KBV in the form (4.7) be geodesic is that either

$$\mathbf{K} = k\mathbf{e}_4, \quad \mathbf{K} = l\mathbf{e}_3, \quad \alpha \neq 0 \Leftrightarrow a, b \text{ both not zero}, \tag{5.14a}$$

or

$$\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2, \quad \overline{K^1} = K^2 \neq 0, \alpha = 0, b = 0, a \neq 0, \tag{5.14b}$$

or

$$\mathbf{K} = K^3\mathbf{e}_3 + K^4\mathbf{e}_4,$$
$$K^3, K^4 \neq 0, \alpha = 0, a = 0, b \neq 0, \quad (5.14c)$$

where k and l are constants.

Examination of (5.14a) shows that since $\mathbf{e}_4$ is shear-free, geodesic, and null, the space must be algebraically special; $\mathbf{K}$ is then a multiple Debever vector. Furthermore, note that the hypothesis of Theorem 3 does not include this case. The proof of Theorem 3 is completed by taking Eqs. (5.14b) and (5.14c) with Killing's equations and integrability conditions to show that each case is incompatible with a working assumption.

Suppose case (5.14b) is examined. Here $K^3 = K^4 = 0$ so that

$$a_{,1} = -a\Gamma_{314} = -a\Gamma_{413}, \quad a_{,2} = -a\Gamma_{423} = -a\Gamma_{324}$$

from (5.6). So $\Gamma_{314} = \Gamma_{413}$ and $\Gamma_{324} = \Gamma_{423}$. Furthermore, $K_{4;3} + K_{3;4} = 0$ yields

$$K^1(\Gamma_{314} + \Gamma_{413}) + K^2(\Gamma_{324} + \Gamma_{423}) = 0.$$

Obviously

$$K^1(\Gamma_{314} - \Gamma_{413}) + K^2(\Gamma_{324} - \Gamma_{423}) \equiv 0,$$

so that

$$K^1\Gamma_{314} + K^2\Gamma_{324} = 0.$$

But $K_{3;4} = a = -(K^1\Gamma_{314} + K^2\Gamma_{324})$. Hence $a = 0$, a contradiction. The case (5.14b) is therefore impossible.

The case (5.14c) remains. Here $K^1 = K^2 = 0$ and

$$ib_{,1} = -ib\Gamma_{314} = -ib\Gamma_{413},$$
$$ib_{,2} = -ib\Gamma_{423} = -ib\Gamma_{324}$$

from (5.6). Therefore $\Gamma_{314} = \Gamma_{423}$ and $\Gamma_{324} = \Gamma_{423}$. The equation $K_{1;2} + K_{2;1} = 0$ yields

$$K^3(\Gamma_{312} + \Gamma_{321}) + K^4(\Gamma_{412} + \Gamma_{421}) = 0,$$

but

$$K^3(\Gamma_{312} - \Gamma_{321}) + K^4(\Gamma_{412} - \Gamma_{421}) \equiv 0$$

so that

$$K^3\Gamma_{312} + K^4\Gamma_{412} = 0.$$

However, $K_{2;1} = ib = K^3\Gamma_{312} + K^4\Gamma_{412}$. Therefore $b = 0$, a contradiction. Hence we have shown cases (5.14b) and (5.14c) to be impossible. QED

A particular kind of Killing vector in a space-time is one which is hypersurface orthogonal; i.e., $K_{[a;b}K_{c]} = 0$. For example, a *static* metric is one having a hypersurface orthogonal timelike Killing vector field. The following theorem is a characterization for this property in the context of nonnull KBV's.

Theorem 4: Suppose K is a Killing vector field with a nonnull Killing bivector. Then $\mathbf{K}$ is hypersurface orthogonal if and only if one of the two following cases is true:

$$K^1 = K^2 = 0 \quad \text{and } K_{\text{II}} \text{ is real}, \quad (5.15a)$$
$$K^3 = K^4 = 0 \quad \text{and } K_{\text{II}} \text{ is pure imaginary}, \quad (5.15b)$$

where $\mathbf{K} = K^a\mathbf{e}_a$. (In terms of the invariants of the next section, $\mathcal{K}$ is real and nonzero.)

Proof: Notice that $K \equiv K_a\epsilon^a$ is hypersurface orthogonal $\Leftrightarrow dK \wedge K = 0$. This means

$$K_{a;b}K_c\epsilon^a \wedge \epsilon^b \wedge \epsilon^c = 0.$$

Hence,

$$0 = 2(K_{\text{II}} + \bar{K}_{\text{II}})(K_1\epsilon^1 \wedge \epsilon^3 \wedge \epsilon^4 + K_2\epsilon^2 \wedge \epsilon^3 \wedge \epsilon^4) + 2(K_{\text{II}} - \bar{K}_{\text{II}})(K_3\epsilon^1 \wedge \epsilon^2 \wedge \epsilon^3 + K_4\epsilon^1 \wedge \epsilon^2 \wedge \epsilon^4).$$

From this equation one sees that either (5.15a) or (5.15b) must be true. Evidently (5.15a) or (5.15b) implies $dK \wedge K = 0$. QED

Notice that reality conditions on (5.6) give $\Gamma_{312} = \Gamma_{321}$, $\Gamma_{412} = \Gamma_{421}$, and $\Gamma_{314} = \Gamma_{413}$, meaning that $\mathbf{e}_3$ and $\mathbf{e}_4$ are hypersurface orthogonal and are 2-surface forming. Hence, the following rather technical result is proved.

Theorem 5: Suppose $\mathbf{K}$ is a Killing vector field (with a nonnull KBV) which is hypersurface orthogonal. Then if the real principal null rays of the KBV are geodesic, they are hypersurface orthogonal and are 2-surface forming.

Corollary: Suppose $\mathbf{K}$ is a Killing vector field (with a nonnull KBV) and $\mathbf{e}_3$ and $\mathbf{e}_4$ are real geodesic principal null rays of the KBV. Suppose also that $K^1 = K^2 = 0$ or $K^3 = K^4 = 0$. Then a necessary and sufficient condition that $\mathbf{K}$ be hypersurface orthogonal is that $\mathbf{e}_3$ and $\mathbf{e}_4$ be hypersurface orthogonal and 2-surface forming.

Proof: Killing's equations imply that, for $\mathbf{e}_4$ and $\mathbf{e}_3$ hypersurface orthogonal (i.e., $\Gamma_{312} = \Gamma_{321}$ and $\Gamma_{421} = \Gamma_{412}$) and 2-surface forming (i.e., $\Gamma_{314} = \Gamma_{413}$),

$$2a = K_{3,4} - K_{4,3} + K_3\Gamma_{344} + K_4\Gamma_{343},$$
$$2ib = K_{1,2} - K_{2,1} + K_1\Gamma_{122} + K_2\Gamma_{121}.$$

Then $K^1 = K^2 = 0 \Rightarrow b = 0$, and so $\mathbf{K}$ is hypersurface orthogonal by Theorem 4; $K^3 = K^4 = 0 \Rightarrow a = 0$ and $\mathbf{K}$ is, again, hypersurface orthogonal. QED

6. INVARIANTS OF R_{abcd} AND $K_{a;b}$

In his paper on a spinor approach to general relativity Penrose[28] introduces the complex invariants[29]

$$\mathfrak{J} \equiv \tfrac{1}{4}(R_{abcd} + iR^*_{abcd})R^{abcd},$$
$$\mathfrak{F} \equiv \tfrac{2}{3}(R_{abcd} + iR^*_{abcd})R^{cd}{}_{mn}R^{mnab}$$

of the Riemann tensor. These quantities are invariant with respect to both coordinate and tetrad transformations. In terms of the conformal scalars,

$$\mathfrak{J} = C^{(5)}C^{(1)} - 4C^{(4)}C^{(2)} + 3C^{(3)^2}, \tag{6.1}$$

$$\mathfrak{F} = 2C^{(4)}C^{(3)}C^{(2)} + C^{(5)}C^{(3)}C^{(1)} - C^{(5)}C^{(2)^2} - C^{(4)^2}C^{(1)} - C^{(3)^3}. \tag{6.2}$$

These independent invariants, a result of the classical study of algebraic invariants, have also been utilized by Géhéniau and Debever,[30] Bel,[31] and Zund.[32] In particular, the space is algebraically special if and only if $\mathfrak{J}^3 = 27\mathfrak{F}^2$. The "harmonic" case for Petrov Type I is obtained whenever $\mathfrak{F} = 0$, $\mathfrak{J} \neq 0$; the "equianharmonic" case of Type I is obtained whenever $\mathfrak{F} \neq 0$, $\mathfrak{J} = 0$.[28]

A larger system can be built up by the addition of $K_{a;b}$ into the scheme. Define

$$\mathcal{K} \equiv \tfrac{1}{2}(K_{a;b} + iK^*_{a;b})K^{a;b},$$
$$\mathfrak{L} \equiv \tfrac{1}{2}K_{a;b}(R^{ab}{}_{cd} + iR^{*ab}{}_{cd})K^{c;d},$$
$$\mathcal{M} \equiv \tfrac{1}{2}K_{a;b}R^{ab}{}_{cd}(R^{cd}{}_{mn} + iR^{*cd}{}_{mn})(K^{m;n} + iK^{*m;n}).$$

Then, for the case examined in Sec. 5 (B is nonnull and reduced to its canonical form),

$$\mathcal{K} = -2K_{\text{II}}^2, \tag{6.3}$$
$$\mathfrak{L} = 4K_{\text{II}}^2C^{(3)}, \tag{6.4}$$
$$\mathcal{M} = 4K_{\text{II}}^2(C^{(4)}C^{(2)} - C^{(3)^2}) = 4K_{\text{II}}^2\Delta_3. \tag{6.5}$$

The condition that a principal null direction for B coincide with one for R_{abcd} is equivalent to $\mathfrak{D} = 0$, where $\mathfrak{D} \equiv 4\mathcal{K}^2\mathfrak{J} - 8\mathcal{K}\mathcal{M} + \mathfrak{L}^2$. In the case at hand

$$\mathfrak{D} = 4K_{\text{II}}^4C^{(5)}C^{(1)}. \tag{6.6}$$

A look at the action of $\mathbf{K}$ on the scalars and invariants mentioned gives the results that

$$\mathbf{K}(C^{(5)}C^{(1)}) = \mathbf{K}(C^{(4)}C^{(2)}) = \mathbf{K}(C^{(4)^2}C^{(1)}) = \mathbf{K}(C^{(5)}C^{(2)^2}) = 0, \tag{6.7}$$

$$\mathbf{K}(\mathfrak{J}) = \mathbf{K}(\mathfrak{F}) = \mathbf{K}(\mathfrak{L}) = \mathbf{K}(\mathcal{M}) = 0. \tag{6.8}$$

since $\mathbf{K}(K_{\text{II}}) = 0$ from (5.4′a).

7. THE HYPERSURFACE ORTHOGONAL KILLING VECTOR FIELD (WITH NONNULL KBV)

It was shown in Sec. 5 that a hypersurface orthogonal Killing vector has a certain representation with regard to the complex null tetrad chosen. The following discussion utilizes this representation and the transformation freedom left on the tetrad [$\alpha = \beta = 0$ in Eq. (2.7)] to get some invariant geometrical results for this special case. The gravitational fields with such a timelike Killing field are the static ones and include the Schwarzschild class[33] and the Weyl–Levi-Civita classes (see, for example, the treatment in Refs. 3 and 4).

Theorem 6: Let $\mathcal{E}$ be a nonflat vacuum Einstein space which admits a Killing vector field $\mathbf{K}$ with a nonnull KBV. If $\mathbf{K}$ is hypersurface orthogonal, then $R^*_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma} = 0$; i.e., the invariant $\mathfrak{J} = \bar{\mathfrak{J}}$. Furthermore, $K^*_{\mu;\nu}K^{\mu;\nu} = 0$ and the invariants $\mathcal{K}$, $\mathfrak{L}$, $\mathcal{M}$, and $\mathfrak{D}$ are real.

Proof: [Case 1, $K^1 = K^2 = 0$ and $\text{Im}(K_{\text{II}}) = 0$.] For simplicity define $a \equiv \text{Re}(K_{\text{II}})$. Equations (5.5a)–(5.5c) reduce here to

$$a_{,1} = C^{(2)}K^3 = -a\Gamma_{314}, \qquad a_{,3} = C^{(3)}K^4 = a\Gamma_{312},$$
$$a_{,2} = -C^{(4)}K^4 = -a\Gamma_{423}, \qquad a_{,4} = -C^{(3)}K^3 = a\Gamma_{421},$$

and

$$a\Gamma_{422} = -C^{(5)}K^4, \qquad a\Gamma_{311} = C^{(1)}K^3,$$
$$a\Gamma_{424} = -C^{(4)}K^3, \qquad a\Gamma_{313} = -C^{(2)}K^4. \tag{7.1}$$

It is apparent from $a_{,3}$ and $a_{,4}$ that $C^{(3)}$ is real. Furthermore $a_{,1}$ and $a_{,2}$ give

$$0 = C^{(2)}K^3 + \overline{C^{(4)}}K^4, \quad 0 = \overline{C^{(2)}}K^3 + C^{(4)}K^4,$$

from which $C^{(4)}C^{(2)} = \overline{C^{(4)}}\,\overline{C^{(2)}}$ is a necessary condition. From the second set in (7.1) we obtain

$$0 = C^{(1)}(K^3)^2 - \overline{C^{(5)}}(K^4)^2,$$
$$0 = \overline{C^{(1)}}(K^3)^2 - \overline{C^{(5)}}(K^4)^2,$$

from which $C^{(5)}C^{(1)} = \overline{C^{(5)}}\,\overline{C^{(1)}}$ is a necessary condition. Hence, by definition, $\mathfrak{J} = \bar{\mathfrak{J}}$.

[Case 2, $K^3 = K^4 = 0$ and $\text{Re}(K_{\text{II}}) = 0$.] Define $b \equiv \text{Im}(K_{\text{II}})$. Equations (5.5a)–(5.5c) become

$$ib_{,1} = C^{(3)}K^2 = -ib\Gamma_{314}, \qquad ib_{,3} = C^{(2)}K^1 = ib\Gamma_{312},$$
$$ib_{,2} = -C^{(3)}K^1 = -ib\Gamma_{423}, \quad ib_{,4} = C^{(4)}K^2 = ib\Gamma_{421},$$

and

$$ib\Gamma_{422} = -C^{(4)}K^1, \qquad ib\Gamma_{311} = -C^{(2)}K^2,$$
$$ib\Gamma_{424} = C^{(5)}K^2, \qquad ib\Gamma_{313} = -C^{(1)}K^1. \tag{7.2}$$

From $b_{,1}$ and $b_{,2}$ one sees that $C^{(3)}$ is real. Also an argument similar to that above gives

$$0 = C^{(2)}K^1 + \overline{C^{(2)}}K^2, \quad 0 = C^{(1)}(K^1)^2 - \overline{C^{(1)}}(K^2)^2$$

and

$$0 = \overline{C^{(4)}}K^1 + C^{(4)}K^2, \quad 0 = \overline{C^{(5)}}(K^1)^2 - C^{(5)}(K^2)^2,$$

so that $C^{(4)}C^{(2)} = \overline{C^{(4)}}\,\overline{C^{(2)}}$ and $C^{(5)}C^{(1)} = \overline{C^{(5)}}\,\overline{C^{(1)}}$ are necessary. Hence $\mathfrak{J} = \bar{\mathfrak{J}}$. From the expressions obtained for $\mathfrak{L}$, $\mathcal{M}$, and $\mathfrak{D}$ in Sec. 6, one sees that these invariants must then be real. From the basic definitions, the invariant $K^*_{a;b}K^{a;b} = K^*_{\mu;\nu}K^{\mu;\nu}$ is proportional to the product ab. Hence, this is zero in both instances. QED

The following theorem states a property of all Einstein spaces with a hypersurface orthogonal spacelike or timelike Killing vector field where

$$\mathcal{K} = \tfrac{1}{2}K_{\mu;\nu}K^{\mu;\nu} \neq 0$$

(one of the indices a or b is zero in the previous discussion).

Theorem 7: Let $\mathcal{E}$ be a nonflat vacuum Einstein space which admits a Killing vector field with a nonnull KBV. If **K** is hypersurface orthogonal and $\mathcal{K} < 0$, then the two principal null rays for $K_{a;b}$ are geodesics; if $\mathcal{K} > 0$, then the two null rays are shear-free.

Proof: The representation has been developed so that $\mathbf{e}_3$ and $\mathbf{e}_4$ are the principal null rays for $K_{a;b}$. We assume then that $\mathbf{K} = K^3\mathbf{e}_3 + K^4\mathbf{e}_4$ and, without loss of generality, that $K^3 \neq 0$. (We know, in fact, that $K^3 = 0$ implies K^4 is a constant, and $\mathbf{K} = K^4\mathbf{e}_4$ is then the null geodesic alluded to in the lemma to Theorem 3.) From the transformation $\mathbf{e}_{3'} = \exp(-A)\mathbf{e}_3$, still allowed, one transforms to $\mathbf{K} = \mathbf{e}_{3'} + K^{4'}\mathbf{e}_{4'}$, taking K^3 as originally greater than zero since a Killing vector field is unique only up to a constant scalar factor. The Γ_{abc} and $C^{(i)}$ are only multiplied by factors of $\exp(-A)$ and K_{II} remains unchanged as relations (3.11) show. Hence, there is still maintained $K_{\mathrm{II}} \equiv a + ib = a$ for $\mathcal{K} < 0$. With the primes removed, the canonical form for $K_{a;b}$ gives (note $K^3 = K_4$)

$$K_{4;4} = K_{4,4} - K_4\Gamma_{344} = 0 \Rightarrow \Gamma_{344} = 0 = K_{4,3} = K_{4,2} = K_{4,1}, \quad (7.3a)$$

$$K_{4;3} = K_{4,3} = K_4\Gamma_{343} = -a \Rightarrow \Gamma_{343} = a, \quad (7.3b)$$

$$K_{4;1} = K_{4,1} - K_4\Gamma_{341} = 0 \Rightarrow \Gamma_{341} = \Gamma_{342} = 0, \quad (7.3c)$$

$$K_{3;1} = K_{3,1} + K_3\Gamma_{341} = 0 \Rightarrow K_{3,1} = K_{3,2} = 0, \quad (7.4a)$$

$$K_{3;3} = K_{3,3} - K_3\Gamma_{433} = 0 \Rightarrow K_{3,3} = -aK_3, \quad (7.4b)$$

$$K_{3;4} = K_{3,4} - K_3\Gamma_{434} = a \Rightarrow K_{3,4} = a. \quad (7.4c)$$

Now Eqs. (7.1) and (7.4c) imply

$$a_{,1} = K_{3,41} = -a\Gamma_{314}, \quad (7.5a)$$

$$a_{,2} = K_{3,42} = -a\Gamma_{423}, \quad (7.5b)$$

$$a_{,3} = K_{3,43} = a\Gamma_{312}, \quad (7.5c)$$

$$a_{,4} = K_{3,44} = a\Gamma_{421}. \quad (7.5d)$$

Commutation relations from Sec. 2 for the tetrad are given by

$$f_{,ab} - f_{,ba} = f_{,m}(\Gamma^m{}_{ab} - \Gamma^m{}_{ba}),$$

where f is any scalar. Consequently, using (7.3c) above, we obtain

$$K_{3,41} - K_{3,14} = K_{3,41} = -K_{3,3}\Gamma_{414} - K_{3,4}\Gamma_{314}.$$

But applying (7.5a) and (7.4c) gives $\Gamma_{414} = \Gamma_{424} = 0$. Therefore, $\mathbf{e}_4$ is geodesic. Hence (7.1) implies $C^{(4)} = 0$ and, since $\Gamma_{314} = \Gamma_{413}$, $C^{(2)} = 0$. Furthermore, Γ_{313} is then zero so that $\mathbf{e}_3$ is also geodesic. Note that it has been shown that $a_{,1} = a_{,2} = 0$ is necessary.

For the second case let $\mathbf{K} = K^1\mathbf{e}_1 + K^2\mathbf{e}_2$, where $\mathbf{e}_3$ and $\mathbf{e}_4$ are again principal null eigenvectors for $K_{a;b}$. Since $K^2 = \overline{K^1}$, neither can be zero. From the transformation $\mathbf{e}_{1'} = \exp(-iB)\mathbf{e}_1$, still allowed, one may transform K^1 and K^2 into *real* components, $K^1 = K^2$. With $b \equiv \mathrm{Im}(K_{\mathrm{II}})$, $K_{\mathrm{II}} = ib$ is still maintained for $\mathcal{K} < 0$ with Γ_{abc} and $C^{(i)}$ being multiplied by factors of $\exp(-iB)$. The primes are removed to give

$$K_{1;1} = K_{1,1} - K_1\Gamma_{211} = 0,$$

$$K_{2;2} = K_{2,2} - K_2\Gamma_{122} = 0,$$

$$K_{1;2} = K_{1,2} + K_1\Gamma_{122} = ib \Rightarrow 2K_{2,2} = ib \text{ and } \Gamma_{122} = \Gamma_{121}, \quad (7.6a)$$

$$K_{1;3} = K_{1,3} + K_1\Gamma_{123} = 0,$$

$$K_{2;3} = K_{2,3} + K_2\Gamma_{213} = 0 \Rightarrow \Gamma_{123} = \Gamma_{213} = 0, \quad (7.6b)$$

$$K_{1;4} = K_{1,4} - K_1\Gamma_{214} = 0,$$

$$K_{2;4} = K_{2,4} - K_2\Gamma_{124} = 0 \Rightarrow \Gamma_{124} = \Gamma_{214} = 0. \quad (7.6c)$$

Hence we conclude that $K_{1,3} = K_{2,3} = K_{1,4} = K_{2,4} = 0$. Consider next the equations from (7.2) and (7.6a)

$$ib_{,1} = 2K_{2,21} = -ib\Gamma_{314}, \quad (7.7a)$$

$$ib_{,2} = 2K_{2,22} = -ib\Gamma_{423}, \quad (7.7b)$$

$$ib_{,3} = 2K_{2,23} = ib\Gamma_{312}, \quad (7.7c)$$

$$ib_{,4} = 2K_{2,24} = ib\Gamma_{421}. \quad (7.7d)$$

The commutation relations on the tetrad give

$$2(K_{2,23} - K_{2,32}) = 2K_{2,23} = 2K_{2,m}(\Gamma^m{}_{23} - \Gamma^m{}_{32}) = ib_{,3} = 2K_{2,1}\Gamma_{322} + ib\Gamma_{312}.$$

Now $K_{2,1} \neq 0$ since $K_{2,1} = K_{1,1} = \overline{K_{2,2}} = -\frac{1}{2}ib$. Therefore, $\Gamma_{322} = 0$ from (7.7c) and $\mathbf{e}_3$ is shear-free. Equations (7.2) further imply that $C^{(2)} = 0$; hence $\Gamma_{312} = \Gamma_{321} = 0 = b_{,3}$. Also consider

$$2(K_{2,24} - K_{2,42}) = 2K_{2,24} = 2K_{2,m}(\Gamma^m{}_{24} - \Gamma^m{}_{21})$$
$$= ib_{,4} = 2K_{2,1}\Gamma_{422} + 2K_{2,2}\Gamma_{412}.$$

Again, since $K_{2,1} \neq 0$, $\Gamma_{422} = 0$. Therefore $\mathbf{e}_4$ is shear-free; $\Gamma_{422} = \Gamma_{411} = 0$. Furthermore, $C^{(4)} = 0$ by (7.2), and $\Gamma_{412} = \Gamma_{421} = 0 = b_{,4}$. QED

The following corollaries provide a look at the hypersurface orthogonal case with regard to Petrov types and the invariants of Sec. 6. Recall that $\mathcal{K} = \overline{\mathcal{K}}$ and $\mathcal{K} \neq 0$.

Corollaries: (Flat space is excluded *a priori.*)

(1) Let $\mathcal{M} = 0$ ($\Leftrightarrow \mathcal{L} = 0$). Then $\mathfrak{J} = 0$. Furthermore $\mathfrak{I} = 0 \Leftrightarrow \mathfrak{D} = 0$, and only Petrov Type N is allowed in this latter instance. If $\mathfrak{D} \neq 0$, then the space is harmonic Petrov Type I.

(2) Let $\mathcal{M} \neq 0$ ($\Leftrightarrow \mathcal{L} \neq 0$). Then $\mathfrak{D} = 0$ implies both $\mathfrak{I}, \mathfrak{J} \neq 0$ and only Petrov Types II and D are allowed. (The case where $\mathfrak{D} \neq 0$ has three possible results, two of which are nonrestrictive and could occur whether or not a Killing vector field is present.)

(3) Let $\mathcal{M} \neq 0$. Then $\mathfrak{D} \neq 0$ allows the harmonic Type I and the equi-anharmonic Type I since here $\mathfrak{J} = 0 \Leftrightarrow \mathfrak{I} \neq 0$. For both $\mathfrak{I}, \mathfrak{J} \neq 0$ the space is Type I for $\mathfrak{I}^3 \neq 27\mathfrak{J}^2$, but for $\mathfrak{I}^3 = 27\mathfrak{J}^2$ the space is restricted to be Type II or Type D.

Proof: This is accomplished by examination of the possibilities allowed the invariants $\mathcal{M}$, $\mathcal{L}$, $\mathfrak{D}$, $\mathfrak{I}$, and $\mathfrak{J}$ when written in terms of the tetrad system, as in Sec. 6. Since $C^{(4)} = C^{(2)} = 0$, these become

$$\mathcal{M} = 2\mathcal{K}C^{(3)^2}, \quad \mathcal{L} = -2\mathcal{K}C^{(3)}, \quad \mathfrak{D} = 4\mathcal{K}^2C^{(5)}C^{(1)},$$
$$\mathfrak{I} = C^{(5)}C^{(1)} + 3C^{(3)^2}, \quad \mathfrak{J} = C^{(3)}(C^{(5)}C^{(1)} - C^{(3)^2}). \tag{7.8}$$

Note that $C^{(5)}C^{(1)} = C^{(3)^2} \Rightarrow \mathfrak{I}^3 \neq 27\mathfrak{J}^2$ since the latter corresponds to $C^{(5)}C^{(1)} = 9C^{(3)^2}$. Putting (7.8) together with the canonical forms for Petrov types (see Sec. 5) results in the statements (1)–(3) above, which are independent of any tetrad system.

The corollaries above are summarized in Table I below, where the asterisk stands for a nonzero value. Note in particular that spaces of Petrov Type III cannot then contain a hypersurface orthogonal Killing vector field which has a nonnull Killing bivector.

TABLE I.

$\mathcal{M}$, $\mathcal{L}$	$\mathfrak{D}$	$\mathfrak{I}$	$\mathfrak{J}$	Petrov type
0	0	0	0	N
0	*	*	0	I (harmonic)
*	0	*	*	II, D
*	*	*	0	I (harmonic)
*	*	0	*	I (equi-anharmonic)
*	*	*	*	I for $\mathfrak{I}^3 \neq 27\mathfrak{J}^2$ II, D for $\mathfrak{I}^3 = 27\mathfrak{J}^2$

One topological result of Theorem 6 is worth mentioning. If a space $\mathcal{E}$ is compact and orientable and satisfies the hypothesis of Theorem 6, then its Pontrjagin number $p[\mathcal{E}] = 0$. This follows from a discussion of Zund.[34] The Euler–Poincaré characteristic $\chi(\mathcal{E})$ can also vanish in such a case whenever $\mathfrak{I} = 0$ (see, for example, Ref. 32). Table I shows when this latter case occurs.

[1] I. Robinson and J. Robinson, "Vacuum Metrics without Symmetry" (unpublished) 1969.

[2] "Space" here and throughout refers to a vacuum Einstein space satisfying $R_{\mu\nu} = 0$.

[3] P. Jordan, J. Ehlers, and W. Kundt, Akad. Wiss. Lit. (Mainz) Abhandl. Math.-Naturwiss. Kl. **23**, 21 (1960).

[4] J. Ehlers and W. Kundt, in *Gravitation*, edited by L. Witten (Wiley, New York, 1962), Chap. 2.

[5] A. Z. Petrov, Sci. Notices. Kazan State Univ. **114**, 55 (1954).

[6] Work on the null case will be reported at a later date if results other than those obtained by R. P. Kerr and the author [G. C. Debney and R. P. Kerr, J. Math. Phys. **11**, 2807 (1970)] (on Killing vectors in algebraically special spaces) prove useful.

[7] Throughout this paper Latin indices refer to components of a tensor with respect to a general basis (tetrad); Greek indices indicate components with respect to a coordinate system.

[8] See R. L. Bishop and S. I. Goldberg, *Tensor Analysis on Manifolds* (Macmillan, New York, 1968), p. 104.

[9] What is being defined here is a complexification of T_P and T_P^*, a formal algebraic generalization of complex numbers. The resulting tetrad is used, however, to generate real tensors.

[10] R. P. Kerr, Phys. Rev. Letters **11**, 237 (1963).

[11] R. K. Sachs, Proc. Roy. Soc. (London) **A264**, 309 (1961).

[12] E. T. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

[13] M. Cahen, R. Debever, and L. Defrise, J. Math. Mech. **16**, 761 (1967).

[14] The "$\wedge$" is the (Grassman) skew-symmetric product operation and "d" stands for the exterior derivation on the algebra thus generated.

[15] See Ref. 8, p. 288.

[16] J. A. Schouten [*Ricci Calculus* (Springer-Verlag, Berlin, 1954), 2nd ed.] gives the name "bivector" to any skew-symmetric contravariant or covariant tensor of order 2. We adopt this convention, noting that here we are dealing mostly with the space of 2-forms over $\mathcal{E}$, i.e., the space of covariant skew-symmetric tensor fields.

[17] If $U = U^{ab}\mathbf{e}_a \wedge \mathbf{e}_b$ and $V = V^{ab}\mathbf{e}_a \wedge \mathbf{e}_b$, then $g(U, V) = g_{abcd} \times U^{ab}V^{cd} = 2U_{ab}V^{ab}$.

[18] This means identical with its complex conjugate.

[19] H. S. Ruse, Proc. London Math. Soc. **41**, 302 (1936).

[20] J. L. Synge, *Relativity: The Special Theory* (North-Holland, Amsterdam, 1965), 2nd ed.

[21] See L. P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1960), p. 243.

[22] See Ref. 21, p. 237.

[23] These cases are sometimes referred to as "singular" and "nonsingular."

[24] I. Robinson, J. Math. Phys. 2, 290 (1961).

[25] J. N. Goldberg and R. K. Sachs, Acta Phys. Polon. 22, 13 (1962).

[26] We note here that e_4 is then a principal null direction for both the Weyl tensor and the KBV.

[27] Some authors have different numerical coefficients on these scalars; this is due to the choice of bivector basis in the original formalism and to a desire to have these fit other invariant schemes.

[28] R. Penrose, Ann. Phys. (N.Y.) **10**, 171 (1960).

[29] There is a difference in numerical factors here from those used in Ref. 28. The factors here merely help some computations to be simpler.

[30] J. Géhéniau and R. Debever, Bull. Acad. Roy. Belg. Cl. Sci. **42**, 114 (1956).

[31] L. Bel, thesis, University of Paris, 1960.

[32] J. D. Zund, Ann. Mat. Pura Appl. **78**, 365 (1968).

[33] K. Schwarzschild, Sitz-Ber. Preuss. Akad. Wiss., 189 (1916).

[34] J. D. Zund, Ann. Mat. Pura Appl. **82**, 381 (1969).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Note on the Electrodynamics of Accelerated Systems*

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(Received 22 October 1970)

Some preliminary results concerning the experimental testability of the free-space constitutive relations are discussed in connection with some recent theoretical developments.

A recent paper by Mo[1] on the electrodynamics of accelerated systems seems to make it desirable to recall some early experimentation that is relevant to free-space constitutive behavior.

There are few experimental tests on record which may be considered as a direct verification of the constitutive behavior observed on accelerated systems in free space. The only experiments known to the present authors are the experiments performed some fifty years ago by Kennard[2] and by Pegram[3]; they constitute experimental tests for rotational motion.

The equipment that was used in both experiments consisted of a tubular cylindrical condensor which was being rotated in a coaxial magnetic field. Kennard found a potential to exist on the condensor when rotated, while Pegram's observation showed that a charge developed on the condensor when it was being shorted by a co-rotating short.

For both experiments it was found that the observations were independent of whether the solenoid generating the coaxial B field was stationary or rotating at the same angular velocity as the cylindrical condensor.

There has been some controversy surrounding these observations. Questions have been raised as to whether the observations were correct and, if so, how should they be interpreted in the light of the circumstance that *the effects still exist even when the solenoid generating the coaxial B field rotates with the same angular velocity as the cylindrical condensor.* It is the latter fact which, in our opinion, makes it desirable to consider these effects as observations of a constitutive nature concerning a frame of reference rotating in free space.

To dispel any uncertainty concerning the reality of the mentioned observations, the present authors constructed a piece of equipment similar to that of Kennard and Pegram. Our as yet preliminary observations show a qualitative agreement with those of Kennard and Pegram. The conditions of our observations were between those of Kennard and Pegram in the sense that our observations were made with an electrometer that had an impedance range intermediate between open circuit (Kennard) and complete short (Pegram).

To the extent that experimental results are available, it seems that the observations can be consistently described by a constitutive relation of the following form (MKS units)

$$\bar{D} = \epsilon_0\bar{E} + \epsilon_0(\bar{\Omega} \times \bar{r}) \times \bar{B} \tag{1}$$

in which $\bar{D}$, $\bar{E}$, $\bar{B}$, and $\bar{r}$, defined on the rotating frame, have the usual meaning, ϵ_0 is the free-space permittivity, and $\bar{\Omega}$ is the angular velocity of the system with respect to inertial space.

For cylindrical symmetry, when using cylinder

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in which $\bar{D}$, $\bar{E}$, $\bar{B}$, and $\bar{r}$, defined on the rotating frame, have the usual meaning, ϵ_0 is the free-space permittivity, and $\bar{\Omega}$ is the angular velocity of the system with respect to inertial space.

For cylindrical symmetry, when using cylinder coordinates, one may write Eq. (1) in the form

$$D_r = \epsilon_0 E_r + \epsilon_0 \Omega r B_z. \tag{2}$$

It is a well-known riddle of EM theory that the second term of (1) [or (2) for that matter] has all by itself a nonvanishing divergence div $(\bar{\Omega} \times \bar{r}) \times \bar{B} = 2\bar{\Omega} \cdot \bar{B} \neq 0$ (see, for instance, Sommerfeld,[4] last page). It would then appear as if an observation made from a rotating frame would record a space charge where none was to begin with. We will make the elimination of this absurdity a cornerstone of the next following considerations, the basic idea being that divergences of individual electric field components $\bar{E}$ contributing to a total electric displacement $\bar{D}$ are not physically meaningful.

Let us instead take the divergence of the "surface" vector $\bar{D}$ and let us insist that its divergence vanish also on the rotating system. We obtain then for conditions of cylindrical symmetry

$$\frac{1}{r}\frac{\partial}{\partial r} r D_r = 0. \tag{3}$$

Solving this equation, we have

$$D_r = A/r \tag{4}$$

with A as a constant of integration.

The ideal Kennard case (open circuit—no displacement) is now characterized by $A = 0$. The Kennard potential can then be obtained from (2) as

$$V_k = \int_{r_1}^{r_2} E_r \, dr = -\tfrac{1}{2}\Omega B_z (r_2^2 - r_1^2), \tag{5}$$

r_1 and r_2 being the radii of the inner and outer cylinder of the tubular condensor.

In the ideal Pegram case, $A \neq 0$. Its value can be calculated from the condition that the potential

$$\int_{r_1}^{r_2} E_r \, dr = 0.$$

One then finds for the integration constant

$$A = \frac{1}{2} \frac{\epsilon_0 \Omega B_z (r_2^2 - r_1^2)}{\ln (r_2/r_1)}. \tag{6}$$

The Pegram charge Q_p on the condensor is obtained by integrating D_r over the surface of the cylinder of length l, say:

$$Q_p = 2\pi A l\,. \tag{7}$$

Substitution of (6) gives

$$Q_p = \frac{\epsilon_0 \pi \Omega l B_z (r_2^2 - r_1^2)}{\ln (r_2/r_1)}. \tag{8}$$

One easily verifies that the ratio of the Pegram charge (8) and the Kennard potential (5) yields (in absolute value) the standard expression for the capacitance of a cylindrical capacitor

$$C = \left| \frac{Q_p}{V_k} \right| = \frac{2\pi\epsilon_0 l}{\ln (r_2/r_1)}. \tag{9}$$

In the light of the mentioned experimental observations and the simple interpretation of these observations in terms of a constitutive relation of the form (1), we summarize the following points as absolutely germane to any theoretical discussion involving accelerated systems in electrodynamics:

(1) The Pegram and Kennard effects are realistic observations that cannot be discounted or disregarded.

(2) A very simple constitutive relation of the form $\bar{D} = \bar{D}(\bar{E}, \bar{B})$ [see Eq. (1)] directly accounts for these observations, rather than the customary relations $\bar{D} = \epsilon_0 \bar{E}$ or $\bar{D} = \bar{E}$, which only hold for inertial systems in matter-free space.

(3) A constitutive relation of the form (1) for a rotating system resolves the difficulty recorded by Sommerfeld that a rotation could give rise to an apparent space-charge div $(\bar{\Omega} \times \bar{r}) \times \bar{B} = 2\bar{\Omega} \cdot \bar{B} \neq 0$.

In the recent paper by Mo[1] we find that the existence of a free-space constitutive dependence of $\bar{D}$ on $\bar{B}$ is considered as a mistaken notion (last paragraph, Sec. 4). We feel that this statement is at variance with the experimental evidence presented by Kennard and Pegram as well as with our own observations. In fact a discussion of the constitutive nature of this evidence appears on p. 490 of Ref. 5 cited by Mo.[1]

The fundamental issues touched upon here go well beyond Mo's paper. The question is not whether the method of "local" inertial tetrads, as used by Mo, can be made equivalent to a method of "global" noninertial references, as used in his Ref. 5. One would expect such an equivalence to exist, at least locally. Remarks to the contrary by Mo are out of context.

The fundamental issue is rather whether or not the method of local tetrads is a suitable mathematical expedient that enhances physical perspicuity such as claimed by its proponents. The presented evidence hardly supports such claims.

* Work supported by NASA Grant NGR 30-002-061.

[1] T. C. Mo, J. Math. Phys. **11**, 2589 (1970).
[2] E. H. Kennard, Phil. Mag. **33**, 179 (1917).
[3] G. B. Pegram, Phys. Rev. **10**, 591 (1917).
[4] A. Sommerfeld, *Lectures on Theoretical Physics, Vol. 3: Electrodynamics*, transl. by E. G. Ramburg (Academic, New York, 1952).

A Nonhomogeneous Boundary-Value Problem for the Linear Transport Equation for a Slab Geometry

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(Received 30 July 1970)

A nonhomogeneous boundary-value problem for the infinite slab of finite thickness is considered. In this problem, the slab receives radiation from a time-dependent source on one of its surfaces. The intensity of this radiation increases from zero at time zero until a later time t_0', after which the intensity is a function of direction only. This problem is solved in the strong sense. The asymptotic behavior of the solution is determined and related to results for steady-state problems in neutron transport theory and radiative transfer.

1. INTRODUCTION

Some time-dependent monoenergetic neutron transport problems have been solved for the plane-parallel slab geometry with isotropic scattering. Lehner and Wing[1,2] used a generalized Laplace transform technique to solve a nonhomogeneous initial-value problem. Bowden and Williams[3] used the normal-mode expansion method of Case to treat this initial-value problem. Recently, Newman and Bowden[4] extended these results to the case of a slab surrounded by infinitely thick reflectors. A nonhomogeneous boundary-value problem was treated by Kuščer and Zweifel.[5] These authors treated the one-speed equation for isotropic scattering in the semi-infinite slab subjected to irradiation of the surface with a monodirectional pulse of neutrons at time $t = 0$.

In this paper,[6] another nonhomogeneous boundary-value problem for the slab is considered. In this problem, the slab receives radiation from a time-dependent source on one of its surfaces. The intensity of this radiation increases from zero at time zero until a later time t_0', after which the intensity is a function of direction only. This problem is solved in the strong sense. The asymptotic behavior of the solution is determined and is related to results for steady-state problems in neutron transport theory and radiative transfer.

2. PRELIMINARY REMARKS

Consider the plane-parallel slab geometry of finite thickness with no independent sources of neutrons. Assume that the neutrons are monoenergetic and produced isotropically inside the slab, which is surrounded by a perfect absorber. Also, assume that the total cross section σ and the expected number c of neutrons which emerge from each collision of a neutron with a nucleus are constant. Let x', $-a' \le x' \le a'$, denote the position coordinate measured from the center of the slab normal to the plane stratification. Let $\mu = \cos\theta$, where θ, $0 \le \theta \le \pi$, is the angle between the direction of neutron motion and the positive x' axis.

The expected distribution $\tilde{N}(x', \mu, t')$ of neutrons at the position x', moving in the direction $\arccos\mu$, at time t', satisfies the linear Boltzmann equation[7] subject to certain boundary conditions. Lehner and Wing[1,2] wrote the system for the initial-value problem in the form

$$u_t = Au, \tag{1}$$

where

$$\begin{gathered} Au \equiv -\mu\frac{\partial u}{\partial x} + \frac{c}{2}\int_{-1}^{1} u(x, \mu', t)\, d\mu', \\ u(\pm a, \mu, t) = 0, \quad \mu \lessgtr 0, \quad t > 0, \\ u(x, \mu, 0) = f_0(x, \mu), \quad |x| \le a, \quad |\mu| \le 1, \\ x = \sigma x' \ (a = \sigma a'), \quad t = \sigma v t', \\ u(x, \mu, t) = e^{\sigma v t'}\tilde{N}(x', \mu, t'). \end{gathered} \tag{2}$$

This formulation leads to a spectral analysis[1] of A on $H = L_2([-a, a] \times [-1, 1])$. The domain $D(A)$ of A is the set of all $f \in H$ such that f is absolutely continuous in x for each μ, $Af \in H$, and $f(\pm a, \mu) = 0$ for $\mu \lessgtr 0$. The spectrum of A is shown to consist of a positive, finite number $m = m(a, c)$ of positive (real) eigenvalues β_i, $i = 1, \cdots, m$, $\beta_i > \beta_j$ for $i < j$, and a left half-plane $\operatorname{Re}\lambda \le 0$ of continuous spectrum. Since each eigenvalue β_i is of multiplicity one [Ref. 1, p. 228, Theorem (5), and Ref. 8, pp. 471–2, Theorem (3)], the normalized eigenfunction corresponding to β_i can be denoted as Ψ_i, $i = 1, \cdots, m$. The β_i are also eigenvalues for the adjoint A^* of A with corresponding eigenfunctions Ψ_i^*, $i = 1, \cdots, m$.

In Ref. 2 the authors showed that A is the infinitesimal generator of a C_0 semigroup $T(t)$, $t \ge 0$, of bounded linear operators on H and that the function

$$u(x, \mu, t) \equiv T(t)f_0(x, \mu)$$

solves the initial-value problem for (1) in the strong sense if $f_0 \in D(A)$. They obtained the expansion

$$u(x, \mu, t) = \sum_{i=1}^{m} (f_0, \Psi_i^*)\Psi_i(x, \mu)e^{\beta_i t} + \zeta(x, \mu, t; f_0), \quad (3)$$

where

$$\zeta(x, \mu, t; f_0) = \underset{\omega \to \infty}{\text{l.i.m.}} \frac{1}{2\pi i} \int_{\delta - i\omega}^{\delta + i\omega} e^{\lambda t}(\lambda - A)^{-1} f_0 \, d\lambda, \quad 0 < \delta < \beta_m. \quad (4)$$

This integral, the strong limit of Riemann sums, can be interpreted as an ordinary Riemann integral if x and μ are fixed.

For convenience, let $H = L_2([-a, a] \times [-1, 1])$ and $H_1 = L_2[-a, a]$. We use the usual notations for an inner product and a norm for these functions on H; for H_1 we add a subscript 1.

3. THE MATHEMATICAL FORMULATION OF THE PROBLEM

We consider the slab subjected to radiation due to a source on the surface at $x' = -a'$. The source of radiation is turned on at time $t' = 0$ and the intensity of the radiation increases in time until $t' = t_0'$. At $t' = t_0'$, the intensity levels off to become a function $\alpha(\mu)$ of direction only. We consider $\alpha \in L_2[-1, 1]$. The increase in intensity from $t' = 0$ to $t' = t_0'$ is indicated by a function $\tilde{E}(t')$ of time which we assume to have the following properties:

(i) $\tilde{E} \in C^2[0, \infty)$,

(ii) $\tilde{E}(0) = d\tilde{E}/dt'(0) = 0$,

(iii) $\tilde{E}(t') \equiv 1$ for all $t' \geq t_0'$.

From (iii), $d\tilde{E}/dt'(t') = 0$ for all $t' \geq t_0'$.

Under these conditions and the above physical assumptions, the expected neutron distribution $\tilde{N}(x', \mu, t')$ in the slab satisfies the linear Boltzmann equation[7] in the form

$$\frac{1}{v}\frac{\partial \tilde{N}}{\partial t'} + \mu \frac{\partial \tilde{N}}{\partial x'} + \sigma \tilde{N} = \frac{c\sigma}{2} \int_{-1}^{1} \tilde{N}(x', \mu', t') \, d\mu' \quad (5)$$

subject to the following conditions:

$$\begin{aligned} &\tilde{N}(x', \mu, 0) = 0, \quad -a' \leq x' \leq a', -1 \leq \mu \leq 1, \\ &\tilde{N}(-a', \mu, t') = \alpha(\mu)\tilde{E}(t'), \quad 0 < \mu \leq 1, 0 \leq t' < \infty, \\ &\qquad \alpha \in L_2[-1, 1], \\ &\tilde{N}(a', \mu, t') = 0, \quad -1 \leq \mu < 0, 0 \leq t' < \infty. \end{aligned} \quad (6)$$

We now obtain an equivalent nonhomogeneous equation with homogeneous initial and boundary values. Define the function $\tilde{f}$ such that

$$\tilde{f}(x', \mu) = \begin{cases} \exp\left[-\dfrac{\sigma(x' + a')}{\mu}\right], & 0 < \mu \leq 1, \\ & -a' \leq x' \leq a', \\ 0, & -1 \leq \mu \leq 0, \\ & -a' \leq x' \leq a', \end{cases}$$

and the function ϕ such that

$$\phi(x', \mu, t') = \tilde{N}(x', \mu, t') - \tilde{E}(t')\tilde{f}(x', \mu)\alpha(\mu).$$

Since $\mu\partial\tilde{f}/\partial x' + \sigma\tilde{f} = 0$, ϕ satisfies the system

$$\begin{aligned} &\frac{1}{\sigma v}\frac{\partial \phi}{\partial t'} + \frac{\mu}{\sigma}\frac{\partial \phi}{\partial x'} + \phi \\ &= \frac{c}{2}\int_{-1}^{1} \phi(x', \mu', t') \, d\mu' + \frac{c}{2}\tilde{E}(t') \\ &\times \int_{-1}^{1} \tilde{f}(x', \mu')\alpha(\mu') \, d\mu' - \frac{\tilde{f}(x', \mu)\alpha(\mu)}{\sigma v}\frac{\partial \tilde{E}}{\partial t'}(t'), \end{aligned} \quad (7)$$

$$\begin{aligned} &\phi(x', \mu, 0) = 0, \quad -a' \leq x' \leq a', -1 \leq \mu \leq 1, \\ &\phi(-a', \mu, t') = 0, \quad 0 < \mu \leq 1, 0 \leq t' < \infty, \\ &\phi(a', \mu, t') = 0, \quad -1 \leq \mu < 0, 0 \leq t' < \infty. \end{aligned} \quad (8)$$

We make the change of space and time variables given in (2) and let

$$u(x, \mu, t) = e^{\sigma v t'}\phi(x', \mu, t').$$

Also, let $f(x, \mu) = \tilde{f}(x', \mu)$, $N(x, \mu, t) = \tilde{N}(x', \mu, t')$, $E(t; \sigma, v) = \tilde{E}(t')$, and $t_0 = v\sigma t_0'$. For convenience, we introduce the functions

$$H_0(x, \mu) = -\alpha(\mu)f(x, \mu)$$

and

$$G_0(x, \mu) = -\frac{c}{2}\int_0^1 H_0(x, s) \, ds$$

for $|x| \leq a$, $|\mu| \leq 1$. Observe that $G_0, H_0 \in H$ from the Cauchy–Schwarz inequality, but neither of these functions is in $D(A)$ because they do not satisfy the boundary conditions required of functions in $D(A)$. Substituting these notations into (7), we obtain the equation

$$u_t = Au + e^t E(t; \sigma, v)G_0 + e^t \frac{dE}{dt}(t; \sigma, v)H_0, \quad (9)$$

where u satisfies the same initial and boundary conditions as ϕ. Observe that the nonhomogeneous part of (9) is the sum of two functions. Each of these functions is the product of three factors: (i) an exponential in t, (ii) a bounded $C^1[0, \infty)$ function of t that is initially zero, and (iii) an H function of x and μ that is not in $D(A)$. In the following, we usually do not indicate the dependence of E on the parameters σ and v.

4. THE SOLUTION OF THE BOUNDARY-VALUE PROBLEM

To solve (9), we first consider the following problem.

Auxiliary problem: Let $K(t)$ be a bounded $C^0(0, \infty)$ function of t that is initially zero. Let $g \in D(A)$. Solve the equation

$$u_t = Au + e^t K(t) g(x, \mu)$$

subject to the condition $u|_{t=0} = 0$.

To solve this problem, we first consider the corresponding homogeneous equation

$$\frac{\partial \psi}{\partial t} = A\psi \tag{10}$$

subject to the condition

$$\psi|_{t=\tau} = e^\tau K(\tau) g, \tag{11}$$

for τ fixed, $0 \le \tau < \infty$. We know (Ref. 2, pp. 128, 129) there exists a semigroup $T(t)$ of bounded linear operators for $t \ge 0$ such that: (i) $T(0) = I$, (ii) $T(t)$ is strongly continuous for $t \ge 0$, and (iii) $T(t)$ is strongly differentiable on $D(A)$ with

$$\frac{dT}{dt}(t) g = AT(t) g = T(t) Ag, \quad g \in D(A). \tag{12}$$

For fixed $\tau \ge 0$, we set

$$\psi_\tau(x, \mu, t) = e^\tau K(\tau) T(t - \tau) g(x, \mu).$$

From (12) we see that $\psi_\tau \in D(A)$ and satisfies (10) in the strong sense. But ψ_τ also satisfies the condition (11) in the strong sense because

$$\|e^\tau K(\tau) T(t - \tau) g(x, \mu) - e^\tau K(\tau) g(x, \mu)\| = e^\tau |K(\tau)| \times \|T(t - \tau) g - g\| \to 0 \quad \text{as} \quad t \to \tau$$

from the strong continuity of the semigroup.

The solution ψ_τ of (10) suggests the following definition:

$$u(t; g, K) = \int_0^t e^\tau K(\tau) T(t - \tau) g \, d\tau, \tag{13}$$

where this integral is to be interpreted as the strong limit of Riemann sums. For u, we can prove the following lemma.

Lemma 1: The function u, defined in (13), is the unique solution in the strong sense of the auxiliary problem.

Proof: To demonstrate the uniqueness, we suppose u_1 and u_2 are solutions. Then

$$\frac{\partial}{\partial t}(u_1 - u_2) = A(u_1 - u_2)$$

and $(u_1 - u_2)|_{t=0} = 0$. Therefore, $u_1 - u_2 \equiv 0$ (Ref. 2, p. 129, Theorem 1).

To show that u satisfies the partial differential equation of the auxiliary problem, we consider the difference quotient for u:

$$\begin{aligned}
&\frac{u(t + \Delta t; g, K) - u(t; g, K)}{\Delta t} \\
&\quad = \int_0^t e^\tau K(\tau) \left[\frac{T(t + \Delta t - \tau) g - T(t - \tau) g}{\Delta t}\right] d\tau \\
&\qquad + \frac{1}{\Delta t} \int_t^{t+\Delta t} e^\tau K(\tau) T(t + \Delta t - \tau) g \, d\tau \\
&\quad \to \int_0^t e^\tau K(\tau) \left.\frac{dT}{dt}\right|_{t-\tau} g \, d\tau + e^t K(t) T(0) g
\end{aligned}$$

from Lebesgue's dominated convergence theorem for Bochner integrals [Ref. 8, p. 48, Theorem 3.6.6] in view of the bound given below. From (12), this is equal to

$$\int_0^t e^\tau K(\tau) A T|_{t-\tau} \, g \, d\tau + e^t K(t) g$$

since $g \in D(A)$; this is also equal to $Au + e^t K(t) g$ (Ref. 9, p. 83, Theorem 3.7.12). Therefore, $u \in D(A)$ and

$$\frac{du}{dt}(t; g, K) = Au(t; g, K) + e^t K(t) g.$$

To apply Lebesgue's theorem above, we use the bound given by the following inequalities:

$$\begin{aligned}
&\left\| \frac{e^\tau K(\tau)}{\Delta t} (T(t + \Delta t - \tau) g - T(t - \tau) g) \right\| \\
&\quad = \left\| e^\tau K(\tau) T(t - \tau) \frac{(T(\Delta t) - I) g}{\Delta t} \right\| \\
&\quad \le e^\tau |K(\tau)| \, e^{c(t-\tau)} \left\| \frac{(T(\Delta t) - I) g}{\Delta t} \right\|
\end{aligned}$$

(from Ref. 10, p. 203, Corollary 2.2, and Ref. 2, pp. 128–129)

$$\begin{aligned}
&\le e^\tau |K(\tau)| \, e^{c(t-\tau)} \left\{ \left\| \frac{(T(\Delta t) - I) g}{\Delta t} - Ag \right\| + \|Ag\| \right\} \\
&\le e^{ct} |K(\tau)| \, e^{(1-c)\tau} \{1 + \|Ag\|\} \quad \text{for} \quad \Delta t < \delta(1).
\end{aligned}$$

Hence, for $\Delta t < \delta(1)$, $\|[e^\tau K(\tau)/\Delta t][T(t + \Delta t - \tau) g - T(t - \tau) g]\|$ is bounded by an integrable function of τ.

The function $u(t; g, K)$ satisfies the initial condition in the strong sense since (Ref. 10, p. 203, Corollary

2.2, and Ref. 2, pp. 128–29)

$$\|u(t; g, K)\| \le \int_0^t e^\tau |K(\tau)| e^{c(t-\tau)} d\tau \|g\|$$
$$\le e^{ct} \max_{0\le\tau\le t_0} [|K(\tau)|] \int_0^t e^{(1-c)\tau} d\tau \|g\|$$

$\to 0$ as $t \to 0$. Therefore, $u(t; g, K)$, as defined in (13), is the solution in the strong sense of the auxiliary problem for $g \in D(A)$. QED

We wish to solve (9), where $G_0, H_0 \in H - D(A)$. The bounded linear operator defined in (13) can be extended to all of H since $D(A)$ is dense in H (Ref. 2, p. 128). Thus, it makes sense to talk about $u(t; G_0, E)$ and $u(t; H_0, dE/dt)$, but it remains to show that $u(t; G_0, E) + u(t; H_0, dE/dt)$ is the solution of (9). From the linearity of (9) and the fact that $G_0, H_0 \in H$, this result follows from the following theorem.

Theorem 1: Let $K(t)$ be a bounded $C^1[0, \infty)$ function of t such that $K(0) = 0$. Let $G \in H$. Then the function $u(t; G, K)$ satisfies uniquely in the strong sense the equation

$$\frac{du}{dt}(t; G, K) = Au(t; G, K) + e^t K(t) G,$$

subject to the initial condition $u|_{t=0} = 0$.

To prove this theorem, we need the following lemma.

Lemma 2: Let $G \in H$. Then $du/dt\,(t; G, K)$ exists and

$$\frac{du}{dt}(t; G, K) = u(t; G, K) + u\left(t; G, \frac{dK}{dt}\right).$$

Proof: Since

$$u(t; G, K) = e^t \int_0^t e^{-s} K(t-s) T(s) G\, ds,$$

the difference quotient

$$\frac{u(t+\Delta t; G, K) - u(t; G, K)}{\Delta t}$$
$$= \left(\frac{e^{\Delta t}-1}{\Delta t}\right) e^t \int_0^t e^{-s} K(t+\Delta t - s) T(s) G\, ds$$
$$+ e^t \int_0^t e^{-s} \left(\frac{K(t+\Delta t - s) - K(t-s)}{\Delta t}\right) T(s) G\, ds$$
$$+ \frac{e^{t+\Delta t}}{\Delta t} \int_t^{t+\Delta t} e^{-s} K(t+\Delta t - s) T(s) G\, ds$$
$$\to e^t \int_0^t e^{-s} K(t-s) T(s) G\, ds$$
$$+ e^t \int_0^t e^{-s} \left.\frac{dK}{dt}\right|_{t-s} T(s) G\, ds$$

from Lebesgue's dominated convergence theorem for Bochner integrals (Ref. 8, p. 48, Theorem 3.6.6). But this sum is $u(t; G, K) + u(t; G, dK/dt)$ as desired. QED

We can now prove Theorem 1.

Proof: The uniqueness and the fact that u satisfies the initial condition in the strong sense follow from the corresponding proofs given for $u(t; g, K)$, $g \in D(A)$, in Lemma 1.

To show $u(t; G, K)$ is a solution of the equation, let $G \in H$ and $\{g_n\}$ be a sequence in $D(A)$ such that $g_n \to G$ in H. For each n,

$$u(t; g_n, K) + u\left(t; g_n, \frac{dK}{dt}\right)$$
$$= \frac{du}{dt}(t; g_n, K) = Au(t; g_n, K) + e^t K(t) g$$

from Lemmas 1 and 2. Therefore,

$$Au(t; g_n, K)$$
$$= u(t; g_n, K) + u\left(t; g_n, \frac{dK}{dt}\right) - e^t K(t) g_n$$
$$\to u(t; G, K) + u\left(t; G, \frac{dK}{dt}\right) - e^t K(t) G$$
$$= \frac{du}{dt}(t; G, K) - e^t K(t) G$$

as $n \to \infty$, from Lemma 2. But, since A is a closed operator (Ref. 2, p. 128), this implies that

$$u(t; G, K) \in D(A)$$

and

$$\frac{du}{dt}(t; G, K) = Au(t; G, K) + e^t K(t) G. \quad \text{QED}$$

For convenience, we introduce the notation

$$J(t; G, K) = \int_0^{t_0} K(\tau) e^\tau T(t-\tau) G(x, \mu)\, d\tau, \quad G \in H,$$

where $K(\tau)$ is a bounded $C^0[0, \infty)$ function of τ such that $K(0) = 0$.

We gather our results in the following theorem.

Theorem 2: There exists a solution N in the strong sense for the system in (5), (6). This solution can be written as

$$N(x, \mu, t) = f(x, \mu)\alpha(\mu) E(t; \sigma, v)$$
$$+ e^{-t} u(t; G_0, E)(x, \mu)$$
$$+ e^{-t} u\left(t; H_0, \frac{dE}{dt}\right)(x, \mu).$$

In particular, for $t > t_0$,

$$N(x, \mu, t) = f(x, \mu)\alpha(\mu) + e^{-t}J(t; G_0, E) + e^{-t}J\left(t; H_0, \frac{dE}{d\tau}\right) + \int_{t_0}^{t} \exp(\tau - t)T(t - \tau)G_0(x, \mu)\, d\tau.$$

5. OTHER REPRESENTATIONS FOR THE SOLUTION N

Since the expression in Theorem 2 does not reveal the asymptotic behavior for N for large t, we now find other representations for N. In the above sections, the only restriction placed on $\alpha(\mu)$ is $\alpha \in L_2[-1, 1]$. In this section and the sections that follow, we require that

$$\alpha \in C^0[-1, 1].$$

Let δ be fixed such that $0 < \delta < \min[\frac{1}{2}, \beta_m]$, where β_m is the smallest eigenvalue for A. To simplify the notation, we define $\zeta(x, \mu, t; G)$ as in (4) for $G \in D(A) \cup \{G_0, H_0\}$. That ζ makes sense follows from the following bound given on the vertical line $\operatorname{Re}\lambda = \delta$

$$|(\lambda - A)^{-1}G(x, \mu)| \le M(\delta, G)/|\lambda|, \qquad (14)$$

$G \in D(A) \cup \{G_0, H_0\}$. $M(\delta, G)$ is a finite constant that depends only on δ and G. Lehner and Wing [Ref. 2, p. 135, (3.6)] give this bound for functions in $D(A)$ and for all $\lambda \in \rho(A)$ with $M = M(\beta, G)$, $\beta = \operatorname{Re}(\lambda)$. In Sec. 8, we give a proof of (14) for G_0 and H_0.

From Theorem 2, a new representation for u provides a new representation for N. A representation for u is obtained from semigroup theory in the following lemma.

Lemma 3: Let $G \in H$. For all $t > t_0$,

$$u(t; G, E) = J(t; G, E) + e^{t_0} \underset{\omega\to\infty}{\text{l.i.m.}} \frac{1}{2\pi i}\int_{\gamma+1-i\omega}^{\gamma+1+i\omega} \frac{\exp[\lambda(t - t_0)]}{\lambda - 1}(\lambda - A)^{-1}G\, d\lambda,$$

where $\gamma > \max[0, \beta_1 - 1]$.

Proof: Let $G \in H$. By definition,

$$u(t; G, E) - J(t; G, E) = e^t \int_0^{t-t_0} e^{-s}T(s)G\, ds.$$

But $Z(s) = e^{-s}T(s)$ is a semigroup of operators whose infinitesimal generator is $A - I$. Therefore, the equation [Ref. 8, p. 232, (11.7.1)] guarantees

$$u(t; G, E) - J(t; G, E) = e^t \underset{\omega\to\infty}{\text{l.i.m.}} \frac{1}{2\pi i}\int_{\gamma-i\omega}^{\gamma+i\omega} \exp[\lambda(t - t_0)][\lambda - (A - I)]^{-1}G\frac{d\lambda}{\lambda}$$
$$= e^{t_0} \underset{\omega\to\infty}{\text{l.i.m.}} \frac{1}{2\pi i}\int_{(\gamma+1)-i\omega}^{(\gamma+1)+i\omega} \frac{\exp[\lambda(t - t_0)]}{\lambda - 1}(\lambda - A)^{-1}G\, d\lambda$$

if $\gamma > \max[0, \beta_1 - 1]$. QED

Now suppose $\beta_i \ne 1$, $i = 1, \cdots, m$. As in Ref. 2, p. 129, Theorem 1, we shift the line of integration of the representation in Lemma 3 to the left. This process, which picks up the contributions of the residues, can be accomplished by means of a rectangular contour C about the poles of the integrand. We know that the singularities of the resolvent are simple poles (Ref. 2, p. 131, Lemma 2). The factor $(\lambda - 1)^{-1}$ introduces another simple pole at $\lambda = 1$.

Since $\lambda - 1$ appears in the denominator of the integral in Lemma 3, the inequality [Ref. 2, p. 135, (3.5)] ensures that the integrals on the horizontal paths approach zero in H as $|\operatorname{Im}\lambda| \to \infty$. Thus, we obtain the following lemma.

Lemma 4: Let $G \in H$. If $\beta_i \ne 1$ for $i = 1, 2, \cdots, m$, then

$$u(t; G, E) = J(t; G, E) + e^t(I - A)^{-1}G + \sum_{i=1}^{m} \frac{e^{(1-\beta_i)t_0}e^{\beta_i t}}{\beta_i - 1}(G, \psi_i^*)\psi_i + e^{t_0} \underset{\omega\to\infty}{\text{l.i.m.}} \frac{1}{2\pi i}\int_{\delta-i\omega}^{\delta+i\omega} \frac{e^{\lambda(t-t_0)}}{\lambda - 1}(\lambda - A)^{-1}G\, d\lambda$$

for all $t > t_0$.

This lemma enables us to write N as in the following theorem.

Theorem 3: If $\beta_i \ne 1$ for $i = 1, \cdots, m$, then

$$\begin{aligned} N(x, \mu, t) &= f(x, \mu)\alpha(\mu) + (I - A)^{-1}G_0 \\ &+ \sum_{i=1}^{m} (G_0, \psi_i^*)\psi_i(x, \mu)\left[\int_0^{t_0} E(\tau)\exp[(1 - \beta_i)\tau]\, d\tau + \frac{\exp[(1 - \beta_i)t_0]}{\beta_i - 1}\right]\exp[(\beta_i - 1)t] \\ &+ \sum_{i=1}^{m} (H_0, \psi_i^*)\psi_i(x, \mu)\int_0^{t_0} \frac{dE}{d\tau}(\tau) \times \exp[(1 - \beta_i)\tau]\, d\tau \exp[(\beta_i - 1)t] \\ &+ e^{-t}\int_0^{t_0} E(\tau)e^{\tau}\zeta(x, \mu, t - \tau; G_0)\, d\tau \\ &+ e^{-t}\int_0^{t_0} \frac{dE}{dt}(\tau)e^{\tau}\zeta(x, \mu, t - \tau; H_0)\, d\tau \\ &+ \frac{\exp(t_0 - t)}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} \frac{\exp[(\lambda)(t - t_0)]}{\lambda - 1}(\lambda - A)^{-1}G_0\, d\lambda \end{aligned}$$

for all $t > t_0$.

Proof: Equation (3) enables us to write $J(t; g, K)$, for $g \in D(A)$, as follows:

$$
\begin{aligned}
J(t; g, K) &= \int_0^{t_0} K(\tau)e^\tau\left(\sum_{i=1}^m (g, \psi_i^*)\psi_i(x, \mu)e^{\beta_i(t-\tau)} + \zeta(x, \mu, t-\tau; g)\right) d\tau \\
&= \sum_{i=1}^m (g, \psi_i^*)\psi_i(x, \mu)e^{\beta_i t}\int_0^{t_0} K(\tau)\exp\left[(1-\beta_i)\tau\right] d\tau \\
&\quad + \int_0^{t_0} K(\tau)e^\tau \zeta(x, \mu, t-\tau; g)\, d\tau. \qquad (15)
\end{aligned}
$$

For the terms in the series in (15), we have fixed x and μ and have interpreted the integral as an ordinary Riemann integral. That this is valid follows from the dominated convergence theorem for Lebesgue integrals since $e^\tau K(\tau)$ is a continuous function of τ. We can extend the bounded linear operators in (15) to all of the Hilbert space H since $D(A)$ is dense in H. The representation remains the same for G_0 and H_0 in view of the bound in (14). Substituting this representation into the expression in Lemma 4, we obtain the series terms above.

Now let t be fixed. Then

$$
\left|\frac{\exp\left[\lambda(t-t_0)\right]}{\lambda-1}(\lambda - A)^{-1}G_0\right| \le \frac{M(\delta, G_0)}{|\lambda|\,|\lambda-1|}\exp\left[\delta(t-t_0)\right]
$$

on the vertical line $\operatorname{Re}\lambda = \delta$, from (14). Therefore, for each t, the

$$
\underset{\omega\to\infty}{\text{l.i.m.}}\int_{\delta-i\omega}^{\delta+i\omega}\frac{\exp\left[\lambda(t-t_0)\right]}{\lambda-1}(\lambda-A)^{-1}G_0\, d\lambda = \int_{\delta-i\infty}^{\delta+i\infty}\frac{\exp\left[\lambda(t-t_0)\right]}{\lambda-1}(\lambda-A)^{-1}G_0\, d\lambda.
$$

The representation for N now follows from Theorem 2 and Lemma 4. QED

If $\beta_i = 1$ for some $i = i_0$, the pole at $\lambda = 1$ produced by the factor $(\lambda - 1)^{-1}$ and the pole produced by the i_0th eigenvalue coalesce. To avoid the difficulty involved in computing the residue for this case, we obtain a different representation for $u(t; G_0, E)$ and $u(t; H_0, dE/dt)$. (Some further remarks are made in Sec. 7 below.) This representation can be obtained by using Eq. (3) and extending the operators to all of H as for J in the proof of Theorem 3. Thus, if $\beta_i = 1$ for some $i = i_0$, then for all $t \ge t_0$

$$
\begin{aligned}
u(t; G_0, E) &= (G_0, \psi_{i_0}^*)\psi_{i_0}(x, \mu)e^t\left(\int_0^{t_0} E(\tau)\, d\tau + E(t_0)(t-t_0)\right) \\
&\quad + \sum_{\substack{i=1\\ i\ne i_0}}^m (G_0, \psi_i^*)\psi_i(x, \mu) \\
&\quad \times \exp(\beta_i t)\left(\int_0^{t_0} E(\tau)\exp\left[(1-\beta_i)\tau\right] d\tau + E(t_0)\frac{(\exp\left[(1-\beta_i)t\right] - \exp\left[(1-\beta_i)t_0\right])}{1-\beta_i}\right) \\
&\quad + \int_0^t e^\tau E(\tau)\zeta(x, \mu, t-\tau; G_0)\, d\tau. \qquad (16)
\end{aligned}
$$

For $t < t_0$, the terms involving $E(t_0)$ must be omitted and the integrations that extend from 0 to t_0 should extend only as far as t. The same argument obtains a similar expression for $u(t; H_0, dE/dt)$. Therefore, we can write N as in the following theorem.

Theorem 4: If $\beta_i = 1$ for some $i = i_0$, then for all $t \ge t_0$

$$
\begin{aligned}
N(x, \mu, t) &= f(x, \mu)\alpha(\mu) \\
&\quad + (G_0, \psi_{i_0}^*)\psi_{i_0}(x, \mu)\left(\int_0^{t_0} E(\tau)\, d\tau + (t-t_0)\right) \\
&\quad + (H_0, \psi_{i_0}^*)\psi_{i_0}(x, \mu)\int_0^{t_0}\frac{dE}{d\tau}(\tau)\, d\tau \\
&\quad + \sum_{\substack{i=1\\ i\ne i_0}}^m (G_0, \psi_i^*)\psi_i(x, \mu) \\
&\quad \times \left(\exp\left[(\beta_i - 1)t\right]\int_0^{t_0} E(\tau)\exp\left[(1-\beta_i)\tau\right] d\tau + \frac{1-\exp\left[(1-\beta_i)t_0\right]\exp\left[(\beta_i-1)t\right]}{1-\beta_i}\right) \\
&\quad + \sum_{\substack{i=1\\ i\ne i_0}}^m (H_0, \psi_i^*)\psi_i(x, \mu)\exp\left[(\beta_i - 1)t\right] \\
&\quad \times \int_0^{t_0}\frac{dE}{d\tau}(\tau)\exp\left[(1-\beta_i)\tau\right] d\tau \\
&\quad + e^{-t}\int_0^t e^\tau E(\tau)\zeta(x, \mu, t-\tau; G_0)\, d\tau \\
&\quad + e^{-t}\int_0^{t_0} e^\tau\frac{dE}{d\tau}(\tau)\zeta(x, \mu, t-\tau; H_0)\, d\tau.
\end{aligned}
$$

To study the asymptotic behavior of the solution N as given in Theorems 3 and 4, we require the following lemma.

Lemma 5: The residual terms for N satisfy

(a) $\int_0^t E(\tau)\exp(\tau - t)\zeta(x, \mu, t-\tau; G_0)\,d\tau = O(1)$,

(b) $\int_0^{t_0} E(\tau)\exp(\tau - t)\zeta(x, \mu, t-\tau; G_0)\,d\tau = O\{\exp[(\delta - 1)t]\}$,

(c) $\int_0^{t_0} \frac{dE}{d\tau}(\tau)\exp(\tau - t)\zeta(x, \mu, t-\tau; H_0)\,d\tau = O\{\exp[(\delta - 1)t]\}$,

(d) $\frac{\exp(t_0 - t)}{2\pi i}\int_{\delta - i\infty}^{\delta + i\infty}\frac{\exp[\lambda(t - t_0)]}{\lambda - 1}(\lambda - A)^{-1}G_0\,d\lambda = O\{\exp[(\delta - 1)t]\}$,

as $t \to \infty$.

Proof: To prove (a), we consider

$$\left|\int_0^t E(\tau)\exp(\tau - t)\zeta(x,\mu,t-\tau;G_0)\,d\tau\right|$$
$$= \left|\operatorname*{l.i.m.}_{\omega\to\infty}\frac{1}{2\pi i}\int_0^t E(\tau) \times \int_{\delta-i\omega}^{\delta+i\omega}\exp[(\lambda-1)(t-\tau)](\lambda - A)^{-1}G_0\,d\lambda\,d\tau\right|$$
$$= \left|\operatorname*{l.i.m.}_{\omega\to\infty}\frac{1}{2\pi i}\int_{\delta-i\omega}^{\delta+i\omega}\int_0^t E(\tau) \times \exp[(\lambda-1)(t-\tau)]\,d\tau(\lambda - A)^{-1}G_0\,d\lambda\right|$$
$$= \frac{1}{2\pi}\left|\int_{-\infty}^{\infty}\left(-E(t) + \int_0^t \frac{dE(\tau)}{d\tau} \times \exp[(\lambda-1)(t-\tau)]\,d\tau\,\frac{(\lambda - A)^{-1}G_0}{\lambda - 1}\,dy\right)\right|$$
$$\le \frac{M(\delta, G_0)}{2\delta}\left[1 + \max_{0\le\tau\le t_0}\left(\left|\frac{dE(\tau)}{d\tau}\right|\right)\frac{1 + \exp[(\delta - 1)t]}{1 - \delta}\right]$$
$$= O(1) \quad \text{as} \quad t \to \infty,$$

by Fubini's Theorem for Bochner integrals (Ref. 9, p. 84). We obtain (b), (c), and (d) from similar arguments. QED

6. ASYMPTOTIC RESULTS

We are now ready to obtain the asymptotic formulas for N. We distinguish three cases: (i) $\beta_1 < 1$, (ii) $\beta_1 = 1$, and (iii) $\beta_1 > 1$. For the first case, we now prove the following theorem.

Theorem 5: For $\beta_1 < 1$, the asymptotic formula for N is

$$N(x, \mu, t) = f(x, \mu)\alpha(\mu) + (I - A)^{-1}G_0 + O\{\exp[(\beta_1 - 1)t]\} \quad \text{as} \quad t \to \infty,$$

where $(I - A)^{-1}G_0$ is given by the resolvent expressions in Ref. 2.

Proof: We consider each term in the representation for N given in Theorem 3. Clearly, the series terms are $O\{\exp[(\beta_1 - 1)t]\}$ as $t \to \infty$. The integral terms are $O\{\exp[(\delta - 1)t]\}$ from Lemma 5(b)–(d). Since the remaining terms are constant in t, the formula now follows. QED

Before we consider the remaining cases, we recall that, even though the number of eigenvalues of A is always positive as a function of $a > 0$ and $c > 0$, there are positive values of a and c for which there is only one eigenvalue β_1. This unique eigenvalue is greater than or equal to one if the product ca is sufficiently small. A graph of β_i/c vs ca, for $ca \le 20$, is given in Ref. 3, p. 1536, Fig. 2.

For the case (ii), we obtain the following theorem.

Theorem 6: For $\beta_1 = 1$, the asymptotic formula for N is

$$N(x, \mu, t) = (G_0, \psi_1^*)\psi_1(x, \mu)t + O(1) \quad \text{as} \quad t \to \infty.$$

That is, N increases linearly with increasing time t.

Proof: We consider the representation for N given in Theorem 4. If $m \ge 2$, there are series terms which are $O\{\exp[(\beta_2 - 1)t]\}$ as $t \to \infty$. From Lemma 5(a) and (c), we know the residual terms are $O(1)$ as $t \to \infty$. The formula now follows. QED

We now consider the remaining case $\beta_1 > 1$, which has subcases that depend on the values of the other eigenvalues of A. The asymptotic formulas, which follow from arguments similar to the above, are given in the following theorem.

Theorem 7:

(a) If $\beta_1 > 1$ and $\beta_2 < 1$, the asymptotic formula for N is

$$N(x, \mu, t) = \left((G_0, \psi_1^*)\int_0^{t_0} E(\tau)\exp[(1 - \beta_1)\tau]\,d\tau + \frac{\exp[(1 - \beta_1)t_0]}{\beta_1 - 1} + (H_0, \psi_1^*)\int_0^{t_0}\frac{dE}{d\tau}(\tau)\exp[(1 - \beta_1)\tau]\,d\tau\right)\psi_1(x, \mu) \times \exp[(\beta_1 - 1)t] + f(x, \mu)\alpha(\mu) + (I - A)^{-1}G_0 + O\{\exp[(\beta_2 - 1)t]\} \quad \text{as} \quad t \to \infty,$$

where $(I - A)^{-1}G_0$ is given by the resolvent expressions in Ref. 2. If β_1 is the only eigenvalue for A, the last term in this formula is $O\{\exp[(\delta - 1)t]\}$ as $t \to \infty$.

(b) If $\beta_1 > 1$ and $\beta_2 = 1$, the asymptotic formula for N is

$$N(x, \mu, t) = \left[(G_0, \psi_1^*)\left(\int_0^{t_0} E(\tau) \exp[(1-\beta_1)\tau]\, d\tau + \frac{\exp[(1-\beta_1)t_0]}{\beta_1 - 1}\right) + (H_0, \psi_1^*)\int_0^{t_0} \frac{dE}{d\tau}(\tau) \exp[(1-\beta_1)\tau]\, d\tau\right]\psi_1(x, \mu) \times \exp[(\beta_1 - 1)t] + (G_0, \psi_2^*)\psi_2(x, \mu)t + O(1) \quad \text{as} \quad t \to \infty.$$

(c) Further subcases depend on the values of other eigenvalues for A in a similar manner.

Hence, N increases exponentially with increasing time t if $\beta > 1$.

We are interested in the time-dependent scattering function $\mathcal{S}$, which is defined such that

$$\mathcal{S}(t, \mu) = \mu N(-a, -\mu, t), \quad 0 < \mu \leq 1.$$

To show the connection between $\mathcal{S}$ for the case $\beta_1 < 1$ and the steady-state scattering function S of Chandrasekhar,[11] we need some information about S.

Consider the steady-state problem of uniform, monodirectional radiation striking the left face of the slab at the incoming angle θ_0, $0 \leq \theta_0 < \pi/2$. Let $\mu_0 = \cos\theta_0$. The diffuse radiation $\psi(x, \mu; \mu_0)$, radiation that has been scattered at least once, for the steady-state problem satisfies [Ref. 11, p. 22, (129)] the equation

$$\mu\frac{\partial\psi}{\partial x} + \psi = \frac{c}{2}\int_{-1}^{1}\psi(x, \mu'; \mu_0)\, d\mu' + \exp\left(-\frac{(x+a)}{\mu_0}\right) \tag{17}$$

and the boundary conditions

$$\psi(-a, \mu; \mu_0) \equiv \psi(a, -\mu; \mu_0) \equiv 0, \quad 0 < \mu \leq 1.$$

It is known that $\psi(-a, -\mu; \mu_0)$ has the representation

$$\mu\psi(-a, -\mu; \mu_0) = S(\mu, \mu_0, 2a) = \frac{\mu\mu_0}{\mu + \mu_0}[X_{2a}(\mu)X_{2a}(\mu_0) - Y_{2a}(\mu)Y_{2a}(\mu_0)],$$

where X_{2a} and Y_{2a} denote the X and Y functions respectively of Chandrasekhar for a slab of thickness $2a$.[11]

In the formula of Theorem 5, we have the term $(I - A)^{-1}G_0$. Defining $\tilde{\psi} = (I - A)^{-1}G_0$, we see that $\tilde{\psi}$ satisfies the equation

$$\mu\frac{\partial\tilde{\psi}}{\partial x} + \tilde{\psi} = \frac{c}{2}\int_{-1}^{1}\tilde{\psi}(x, \mu')\, d\mu' + \frac{c}{2}\int_0^1 \alpha(s)\exp\left(-\frac{(x+a)}{s}\right) ds.$$

From the linearity of this equation,

$$\tilde{\psi}(x, \mu) = \frac{c}{2}\int_0^1 \alpha(\mu_0)\psi(x, \mu; \mu_0)\, d\mu_0, \tag{18}$$

where ψ denotes the solution of (17). Hence,

$$\mu\tilde{\psi}(-a, -\mu) = \frac{c}{2}\int_0^1 \alpha(\mu_0)S(\mu, \mu_0, 2a)\, d\mu, \quad 0 < \mu \leq 1. \tag{19}$$

Since $f(x, -\mu) \equiv 0$ for $\mu > 0$, Theorem 5 and Eq. (19) provide the asymptotic formula in the following theorem.

Theorem 8: If $\beta_1 < 1$, the asymptotic formula for the time-dependent scattering function is

$$\mathcal{S}(t, \mu) = \frac{c}{2}\int_0^1 \alpha(\mu_0)S(\mu, \mu_0, 2a)\, d\mu_0 + O\{\exp[(\beta_1 - 1)t]\} = \frac{c}{2}\mu X_{2a}(\mu)\int_0^1 \frac{\mu_0\alpha(\mu_0)X_{2a}(\mu_0)\, d\mu_0}{\mu + \mu_0} - \frac{c}{2}\mu Y_{2a}(\mu)\int_0^1 \frac{\mu_0\alpha(\mu_0)Y_{2a}(\mu_0)\, d\mu_0}{\mu + \mu_0} + O\{\exp[(\beta_1 - 1)t]\}, \quad 0 < \mu \leq 1, \quad \text{as} \quad t \to \infty.$$

In the just critical case, $\beta_1 = 1$, the asymptotic formula for N in Theorem 6 provides the following theorem.

Theorem 9: If $\beta_1 = 1$, the asymptotic formula for the time-dependent scattering function is

$$\mathcal{S}(t, \mu) = (G_0, \psi_1^*)\mu\psi_1(-a, -\mu)t + O(1), \quad 0 < \mu \leq 1, \quad \text{as} \quad t \to \infty.$$

That is, $\mathcal{S}$ increases linearly with increasing time t.

Theorem 7 provides the formulas for the remaining case in the following theorem.

Theorem 10:

(a) If $\beta_1 > 1$ and $\beta_2 < 1$, the asymptotic formula for $\mathcal{S}$ is

$$\mathcal{S}(t, \mu) = \left[(G_0, \psi_1^*)\left(\int_0^{t_0} E(\tau)\exp[(1-\beta_1)\tau]\, d\tau + \frac{\exp[(1-\beta_1)t_0]}{\beta_1 - 1}\right) + (H_0, \psi_1^*) \times \int_0^{t_0}\frac{dE}{d\tau}(\tau)\exp[(1-\beta_1)\tau]\, d\tau\right] \times \mu\psi_1(-a, -\mu)\exp[(\beta_1 - 1)t] + \mu(I - A)^{-1}G_0(-a, -\mu) + O\{\exp[(\beta_2 - 1)t]\}, \quad 0 < \mu \leq 1, \quad \text{as} \quad t \to \infty.$$

If β_1 is the only eigenvalue for A, the last term in this formula is $O\{\exp[(\delta - 1)t]\}$ as $t \to \infty$.

(b) If $\beta_1 > 1$ and $\beta_2 = 1$, the asymptotic formula for $\mathcal{S}$ is

$$\begin{aligned}\mathcal{S}(t,\mu) = \Bigg[&(G_0, \psi_1^*)\left(\int_0^{t_0} E(\tau)\exp[(1-\beta_1)\tau]\,d\tau + \frac{\exp[(1-\beta_1)t_0]}{\beta_1 - 1}\right) + (H_0, \psi_1^*) \\ &\times \int_0^{t_0} \frac{dE}{d\tau}(\tau)\exp[(1-\beta_1)\tau]\,d\tau\Bigg] \\ &\times \mu\psi_1(-a, -\mu)\exp[(\beta_1 - 1)t] \\ &+ (G_0, \psi_2^*)\mu\psi_2(-a, -\mu)t + O(1), \\ &\qquad 0 < \mu \le 1, \quad \text{as} \quad t \to \infty.\end{aligned}$$

(c) Further subcases for $\mathcal{S}$ depend on the values of other eigenvalues for A in a similar manner.

Therefore, $\mathcal{S}$ increases exponentially with increasing time t if $\beta_1 > 1$.

In order to write $(I - A)^{-1}G_0$ in terms of the X and Y functions as in the case $\beta_1 < 1$, it is necessary to extend the theory of the X and Y functions. We do not give this extension to the case $\beta_1 > 1$.

The time-dependent transmission function $\mathcal{T}$ is defined such that

$$\mathcal{T}(t,\mu) = \mu N(a, \mu, t), \quad 0 < \mu \le 1.$$

We can now obtain the asymptotic formulas for $\mathcal{T}$ and indicate the connection between $\mathcal{T}$ and the steady-state transmission function T of Chandrasekhar[11] for the case $\beta_1 < 1$.

It is known that the solution ψ of (17) has the representation

$$\begin{aligned}\mu\psi(a, \mu; \mu_0) &= T(\mu, \mu_0, 2a) \\ &= \frac{\mu\mu_0}{\mu - \mu_0}[X_{2a}(\mu)Y_{2a}(\mu_0) - Y_{2a}(\mu)X_{2a}(\mu_0)].\end{aligned}$$

Therefore, we obtain from (18)

$$\mu\tilde{\psi}(a,\mu) = \frac{c}{2}\int_0^1 \alpha(\mu_0)T(\mu, \mu_0, 2a)\,d\mu_0, \quad 0 < \mu \le 1.$$

Since $f(a, \mu) = \exp(-2a/\mu)$ for $0 < \mu \le 1$, this representation for $\tilde{\psi}(a, \mu)$ and Theorem 5 provide the following theorem.

Theorem 11: If $\beta_1 < 1$, the asymptotic formula for time-dependent transmission function is

$$\begin{aligned}\mathcal{T}(t,\mu) &= \mu\alpha(\mu)\exp(-2a/\mu) \\ &\quad + \frac{c}{2}\int_0^1 \alpha(\mu_0)T(\mu, \mu_0, 2a)\,d\mu_0 \\ &\quad + O\{\exp[(\beta_1 - 1)t]\} \\ &= \mu\alpha(\mu)\exp(-2a/\mu) \\ &\quad + \frac{c}{2}\mu X_{2a}(\mu)\int_0^1 \frac{\mu_0\alpha(\mu_0)Y_{2a}(\mu_0)}{\mu - \mu_0}\,d\mu_0 \\ &\quad - \frac{c}{2}\mu Y_{2a}(\mu)\int_0^1 \frac{\mu_0\alpha(\mu_0)X_{2a}(\mu_0)}{\mu - \mu_0}\,d\mu_0 \\ &\quad + O\{\exp[(\beta_1 - 1)t]\}, \\ &\qquad 0 < \mu \le 1, \quad \text{as} \quad t \to \infty.\end{aligned}$$

From Theorem 6, we obtain the following theorem.

Theorem 12: If $\beta_1 = 1$, the asymptotic formula for the time-dependent transmission function is

$$\mathcal{T}(t,\mu) = (G_0, \psi_1^*)\mu\psi_1(a, \mu)t + O(1), \quad 0 < \mu \le 1, \quad \text{as} \quad t \to \infty.$$

That is, $\mathcal{T}$ increases linearly with increasing time t.

Theorem 7 provides the formulas for the remaining case given in the following theorem.

Theorem 13:

(a) If $\beta_1 > 1$ and $\beta_2 < 1$, the asymptotic formula for the time-dependent transmission function is

$$\begin{aligned}\mathcal{T}(t,\mu) = \Bigg[&(G_0, \psi_1^*)\left(\int_0^{t_0} E(\tau)\exp[(1-\beta_1)\tau]\,d\tau + \frac{\exp[(1-\beta_1)t_0]}{\beta_1 - 1}\right) + (H_0, \psi_1^*) \\ &\times \int_0^{t_0} \frac{dE}{d\tau}(\tau)\exp[(1-\beta_1)\tau]\,d\tau\Bigg] \\ &\times \mu\psi_1(a, \mu)\exp[(\beta_1 - 1)t] \\ &+ \mu\alpha(\mu)\exp(-2a/\mu) + \mu(I - A)^{-1}G_0(a, \mu) \\ &+ O\{\exp[(\beta_2 - 1)t]\}, \\ &\qquad 0 < \mu \le 1, \quad \text{as} \quad t \to \infty.\end{aligned}$$

If β_1 is the only eigenvalue for A, the last term in this formula is $O\{\exp[(\delta - 1)t]\}$ as $t \to \infty$.

(b) If $\beta_1 > 1$ and $\beta_2 = 1$, the asymptotic formula for $\mathcal{T}$ is

$$\begin{aligned}\mathcal{T}(t,\mu) = \Bigg[&(G_0, \psi_1^*)\left(\int_0^{t_0} E(\tau)\exp[(1-\beta_1)\tau]\,d\tau + \frac{\exp[(1-\beta_1)t_0]}{\beta_1 - 1}\right) + (H_0, \psi_1^*) \\ &\times \int_0^{t_0} \frac{dE}{d\tau}(\tau)\exp[(1-\beta_1)\tau]\,d\tau\Bigg] \\ &\times \mu\psi_1(a, \mu)\exp[(\beta_1 - 1)t] \\ &+ (G_0, \psi_2^*)\mu\psi_2(a, \mu)t + O(1), \\ &\qquad 0 < \mu \le 1, \quad \text{as} \quad t \to \infty.\end{aligned}$$

(c) Further subcases for $\mathcal{T}$ depend on the values of other eigenvalues for A in a similar manner.

Therefore, $\mathcal{T}$ increases exponentially with increasing time t if $\beta_1 > 1$.

7. FURTHER REMARKS ABOUT THE CASE $\beta_i = 1$ FOR SOME i

We now discuss a representation like that in Theorem 3 for the case $\beta_i = 1$ for some $i = i_0$. Moving the contour C of integration for the integral in $u(t; G, E) - J(t; G_0, E)$ past β_i, $i = 1, 2, \cdots, (i_0 - 1)$, picks up the contributions of the residues at these eigenvalues.

Let

$$L(\lambda) = \frac{\exp[\lambda(t - t_0)]}{\lambda - 1}(\lambda - A)^{-1}G_0(x, \mu)$$

for x, μ, and t fixed. The function $L(\lambda)$ is an analytic function of λ on $\rho(A)$ (Ref. 2, p. 138, Lemma 10). (Observe that this analyticity is not vector analyticity.) For the case $\beta_{i_0} = 1$, it can be shown that $L(\lambda)$ has a pole of order 2 at $\lambda = 1$. Hence, we can shift the contour of integration further to the left to pick up the contribution of the residue at $\lambda = 1$, provided we can compute this residue.

Consider the expansion for the resolvent given in Ref. 12, p. 213, as follows:

$$(\lambda - A)^{-1}G = \frac{B_1(G)}{\lambda - 1} + \sum_{n=0}^{\infty} A_n(\lambda - 1)^n G$$

for $G \in H$ and $|\lambda - 1|$ sufficiently small, where B_1 and A_n, $n = 0, 1, \cdots$, are bounded linear operators on H. The limit for the series is taken in the sense of the topology induced by the operator norm.

It can be shown that the coefficient of $(\lambda - 1)^{-2}$ in the expansion of $L(\lambda)$ about $\lambda = 1$ is

$$\exp(t - t_0)B_1[G_0(x, \mu)].$$

Hence, $\operatorname{Res}_{\lambda=1} L(\lambda)$ can be computed as

$$\lim_{\lambda(\text{real})\to 1}\left((\lambda - 1)L(\lambda) - \frac{\exp(t - t_0)B_1[G_0(x, \mu)]}{\lambda - 1}\right).$$

Since this limit can be computed, the contour C of integration can be moved past $\beta_{i_0} = 1$ and then moved past the other eigenvalues β_i, $i = (i_0 + 1), \cdots, m$.

Recall that the operator

$$\Lambda_\lambda \cdot = \frac{c}{2}\int_{-a}^{a} E_1(\lambda|x - y|) \cdot dy$$

is a self-adjoint, completely continuous operator on $L_2[-a, a]$ for real $\lambda > 0$ (Ref. 1, pp. 224–25). The eigenvalues $l_i(\lambda)$ and the eigenfunctions $\rho_i(x; \lambda)$ of Λ_λ are analytic functions of λ with the analyticity of ρ_i being vector-analyticity in $L_2[-a, a]$ (Ref. 13, p. 610, Theorem 2). Also, $l_{i_0}(1) = 1$ and $l'_{i_0}(1) = -1$. The latter fact can be shown in the calculation of $\operatorname{Res}_{\lambda=1} L(\lambda)$.

For convenience, we also define the step functions $x_1(\mu)$ and $x_2(\mu)$ such that

$$x_1(\mu) = \begin{cases} x, & \mu < 0, \\ -a, & \mu > 0, \end{cases} \quad \text{and} \quad x_2(\mu) = \begin{cases} a, & \mu < 0, \\ x, & \mu > 0, \end{cases}$$

for each x fixed.

After we perform the necessary calculations, Theorem 2, Lemma 3, and the representation for $J(t; G_0, E)$ given in the proof of Theorem 3 enable us to state the following theorem.

Theorem 4': Let $\beta_i = 1$ for some $i = i_0$. Then

$$\begin{aligned}
N(x, \mu, t) = {} & \left(t - t_0 - 2 + \frac{l''_{i_0}(1)}{2} + \int_0^{t_0} E(\tau)\, d\tau\right) \\
& \times (G_0, \psi_{i_0}^*)\psi_{i_0}(x, \mu) \\
& + \left(G_0, \frac{\partial \rho_{i_0}}{\partial \lambda}(\cdot; 1)\right)_1 \psi_{i_0}(x, \mu) \\
& \pm (G_0, \psi_{i_0}^*)\int_{x_1}^{x_2}\left(\frac{x' - x}{\mu}\right) \\
& \times \exp[(x' - x)/\mu]\rho_{i_0}(x'; 1)\, dx' \\
& \pm (G_0, \psi_{i_0}^*)\int_{x_1}^{x_2}\exp\left(\frac{x' - x}{\mu}\right)\frac{\partial \rho_{i_0}}{\partial \lambda}(x'; 1)\, dx' \\
& \pm \frac{1}{\mu}\int_{x_1}^{x_2}\exp\left(\frac{x' - x}{\mu}\right)G_0(x', \mu)\, dx' \\
& \pm \frac{c}{2\mu}\int_{x_1}^{x_2}\exp\left(\frac{x' - x}{\mu}\right)\Lambda_1(G_0)(x', \mu)\, dx' \\
& \pm \frac{c}{2\mu}\sum_{\substack{i=1 \\ i \neq i_0}}^{\infty}\frac{l_i^2(1)}{1 - l_i(1)}(G_0, \rho_i(\cdot; 1))_1 \\
& \times \int_{x_1}^{x_2}\exp\left(\frac{x' - x}{\mu}\right)\rho_i(x'; 1)\, dx' \\
& + f(x, \mu)\alpha(\mu) \\
& + \sum_{\substack{i=1 \\ i \neq i_0}}^{m}\left(\int_0^{t_0} E(\tau)\exp[(1 - \beta_i)\tau]\, d\tau\right. \\
& \left. + \frac{\exp[(1 - \beta_i)t_0]}{\beta_i - 1}\right)(G_0, \psi_i^*)\psi_i(x, \mu) \\
& \times \exp[(\beta_i - 1)t] + \sum_{i=1}^{m}(H_0, \psi_i^*)\psi_i(x, \mu) \\
& \times \int_0^{t_0}\frac{dE}{d\tau}(\tau)\exp[(1 - \beta_i)\tau]\, d\tau \\
& \times \exp[(\beta_i - 1)t] \\
& + \int_0^{t_0} E(\tau)\exp(\tau - t)\zeta(x, \mu, T - \tau; G_0)\, d\tau \\
& + \int_0^{t_0}\frac{dE}{d\tau}(\tau)\exp(\tau - t)\zeta(x, \mu, t - \tau; H_0)\, d\tau \\
& + \frac{\exp(t_0 - t)}{2\pi i}\int_{\delta - i\infty}^{\delta + i\infty}\frac{\exp[\lambda(t - t_0)]}{\lambda - 1} \\
& \times (\lambda - A)^{-1}G_0\, d\lambda,
\end{aligned}$$

where the upper signs correspond to $\mu > 0$ and the lower signs to $\mu < 0$.

From this theorem and Lemma 5(b)–(d), we obtain the following theorem.

Theorem 6′: If $\beta_1 = 1$ and $\beta_2 < 1$, the asymptotic formula for N is

$$\begin{aligned}
N(x, \mu, t) = &\left(t - t_0 - 2 + \frac{l_1''(1)}{2} + \int_0^{t_0} E(\tau)\, d\tau\right) \\
&\times (G_0, \psi_1^*)\psi_1(x, \mu) \\
&+ \left(G_0, \frac{\partial \rho_1}{\partial \lambda}(\cdot; 1)\right)_1 \psi_1(x, \mu) \\
&\pm (G_0, \psi_1^*)\int_{x_1}^{x_2} \left(\frac{x' - x}{\mu}\right) \\
&\times \exp\left(\frac{x' - x}{\mu}\right)\rho_1(x'; 1)\, dx' \\
&\pm (G_0, \psi_1^*)\int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right)\frac{\partial \rho_1}{\partial \lambda}(x'; 1)\, dx' \\
&\pm \frac{1}{\mu}\int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right) G_0(x', \mu)\, dx' \\
&\pm \frac{c}{2\mu}\int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right)\Lambda_1(G_0)(x', \mu)\, dx' \\
&\pm \frac{c}{2\mu}\sum_{i=2}^{\infty} \frac{l_i^2(1)}{1 - l_i(1)}(G_0, \rho_i(\cdot; 1))_1 \\
&\times \int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right)\rho_i(x'; 1)\, dx' \\
&+ f(x, \mu)\alpha(\mu) + (H_0, \psi_1^*)\psi_1(x, \mu) \\
&\times \int_0^{t_0} \frac{dE}{d\tau}(\tau)\, d\tau + O\{\exp[(\beta_2 - 1)t]\} \\
&\qquad \text{as} \quad t \to \infty.
\end{aligned}$$

If β_1 is the only eigenvalue for A, then the last term in this formula is $O\{\exp[(\delta - 1)t]\}$ as $t \to \infty$.

In a similar manner, we obtain the following theorem.

Theorem 7′: If $\beta_1 > 1$, $\beta_2 = 1$, and $\beta_3 < 1$, the asymptotic formula for N is

$$\begin{aligned}
N(x, \mu, t) = &\left[(G_0, \psi_1^*)\left(\int_0^{t_0} E(\tau)\exp[(1 - \beta_1)\tau]\, d\tau \right.\right. \\
&\left.+ \frac{\exp[(1 - \beta_1)t_0]}{\beta_1 - 1}\right) + (H_0, \psi_1^*) \\
&\left.\times \int_0^{t_0} \frac{dE}{d\tau}(\tau)\exp[(1 - \beta_1)\tau]\, d\tau\right] \\
&\times \psi_1(x, \mu)\exp[(\beta_1 - 1)t] \\
&+ \left(t - t_0 - 2 + \frac{l_2''(1)}{2} + \int_0^{t_0} E(\tau)\, d\tau\right) \\
&\times (G_0, \psi_2^*)\psi_2(x, \mu) \\
&+ \left(G_0, \frac{\partial \rho_2}{\partial \lambda}(\cdot; 1)\right)_1 \psi_2(x, \mu) \\
&\pm (G_0, \psi_2^*)\int_{x_1}^{x_2} \left(\frac{x' - x}{\mu}\right) \\
&\times \exp\left(\frac{x' - x}{\mu}\right)\rho_2(x'; 1)\, dx' \\
&\pm (G_0, \psi_2^*)\int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right)\frac{\partial \rho_2}{\partial \lambda}(x'; 1)\, dx' \\
&\pm \frac{1}{\mu}\int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right) G_0(x', \mu)\, dx' \\
&\pm \frac{c}{2\mu}\int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right)\Lambda_1(G_0)(x', \mu)\, dx' \\
&\pm \frac{c}{2\mu}\sum_{\substack{i=1\\ i\neq 2}}^{\infty} \frac{l_i^2(1)}{1 - l_i(1)}(G_0, \rho_i(\cdot; 1))_1 \\
&\times \int_{x_1}^{x_2} \exp\left(\frac{x' - x}{\mu}\right)\rho_i(x'; 1)\, dx' \\
&+ f(x, \mu)\alpha(\mu) + (H_0, \psi_2^*)\psi_2(x, \mu) \\
&\times \int_0^{t_0} \frac{dE}{d\tau}(\tau)\, d\tau + O\{\exp[(\beta_3 - 1)t]\}
\end{aligned}$$

as $t \to \infty$. If β_1 and β_2 are the only eigenvalues for A, then the last term in this formula is $O\{\exp[(\delta - 1)t]\}$ as $t \to \infty$.

Further subcases depend on the values of eigenvalues less than β_2 in a similar manner.

This theorem in turn provides more complete formulas for $\mathcal{S}$ and $\mathcal{T}$ than those given in Theorems 9, 10(b), 12, and 13(b).

8. THE PROOF OF THE INEQUALITY (14) FOR G_0 AND H_0

To prove (14), we consider the resolvent for A as given in Ref. 1, pp. 231–32, Lemma 10. Let $G \in H$ and let $\xi(x; \lambda)$ denote the unique solution in $L_2[-a, a]$ of the integral equation

$$\frac{2}{c}\xi(x; \lambda) + \int_{-a}^{a} E_1(\lambda|x - y|)\xi(y; \lambda)\, dy + F(x; \lambda, G), \tag{20}$$

where

$$E_1(z) = \int_1^\infty \frac{e^{-zs}}{s}\, ds \quad \text{for} \quad \mathrm{Re}(z) \geq 0, \quad z \neq 0,$$

and

$$\begin{aligned}
F(x; \lambda, G) = &\int_0^1 \frac{d\mu}{\mu}\int_{-a}^{x} \exp\left(\frac{-\lambda}{\mu}(x - y)\right) G(y, \mu)\, dy \\
&- \int_{-1}^{0} \frac{d\mu}{\mu}\int_{x}^{a} \exp\left(\frac{-\lambda}{\mu}(x - y)\right) G(y, \mu)\, dy.
\end{aligned}$$

Then

$$(\lambda - A)^{-1}G(x, \mu) = \begin{cases} \dfrac{c}{2\mu}\displaystyle\int_{-a}^{x} \exp\left(\frac{-\lambda}{\mu}(x-y)\right)\xi(y;\lambda)\,dy + \frac{1}{\mu}\int_{-a}^{x}\exp\left(\frac{-\lambda}{\mu}(x-y)\right)G(y,\mu)\,dy, & \mu > 0, \\ \dfrac{-c}{2\mu}\displaystyle\int_{x}^{a} \exp\left(\frac{-\lambda}{\mu}(x-y)\right)\xi(y;\lambda)\,dy - \frac{1}{\mu}\int_{x}^{a}\exp\left(\frac{-\lambda}{\mu}(x-y)\right)G(y,\mu)\,dy, & \mu < 0. \end{cases} \tag{21}$$

For fixed x, $(\lambda - A)^{-1}G(x, \mu)$ is a continuous function of μ at $\mu = 0$; and in fact

$$(\lambda - A)^{-1}G(x, 0) = [(c/2)\xi(x;\lambda) + G(x, 0)]\lambda^{-1}, \tag{22}$$

provided $\lim_{\mu\to 0} G(x,\mu) = G(x, 0)$ (Ref. 2, pp. 141–42).

Concerning the exponential function E_1, we note

$$\int_{-\infty}^{\infty} E_1^2(|s|)\,ds = 4\ln 2. \tag{23}$$

Let δ be fixed, $0 < \delta < \min[\frac{1}{2}, \beta_m]$. The proof that follows is applicable to a larger set in the λ plane, but for simplicity we will not consider this generalization. For convenience, let $c_1 = \max[|\alpha(\mu)|]$, $-1 \le \mu \le 1$. We prove the inequality (14) for every function G that possesses the following five properties of G_0 and H_0:

(i) There exists a constant $c_2(G)$ such that $|G(x,\mu)| \le c_2$ for all x, μ and $\int_{-a}^{a} |\partial G/\partial x(x,\mu)|\,dx \le c_2$ for all μ.

(ii) $(\partial/\partial x)\int_{-1}^{1} G(x,\mu)\,d\mu = \int_{-1}^{1}(\partial/\partial x)G(x,\mu)\,d\mu$ for all x.

(iii) The derivative $(dF/dx)(x;\lambda, G)$ exists and is a continuous function of x in $-a < x < a$ with a finite limit at $x = a$ and at worst a logarithmic singularity at $x = -a$.

(iv) There exists a constant $c_3(\delta, G)$ such that

$$\left\| F\left(x;\lambda,\frac{\partial G}{\partial x}\right)\right\|_1 \le c_3(\delta, G).$$

(v) G satisfies the inequality

$$|(\lambda - A)^{-1}G(x,0)| \le \frac{1}{|\lambda|}\left(\frac{c}{2}|\xi(x;\lambda)| + c_2\right),$$

for each x.

We can take $c_2(G_0) = cc_1/2$, $c_2(H_0) = c_1$, $c_3(\delta, G_0) = 4cc_1((a/\delta)\ln 2)^{\frac{1}{2}}$, and $c_3(\delta, H_0) = 2(1+\beta_m)c_1(\ln 2)^{\frac{1}{2}}/[\delta(1-\delta)]$. Property (v) for G_0 and H_0 follows from (22), except possibly for H_0 at $x = -a$. But

$$(\lambda - A)^{-1}H_0(-a, 0) = \frac{c}{2\lambda}\xi(-a;\lambda)$$

from (21) so that the inequality is satisfied for all x.

We now obtain (14) for functions that satisfy (i)–(v) from the representation for the resolvent by integration by parts. We first consider $\mu > 0$. It follows immediately from property (i) that

$$\left|\frac{1}{\mu}\int_{-a}^{x}\exp\left(-\frac{\lambda}{\mu}(x-y)\right)G(y,\mu)\,dy\right| \le \frac{3c_2}{|\lambda|}, \quad \mu > 0. \tag{24}$$

For the other integral in (21) for $\mu > 0$, we obtain

$$\left|\frac{c}{2\mu}\int_{-a}^{x}\exp\left(-\frac{\lambda}{\mu}(x-y)\right)\xi(y;\lambda)\,dy\right| \le \frac{c}{2\lambda}\left(|\xi(x;\lambda)| + |\xi(-a;\lambda)| + \int_{-a}^{x}\left|\frac{\partial\xi}{\partial y}(y;\lambda)\right|dy\right). \tag{25}$$

To bound this quantity, we obtain bounds for $|\xi(x;\lambda)|$ and $\int_{-a}^{a}|(\partial\xi/\partial y)(y;\lambda)|\,dy$.

For the former,

$$\begin{aligned}|\xi(x,\lambda)| &\le \frac{c}{2}\int_{-a}^{a} E_1(\beta|x-y|)\,|\xi(y;\lambda)|\,dy + \frac{c}{2}|F(x;\lambda,G)| \\ &\le \frac{c}{2\delta}\left(\int_{-\infty}^{\infty}E_1^2(|s|)\,ds\right)^{\frac{1}{2}}\left(\int_{-a}^{a}|\xi(y;\lambda)|^2\,dy\right)^{\frac{1}{2}} + \frac{c}{2}|F(x;\lambda,G)| \\ &\le \frac{cc_4(\delta)\,\|G\|\,(\ln 2)^{\frac{1}{2}}}{\delta^2} + \frac{c}{2}|F(x;\lambda,G)|\end{aligned} \tag{26}$$

from (23) and the inequality (Ref. 2, p. 135)

$$\|\xi\|_1 \le \frac{c_4(\delta)}{\delta}\|G\|.$$

[In Ref. 2 the closed region $\{\lambda = \beta + iy: 0 \le \beta \le \beta' < \infty,\ |\lambda| \ge \lambda_1,\ |\lambda - \beta_i| \ge \epsilon,\ i = 1, \cdots, m\}$ is considered. The constant $c_4(\delta)$ depends on this set, and ϵ and λ_1 must be chosen small enough that $\epsilon < \beta_m - \delta$, $\lambda_1 < \delta$ and a certain inequality is satisfied (Ref. 2, pp. 133–34, Lemma 6). Hence, c_4 depends on δ.] But

$$\begin{aligned}F(x;\lambda,G) &= \frac{1}{\lambda}\int_{-1}^{1}G(x,\mu)\,d\mu - \frac{1}{\lambda}\int_{0}^{1}e^{-\lambda(x+a)/\mu}G(-a,\mu)\,d\mu \\ &\quad - \frac{1}{\lambda}\int_{-1}^{0}e^{-\lambda(x-a)/\mu}G(a,\mu)\,d\mu \\ &\quad - \frac{1}{\lambda}\int_{0}^{1}\int_{-a}^{x}e^{-\lambda(x-y)/\mu}\frac{\partial G}{\partial y}(y,\mu)\,dy\,d\mu \\ &\quad + \frac{1}{\lambda}\int_{-1}^{0}\int_{x}^{a}e^{-\lambda(x-y)/\mu}\frac{\partial G}{\partial y}(y,\mu)\,dy\,d\mu.\end{aligned} \tag{27}$$

Hence,

$$|F(x;\lambda,G)| \le 6c_2/|\lambda|$$

from property (i). Therefore, we have from (26),

$$|\xi(x;\lambda)| \le \frac{cc_4(\delta)\,\|G\|\,(\ln 2)^{\frac{1}{2}}}{\delta^2} + \frac{3cc_2}{\delta}. \tag{28}$$

We denote this constant as $c_5(\delta, G)$.

We now turn to the existence of $\partial\xi/\partial x$ and of a bound for $\int_{-a}^{a} |(\partial\xi/\partial x)(x;\lambda)|\,dx$. Recalling Eq. (20), we can write

$$\frac{2}{c}\frac{\partial\xi}{\partial x}(x;\lambda) = \int_{-a}^{a} E_1(\lambda\,|x-y|)\frac{\partial\xi}{\partial y}(y;\lambda)\,dy + K(x;\lambda,G), \quad (29)$$

where

$$K(x;\lambda,G) = \frac{dF}{dx}(x;\lambda,G) + \xi(-a;\lambda)E_1(\lambda\,|x+a|) - \xi(a;\lambda)E_1(\lambda\,|x-a|).$$

That $\partial\xi/\partial x$ exists and is the solution of (29) follows from property (iii) and the proof of Theorem 35.1 on pp. 85–87 of Ref. 14. (The theorem stated in this reference would require dF/dx to be continuous in $-a < x < a$ and have finite limits at the end points approached from inside the interval. However, the proof given there allows dF/dx to have logarithmic singularities at the end points.) We use (29) to obtain the necessary bound for $\int_{-a}^{a} |(\partial\xi/\partial x)(x;\lambda)|\,dx$.

The function $K(x;\lambda,G)\in L_2[-a,a]$, for each λ, because it only has logarithmic singularities. Hence, (29) is of the same form as (20). Also,

$$\|K(x;\lambda,G)\|_1 \le \left\|\frac{dF}{dx}(x;\lambda,G)\right\|_1 + \frac{4}{\delta}c_5(\delta,G)(\ln 2)^{\frac{1}{2}} \quad (30)$$

from (23) and (28). To bound $\|dF/dx\,(x;\lambda,G)\|_1$, we use property (ii) to differentiate F as it is given in (27) to obtain

$$\frac{dF}{dx}(x;\lambda,G) = \int_0^1 \frac{e^{-\lambda(x+a)/\mu}}{\mu}G(-a,\mu)\,d\mu - \int_0^1 \frac{e^{\lambda(x-a)/\mu}}{\mu}G(a,-\mu)\,d\mu + F\left(x;\lambda,\frac{\partial G}{\partial x}\right).$$

Property (iv) now gives

$$\left\|\frac{dF}{dx}(x;\lambda,G)\right\|_1 \le c_2\,\|E_1(\delta\,|x+a|)\|_1 + c_2\,\|E_1(\delta\,|a-x|)\|_1 + c_3(\delta,G) \le \frac{4c_2(\ln 2)^{\frac{1}{2}}}{\delta} + c_3(\delta,G).$$

Therefore, from (30),

$$\|K(x;\lambda,G)\|_1 \le \frac{4(\ln 2)^{\frac{1}{2}}}{\delta}[c_5(\delta,G)+c_2] + c_3(\delta,G). \quad (31)$$

We are now ready to use (29) to obtain

$$\left\|\frac{\partial\xi}{\partial x}(x;\lambda)\right\|_1 \le \frac{c}{2\delta}\left(\int_{-\infty}^{\infty}E_1^2(|s|)\,ds\right)^{\frac{1}{2}}\left\|\frac{\partial\xi}{\partial x}\right\|_1 + \frac{c}{2}\|K\|_1$$
$$\le [c_4(\delta)/\delta^2](\ln 2)^{\frac{1}{2}}\,\|K\|_1 + (c/2)\,\|K\|_1 \quad \text{(Ref. 2, p. 135)}$$
$$\le (cc_4(\delta)(\ln 2)^{\frac{1}{2}} + c/2) \times \{[4(\ln 2)^{\frac{1}{2}}/\delta][c_5(\delta,G)+c_2] + c_3(\delta,G)\}$$

from (31). Denote this constant as $c_6(\delta,G)$. Then, from the Cauchy–Schwarz inequality,

$$\int_{-a}^{a}\left|\frac{\partial\xi}{\partial x}(x;\lambda)\right|dx \le (2a)^{\frac{1}{2}}\left\|\frac{\partial\xi}{\partial x}\right\|_1 \le (2a)^{\frac{1}{2}}c_6(\delta,G). \quad (32)$$

We can now return to (25) and write, for $\mu > 0$,

$$\left|\frac{c}{2\mu}\int_{-a}^{x}\exp\left(-\frac{\lambda}{\mu}(x-y)\right)\xi(y;\lambda)\,dy\right| \le \frac{c}{2\,|\lambda|}[2c_5(\delta,G) + (2a)^{\frac{1}{2}}c_6(\delta,G)] \quad (33)$$

from (28) and (32).

Therefore, for $\mu > 0$,

$$|(\lambda - A)^{-1}G(x,\mu)| \le (1/|\lambda|)[cc_5(\delta,G) + c(a/2)^{\frac{1}{2}}c_6(\delta,G) + 3c_2]$$

from (24) and (33). Similar arguments obtain the same inequality for $\mu < 0$. Also,

$$|(\lambda - A)^{-1}G(x,0)| \le (1/|\lambda|)[(c/2)\,|\xi(x;\lambda)| + c_2],$$

by property (v),

$$\le (1/|\lambda|)[(c/2)c_5(\delta,G) + c_2],$$

by (28).

We now define

$$M(\delta,G) = \max\,[(cc_5(\delta,G) + c(a/2)^{\frac{1}{2}}c_6(\delta,G) + 3c_2), ((c/2)c_5(\delta,G) + c_2)].$$

This definition completes the proof of the inequality (14) for all functions that satisfy the properties (i)–(v) with $\operatorname{Re}\lambda = \delta$ fixed in $0 < \delta < \beta_m$.

ACKNOWLEDGMENT

The author wishes to thank Professor T. W. Mullikin for all of his assistance.

* This research was supported by NASA Contract No. NGL 15-005-021 (Purdue University Institutional Grant). The author is now employed by the Jet Propulsion Laboratory, California Institute of Technology.

[1] J. Lehner and G. M. Wing, Commun. Pure Appl. Math. **8**, 217 (1955).
[2] J. Lehner and G. M. Wing, Duke Math. J. **23**, 125 (1956).
[3] R. L. Bowden and C. D. Williams, J. Math. Phys. **5**, 1527 (1964).
[4] P. A. Newman and R. L. Bowden, J. Math. Phys. **11**, 2445 (1970).
[5] K. Kuščer and P. F. Zweifel, J. Math. Phys. **6**, 1125 (1965).
[6] G. R. Hintz, Ph.D. thesis, Purdue University, 1969.
[7] B. Davison, *Neutron Transport Theory* (Oxford U.P., Oxford, 1957).
[8] E. Hille, *Functional Analysis and Semi-Groups* (Am. Math. Soc. Colloq. Publ., Providence, R.I., 1948), Vol. 31.
[9] E. Hille and R. S. Phillips, *Functional Analysis and Semi-Groups* (Am. Math. Soc. Colloq. Publ., Providence, R.I., 1957), Vol. 31, rev. ed.
[10] R. S. Phillips, Trans. Am. Math. Soc. **74**, 199 (1953).
[11] S. Chandrasekhar, *Radiative Transfer* (Dover, N.Y., 1960).
[12] A. E. Taylor, Acta Math. **84**, 189 (1951).
[13] F. Rellich, Math. Ann. **113**, 600 (1936).
[14] I. W. Busbridge, *The Mathematics of Radiative Transfer*, Cambridge Tracts, No. 50 (Cambridge U.P., Cambridge, 1960).

Simplified Intrinsic Proof of the Rainich Differential Relation

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(Received 19 November 1970)

The necessity and sufficiency of the Rainich differential relation, a basic equation of the "already unified field theory," is proved in a simplified way by intrinsic techniques. Some tensor identities of interest in their own right are derived and used in this proof. The results in this paper generalize those given in a previous paper [Ann. Phys. (N.Y.) **60**, 384 (1970)], where only the necessity of the Rainich differential condition was proved.

I. INTRODUCTION

In a recent paper[1] (hereafter referred to as I), we used intrinsic techniques to achieve considerable simplification in the derivation of the equations of the "already unified field theory" of Maxwell, Einstein, and Rainich. First, we gave a proof of the necessity and sufficiency of the Rainich algebraic conditions on the Ricci tensor R in order that the energy–momentum tensor T (related to R by the Einstein field equation[2] $R - \frac{1}{2}R_s I_4 = \kappa T$, where κ is a constant) can be expressed in the form[3]

$$T = (8\pi)^{-1} G \cdot G^*, \tag{1}$$

where G is an antisymmetric complex dyadic function satisfying

$$\star G = iG. \tag{2}$$

Secondly, in the case $R : R \neq 0$, we gave a proof of the necessity but not of the sufficiency of the Rainich differential relation in order that the dyadic function G of Eq. (1) can be restricted to satisfy the additional condition[4]

$$\mathbf{D} \cdot G = 0. \tag{3}$$

The purpose of the present paper is to generalize this proof to show both the necessity and sufficiency of the differential relation. In addition to presenting a proof somewhat simpler and more direct than others previously published (including the one given in I), we derive several identities of interest in themselves, some of which we believe to be new. We begin by obtaining these identities in Sec. II. In Sec. III we make use of them to show, in a completely intrinsic manner, the necessity and sufficiency of the Rainich differential relation in the case $R : R \neq 0$.

II. SOME INTRINSIC TENSOR IDENTITIES

The purpose of this section is to derive some identities which are of interest in their own right as well as being very useful in the discussion in the next section.

We being by showing, as a generalization of Eqs. (21) and (22) of I, that if M and N are any antisymmetric complex dyadics such that

$$\star M = iM, \tag{4a}$$

$$\star N = iN, \tag{4b}$$

then

$$M : N^* = 0, \tag{5}$$

$$M \cdot N^* = N^* \cdot M. \tag{6}$$

Proof: Recall Eqs. (11) and (12) of I, which read

$$\star A : \star C = -A : C, \tag{7a}$$

$$C \cdot \star B + B \cdot \star C = -\tfrac{1}{2}(B : \star C) I_4, \tag{7b}$$

where A, B, and C are arbitrary antisymmetric complex dyadics. If we set $A = M$ and $C = N^*$ in Eq. (7a), then Eq. (5) results after using Eq. (4a) and the complex conjugate of Eq. (4b). Similarly, by setting $C = M$ and $B = N^*$ in Eq. (7b), we arrive at Eq. (6) after making use of Eq. (4a), the complex conjugate of Eq. (4b), and Eq. (5).

Also for future use, we state Eq. (23) of I, which is

$$M \cdot M = -\tfrac{1}{4} M : M I_4, \tag{8}$$

where M satisfies Eq. (4a).

Now we show that

$$B \cdot A = A \cdot B + \boldsymbol{\Gamma} : (\star A \cdot B), \tag{9}$$

where A and B are any antisymmetric complex dyadics.

Proof: Recall Eq. (4b) of I:

$$\boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma} \,\vdots\, \mathbf{uvw} = \mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w}, \tag{10}$$

where **u**, **v**, and **w** are arbitrary 4-vectors. Making use of this expression, we can write

$$\begin{aligned}\mathbf{\Gamma} : \{[\mathbf{\Gamma} : (\mathbf{uv})] \cdot (\mathbf{wz})\} &= -\mathbf{z} \cdot \mathbf{\Gamma} \cdot \mathbf{\Gamma} \vdots (\mathbf{uvw}) \\ &= -\mathbf{z} \cdot (\mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w}) \\ &= (\mathbf{u} \wedge \mathbf{v}) \cdot \mathbf{zw} + \mathbf{wz} \cdot (\mathbf{u} \wedge \mathbf{v}) \\ &\quad - \mathbf{z} \cdot \mathbf{w}\, (\mathbf{u} \wedge \mathbf{v}),\end{aligned}$$

where $\mathbf{z}$ is also an arbitrary 4-vector. Thus it follows that

$$\begin{aligned}\mathbf{\Gamma} : \{[\mathbf{\Gamma} : (\mathbf{u} \wedge \mathbf{v})] \cdot (\mathbf{w} \wedge \mathbf{z})\} &= -2\, (\mathbf{u} \wedge \mathbf{v}) \cdot (\mathbf{w} \wedge \mathbf{z}) \\ &\quad + 2\, (\mathbf{w} \wedge \mathbf{z}) \cdot (\mathbf{u} \wedge \mathbf{v}),\end{aligned}$$

which can be immediately generalized to give Eq. (9).

Next we shall prove the identity

$$\mathbf{D}(\mathsf{B} \cdot \mathsf{A}) = (\mathbf{D}\mathsf{B}) \cdot \mathsf{A} + (\mathbf{D}\mathsf{A}) \cdot \mathsf{B} + [\mathbf{D}(\mathbf{\Gamma} \cdot {}^{\star}\mathsf{A})] : \mathsf{B} \tag{11}$$

for antisymmetric complex dyadic functions A and B.

Proof: Note first that, from the properties of covariant differentiation,

$$\mathbf{a} \cdot \mathbf{D}\mathbf{\Gamma} = 0, \tag{12a}$$

$$\mathbf{a} \cdot \mathbf{D}\mathsf{A}_{\mathrm{T}} = (\mathbf{a} \cdot \mathbf{D}\mathsf{A})_{\mathrm{T}}, \tag{12b}$$

$$\mathbf{a} \cdot \mathbf{D}\mathsf{A}^* = (\mathbf{a} \cdot \mathbf{D}\mathsf{A})^*, \tag{12c}$$

where $\mathbf{a}$ is an arbitrary 4-vector function. It follows from Eq. (12b) that if A is antisymmetric, $\mathbf{a} \cdot \mathbf{D}\mathsf{A}$ is also antisymmetric. From Eq. (12a) we also get

$$\mathbf{D}\mathbf{\Gamma} = 0, \tag{12d}$$

$$\mathbf{a} \cdot \mathbf{D}\, {}^{\star}\mathsf{A} = {}^{\star}(\mathbf{a} \cdot \mathbf{D}\mathsf{A}). \tag{12e}$$

Now, making use of Eq. (9) with A replaced by $\mathbf{a} \cdot \mathbf{D}\mathsf{A}$, together with Eqs. (12e) and (12a), we find

$$\begin{aligned}\mathbf{a} \cdot \mathbf{D}(\mathsf{B} \cdot \mathsf{A}) &= (\mathbf{a} \cdot \mathbf{D}\mathsf{B}) \cdot \mathsf{A} + \mathsf{B} \cdot (\mathbf{a} \cdot \mathbf{D}\mathsf{A}) \\ &= (\mathbf{a} \cdot \mathbf{D}\mathsf{B}) \cdot \mathsf{A} + (\mathbf{a} \cdot \mathbf{D}\mathsf{A}) \cdot \mathsf{B} \\ &\quad + \mathbf{\Gamma} : [(\mathbf{a} \cdot \mathbf{D}\, {}^{\star}\mathsf{A}) \cdot \mathsf{B}] \\ &= (\mathbf{a} \cdot \mathbf{D}\mathsf{B}) \cdot \mathsf{A} + (\mathbf{a} \cdot \mathbf{D}\mathsf{A}) \cdot \mathsf{B} \\ &\quad + [\mathbf{a} \cdot \mathbf{D}(\mathbf{\Gamma} \cdot {}^{\star}\mathsf{A})] : \mathsf{B},\end{aligned}$$

and, since $\mathbf{a}$ is arbitrary, Eq. (11) results. QED

Contraction of Eq. (11) on the first two files gives the identity

$$\begin{aligned}\mathbf{D} \cdot (\mathsf{B} \cdot \mathsf{A}) &= (\mathbf{D} \cdot \mathsf{B}) \cdot \mathsf{A} + (\mathbf{D} \cdot \mathsf{A}) \cdot \mathsf{B} \\ &\quad - \mathbf{\Gamma} \vdots [(\mathbf{D}\, {}^{\star}\mathsf{A}) \cdot \mathsf{B}]\end{aligned} \tag{13}$$

with the help of Eq. (12d).

A special case of Eq. (11) is obtained when $\mathsf{B} = \mathsf{M}$, $\mathsf{A} = \mathsf{N}^*$, with M and N satisfying Eqs. (4). We then have

$$\mathbf{D}(\mathsf{M} \cdot \mathsf{N}^*) = (\mathbf{D}\mathsf{M}) \cdot \mathsf{N}^* + (\mathbf{D}\mathsf{N}^*) \cdot \mathsf{M}. \tag{14}$$

Proof: By operating on both sides of Eq. (4b) with $\mathbf{a} \cdot \mathbf{D}$ and using Eq. (12e), we get

$${}^{\star}(\mathbf{a} \cdot \mathbf{D}\mathsf{N}) = i(\mathbf{a} \cdot \mathbf{D}\mathsf{N}). \tag{15}$$

Consequently, from Eq. (6), with N replaced by $\mathbf{a} \cdot \mathbf{D}\mathsf{N}$ and with the aid of Eq. (12c), we have

$$\mathsf{M} \cdot (\mathbf{a} \cdot \mathbf{D}\mathsf{N}^*) = (\mathbf{a} \cdot \mathbf{D}\mathsf{N}^*) \cdot \mathsf{M}. \tag{16}$$

Using this result yields[5]

$$\begin{aligned}\mathbf{a} \cdot \mathbf{D}(\mathsf{M} \cdot \mathsf{N}^*) &= (\mathbf{a} \cdot \mathbf{D}\mathsf{M}) \cdot \mathsf{N}^* + \mathsf{M} \cdot (\mathbf{a} \cdot \mathbf{D}\mathsf{N}^*) \\ &= (\mathbf{a} \cdot \mathbf{D}\mathsf{M}) \cdot \mathsf{N}^* + (\mathbf{a} \cdot \mathbf{D}\mathsf{N}^*) \cdot \mathsf{M},\end{aligned}$$

and, since $\mathbf{a}$ is arbitrary, this implies Eq. (14). QED

Contraction on the first two files of Eq. (14) gives[6]

$$\mathbf{D} \cdot (\mathsf{M} \cdot \mathsf{N}^*) = (\mathbf{D} \cdot \mathsf{M}) \cdot \mathsf{N}^* + (\mathbf{D} \cdot \mathsf{N}^*) \cdot \mathsf{M}, \tag{17}$$

which is a special case of Eq. (13).

An additional corollary to Eq. (13) follows by setting $\mathsf{B} = \mathsf{A} = \mathsf{M}$ with M again satisfying Eq. (4a). We thus obtain

$$-\tfrac{1}{4}\mathbf{D}(\mathsf{M} : \mathsf{M}) = 2(\mathbf{D} \cdot \mathsf{M}) \cdot \mathsf{M} - i\mathbf{\Gamma} \vdots [(\mathbf{D}\mathsf{M}) \cdot \mathsf{M}] \tag{18}$$

after resorting to Eq. (8).

III. NECESSITY AND SUFFICIENCY OF THE RAINICH DIFFERENTIAL CONDITION

For the case $\mathsf{R} : \mathsf{R} \neq 0$, suppose the Ricci tensor R satisfies the Rainich algebraic conditions and, consequently, can be expressed in the form

$$\mathsf{R} = \kappa\mathsf{T} = (8\pi)^{-1}\kappa\mathsf{K} \cdot \mathsf{K}^*, \tag{19}$$

where K is an antisymmetric complex dyadic function[7] for which ${}^{\star}\mathsf{K} = i\mathsf{K}$. It immediately follows from Eqs. (6) and (8) that

$$\mathsf{R} : \mathsf{R} = (\mathsf{R} \cdot \mathsf{R})_s = (16\pi)^{-2}\kappa^2\mathsf{K} : \mathsf{K}\mathsf{K}^* : \mathsf{K}^*, \tag{20}$$

and thus $\mathsf{K} : \mathsf{K} \neq 0$.

Define now

$$\mathsf{G} = e^{-i\varphi}\mathsf{K}, \tag{21}$$

where φ is a real-valued function. We shall show that the following equations are equivalent:

$$\mathbf{D} \cdot \mathsf{G} = 0, \tag{3}$$

$$\mathbf{D} \cdot \mathsf{K} = i(\mathbf{D}\varphi) \cdot \mathsf{K}, \tag{22a}$$

$$\mathbf{D}\varphi = 4i(\mathsf{K} : \mathsf{K})^{-1}(\mathbf{D} \cdot \mathsf{K}) \cdot \mathsf{K}, \tag{22b}$$

$$\mathbf{D}\varphi = \tfrac{1}{4}i\mathbf{D} \ln [(\mathsf{K}^* : \mathsf{K}^*)(\mathsf{K} : \mathsf{K})^{-1}] + \mathbf{f}, \tag{22c}$$

where

$$\mathbf{f} \equiv (\mathsf{R} : \mathsf{R})^{-1}\mathbf{\Gamma} \vdots [(\mathbf{D}\mathsf{R}) \cdot \mathsf{R}]. \tag{23}$$

Note that taking the exterior derivative of Eq. (22c) gives

$$\mathbf{D} \wedge \mathbf{f} = 0, \tag{24}$$

which is the Rainich differential relation. On the other hand, Eq. (24) implies that there exists a real function φ such that Eq. (22c) holds.

By making a substitution from Eq. (21), one can get Eq. (22a) from (3) and vice versa. By taking a dot product with K and using Eq. (8), one can get Eq. (22b) from (22a) and vice versa.

We shall now show the equivalence of Eqs. (22b) and (22c). One-half the imaginary part of Eq. (22b) is

$$0 = (\mathsf{K} : \mathsf{K})^{-1}(\mathbf{D} \cdot \mathsf{K}) \cdot \mathsf{K} + (\mathsf{K}^* : \mathsf{K}^*)^{-1}(\mathbf{D} \cdot \mathsf{K}^*) \cdot \mathsf{K}^*, \tag{25a}$$

and the real part is

$$\mathbf{D}\varphi = 2i[(\mathsf{K} : \mathsf{K})^{-1}(\mathbf{D} \cdot \mathsf{K}) \cdot \mathsf{K} - (\mathsf{K}^* : \mathsf{K}^*)^{-1} \times (\mathbf{D} \cdot \mathsf{K}^*) \cdot \mathsf{K}^*]. \tag{25b}$$

With the aid of Eqs. (8), (6), (17), (19), and (20), Eq. (25a) becomes

$$\begin{aligned} 0 &= 4(\mathsf{K} : \mathsf{K}\mathsf{K}^* : \mathsf{K}^*)^{-1}[(\mathbf{D} \cdot \mathsf{K}) \cdot \mathsf{K} \cdot \mathsf{K}^* \cdot \mathsf{K}^* + (\mathbf{D} \cdot \mathsf{K}^*) \cdot \mathsf{K}^* \cdot \mathsf{K} \cdot \mathsf{K}] \\ &= 4(\mathsf{K} : \mathsf{K}\mathsf{K}^* : \mathsf{K}^*)^{-1}[\mathbf{D} \cdot (\mathsf{K} \cdot \mathsf{K}^*)] \cdot \mathsf{K} \cdot \mathsf{K}^* \\ &= (\mathsf{R} : \mathsf{R})^{-1}(\mathbf{D} \cdot \mathsf{R}) \cdot \mathsf{R}. \end{aligned} \tag{26}$$

However, the Ricci tensor always satisfies $\mathbf{D} \cdot (\mathsf{R} - \frac{1}{2}\mathsf{R}_s\mathsf{I}_4) = 0$, and one of the Rainich algebraic conditions is $\mathsf{R}_s = 0$; thus $\mathbf{D} \cdot \mathsf{R} = 0$. Consequently, Eq. (26) is always true and imposes no new restrictions on R. We now turn to Eq. (25b), which, by virtue of Eq. (18), can be expressed as

$$\begin{aligned} \mathbf{D}\varphi = \tfrac{1}{4}i\mathbf{D} \ln [(\mathsf{K}^* : \mathsf{K}^*)(\mathsf{K} : \mathsf{K})^{-1}] \\ - (\mathsf{K} : \mathsf{K}\mathsf{K}^* : \mathsf{K}^*)^{-1}\boldsymbol{\Gamma} \vdots [\mathsf{K}^* : \mathsf{K}^*(\mathbf{D}\mathsf{K}) \cdot \mathsf{K} \\ + \mathsf{K} : \mathsf{K}(\mathbf{D}\mathsf{K}^*) \cdot \mathsf{K}^*]. \end{aligned} \tag{27}$$

Proceeding in a similar fashion as before and using Eqs. (8), (6), (14), and (19), we get

$$\begin{aligned} -[(\mathbf{D}\mathsf{K}) \cdot \mathsf{K}\mathsf{K}^* : \mathsf{K}^* + (\mathbf{D}\mathsf{K}^*) \cdot \mathsf{K}^*\mathsf{K} : \mathsf{K}] \\ = 4[(\mathbf{D}\mathsf{K}) \cdot \mathsf{K} \cdot \mathsf{K}^* \cdot \mathsf{K}^* + (\mathbf{D}\mathsf{K}^*) \cdot \mathsf{K}^* \cdot \mathsf{K} \cdot \mathsf{K}] \\ = 4[(\mathbf{D}\mathsf{K}) \cdot \mathsf{K}^* + (\mathbf{D}\mathsf{K}^*) \cdot \mathsf{K}] \cdot \mathsf{K} \cdot \mathsf{K}^* \\ = 4[\mathbf{D}(\mathsf{K} \cdot \mathsf{K}^*)] \cdot \mathsf{K} \cdot \mathsf{K}^* = (16\pi)^2\kappa^{-2}(\mathbf{D}\mathsf{R}) \cdot \mathsf{R}. \end{aligned}$$

Substituting this result back into Eq. (27) and using Eq. (20), we arrive at Eq. (22c).

Finally, substitution of Eq. (21) into Eq. (19) gives Eq. (1). This completes the proof of the necessity and sufficiency of the Rainich differential relation on R in order that the dyadic function G satisfying Eqs. (1) and (2) can be further restricted to satisfy Eq. (3). In particular, K can be modified to make $\mathsf{K} : \mathsf{K}$ real without changing Eq. (19) [for example, by choosing $\mathsf{K} = (8\pi\tau/\kappa)^{\frac{1}{2}}\hat{\mathsf{G}}$ with $\hat{\mathsf{G}}$ defined in accordance with Eq. (58) of I]; then Eq. (22c) becomes

$$\mathbf{D}\varphi = \mathbf{f}, \tag{28}$$

and integration of Eq. (28) gives

$$\varphi(x) = \int_{x_0}^{x} \mathbf{f}(x) \cdot \mathbf{d}x + \varphi(x_0), \tag{29}$$

which determines $\varphi(x)$ to within an additive constant.

[1] M. Rosenbaum and C. P. Luehr, Ann. Phys. (N.Y.) **60**, 384 (1970).

[2] Either $\mathsf{R}_s = 0$ or $\mathsf{T}_s = 0$ implies that the Einstein field equation reduces to $\mathsf{R} = \kappa\mathsf{T}$.

[3] The complex conjugate of a complex dyadic C is denoted by C^*. The dual $^\star\mathsf{A}$ of an antisymmetric dyadic A is given by $^\star\mathsf{A} = \frac{1}{2}\boldsymbol{\Gamma} : \mathsf{A}$, where $\boldsymbol{\Gamma}$ is the totally antisymmetric tetradic defined intrinsically in I. Additional notation used in this paper are the transpose B_T of a dyadic B, the scalar invariant C_s of a dyadic C, the unit dyadic I_4, and the covariant gradient operator **D**.

[4] Equation (3) is a form of Maxwell's equation. This equation and its complex conjugate equation $\mathbf{D} \cdot \mathsf{G}^* = 0$ are easily seen to be equivalent to the more familiar form of Maxwell's equations, $\mathbf{D} \cdot \mathsf{F} = 0$ and $\mathbf{D} \cdot {}^\star\mathsf{F} = 0$, in terms of the electromagnetic field tensor F, if we set $\mathsf{G} = \mathsf{F} - i\,{}^\star\mathsf{F}$ and $\mathsf{G}^* = \mathsf{F} + i\,{}^\star\mathsf{F}$. It also follows that Eq. (1) is equivalent to a better known expression $\mathsf{T} = (8\pi)^{-1}(\mathsf{F} \cdot \mathsf{F} + {}^\star\mathsf{F} \cdot {}^\star\mathsf{F})$ for the electromagnetic energy-momentum tensor.

[5] Note that, by virtue of Eq. (16), $(\mathbf{a} \cdot \mathbf{D}\mathsf{N}^*) \cdot \mathsf{M}$ is symmetric; therefore, $\boldsymbol{\Gamma} : [(\mathbf{a} \cdot \mathbf{D}\mathsf{N}^*) \cdot \mathsf{M}] = 0$. This explains why the last term in Eq. (11) does not occur in the particular case given by Eq. (14).

[6] Equation (17) makes possible a very easy proof of $\mathbf{D} \cdot \mathsf{T} = 0$ from the expression for T given by Eq. (1), where G satisfies Eqs. (2) and (3). The proof is

$$\mathbf{D} \cdot \mathsf{T} = (8\pi)^{-1}\mathbf{D} \cdot (\mathsf{G} \cdot \mathsf{G}^*) = (8\pi)^{-1}[(\mathbf{D} \cdot \mathsf{G}) \cdot \mathsf{G}^* + (\mathbf{D} \cdot \mathsf{G}^*) \cdot \mathsf{G}] = 0.$$

[7] L. Witten ["A Geometric Theory of the Electromagnetic and Gravitational Fields," in *Gravitation: An Introduction to Current Research*, edited by L. Witten (Wiley, New York, 1962)] also used the dyadic function K (in component form) in his proof of the necessity and sufficiency of the Rainich differential relation.

Eigenvalue Problem for Lagrangian Systems. IV

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(Received 21 September 1970)

The constants of the motion of the linear Lagrangian system $\ddot{\xi} + A\dot{\xi} + H\xi(t) = 0$ are shown to generate a useful class of orthogonality relations. For systems with complete sets of eigenvectors, these are used to derive the expansion coefficients for arbitrary initial data. We show that every stable system possesses a complete set of eigenvectors and that this set is the union of two basis sets.

I. INTRODUCTION

In several earlier papers,[1-3] we established orthogonality and completeness properties for the eigenvectors of the gyroscopic Lagrangian system

$$\ddot{\xi} + A\dot{\xi} + H\xi(t) = 0 \tag{1}$$

in the special case $H \geq 0$. The present article assumes, as before, that H and iA are linear time-independent Hermitian operators on and into the complex Hilbert space E; however, we now drop the restriction that $H \geq 0$ and assume E to be finite dimensional with $\dim E = n$. We consider the class V of Hermitian operators which are constants of the motion of the system, construct infinitely many of these, and show that the eigenvectors possess useful and general orthogonality relations with respect to the operators in V. For systems with complete sets of eigenvectors, the expansion coefficients are determined for arbitrary initial data. We find that the orthogonality and completeness properties obtained previously for systems with $H > 0$ generalize to arbitrary stable systems. In particular, it is shown that every stable system admits of a complete set S of $2n$ eigenvectors with real eigenvalues, where S is the union of two sets S_1 and S_2, each of which forms a basis for E. The sets S_1 and S_2 are orthonormal with respect to a positive definite "weight" operator P, and the contents of these sets are shown to satisfy self-adjoint eigenvalue problems of the form $\omega P\xi = Q\xi$, where Q is Hermitian, so that the usual variational principles obtain.

We shall employ the following notation: The inner product on E will be denoted by $(\ ,\ )$, the norm by $\|\ \|$, and the adjoint of a linear operator G will be denoted by $G^\dagger$.

II. THE EQUIVALENT FIRST-ORDER SYSTEM AND ITS CONSTANTS OF MOTION

We begin by converting Eq. (1) to an equivalent first-order system in the Hilbert space $E^2 \equiv E \times E$. The elements of E^2 will be denoted by two-component column vectors $\zeta = \binom{\zeta_1}{\zeta_2}$, where $\zeta_1, \zeta_2 \in E$, the inner product in E^2 will be denoted by $\langle \zeta, \eta\rangle = (\zeta_1, \eta_1) + (\zeta_2, \eta_2)$, and the norm in E^2 will be denoted by $\|\ \|_2$.

Let $\xi(t) \in E$ for $t \geq 0$ be a solution of the system $\ddot{\xi} + A\dot{\xi} + H\xi(t) = 0$ for $t \geq 0$ satisfying the initial data $\xi(0+) = \xi_0$, $\dot{\xi}(0+) = \dot{\xi}_0$. Then it is readily verified that $\zeta(t) \equiv \binom{\xi(t)}{\dot{\xi}(t)} \in E^2$ for $t \geq 0$ is a solution of the system

$$\dot{\zeta} = W\zeta(t), \quad t \geq 0, \tag{2}$$

satisfying the initial data $\zeta(0+) = \zeta_0 \equiv \binom{\xi_0}{\dot{\xi}_0}$, where $W \equiv \begin{pmatrix} 0 & I \\ -H & -A\end{pmatrix}$ maps E^2 into itself. We note that the unique solution of Eq. (2) for the initial data S_0 is given by $\zeta(t) = e^{Wt}\zeta_0$, exists for every $\zeta_0 \in E^2$, and is infinitely often differentiable. If $\zeta(t) = \binom{\zeta_1(t)}{\zeta_2(t)}$ satisfies Eq. (2) and the initial data $\zeta(0+) = \binom{\xi_0}{\dot{\xi}_0}$, then $\xi(t) = \zeta_1(t)$ satisfies Eq. (1) and the initial data $\xi(0+) = \xi_0$, $\dot{\xi}(0+) = \dot{\xi}_0$. Furthermore, $\xi(t) = \zeta_2(t)$ also satisfies Eq. (1). It follows that our first- and second-order systems are both stable or both unstable, i.e., each solution $\xi(t)$ of Eq. (1) satisfies $\|\xi(t)\| \leq M$ for some constant M and all $t \geq 0$ if and only if each solution $\zeta(t)$ of Eq. (2) satisfies $\|\zeta(t)\|_2 \leq N$ for some constant N and all $t \geq 0$. We summarize these results in the following theorem.

Theorem 1: Let $\xi(t)$ and $\zeta(t)$ be solutions of Eqs. (1) and (2), respectively, and let them satisfy the initial data $\zeta(0+) = \binom{\xi(0+)}{\dot{\xi}(0+)} = \binom{\xi_0}{\dot{\xi}_0} \in E^2$. Then

$$\zeta(t) = \begin{pmatrix}\xi(t)\\ \dot{\xi}(t)\end{pmatrix} = e^{Wt}\begin{pmatrix}\xi_0\\ \dot{\xi}_0\end{pmatrix}, \quad t \geq 0. \tag{3}$$

Solutions of Eqs. (1) and (2) exist for arbitrary initial data $\binom{\xi_0}{\dot{\xi}_0} \in E^2$, are unique, and are infinitely often differentiable. The system (1) is stable if and only if the system (2) is stable.

The orthogonality relations derived in Sec. III depend upon the existence of a certain class V of Hermitian operators which are constants of the motion of the system $\dot{\zeta} = W\zeta$. To be precise, we define V to be the class of all Hermitian operators G on and into E^2 such that $d\langle\zeta, G\zeta\rangle/dt \equiv 0$ for every solution $\zeta(t)$ of Eq. (2). One important element of V is the operator

$L \equiv \begin{pmatrix} -iA & -i \\ i & 0 \end{pmatrix}$, with the inverse $L^{-1} = \begin{pmatrix} 0 & -i \\ i & iA \end{pmatrix}$. Some useful properties of the class V are given in the next theorem.

Theorem 2:

(A) V is a linear vector space over the real numbers.

(B) $G \in V$ if and only if G and iGW are both Hermitian.

(C) $L \in V$.

(D) $G \in V$ if and only if $G = LF + F^\dagger L$, where F commutes with W.

(E) If $G \in V$, then $G(iW)^n \in V$ for all $n = 1, 2, 3, \cdots$.

Proof: Statement (A) is obvious. Let $\zeta(t)$ satisfy $\dot{\zeta} = W\zeta$ for $t \geq 0$, with $\zeta(0+) = \zeta_0$, and let M and F be two linear operators on and into E^2. Then

$$\begin{aligned}\frac{d}{dt}\langle \zeta, MF\zeta\rangle &= \langle \dot{\zeta}, MF\zeta\rangle + \langle \zeta, MF\dot{\zeta}\rangle \\ &= \langle W\zeta, MF\zeta\rangle + \langle \zeta, MFW\zeta\rangle \\ &= \langle \zeta, [W^\dagger MF + MFW]\zeta\rangle \\ &= \langle \zeta, \{M[FW - WF] + [MW + W^\dagger M]F\}\zeta\rangle, \\ & \qquad t \geq 0. \quad (4)\end{aligned}$$

We set $M = G$ and $F = I$ to obtain

$$\frac{d}{dt}\langle \zeta, G\zeta\rangle = \langle \zeta, [GW + W^\dagger G]\zeta\rangle, \quad t \geq 0. \quad (5)$$

Let G and iGW be Hermitian. Then $GW + W^\dagger G = 0$ so that $G \in V$ by Eq. (5).

Conversely, suppose $G \in V$, so that the left-hand side of Eq. (5) vanishes. Therefore, $\langle \zeta_0, [GW + W^\dagger G]\zeta_0\rangle = 0$ for every solution $\zeta(t)$ of Eq. (2), and, since solutions of (2) exist for arbitrary initial data $\zeta_0 \in E^2$, we must have $GW + W^\dagger G = 0$, which implies that iGW is Hermitian. This proves (B). Statement (C) follows from (B) since L and $iLW = -\begin{pmatrix} H & 0 \\ 0 & I \end{pmatrix}$ are both Hermitian. Now suppose that $G = LF + F^\dagger L$, where F commutes with W. Then G is Hermitian, and Eq. (4) with $M = L$ gives $d\langle \zeta, LF\zeta\rangle/dt = 0$. Hence $0 = d(2\,\mathrm{Re}\,\langle \zeta, LF\zeta\rangle)/dt = d\langle \zeta, [LF + F^\dagger L]\zeta\rangle/dt$, so that $G \in V$. Conversely, let $G \in V$. Define $F \equiv \frac{1}{2}L^{-1}G$, so that $LF = \frac{1}{2}G = F^\dagger L$ and $G = LF + F^\dagger L$. Equation (4) with $M = L$ and $t = 0+$ yields

$$\begin{aligned}0 = \frac{1}{2}\frac{d}{dt}\langle \zeta, G\zeta\rangle &= \frac{d}{dt}\langle \zeta, LF\zeta\rangle \\ &= \langle \zeta_0, L[FW - WF]\zeta_0\rangle,\end{aligned}$$

and therefore the right-hand side must vanish for all $\zeta_0 \in E^2$. This implies that $FW = WF$, which completes the proof of (D). Finally, if $G \in V$, $G(iW)$ is Hermitian by (B). Setting $M = G$ and $F = iW$ in Eq. (4), we obtain $d\langle \zeta, GiW\zeta\rangle/dt = 0$; thus $G \in V$ implies $GiW \in V$, so that $G(iW)^n \in V$ for all positive integers n.

The existence of a positive-definite operator $P \in V$ implies that the system (2) is stable and that its solution can be reduced to an eigenvalue problem of the form $\omega P\eta = Q\eta$, where Q is Hermitian. Indeed, if such a P exists, then for every solution $\zeta(t)$ of Eq. (2), we have

$$\delta\, \|\zeta(t)\|_2^2 \leq \langle \zeta, P\zeta\rangle = \langle \zeta_0, P\zeta_0\rangle, \quad t \geq 0,$$

where

$$\delta \equiv \inf_{E^2} \frac{\langle \eta, P\eta\rangle}{\langle \eta, \eta\rangle} > 0.$$

The insertion of a solution of the form $\zeta(t) = \eta \exp(i\omega t)$ into Eq. (2) yields, after multiplication by P, $\omega P\eta = -iPW\eta$, where $-iPW$ is Hermitian by Theorem 2(B). Thus the construction of a positive-definite element of V is, whenever possible, obviously highly desirable. Unfortunately, although we show in Sec. IV that V always contains a positive-definite P if the system is stable, there seems to be at this moment no direct way of computing P in the general case without first computing the eigenvalues and eigenvectors of W. In any given case one might try his luck with polynomials of the form $L[\sum_0^N a_k(iW)^k]$ with a_k real [every such operator is in V by Theorem 2(A) and (E)]; indeed, a positive-definite operator of this form always exists with $N \leq 2n$ if the system is stable and the eigenvalues of W are distinct. For example, if there should exist a real number α such that $\alpha iA + H > \alpha^2$, then one can readily verify that $L(-\alpha - iW)$ is positive definite.

III. ORTHOGONALITY RELATIONS

We assume solutions to Eq. (2) with a time dependence of the form $\exp(i\omega t)$, where ω is a real or complex number, and Eq. (2) yields the eigenvalue problem

$$\omega\zeta = T\zeta \quad (6)$$

for the eigenvalue ω and corresponding eigenvector $\zeta\ (\neq 0)$, where $T \equiv -iW = \begin{pmatrix} 0 & -i \\ iH & iA \end{pmatrix}$. We note that the adjoint of T is given by $T^\dagger = \begin{pmatrix} 0 & -iH \\ i & iA \end{pmatrix}$, $LT = K \equiv \begin{pmatrix} H & 0 \\ 0 & I \end{pmatrix} \in V$, and that the class V consists of all Hermitian operators G on and into E^2 such that GT is Hermitian [by Theorem 2(B)].

We define $S_\omega \equiv \{\zeta \mid \zeta \in E^2,\ \omega\zeta = T\zeta\}$ and $S_\omega^\dagger \equiv \{\zeta \mid \zeta \in E^2,\ \omega\zeta = T^\dagger\zeta\}$. If $S \subset E^2$ and G is any linear operator on and into E^2, then $G(S) \equiv \{\zeta \mid \zeta = G(\xi)$ for some $\xi \in S\}$. The complex conjugate of ω is denoted by $\bar{\omega}$.

Theorem 3:

(A) $\dim S_\omega^\dagger = \dim S_\omega$.
(B) $\dim S_{\bar{\omega}} = \dim S_\omega$.

Let $G \in V$. Then:

(C) S_λ is orthogonal to $G(S_\omega)$ if $\lambda \neq \bar{\omega}$.
(D) $S_\omega^\dagger \supset G(S_\omega)$. If G is invertible, then $S_\omega^\dagger = G(S_\omega)$.
(E) For real ω, there exists a basis for S_ω consisting of $m \equiv \dim S_\omega$ vectors $\zeta_1, \cdots, \zeta_m$ such that $\langle \zeta_k, G\zeta_l\rangle = \gamma_l\delta_{kl}$, where $\gamma_l = \pm 1$ or 0, $l = 1, 2, \cdots, m$.
(F) For nonreal ω, there exist bases $\{\zeta_1, \cdots, \zeta_m\}$ and $\{\hat{\zeta}_1, \cdots, \hat{\zeta}_m\}$ ($m \equiv \dim S_\omega = \dim S_{\bar{\omega}}$) of S_ω and $S_{\bar{\omega}}$, respectively, such that $\langle \zeta_k, G\zeta_l\rangle = 0$, $\langle \hat{\zeta}_k, G\hat{\zeta}_l\rangle = 0$, and $\langle \hat{\zeta}_k, G\zeta_l\rangle = \rho_k\delta_{kl}$, $k, l = 1, \cdots, m$, where $\rho_k = 1$ or 0, $k = 1, \cdots, m$.

Proof: Let $G \in V$ and $\zeta \in G(S_\omega)$. Then $\zeta = G\xi$, where $\omega\xi = T\xi$. Hence

$$\omega\zeta = \omega G\xi = GT\xi = T^\dagger G\xi = T^\dagger\zeta, \tag{7}$$

which implies that $\zeta \in S_\omega^\dagger$. Now suppose that G^{-1} exists, let $\eta \in S_\omega^\dagger$, and set $\rho \equiv G^{-1}\eta$. Then $\omega G\rho = \omega\eta = T^\dagger\eta = T^\dagger G\rho = GT\rho$. Hence $\rho \in S_\omega$ and $\eta = G\rho \in G(S_\omega)$, which proves (D). Since $L \in V$ and L^{-1} exists, we have $L(S_\omega) = S_\omega^\dagger$ and $\dim S_\omega = \dim S_\omega^\dagger$. Statement (B) now follows at once from the well-known theorem that the null spaces of a linear transformation and its adjoint have the same dimension (for finite-dimensional E). Now suppose $\zeta \in G(S_\omega)$ and $r \in S_\lambda$. We form the inner product of Eq. (7) with r to obtain $\bar{\omega}\langle\zeta, r\rangle = \langle T^\dagger\zeta, r\rangle = \langle\zeta, Tr\rangle = \lambda\langle\zeta, r\rangle$, which yields (C). Let ω be real, and let P_1 be the projector onto S_ω. Then S_ω is an invariant subspace for the Hermitian operator P_1GP_1, and there exists a basis for S_ω consisting of $m = \dim S_\omega$ orthonormal eigenvectors $\xi_1, \cdots, \xi_m$ of P_1GP_1 satisfying $\lambda_k\xi_k = P_1GP_1\xi_k$, λ_k real, $k = 1, 2, \cdots, m$. We define

$$\zeta_k = \begin{cases} \xi_k, & \lambda_k = 0 \\ \lambda_k^{-\frac{1}{2}}\xi_k, & \lambda_k \neq 0 \end{cases}, \quad k = 1, 2, \cdots, m.$$

Then $\langle\zeta_k, G\zeta_l\rangle = \langle\zeta_k, P_1GP_1\zeta_l\rangle = \gamma_k\delta_{kl}$, where

$$\gamma_k = \begin{cases} 0, & \lambda_k = 0 \\ 1, & \lambda_k > 0, \\ -1, & \lambda_k < 0 \end{cases}$$

which verifies (E). It remains to prove (F). Suppose that ω is not real. Let $m \equiv \dim S_{\bar{\omega}} = \dim S_\omega$, $r \equiv \dim G(S_\omega)$, $N \equiv \{\xi \mid \xi \in S_\omega,\ G\xi = 0\}$, $S \equiv \{\xi \mid \xi\ G(S_\omega),\ \xi \perp S_{\bar{\omega}}\}$, $\tilde{S}$ be the orthogonal complement of S with respect to $G(S_\omega)$, $q \equiv \dim \tilde{S}$, and P be the projector onto $S_{\bar{\omega}}$. Then $\dim N = m - r$, $\dim S = r - q$, and $\|P\eta\|_2 > 0$ for all nonzero $\eta \in \tilde{S}$. If $q = 0$, $G(S_\omega) \perp S_{\bar{\omega}}$, and we simply choose $\hat{\zeta}_1, \cdots, \hat{\zeta}_m$ and $\zeta_1, \cdots, \zeta_m$ to be any orthonormal bases of $S_{\bar{\omega}}$ and S_ω, respectively. Suppose $q > 0$. Choose $\eta_1 \in \tilde{S}$ so that $\|P\eta_1\|_2 = 1$, and take $\hat{\zeta}_1 = P\eta_1$. For $l = 2, \cdots, q$, choose $\eta_l \in \tilde{S}$ so that $\langle\eta_l, \hat{\zeta}_k\rangle = 0$ for $k = 1, 2, \cdots, l - 1$, where $\hat{\zeta}_k \equiv P\eta_k$, $k = 1, \cdots, q$. Let $\{\hat{\zeta}_{q+1}, \cdots, \hat{\zeta}_m\}$ be an orthonormal basis for the orthogonal complement of the span of $\{\hat{\zeta}_1, \cdots, \hat{\zeta}_q\}$ with respect to $S_{\bar{\omega}}$, let $\{\eta_{q+1}, \cdots, \eta_r\}$ be an orthonormal basis for S, choose $\zeta_1, \cdots, \zeta_r$ from S_ω so that $\eta_k = G(\zeta_k)$, $k = 1, 2, \cdots, r$, and let $\{\zeta_{r+1}, \cdots, \zeta_m\}$ be an orthonormal basis for N. Then $\{\eta_1, \cdots, \eta_r\}$ is a basis for $G(S_\omega)$, $\{\zeta_1, \cdots, \zeta_m\}$ is a basis for S_ω, $\{\hat{\zeta}_1, \cdots, \hat{\zeta}_m\}$ is an orthonormal basis for $S_{\bar{\omega}}$, and $\langle\hat{\zeta}_k, G\zeta_l\rangle = \rho_k\delta_{kl}$, where

$$\rho_k = \begin{cases} 1, & k = 1, \cdots, q \\ 0, & k = q + 1, \cdots, m \end{cases}.$$

Since $\omega \neq \bar{\omega}$, (C) implies that $\langle\zeta_k, G\zeta_l\rangle = 0$ and $\langle\hat{\zeta}_k, G\hat{\zeta}_l\rangle = 0$ for $k, l = 1, 2, \cdots, m$. This completes the proof of Theorem 3.

In general, since eigenvectors corresponding to distinct eigenvalues are linearly independent, $d \equiv \sum_\omega \dim S_\omega \leq 2n$. Let $G \in V$. Theorem 3 permits us to select our eigenvectors as follows: For each eigenvalue ω with $\operatorname{Im}\omega > 0$, choose bases for S_ω and $S_{\bar{\omega}}$ so that (F) holds, while, for each real eigenvalue ω, choose a basis for S_ω so that (E) holds. Let C denote the union of the bases thereby selected for the eigenspaces S_ω with $\operatorname{Im}\omega > 0$, let $\hat{C}$ denote the union of those bases selected for the corresponding eigenspaces $S_{\bar{\omega}}$, and let R denote the union of the bases selected for the S_ω with $\operatorname{Im}\omega = 0$. Then C and $\hat{C}$ each consist of

$$r \equiv \sum_{\operatorname{Im}\omega > 0} \dim S_\omega$$

linearly independent eigenvectors, and we enumerate the contents of these sets as $C = \{\eta_1, \eta_2, \cdots, \eta_r\}$ and $\hat{C} = \{\hat{\eta}_1, \cdots, \hat{\eta}_r\}$ so that $\langle\eta_k, G\hat{\eta}_l\rangle = \rho_k\delta_{kl}$ for $k, l = 1, 2, \cdots, r$. The set R consists of $d - 2r$ linearly independent vectors, which we enumerate as $R = \{\zeta_1, \cdots, \zeta_{d-2r}\}$ so that $\langle\zeta_k, G\zeta_l\rangle = \gamma_l\delta_{kl}$ for $k, l = 1, 2, \cdots, d - 2r$. By combining these results and using Theorem 3(C), the d eigenvectors thereby selected are linearly independent and satisfy the following orthogonality relations:

$$\left.\begin{aligned}\langle\eta_k, G\eta_l\rangle = 0, \langle\hat\eta_k, G\hat\eta_l\rangle = 0\\ \langle\eta_k, G\hat\eta_l\rangle = \rho_k\delta_{kl}\end{aligned}\right\}, \quad k, l = 1, \cdots, r, \tag{8}$$

$$\langle\eta_k, G\zeta_l\rangle = 0, \langle\hat\eta_k, G\zeta_l\rangle = 0, \quad k = 1, \cdots, r, \quad l = 1, \cdots, d - 2r,$$

$$\langle\zeta_k, G\zeta_l\rangle = \gamma_k\delta_{kl}, \quad k, l = 1, \cdots, d - 2r,$$

where $\rho_k = 1$ or 0 and $\gamma_k = \pm 1$ or 0. This leads us to the following definition: A set of d linearly independent eigenvectors $\{\eta_1, \cdots, \eta_r, \hat\eta_1, \cdots, \hat\eta_r, \zeta_1, \cdots, \zeta_{d-2r}\}$ such that

$$T\eta_k = \Omega_k\eta_k, \quad \operatorname{Im}\Omega_k > 0, \quad k = 1, \cdots, r,$$

$$T\hat\eta_k = \bar\Omega_k\hat\eta_k, \quad k = 1, \cdots, r,$$

$$T\zeta_k = \omega_k\zeta_k, \quad \operatorname{Im}\omega_k = 0, \quad k = 1, \cdots, d - 2r,$$

and satisfying Eqs. (8) for some $G \in V$ is said to be G-canonical. If, in addition, $d = 2n$, then we say that the set is a complete G-canonical set. Note that if ξ is an element of a G-canonical set, then $G\xi$ is orthogonal to all elements of the set except possibly one; hence, if G is invertible and if the set is complete, then no γ_k or ρ_k can be zero, i.e., $\gamma_l = \pm 1$ and $\rho_k = 1$ for $l = 1, \cdots, d - 2r$ and $k = 1, \cdots, r$.

Theorem 4: Let $d \equiv \sum_\omega \dim S_\omega = 2n$ (i.e., suppose that the eigenvectors of T span E^2) and let $G \in V$ be invertible. Then there exists a complete G-canonical set of eigenvectors $\{\eta_1, \cdots, \eta_r, \hat\eta_1, \cdots, \hat\eta_r, \zeta_1, \cdots, \zeta_{2(n-r)}\}$ satisfying Eqs. (8) with $\rho_k = 1$, $k = 1, \cdots, r$ and $\gamma_k = \pm 1$, $k = 1, \cdots, 2(n - r)$. For every $\zeta \in E^2$, we have

$$\zeta = \sum_1^{2(n-r)} \alpha_k\zeta_k + \sum_1^r (\beta_k\eta_k + \hat\beta_k\hat\eta_k) \tag{9}$$

and

$$\langle\zeta, G\zeta\rangle = \sum_1^{2(n-r)} |\alpha_k|^2 \gamma_k + 2 \operatorname{Re} \sum_1^r \bar\beta_k\hat\beta_k, \tag{10}$$

where

$$\alpha_k = \langle\zeta_k, G\zeta\rangle\gamma_k^{-1}, \quad \beta_k = \langle\hat\eta_k, G\zeta\rangle, \quad \hat\beta_k = \langle\eta_k, G\zeta\rangle. \tag{11}$$

Proof: It only remains to verify Eqs. (10) and (11), which follow immediately from Eqs. (8).

The operator L is always invertible and is a convenient element of V with which to form a canonical set of eigenvectors. The operator K might also be used, but K suffers from the limitation that K^{-1} exists only if H is invertible; furthermore, since $K = LT$, the eigenvectors of an L-canonical set exhibit their useful orthogonality properties with respect to K as well as L. The orthogonality relations of an L-canonical set can be rewritten in terms of E alone without any reference to E^2 by noting that ζ is an eigenvector of T with eigenvalue ω if and only if $\zeta = \binom{\xi}{i\omega\xi}$, where $\xi \neq 0$ and $H_\omega\xi \equiv (\omega^2 I - \omega iA - H)\xi = 0$. Such a nonzero ξ satisfying $H_\omega\xi = 0$ will be called an eigenvector of Eq. (1) with eigenvalue ω, since $\xi e^{i\omega t}$ satisfies Eq. (1). Thus, if $\{\eta_1, \cdots, \eta_r, \hat\eta_1, \cdots, \hat\eta_r, \zeta_1, \cdots, \zeta_{d-2r}\}$ is an L-canonical set, we have

$$\eta_k = \begin{pmatrix}\phi_k\\ i\Omega_k\phi_k\end{pmatrix}, \quad \hat\eta_k = \begin{pmatrix}\hat\phi_k\\ i\bar\Omega_k\hat\phi_k\end{pmatrix}, \quad k = 1, \cdots, r,$$

$$\zeta_l = \begin{pmatrix}\xi_l\\ i\omega_l\xi_l\end{pmatrix}, \quad l = 1, \cdots, d - 2r, \tag{12}$$

where ϕ_k, $\hat\phi_k$, and ξ_l are eigenvectors of Eq. (1) with eigenvalues Ω_k, $\bar\Omega_k$, and ω_l, respectively. The orthogonality relations (8) can now be expressed directly in terms of E; for example, the last of Eqs. (8) becomes

$$(\omega_k + \omega_l)(\xi_k, \xi_l) - (\xi_k, iA\xi_l) = \gamma_k\delta_{kl}, \quad k, l = 1, \cdots, d - 2r. \tag{13}$$

For a complete L-canonical set and $\zeta_0 = \binom{x}{\dot x} \in E^2$, Eqs. (8)–(11) give

$$x = \sum_1^{2(n-r)} \alpha_k\xi_k + \sum_1^r (\beta_k\phi_k + \hat\beta_k\hat\phi_k), \tag{14}$$

$$\dot x = \sum_1^{2(n-r)} \alpha_k i\omega_k\xi_k + \sum_1^r (\beta_k i\Omega_k\phi_k + \hat\beta_k i\bar\Omega_k\hat\phi_k), \tag{15}$$

$$2 \operatorname{Im}(x, \dot x) - (x, iAx) = \langle\zeta_0, L\zeta_0\rangle = \sum_1^{2(n-r)} |\alpha_k|^2 \gamma_k + 2 \operatorname{Re} \sum_1^r \bar\beta_k\hat\beta_k, \tag{16}$$

$$(x, Hx) + (\dot x, \dot x) = \langle\zeta_0, K\zeta_0\rangle = \sum_1^{2(n-r)} |\alpha_k|^2 \omega_k\gamma_k + 2 \operatorname{Re} \sum_1^r \bar\beta_k\hat\beta_k\bar\Omega_k, \tag{17}$$

with

$$\alpha_k = (\xi_k, (\omega_k x - iAx - i\dot x))\gamma_k^{-1}, \quad k = 1, \cdots, 2(n - r), \tag{18}$$

$$\beta_k = (\hat\phi_k, (\Omega_k x - iAx - i\dot x)), \quad k = 1, \cdots, r, \tag{19}$$

$$\hat\beta_k = (\phi_k, (\bar\Omega_k x - iAx - i\dot x)), \quad k = 1, \cdots, r, \tag{20}$$

and

$$\xi(t) = \sum_1^{2(n-r)} \alpha_k\xi_k \exp(i\omega_k t) + \sum_1^r [\beta_k\phi_k \exp(i\Omega_k t) + \hat\beta_k\hat\phi_k \exp(i\bar\Omega_k t)]$$

is the unique solution of Eq. (1) satisfying the initial data $\xi(0+) = x$, $\dot\xi(0+) = \dot x$. Equations (16) and (17) are equal, respectively, to the constants of motion

$$\left\langle \begin{pmatrix}\xi\\ \dot\xi\end{pmatrix}, L\begin{pmatrix}\xi\\ \dot\xi\end{pmatrix}\right\rangle = 2\,\mathrm{Im}\,(\xi, \dot\xi) - (\xi, iA\xi)$$

and

$$\left\langle \begin{pmatrix}\xi\\ \dot\xi\end{pmatrix}, K\begin{pmatrix}\xi\\ \dot\xi\end{pmatrix}\right\rangle = (\xi, H\xi) + (\dot\xi, \dot\xi).$$

IV. STABLE SYSTEMS

We now turn our attention to an important class of systems which always possess complete canonical sets of eigenvectors, namely, the class of stable systems. This fact is demonstrated in Theorem 5, and we show in the sequel that the eigenvectors of a complete L-canonical set possessing positive γ's form a basis for E, as do those with negative γ's. Finally, we show that $H_\omega \equiv \omega^2 - \omega iA - H$ factors into $(\omega - D_2^\dagger)(\omega - D_1)$, where D_1 and D_2 can be used to put the eigenvalue problem into self-adjoint form [see Eqs. (30)–(36)]. This provides variational principles for the eigenvalues; unfortunately, the construction of the pertinent operators requires (at least at the present stage of development) the knowledge of one or the other of the basis sets of eigenvectors. Duffin[4,5] has given minimax principles for the special subclass of stable systems where A and H satisfy $(\xi, iA\xi)^2 + 4(\xi, \xi)(\xi, H\xi) > 0$ for all $\xi \neq 0$, and these minimax principles are formulated directly in terms of A and H; however, it is a simple matter to find examples which show that these minimax principles are not valid for the general class of stable systems.

Theorem 5: The following statements are equivalent:

(A) System (2) [or system (1)] is stable.

(B) All the eigenvalues of T are real and, for any $G \in V$, there exists a complete G-canonical set of eigenvectors.

(C) V contains a positive-definite operator P.

Proof: We show that (A) implies (B), (B) implies (C), and (C) implies (A). Suppose the system is stable. By Theorem 3(B), the eigenvalues of T occur in complex conjugate pairs; hence, if all the eigenvalues of T are not real, there exists an eigenvalue ω with $\mathrm{Im}\,\omega < 0$. Let η be the corresponding eigenvector. Then $\zeta(t) = \eta e^{i\omega t}$ satisfies Eq. (2) and is exponentially unbounded. Thus (A) implies that all the eigenvalues of T are real. Now E^2 is the direct sum of the subspaces of generalized eigenvectors of T corresponding to the eigenvalues ω; hence, if $\sum_\omega \dim S_\omega < 2n$, there exists a generalized eigenvector η of rank 2, i.e., for some eigenvalue ω there exists $\eta \in E^2$ such that $(T - \omega)\eta \neq 0$ and $(T - \omega)^2\eta = 0$. Then $\zeta(t) \equiv [it(T - \omega)\eta + \eta]\exp i\omega t$ satisfies Eq. (2) and is unbounded since ω is real. Thus (A) implies (B). Suppose now that (B) holds, so that there exists a complete L-canonical set of eigenvectors $\{\zeta_1, \cdots, \zeta_{2n}\}$ with real eigenvalues $\omega_1, \cdots, \omega_{2n}$. For $\zeta \in E^2$, we define the linear operator P by

$$P\zeta \equiv \sum_1^{2n} \langle L\zeta_k, \zeta\rangle L\zeta_k. \tag{21}$$

Then

$$\langle \zeta, P\zeta\rangle = \sum_1^{2n} \langle L\zeta_k, \zeta\rangle\langle \zeta, L\zeta_k\rangle = \sum_1^{2n} |\langle L\zeta_k, \zeta\rangle|^2 \geq 0,$$

where the equality holds if and only if $\zeta = 0$, since the ζ_k are linearly independent and L is invertible. Furthermore,

$$\begin{aligned}\langle \zeta, PT\zeta\rangle &= \sum_1^{2n} \langle L\zeta_k, T\zeta\rangle\langle \zeta, L\zeta_k\rangle\\ &= \sum_1^{2n} \langle \zeta_k, LT\zeta\rangle\langle \zeta, L\zeta_k\rangle\\ &= \sum_1^{2n} \langle LT\zeta_k, \zeta\rangle\langle \zeta, L\zeta_k\rangle\\ &= \sum_1^{2n} \omega_k\langle L\zeta_k, \zeta\rangle\langle \zeta, L\zeta_k\rangle\\ &= \sum_1^{2n} \omega_k\, |\langle L\zeta_k, \zeta\rangle|^2,\end{aligned}$$

which is real. Thus P and PT are Hermitian and P is positive definite. By Theorem 2(B), $P \in V$. That (C) implies (A) was demonstrated at the end of Sec. II.

Lemma 1: Let $\xi_1, \cdots, \xi_m$ be m linearly independent eigenvectors of Eq. (1) with real eigenvalues ω_k, where

$$(\omega_k + \omega_l)(\xi_k, \xi_l) - (\xi_k, iA\xi_l) = \gamma_k\delta_{kl}, \quad k, l = 1, \cdots, m. \tag{22}$$

Let $F(x)$ be the $m \times m$ matrix defined for all $x \in (-\infty, \infty)$ by

$$F_{kl}(x) \equiv x^2(\xi_k, \xi_l) - x(\xi_k, iA\xi_l) - (\xi_k, H\xi_l), \quad k, l = 1, \cdots, m. \tag{23}$$

Then, if $\gamma_k > 0$ for all $k = 1, \cdots, m$, $F(x)$ is positive definite for $x > \max_{1\leq k\leq m}\omega_k$, while if $\gamma_k < 0$ for all $k = 1, \cdots, m$, then $F(x)$ is positive definite for $x < \min_{1\leq k\leq m}\omega_k$.

Proof: Equation (22) implies $\langle \zeta_k, L\zeta_l\rangle = \gamma_k\delta_{kl}$, where

$$\zeta_k = \begin{pmatrix}\xi_k\\ i\omega_k\xi_k\end{pmatrix}, \quad k = 1, \cdots, m.$$

Then

$$(\xi_k, H\xi_l) + \omega_k\omega_l(\xi_k, \xi_l) = \langle\zeta_k, K\zeta_l\rangle = \langle\zeta_k, LT\zeta_l\rangle = \omega_l\langle\zeta_k, L\zeta_l\rangle = \omega_l\gamma_k\delta_{kl}. \quad (24)$$

Eliminating $(\xi_k, H\xi_l)$ and $(\xi_k, iA\xi_l)$ from Eq. (23) by means of Eqs. (22) and (24), we obtain

$$F_{kl}(x) = (r_k, r_l) + (x - \omega_l)\gamma_k\delta_{kl}, \quad (25)$$

where $r_k \equiv (x - \omega_k)\xi_k$, $k = 1, \cdots, m$. The vectors $\xi_1, \cdots, \xi_m$ are linearly independent; thus, if $x \neq \omega_k$ for all $k = 1, \cdots, m$, the m vectors r_k are also linearly independent and therefore the $m \times m$ matrix $R(x)$ defined by $R_{kl} \equiv (r_k, r_l)$, $k, l = 1, \cdots, m$, is positive definite. The $m \times m$ matrix $M(x)$ defined by $M_{kl} \equiv (x - \omega_l)\gamma_k\delta_{kl}$, $k, l = 1, \cdots, m$, will be positive definite if either of the following holds: (1) $x > \max_{1\leq k\leq m} \omega_k$ and $\gamma_k > 0$ for all $k = 1, \cdots, m$ or (2) $x < \min_{1\leq k\leq m} \omega_k$ and $\gamma_k < 0$ for all $k = 1, \cdots, m$. Thus the hypothesis of the lemma implies that $F(x)$ is the sum of two positive-definite matrices, and the proof is complete.

Lemma 2: Let $\xi_1, \cdots, \xi_q$ be q eigenvectors of Eq. (1) with distinct real eigenvalues $\omega_1, \cdots, \omega_q$.

(A) If $\gamma_k \equiv 2\omega_k(\xi_k, \xi_k) - (\xi_k, iA\xi_k) > 0$ for all $k = 1, \cdots, q$, then the vectors $\xi_1, \cdots, \xi_q$ are linearly independent.

(B) If $\gamma_k < 0$ for all $k = 1, \cdots, q$, then the vectors $\xi_1, \cdots, \xi_q$ are linearly independent.

Proof: (A) The proof is by induction. Suppose that $\gamma_k > 0$ for all $k = 1, \cdots, q$. We assume for convenience that $\omega_1 < \omega_2 < \cdots < \omega_q$. The vector ξ_1 forms a linearly independent set. Suppose that the vectors $\xi_1, \cdots, \xi_m$ are linearly independent for some $m < q$. Since the ω_k are distinct, Theorem 3(C) implies that Eq. (22) holds, and therefore the previous lemma guarantees that the $m \times m$ matrix $F(x)$, defined by Eq. (23), is positive definite for $x > \omega_m$. If the set $\{\xi_1, \cdots, \xi_{m+1}\}$ is linearly dependent, then $\xi_{m+1} = \sum_1^m \alpha_k\xi_k$, and the product of $F(\omega_{m+1})$ with the nonzero column vector

$$\alpha \equiv \begin{pmatrix} \alpha_1 \\ \cdot \\ \cdot \\ \cdot \\ \alpha_m \end{pmatrix}$$

gives

$$[F(\omega_{m+1})\alpha]_k = \sum_{l=1}^m \alpha_l[\omega_{m+1}^2(\xi_k, \xi_l) - \omega_{m+1}(\xi_k, iA\xi_l) - (\xi_k, H\xi_l)] = (\xi_k, (\omega_{m+1}^2 - \omega_{m+1}iA - H)\xi_{m+1}) = 0, \quad (26)$$

$k = 1, \cdots, m$, i.e., $F(\omega_{m+1})\alpha = 0$ for $\alpha \neq 0$, which contradicts $F(\omega_{m+1}) > 0$. Hence the linear independence of the vectors $\xi_1, \cdots, \xi_m$ implies the linear independence of the vectors $\xi_1, \cdots, \xi_{m+1}$. The proof of (B) is similar, except that it is more convenient to assume here that $\omega_1 > \omega_2 > \cdots > \omega_q$.

Theorem 6: Let $\xi_1, \cdots, \xi_m$ be m eigenvectors of Eq. (1) with real eigenvalues ω_k satisfying Eq. (22). If the γ_k are either all positive or all negative, then $\{\xi_1, \cdots, \xi_m\}$ is linearly independent.

Proof: Let all the γ_k be of one sign. The set $\{\omega_1, \cdots, \omega_m\}$ consists of $r \leq m$ distinct real numbers $\Omega_1, \cdots, \Omega_r$. For each eigenvalue

$$\omega \in \{\omega_1, \cdots, \omega_m\} = \{\Omega_1, \cdots, \Omega_r\},$$

we define $J(\omega) \equiv \{k \mid \omega_k = \omega, 1 \leq k \leq m\}$. Let $\sum_1^m \alpha_k\xi_k = 0$. Then $\sum_1^r \psi_l = 0$, where

$$\psi_l \equiv \sum_{J(\Omega_l)} \alpha_k\xi_k, \quad l = 1, \cdots, r. \quad (27)$$

Suppose some $\psi_l \neq 0$. We may then assume, without loss of generality, that $\psi_l \neq 0$ for $l = 1, \cdots, q$ and $\psi_l = 0$ for $l = q + 1, \cdots, r$, so that $\sum_1^q \psi_l = 0$. The $\psi_1, \cdots, \psi_q$ are eigenvectors of Eq. (1) with distinct real eigenvalues $\Omega_1, \cdots, \Omega_q$, and Eq. (27) gives

$$\Gamma_l \equiv 2\Omega_l(\psi_l, \psi_l) - (\psi_l, iA\psi_l) = \sum_{j,k\in J(\Omega_l)} \bar{\alpha}_j\alpha_k[2\Omega_l(\xi_j, \xi_k) - (\xi_j, iA\xi_k)] = \sum_{J(\Omega_l)} |\alpha_k|^2 \gamma_k, \quad l = 1, \cdots, r$$

by Eq. (22), so that the Γ_l have the same sign as the γ_k. Therefore, Lemma 2 implies that $\{\psi_1, \cdots, \psi_q\}$ is linearly independent, which contradicts $\sum_1^q \psi_l = 0$. Hence

$$0 = \psi_l = \sum_{J(\Omega_l)} \alpha_j\xi_j, \quad l = 1, \cdots, r.$$

Therefore, for each $k \in J(\Omega_l)$,

$$0 = \left(\xi_k, [2\Omega_l - iA] \sum_{J(\Omega_l)} \alpha_j\xi_j\right) = \sum_{J(\Omega_l)} \alpha_j[2\Omega_l(\xi_k, \xi_j) - (\xi_k, iA\xi_j)] = \alpha_k\gamma_k$$

by Eq. (22), so that $\alpha_k = 0$ for $k = 1, \cdots, m$, and $\{\xi_1, \cdots, \xi_m\}$ is linearly independent.

Theorem 7: Every complete L-canonical set of eigenvectors

$$\zeta_k = \begin{pmatrix} \xi_k \\ i\omega_k\xi_k \end{pmatrix}$$

with real eigenvalues ω_k can be enumerated so that

$$\langle\zeta_k, L\zeta_l\rangle = \gamma_k\delta_{kl}, \quad k, l = 1, \cdots, 2n, \quad (28)$$

where

$$\gamma_k = \begin{cases} 1 & k = 1, \cdots, n \\ -1 & k = n+1, \cdots, 2n \end{cases}. \quad (29)$$

Each of the sets $\{\xi_1, \cdots, \xi_n\}$ and $\{\xi_{n+1}, \cdots, \xi_{2n}\}$ is a basis for E, and there exist linear operators D_1 and D_2 from E into E with the following properties:

$$D_1 + D_2^\dagger = iA, \quad D_2^\dagger D_1 = -H, \quad (30)$$

$$\omega^2 - \omega iA - H = (\omega - D_2^\dagger)(\omega - D_1), \quad (31)$$

$$P \equiv D_1 - D_2 > 0, \quad (32)$$

$$(\xi_k, P\xi_l) = \delta_{kl},$$

$$k, l = 1, \cdots, n, \quad \text{and} \quad k, l = n+1, \cdots, 2n, \quad (33)$$

$$D_1\xi_k = \omega_k\xi_k, \quad D_2\xi_{k+n} = \omega_{k+n}\xi_{k+n}, \quad k = 1, \cdots, n, \quad (34)$$

$$\omega_k P\xi_k = (H + D_1^\dagger D_1)\xi_k, \qquad k = 1, \cdots, n, \quad (35)$$

$$\omega_k P\xi_k = -(H + D_2^\dagger D_2)\xi_k, \quad k = n+1, \cdots, 2n. \quad (36)$$

Proof: The $2n$ numbers γ_k of a complete L-canonical set of eigenvectors

$$\zeta_k = \begin{pmatrix} \xi_k \\ i\omega_k\xi_k \end{pmatrix}$$

with real eigenvalues ω_k assume the values ± 1, $k = 1, \cdots, 2n$, and the ξ_k satisfy Eq. (22) for $k, l = 1, \cdots, 2n$. The number of vectors in each of the disjoint sets $S_1 \equiv \{\xi_k \mid \gamma_k = 1\}$ and $S_2 \equiv \{\xi_k \mid \gamma_k = -1\}$ totals $2n$; by Theorem 6, S_1 and S_2 are linearly independent subsets of E and hence contain no more than n vectors each, which implies that S_1 and S_2 both contain precisely n vectors. We can always label the ζ_k so that $S_1 = \{\xi_1, \cdots, \xi_n\}$ and $S_2 = \{\xi_{n+1}, \cdots, \xi_{2n}\}$, in which case Eqs. (28) and (29) hold. Let $\xi \in E$. Since $S_1 = \{\xi_1, \cdots, \xi_n\}$ is a basis for E, $\xi = \sum_1^n \alpha_k\xi_k$, where the α_k are uniquely determined. We define D_1 by $D_1\xi \equiv \sum_1^n \alpha_k\omega_k\xi_k$. Thus $D_1\xi_k = \omega_k\xi_k, k = 1, \cdots, n$, and

$$(D^2 - iAD_1 - H)\xi = \sum_1^n \alpha_k(D_1^2 - iAD_1 - H)\xi_k$$
$$= \sum_1^n \alpha_k(\omega_k^2 - \omega_k iA - H)\xi_k = 0$$

for all $\xi \in E$, so that $H = (D_1 - iA)D_1$. Equations (30) and (31) are now immediate consequences of the definition $D_2 \equiv iA - D_1^\dagger$. Let $P \equiv D_1 - D_2 = D_1^\dagger + D_1 - iA$. Then

$$(\xi_k, P\xi_l) = (D_1\xi_k, \xi_l) + (\xi_k, [D_1 - iA]\xi_l)$$
$$= (\xi_k, [\omega_k + \omega_l - iA]\xi_l) = \delta_{kl},$$
$$k, l = 1, \cdots, n,$$

and

$$(\xi, P\xi) = \sum_1^n \bar{\alpha}_k\alpha_l(\xi_k, P\xi_l) = \sum_1^n |\alpha_k|^2 > 0 \quad \text{for} \quad \xi \neq 0.$$

Now $PD_1 = (D_1^\dagger + D_1 - iA)D_1 = D_1^\dagger D_1 + (D_1 - iA)D_1 = D_1^\dagger D_1 + H$, and therefore

$$\omega_k P\xi_k = PD_1\xi_k = (H + D_1^\dagger D_1)\xi_k, \quad k = 1, \cdots, n.$$

Let $1 \leq k \leq n$, $n + 1 \leq j \leq 2n$; then

$$(\xi_k, [\omega_j - D_2]\xi_j) = (\xi_k, [\omega_j + D_1^\dagger - iA]\xi_j)$$
$$= (D_1\xi_k, \xi_j) + (\xi_k, [\omega_j - iA]\xi_j)$$
$$= (\xi_k, [\omega_k + \omega_j - iA]\xi_j) = 0,$$

so that $(\omega_j - D_2)\xi_j$ is orthogonal to every vector in the basis S_1. Hence $(D_2 - \omega_j)\xi_j = 0, j = n + 1, \cdots, 2n$. Note that $P = D_1 - D_2 = D_1^\dagger - D_2^\dagger = iA - D_2 - D_2^\dagger$ and thus, for $n + 1 \leq k, l \leq 2n$, we have

$$(\xi_k, P\xi_l) = -(\xi_k, (D_2^\dagger + D_2 - iA)\xi_l)$$
$$= -(\xi_k, (\omega_k + \omega_l - iA)\xi_l) = -\gamma_k\delta_{kl} = \delta_{kl},$$

which completes the proof of Eq. (33). Since $H = (D_1 - iA)D_1 = D_1^\dagger(D_1^\dagger - iA) = (D_2 - iA)D_2$,

$$PD_2 = -(D_2^\dagger + D_2 - iA)D_2 = -D_2^\dagger D_2 - H,$$

which implies Eq. (36).

ACKNOWLEDGMENT

The work presented here was sponsored by the U.S. Atomic Energy Commission.

[1] E. M. Barston, J. Math. Phys. **8**, 523 (1967).
[2] E. M. Barston, J. Math. Phys. **8**, 1886 (1967).
[3] E. M. Barston, J. Math. Phys. **9**, 2069 (1968).
[4] R. J. Duffin, J. Ratl. Mech. Anal. **4**, 221 (1955).
[5] R. J. Duffin, Quart. J. Appl. Math. **18**, 215 (1960).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Some General Inequalities in Quantum Statistical Mechanics*

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(Received 17 December 1970)

Let $H = H_0 + \lambda H_1$ be the Hamiltonian of a system where λ is a coupling parameter for the interaction H_1. The partition function $Z = \text{Tr} \exp(-\beta H)$ is then a function of both λ and β. We investigate various general inequalities involving derivatives of $\log Z$ with respect to β and λ.

I. INTRODUCTION AND SUMMARY OF RESULT

Let us consider a Hamiltonian of form

$$H = H_0 + \lambda H_1, \tag{1}$$

where H_0 is an unperturbed (not necessarily free) Hamiltonian and λH_1 is an unspecified interaction with coupling parameter λ. The thermodynamical partition function Z defined by

$$Z = \text{Tr} \exp(-\beta H) \tag{2}$$

is obviously a function of λ as well as of $\beta = 1/kT$, where k and T are the Boltzmann constant and the temperature, respectively. It is known[1] that the inequality

$$\frac{\partial^2}{\partial \lambda^2} \log Z \geq 0 \tag{3}$$

is valid irrespective of any dynamical detail. This inequality can also be derived as a direct consequence of the convexity theorem.[2]

Equation (3) has been applied by Bogoliubov[1] in proving asymptotic exactness of the free energy expression for a system with four-fermion positive interaction. Kadanoff and Baym[3] have shown an inconsistency of the random phase approximation and Hartree–Fock methods in some physical problems by means of this inequality. Also, if λH_1 represents the electromagnetic interaction of an isotropic medium with a constant external magnetic (or electric) field whose field strength is λ, then Eq. (3) implies that the magnetic (or electric) susceptibility is always nonnegative, a result known[4] for the case of the zero field limit.

The purpose of this paper is to show that we can derive some generalizations of this inequality. Defining the expectation value of an operator Q by the standard formula

$$\langle Q \rangle = (1/Z) \text{Tr} [Q \exp(-\beta H)], \tag{4}$$

we can first prove inequalities

$$M \geq \frac{\partial^2}{\partial \lambda^2} \log Z \geq \max(M_1, M_2) \geq 0, \tag{5}$$

where M, M_1, and M_2 are given by

$$M = \beta^2 \langle \bar{H}_1 \bar{H}_1 \rangle, \quad \bar{H}_1 = H_1 - \langle H_1 \rangle, \tag{6}$$

$$M_1 = M - \tfrac{1}{12}\beta^4 \langle KK \rangle, \quad K = i[H_0, H_1], \tag{7}$$

$$M_2 = \beta\, |\langle [C, H_1] \rangle|^2 / \langle [[C, H], C^+] \rangle \geq 0. \tag{8}$$

In Eq. (8), the operator C is arbitrary. The upper bound $(\partial^2/\partial\lambda^2) \log Z = M$ in Eq. (5) is attainable if and only if H_0 and H_1 commute[3] with each other as in classical mechanics. Also, Eq. (7) indicates a measure of the deviation from the maximally possible value M for $(\partial^2/\partial\lambda^2) \log Z$. Indeed, it suggests that the latter will asymptotically approach the maximal value M in the extreme high temperature limit $\beta \to 0$. We will give an application of Eq. (8) in the next section.

With respect to the temperature dependence, we can prove inequalities

$$\xi \frac{\partial^2}{\partial \beta^2} \log Z \geq \beta \left(\frac{\partial^2 F}{\partial \lambda \partial \beta} \right)^2, \tag{9}$$

$$\frac{\partial^2}{\partial \beta^2} \log \xi + 2 \frac{\partial^2}{\partial \beta^2} \log Z + \frac{1}{\beta^2} \geq 0, \tag{10}$$

$$\frac{\partial^2}{\partial \beta^2} \log \xi + \frac{\partial^2}{\partial \beta^2} \log Z + \frac{1}{\beta^2} + \frac{2}{\xi} \beta \left(\frac{\partial^2 F}{\partial \beta \partial \lambda} \right)^2 \geq 0, \tag{11}$$

$$\frac{\partial^2}{\partial \beta^2} \log \left[\xi + \beta \left(\frac{\partial F}{\partial \lambda} \right)^2 \right] + \frac{\partial^2}{\partial \beta^2} \log Z + \frac{1}{\beta^2} \geq 0, \tag{12}$$

where, for simplicity, we have set

$$\xi \equiv \beta^{-1} \frac{\partial^2}{\partial \lambda^2} \log Z \geq 0, \tag{13}$$

$$F \equiv -\beta^{-1} \log Z. \tag{14}$$

Notice that F is the Helmholtz energy. In particular, Eq. (9) leads to an inequality

$$\frac{1}{4\pi} (\mu - 1) C_v \geq k \beta^3 \left(\frac{\partial M}{\partial \beta} \right)_v^2, \tag{15}$$

where μ, C_v, and M are the permeability, specific heat at constant volume, and magnetization of the system, respectively.

If $\sigma(\omega)$ represents any diagonal component of an electric conductivity tensor for frequency ω, then we can also show an inequality

$$\frac{\partial^2}{\partial\beta^2}\log \operatorname{Re}\sigma(\omega) + \frac{\partial^2}{\partial\beta^2}\log Z + \frac{\hbar^2\omega^2}{4}\left(\frac{1}{\sinh(\hbar\omega\beta/2)}\right)^2 \geq 0. \quad (16)$$

Finally, if E_0 is the ground state energy of the Hamiltonian H, then we find

$$\frac{\partial}{\partial\beta}\log\xi + \left(E_0 + \frac{\partial}{\partial\beta}\log Z\right) \leq \frac{1}{\beta}, \quad (17)$$

$$\frac{\partial}{\partial\beta}\log \operatorname{Re}\sigma(\omega) + \left(E_0 + \frac{\partial}{\partial\beta}\log Z\right) \leq \frac{\hbar\omega}{1-\exp(-\hbar\beta\omega)}. \quad (18)$$

Details of these derivations as well as some more general inequalities will be given in the next section.

II. FORMULATION AND DERIVATION

In order to maintain generality, we will consider a general Hamiltonian of form

$$H = H_0 + \sum_{j=1}^{n}\lambda_j H_j \quad (19)$$

rather than Eq. (1). If we choose $n = 1$, it will reduce to Eq. (1) and we will always then set $\lambda_1 = \lambda$.

First, taking a derivative of Z with respect to the jth coupling parameter λ_j, we find

$$\frac{\partial Z}{\partial\lambda_j} = -\beta\operatorname{Tr}(H_j\exp(-\beta H)). \quad (20)$$

Notice that in obtaining Eq. (20) we need not worry[5] about possible effects of noncommutativity among operators H_j and H_i, $i = 0, 1, \cdots, n$, because of the cyclic invariance of the trace. Another way of deriving Eq. (20) is to start with the eigenvalue problem

$$H|n\rangle = E_n|n\rangle. \quad (21)$$

Although both E_n and $|n\rangle$ depend in general upon the parameter λ_j, the well-known variational principle enables us[5,6] to have

$$\frac{\partial E_n}{\partial\lambda_j} = \langle n|H_j|n\rangle, \quad (22)$$

where we normalized the state vector by $\langle n|n\rangle = 1$. Rewriting Z as

$$Z = \sum_n \exp(-\beta E_n) \quad (23)$$

and taking its derivative with respect to λ_j, we obtain Eq. (20) again when we use Eq. (22).

Next, we would like to compute the second-order derivative. To achieve this, we use the imaginary time formulation[7,8] and introduce the interaction and Heisenberg operators, respectively, by

$$Q^{\text{in}}(\tau) = \exp(H_0\tau)Q\exp(-H_0\tau),$$
$$Q(\tau) = \exp(H\tau)Q\exp(-H\tau) \quad (24)$$

for an arbitrary Schrödinger operator Q. The well-known operator technique[7,8] then enables us to rewrite Eq. (20) as

$$\frac{\partial Z}{\partial\lambda_j} = -\beta\operatorname{Tr}[\exp(-\beta H_0)U(\beta,0)H_j^{in}(0)], \quad (25)$$

where the transformation function $U(\beta, 0)$ is given by

$$U(\beta,0) \equiv \exp(\beta H_0)\exp(-\beta H) = T\exp\left(-\int_0^\beta d\tau\sum_{j=1}^{n}\lambda_j H_j^{in}(\tau)\right). \quad (26)$$

Taking the derivative of both sides of Eq. (25) with respect to λ_i and re-expressing the final result in terms of Heisenberg operators, we find

$$\frac{\partial^2 Z}{\partial\lambda_i\partial\lambda_j} = \beta\int_0^\beta d\tau\operatorname{Tr}[\exp(-\beta H)H_i(\tau)H_j(0)] = \beta Z\int_0^\beta d\tau\langle H_i(\tau)H_j(0)\rangle. \quad (27)$$

From this, we now compute

$$\frac{\partial^2\log Z}{\partial\lambda_i\partial\lambda_j} = \beta\int_0^\beta d\tau\langle\bar{H}_i(\tau)\bar{H}_j(0)\rangle, \quad (28)$$

where $\bar{H}_j(\tau)$ is defined by

$$\bar{H}_j(\tau) = \exp(H\tau)\bar{H}_j\exp(-H\tau) = H_j(\tau) - \langle H_j\rangle. \quad (29)$$

By means of Eq. (28), we could compute

$$\partial^2\log Z/\partial\lambda_i\partial\lambda_j$$

in terms[7,8] of the familiar Feynman diagram technique. However, we avoid the use of the perturbation method in this paper.

Inserting the completeness condition $\sum_n |n\rangle\langle n| = 1$ in the calculation of the integral in Eq. (28), we obtain

$$\frac{\partial^2}{\partial\lambda_i\partial\lambda_j}\log Z = Z^{-1}\beta^2\sum_{n,m}\varphi(-\beta E_n, -\beta E_m)\langle n|\bar{H}_i|m\rangle\langle m|\bar{H}_j|n\rangle, \quad (30)$$

where for simplicity we have set

$$\varphi(x, y) \equiv [1/(x - y)](e^x - e^y). \tag{31}$$

This equation is the starting point of our method. We may remark that Eq. (30) can also be obtained directly from Eq. (23) if we use a formula[9]

$$\frac{\partial^2 E_n}{\partial \lambda_i \partial \lambda_j} = -\sum_m{}' \frac{1}{E_m - E_n} [\langle n| H_i |m\rangle\langle m| H_j |n\rangle + (i \leftrightarrow j)], \tag{32}$$

where the summation over m excludes the state $m = n$, and we have assumed that there is no degeneracy of eigenvalues. The formula Eq. (30) reduces to the familiar second-order perturbation result[4] if we set $\lambda = 0$ with $n = 1$. (This n should not be confused with those specifying the energy eigenstates.)

First, let us observe that $\varphi(x, y)$ defined by Eq. (31) satisfies a well-known inequality

$$\tfrac{1}{2}(e^x + e^y) \geq \varphi(x, y) \geq 0 \tag{33}$$

for arbitrary real numbers x and y. Then, after some simple algebra, it is easy to see that Eq. (30) gives us inequalities

$$\sum_{i,j=1}^{n} C_i^* \frac{\partial^2 \log Z}{\partial \lambda_i \partial \lambda_j} C_j \geq 0, \tag{34}$$

$$\sum_{i,j=1}^{n} C_i^* \left(\beta^2 \langle \bar{H}_i \bar{H}_j\rangle - \frac{\partial^2 \log Z}{\partial \lambda_i \partial \lambda_j}\right) C_j \geq 0 \tag{35}$$

for arbitrary real or complex numbers C_j, $j = 1, \cdots, n$.

Moreover, if we note another inequality

$$0 \geq \varphi(x, y) - \tfrac{1}{2}(e^x + e^y) \geq -\tfrac{1}{24}(x - y)^2(e^x + e^y), \tag{36}$$

we can derive analogously

$$\sum_{i,j=1}^{n} C_i^* \left(\frac{\partial^2 \log Z}{\partial \lambda_i \partial \lambda_j} - \beta^2 \langle \bar{H}_i \bar{H}_j\rangle + \tfrac{1}{12}\beta^4 \langle K_i K_j\rangle\right) C_j \geq 0, \tag{37}$$

where K_j is given by a commutator

$$K_j \equiv i[H, H_j]. \tag{38}$$

In particular, when we restrict ourselves to the case $n = 1$ with $\lambda_1 = \lambda$, then these inequalities give us

$$M \geq \frac{\partial^2}{\partial \lambda^2} \log Z \geq \max(0, M_1) \geq 0,$$

where M and M_1 are defined by Eqs. (6) and (7). The upper bound $\varphi(x, y) = \frac{1}{2}(e^x + e^y)$ in Eq. (33) is now possible only for $x = y$. Hence, the equality in Eq. (35) is possible if and only if $\sum_{j=1}^{n} C_j \bar{H}_j$ has no nondiagonal matrix element, i.e., we must have $\sum_{j=1}^{n} C_j [H, \bar{H}_j] = 0$. Especially for $n = 1$, this implies that the upper bound M in Eq. (5) is attainable if and only if H_0 commutes with H_1.[3] Similarly, an equality in Eq. (34) is possible only when we have $\sum_{j=1}^{n} C_j \bar{H}_j = 0$. Since we can eliminate all linearly dependent interactions, if any, from the beginning, we can assume without loss of generality that the n operators $\bar{H}_j$, $j = 1, \cdots, n$, are linearly independent. Therefore, the equality in Eq. (34) is possible solely if we have $C_j = 0$ for all $j = 1, \cdots, n$. Hence, we conclude that $\partial^2 \log Z/\partial\lambda_i \partial\lambda_j$, $i, j = 1, \cdots, n$, regarded as an $n \times n$ matrix is a symmetric and strictly positive matrix. As a consequence, $\log Z$ is a convex function of the parameters λ_j, $j = 1, \cdots, n$. Therefore, if we define

$$Z(V) \equiv \operatorname{Tr} \exp[-\beta(H_0 + V)] \tag{39}$$

for an arbitrary operator V, we must then have an inequality

$$\sum_{j=1}^{n} x_j \log Z(V_j) \geq \log Z\left(\sum_{j=1}^{n} x_j V_j\right), \tag{40}$$

where the x_j, $j = 1, \cdots, n$, are arbitrary nonnegative numbers satisfying the condition $\sum_{j=1}^{n} x_j = 1$, $1 \geq x_j \geq 0$. Equation (40) can also be derived by means of the convexity theorem.[2]

For simplicity, let us set

$$\xi_{ij} \equiv \frac{1}{\beta} \frac{\partial^2}{\partial \lambda_i \partial \lambda_j} \log Z. \tag{41}$$

Since Eq. (34) is valid for arbitrary constants C_j, we must have inequalities

$$\xi_{ii}\xi_{jj} \geq (\xi_{ij})^2, \quad \xi_{jj} \geq 0 \tag{42}$$

for all $i, j = 1, \cdots, n$. As an application of these inequalities, let us consider the case $n = 3$ and identify $\sum_{j=1}^{3} \lambda_j H_j$ as the electromagnetic interaction of an anisotropic medium with a constant external magnetic (or electric) field whose jth component is given by λ_j, $j = 1, 2, 3$. Since the magnetic (or electric) susceptibility tensor of the medium is given by ξ_{ij}, we find that Eq. (34) or (42) shows the tensor to be always positive.

Also, when we choose $H_4 = N$ to be the occupation number operator with $-\lambda_4 = \mu$ being the chemical potential of the system, Eq. (42) gives

$$\xi_{jj}\left(\frac{\partial n}{\partial \mu}\right) \geq \left(\frac{\partial n}{\partial \lambda_j}\right)^2, \tag{43}$$

where $n = -\partial F/\partial \mu$ is the particle number.

Next let x and y be two arbitrary real numbers and consider a quadratic form of x and y defined by

$$Q(x, y) = Z^{-1}\beta^2 \sum_{n,m} \varphi(-\beta E_n, -\beta E_m) \times |\langle n| (\bar{H}_j - x - yH) |m\rangle|^2.$$

This is obviously nonnegative because of Eq. (33). When we minimize this expression with respect to x and y, we find

$$\frac{\partial^2}{\partial\beta^2}\log Z \frac{\partial^2}{\partial\lambda^2}\log Z \geq \left(\frac{\partial^2 \log Z}{\partial\lambda\partial\beta} - \frac{1}{\beta}\frac{\partial}{\partial\lambda}\log Z\right)^2. \quad (44)$$

This proves Eq. (9). Again if we identify λH_1 to be the external magnetic interaction, then it leads to the inequality (15).

In order to derive the inequalities (5) and (8), we consider an inner product

$$(A, B) = Z^{-1}\beta^2 \sum_{n,m} \varphi(-\beta E_n, -\beta E_m) \times \langle n| A^+ |m\rangle\langle m| B |n\rangle \quad (45)$$

for two arbitrary operators A and B. Since $\varphi(x, y)$ is nonnegative, the familiar Schwarz inequality gives us

$$(A, A)(B, B) \geq |(A, B)|^2. \quad (46)$$

Following the usual technique,[10,11] let us, moreover, set $B = [C, H]$ for another operator C. After a simple calculation, we find

$$Z(A, A)\,\mathrm{Tr}\,[C^+, [H, C]] \geq \beta\,|\mathrm{Tr}\,[C, A^+]|^2. \quad (47)$$

If we use the upper bound (33) for $\varphi(x, y)$, this gives the usual Bogoliubov inequality[10,11]

$$\tfrac{1}{2}\beta\langle AA^+ + A^+A\rangle\langle[[C, H], C^+]\rangle \geq |\langle[C, A]\rangle|^2. \quad (48)$$

In our case, we choose $A = H_j$ in Eq. (47) and note that $(H_j, H_i) = \partial^2 \log Z/\partial\lambda_i\partial\lambda_j$ so that Eq. (47) leads to

$$\frac{\partial^2 \log Z}{\partial\lambda_j\partial\lambda_j} \geq \beta\frac{|\langle[C, H_j]\rangle|^2}{\langle[[C, H], C^+]\rangle} \geq 0. \quad (49)$$

This establishes Eqs. (5) and (8). It should be noted that C is an arbitrary operator. As an application of Eq. (49), let us consider an electromagnetic interaction of an isotropic medium where both constant external electric and magnetic fields are simultaneously applied. Then, choosing λ_j to be the magnetic field strength in the z direction, we have

$$H_1 = \sum_i (Q_i/2m_ic)[(\mathbf{x}_i \times \mathbf{p}_i) + \boldsymbol{\sigma}_i]_3, \quad (50)$$

where the summation is extended to all particles with electric charge Q_i and mass m_i in the medium and $\boldsymbol{\sigma}$ is the Pauli spin matrix. If we choose the arbitrary operator C specially to be equal to the center-of-mass operator

$$C = \sum_i m_i\mathbf{x}_i \Big/ \sum_i m_i,$$

then Eq. (49) gives

$$(1/4\pi)(\mu - 1) \geq (1/4mc^2)[(\epsilon - 1)/4\pi]^2E_\perp \geq 0, \quad (51)$$

where μ, ϵ, m, c, and $E_\perp$ are the permeability, dielectric constant, mass density, velocity of light, and the electric field component perpendicular to the magnetic field, respectively. If the electric field is applied perpendicular to the magnetic field, then Eq. (51) can be rewritten as

$$2(\mu - 1)/(\epsilon - 1)^2 \geq E_2/E_1 \geq 0, \quad (52)$$

where E_2 is the total electric field energy contained in the medium and E_1 is the total rest mass energy of all charged particles in the matter. Since E_2/E_1 is extremely small in general, Eq. (52) is not practically useful. However, it demonstrates the fact that the permeability μ must at least increase quadratically with the electric field.

Finally, in order to derive inequalities involving derivatives with respect to β, we may state a corollary[12] of Bernstein's theorem for absolutely monotonic functions. A real function $f(x)$ of a real variable x is called an absolute monotonic function of x in the interval $a < x < b$ if we have $d^nf(x)/dx^n \geq 0$ for $a < x < b$ and for all nonnegative integers $n = 0, 1, 2, \cdots$. We obviously have an inequality

$$\frac{d}{dx}\log f(x) \geq 0. \quad (53)$$

But a corollary[12] of Bernstein's theorem demands a less obvious fact, that if $f(x)$ is absolutely monotonic over the whole negative axis $0 > x > -\infty$, then $\log f(x)$ is a convex function in the interval, i.e., we must have

$$\frac{d^2}{dx^2}\log f(x) \geq 0, \quad 0 > x > -\infty. \quad (54)$$

To illustrate this theorem, let E_0 be the ground state energy of H so that we have $E_n \geq E_0$ for all states $|n\rangle$. Moreover, by identifying $x = -\beta$ and setting

$$f(x) = Z\exp(\beta E_0) = \sum_n \exp[x(E_n - E_0)],$$

it is apparent that $d^nf(x)/dx^n \geq 0$ for all $n = 0, 1, 2, \cdots$ in the interval $0 \geq x > -\infty$. Hence, $f(x)$ is absolutely monotonic in the interval, and by the above theorem we must have Eq. (54), which is equivalent to

$$\frac{\partial^2}{\partial\beta^2}\log Z \geq 0. \quad (55)$$

Of course, this relation can be easily obtained by a direct calculation since we have

$$\frac{\partial^2}{\partial\beta^2}\log Z = \langle\bar{H}\bar{H}\rangle, \quad \bar{H} = H - \langle H\rangle. \tag{56}$$

However, we can derive more complicated inequalities as follows. First we note that a function defined by

$$\varphi_{nm}(x) = \varphi(-\beta E_n, -\beta E_m)\exp(\beta E_0), \quad x = -\beta, \tag{57}$$

is absolutely monotonic in the negative interval $0 \geq x > -\infty$, since we can rewrite

$$\varphi_{nm}(x) = \int_0^1 dt \times \exp\{x[t(E_n - E_0) + (1-t)(E_m - E_0)]\}. \tag{58}$$

Now, let us consider a function

$$g_{ij}(x) = \sum_{n,m}\sum_{l,k}\varphi_{nm}(x)\varphi_{lk}(x) \times |\langle n| H_j |m\rangle\,\delta_{lk} - \langle l| H_i |k\rangle\,\delta_{nm}|^2. \tag{59}$$

This function is also absolutely monotonic since products and sums of absolutely monotonic functions have the same property. Therefore, we must have

$$\frac{d^2}{dx^2}\log g_{ij}(x) \geq 0. \tag{60}$$

But Eq. (59) can be evaluated to be

$$g_{ij}(x) = \beta^{-1}Z^2\left[\xi_{ii} + \xi_{jj} + \beta\left(\frac{\partial F}{\partial\lambda_i} - \frac{\partial F}{\partial\lambda_j}\right)^2\right]\exp(2\beta E_0), \tag{61}$$

where ξ_{ij} is defined by Eq. (41). Especially, when we set $i = j = 1$ with $n = 1$, we find

$$\frac{\partial^2}{\partial\beta^2}\log\left(\frac{\partial^2}{\partial\lambda^2}\log Z\right) + 2\frac{\partial^2}{\partial\beta^2}\log Z + \frac{2}{\beta^2} \geq 0. \tag{62}$$

This is nothing but Eq. (10).

Similarly, another function $h_j(x)$ given by

$$h_j(x) = \sum_{n,m}\varphi_{nm}(x)\,|\langle n| H_j |m\rangle - b\delta_{nm}|^2 \tag{63}$$

is absolutely monotonic for arbitrary constant b, so that we derive an inequality

$$\frac{\partial^2}{\partial\beta^2}\log[\beta^{-1}\xi_{jj} + (b - \langle H_j\rangle)^2] + \frac{\partial^2}{\partial\beta^2}\log Z \geq 0. \tag{64}$$

Since b is arbitrary, we can set $b = +\langle H_j\rangle$ to obtain

$$\frac{\partial^2}{\partial\beta^2}\log\xi_{jj} + \frac{\partial^2}{\partial\beta^2}\log Z + \frac{1}{\beta^2} + \frac{2}{\xi_{jj}}\beta\left(\frac{\partial^2 F}{\partial\beta\partial\lambda_j}\right)^2 \geq 0. \tag{65}$$

This proves Eq. (11). Moreover, if we set $b = 0$ in Eq. (64), we derive

$$\frac{\partial^2}{\partial\beta^2}\log\left[\xi_{jj} + \beta\left(\frac{\partial F}{\partial\lambda_j}\right)^2\right] + \frac{\partial^2}{\partial\beta^2}\log Z + \frac{1}{\beta^2} \geq 0. \tag{66}$$

This is Eq. (12). Also, since Eq. (53) must be valid for $f(x) = h_j(x)$, it leads to

$$-\frac{\partial}{\partial\beta}h_j(\beta) \geq 0. \tag{67}$$

Choosing $b = -\langle H_j\rangle$, we arrive at Eq. (17).

Finally, Kubo's formula[13] for the electric conductivity tensor $\sigma_{\mu\nu}(\omega)$ is given by

$$\sigma_{\mu\nu}(\omega) = \int_0^\infty dt\exp(-i\omega t)\int_0^\beta d\tau\langle J_\nu(-i\hbar\tau)J_\mu(t)\rangle, \tag{68}$$

where $J_\mu(t)$ is here defined by

$$J_\mu(t) = \exp(iHt/\hbar)J_\mu\exp(-iHt/\hbar). \tag{69}$$

Integrating Eq. (68), we find

$$\sigma_{\mu\nu}(\omega) = (i\hbar\beta/Z)\sum_{n,m}(E_n - E_m - \hbar\omega + i\eta)^{-1} \times \varphi(-\beta E_n, -\beta E_m)\,\langle n| J_\mu| |m\rangle\langle m| J_\nu |n\rangle, \tag{70}$$

where η is the vanishingly small positive number. Taking the real part of both sides, we obtain

$$\mathrm{Re}\,\sigma_{\mu\nu}(\omega) = (\hbar\beta/Z)\pi\sum_{n,m}\delta(E_n - E_m - \hbar\omega) \times \varphi(-\beta E_n, -\beta E_m)\,\langle n| J_\mu |m\rangle\langle m| J_\nu |n\rangle. \tag{71}$$

Due to the presence of the delta function inside Eq. (71), this expression is further reduced to

$$\mathrm{Re}\,\sigma_{\mu\nu}(\omega) = \pi(Z\omega)^{-1}[\exp(\hbar\beta\omega) - 1] \times \sum_{n,m}\delta(E_n - E_m - \hbar\omega) \times \exp(-\beta E_n)\,\langle n| J_\mu |m\rangle\langle m| J_\nu |n\rangle. \tag{72}$$

Therefore, if $\sigma(\omega)$ represents any diagonal component $\sigma_{\mu\mu}(\omega)$, then a function

$$G(-\beta) = \omega[\exp(\hbar\beta\omega) - 1]^{-1}Z\,\mathrm{Re}\,\sigma(\omega)\exp(\beta E_0) \tag{73}$$

is absolutely monotonic with respect to $x = -\beta$. Hence, the corollary of Bernstein's theorem gives

$$\frac{\partial^2}{\partial\beta^2}\log\mathrm{Re}\,\sigma(\omega) + \frac{\partial^2}{\partial\beta^2}\log Z - \frac{\partial^2}{\partial\beta^2}\log[\exp(\hbar\beta\omega) - 1] \geq 0, \tag{74}$$

which is nothing but Eq. (16). Finally, Eq. (18) can be obtained from Eq. (53), i.e.,

$$\frac{\partial}{\partial(-\beta)} \log G(-\beta) \geq 0. \tag{75}$$

Last, we may remark that, for arbitrary operators A and B, we have a formal identity

$$\langle[[A^+, H], B]\rangle = (\beta/Z) \sum_{n,m} \varphi(-\beta E_n, -\beta E_m) \times \langle n| [A^+, H] |m\rangle\langle m| [H, B] |n\rangle. \tag{76}$$

Choose $A = c^{-1} \sum_i Q_i x_{\mu i}$ and $B = c^{-1} \sum_i Q_i x_{\nu i}$, where Q_i is the electric charge of the ith particle. If we note that the electric current J_μ is given by

$$J_\mu = (i/\hbar)[H, A] = \sum_i (Q_i/m_i c) p_{\mu i},$$

then Eqs. (76) and (71) lead to the Kubo sum rule[13]

$$\pi^{-1} \int_0^\infty d\omega \,\mathrm{Re}\, [\sigma_{\mu\nu}(\omega) + \sigma_{\nu\mu}(\omega)] = \sum_i (Q_i^2/m_i c^2) \delta_{\nu\mu}, \tag{77}$$

where we have used the relation

$$\mathrm{Re}\, \sigma_{\mu\nu}(\omega) = \mathrm{Re}\, \sigma_{\nu\mu}(-\omega). \tag{78}$$

If H_1 represents the electric dipole interaction, i.e., if we have $H_1 = \sum_i Q_i \mathbf{x}_i$, then Eq. (71) leads to a formal relation

$$\beta \xi_{\mu\nu} = \frac{c^2}{\pi} \int_{-\infty}^\infty d\omega \frac{1}{\omega^2} \mathrm{Re}\, \sigma_{\mu\nu}(\omega) \tag{79}$$

since we have $\mathbf{J} = (i/c\hbar)[H, H_1] = (1/c\hbar)K$ in this case. By this formula, we could compute the electric susceptibility tensor $\xi_{\mu\nu}$. However, this integral is ambiguous at $\omega = 0$ and should be interpreted as an integral for generalized functions. Hence, for any small positive number η, we interpret

$$\int_{-\eta}^{\eta} d\omega \frac{1}{\omega^2} f(\omega) = -\frac{2}{\eta^2} f(0) + f''(0)\eta + \int_{-\eta}^{\eta} d\omega \frac{1}{\omega^2} [f(\omega) - f(0) - f'(0)\omega - \tfrac{1}{2} f''(0)\omega^2].$$

Similarly, from Eq. (72) we compute

$$\frac{1}{\pi} \int_{-\infty}^\infty d\omega \,\mathrm{Re}\, \sigma_{\mu\nu}(\omega)\omega[\exp(\hbar\beta\omega) - 1]^{-1} = \langle J_\mu J_\nu \rangle. \tag{80}$$

The right-hand side of this equation is related to M_1 defined by Eq. (7) when we note $K = c\hbar \mathbf{J}$.

Some applications to problems of particle physics by an analogous technique will be given elsewhere.[9,14]

ACKNOWLEDGMENTS

The author would like to express his gratitude to Professor K. H. Bennemann and Professor K. H. Nussenzveig for discussions and useful comments.

* Work supported in part by the U.S. Atomic Energy Commission.

[1] N. N. Bogoliubov, Jr., Physica **32**, 933 (1966).

[2] D. Ruelle, *Statistical Mechanics* (Benjamin, New York, 1966), p. 27; A. Huber, in *Methods and Problems of Theoretical Physics* (North-Holland, Amsterdam, 1970), p. 37. These articles give mathematically rigorous treatment of deriving the convexity theorem. The present author would like to express his gratitude to Professor K. H. Nussenzveig for calling his attention to these references as well as many other points.

[3] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962), p. 83. In this case, H_1 represents the occupation number operator so that H_1 commutes with H_0. Then, the proof of Eq. (3) is much simplified.

[4] L. D. Landau and E. M. Lifshitz, *Electromagnetism of Continuous Media*, transl. by J. D. Sykes and J. S. Bell from Russian (Pergamon, New York, 1960), p. 63.

[5] L. P. Kadanoff and G. Baym, Ref. 3, pp. 15–16. This statement is obviously correct if the underlying Hilbert space is of finite dimension. We are implicitly assuming here and hereafter that all possible complications due to infinite dimensionality of the Hilbert space will not affect the final results.

[6] K. Sawada, Phys. Rev. **106**, 372 (1957); R. P. Feynman, *ibid.* **56**, 72 (1939).

[7] T. Matsubara, Progr. Theoret. Phys. (Kyoto) **14**, 351 (1955).

[8] A. A. Abrikosov, L. P. Gorkov, and Z. E. Dzyloshinski, *Methods of Quantum Field Theory in Statistical Physics*, transl. by R. A. Silverman (Prentice-Hall, London, 1963).

[9] S. Okubo, Nuovo Cimento **1A**, 717 (1971); S. T. Epstein, Am. J. Phys. **22**, 613 (1954).

[10] N. N. Bogoliubov, Physik. Abhandl. Sowjetunion **6**, 1, 113, 229 (1962).

[11] N. D. Mermin and H. Wagner, Phys. Rev. Letters **17**, 1133 (1966); D. Ruelle, Ref. 2.

[12] See, e.g., D. V. Widder, *Laplace Transform* (Princeton U.P., Princeton, N.J., 1941), p. 167.

[13] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).

[14] Here, we simply state as an application of Bernstein's theorem (see Ref. 12) that the Pomeron Regge trajectory function $\alpha(t)$ must satisfy an inequality $t\alpha''(t) + \alpha'(t) \geq 0$ in the interval $4m_\pi^2 \geq t \geq 0$, where m_π is the pion mass. For $t = 0$, this reproduces the familiar inequality $\alpha'(0) \geq 0$.

Phase Transitions in Binary Lattice Gases*

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(Received 2 November 1970)

We prove the existence of phase transitions in several kinds of two-component lattice gases: Some of these are isomorphic to spin systems and/or to fluids composed of asymmetrical molecules which can have different orientations. Among the models studied is one with infinite repulsion between particles of different species (hard cores), extending over arbitrarily many neighboring lattice sites. Some of these systems have been investigated previously in the mean field approximation and numerically.

1. INTRODUCTION

Among the most striking aspects of the behavior of macroscopic systems are the ubiquity and variety of the phase transitions they undergo. The demonstration that the nonsmooth behavior of the thermodynamic functions, which characterizes phase transitions, follows from the rules of statistical mechanics for the computation of these quantities is one of the most interesting aspects of the latter study.

The first demonstration of this kind was Peierls' proof of the existence of spontaneous magnetization in a two-dimensional Ising spin system with nearest-neighbor ferromagnetic interactions.[1] Peierls' results have been made rigorous and his method generalized and used to prove the existence of phase transitions for various lattice systems without having (or being able) to compute the thermodynamic functions explicitly.[2] In recent work along this line Dobrushin was able to prove the existence of a phase transition in a ν-dimensional lattice gas, $\nu \geq 2$, with hard cores which exclude the occupancy, by any particle, of the 2ν nearest-neighbor sites of an occupied site.[3] This required a new extension of the Peierls' method since this system does not have the symmetry (between "up" and "down" spins) of the spin system.[4]

In this paper we extend the Peierls' method further and prove the existence of phase transitions in four binary lattice-gas models described below. In one of these models the particles have arbitrarily extended hard cores: a type of system for which the existence of a phase transition has not been proven rigorously before.

2. DESCRIPTION OF MODELS

Consider a ν-dimensional square lattice Z^ν, $\nu \geq 2$, and let V be a cubic box containing $|V|$ lattice points. Suppose that the sites of V can be occupied by two types of particles called A and B.

Model 1 is described by the activities z_A, z_B, and the following interaction potentials:

$$\varphi_{AA}(\mathbf{r}) = \varphi_{BB}(\mathbf{r}) = \begin{cases} 0 & \text{for } \mathbf{r} \neq 0 \\ +\infty & \text{for } \mathbf{r} = 0 \end{cases} \quad (2.1)$$

and

$$\varphi_{AB}(\mathbf{r}) = \begin{cases} 0 & \text{for } |\mathbf{r}| > d \\ +\infty & \text{for } |\mathbf{r}| \leq d \end{cases}, \quad (2.2)$$

where $\mathbf{r}$ is a vector between lattice sites occupied by different particles and d is the lattice spacing. We shall call *model 2* the generalization of model 1 obtained by allowing $\varphi_{AB}(\mathbf{r}) = +\infty$ for $\mathbf{r}$ in some symmetric convex set.

Let α be a configuration containing $N_A(\alpha)$ and $N_B(\alpha)$ particles of type A and B, respectively. If α is allowed, i.e., if on each lattice site there is at most one particle and no A particle is within the hard core of any B particle, then the Boltzmann factor for α is simply

$$z_A^{N_A(\alpha)} z_B^{N_B(\alpha)}. \quad (2.3)$$

We can observe that the line $z_A = z_B$ is a symmetry line for the problem, and we may expect that as $z_A = z_B = z \to \infty$, this symmetry is spontaneously broken and that there are two distinct equilibrium states, one A-rich and the other B-rich. If this happens, the system will show a first-order phase transition when one passes from the $z_A > z_B$ region to the $z_B > z_A$ region through a point z on the diagonal $z_A = z_B$ with z large enough.

The technique for showing the spontaneous breakdown of the symmetry will be the Peierls' technique of introducing a nonsymmetric "surface term" in the Boltzmann factor of a configuration and showing that its influence will not disappear even for very large systems when z is large enough.

Calling D the "diameter" of the hard cores in model 2, we find an upper bound on the lattice gas fugacity above which there is some phase transition. This upper bound tends to zero, as it should, when $D \to \infty$. Unfortunately, however, it only goes to zero as D^{-1}, which means that if one tries to go to the limit of a continuum gas by keeping the hard core length D fixed while letting the lattice spacing d go to zero, the upper bound on the critical continuum fugacity would go to infinity as $d^{-(\nu-1)}$ since the continuum fugacity z_c behaves as $zd^{-\nu}$ (z the lattice gas fugacity) in the lattice $\leftrightarrow$ continuum transformation. We are thus unable to prove the existence of a phase transition at some finite fugacity, in a continuum system: a proof sadly lacking at the present time. (The only proofs of the existence of phase transitions for continuum systems available at present are for systems with infinite range "Kac potentials" which exhibit classical van der Waals type phase transitions.[5]) Whether the kind of technique employed in this paper will eventually prove useful for continuum systems remains to be seen.

Model 1 may also be interpreted as a model for orientational phase transitions in two dimensions. To do this, we imagine a two-dimensional square lattice where molecules with two different orientations "horizontal" and "vertical" can be situated at the center of each bond. Some sites (bonds) may also be empty. When there is a particle in a horizontal (vertical) position on some site, then it excludes vertical (horizontal) particles from its four neighbor sites. We may picture the molecules as narrow rods of the same length as the bonds with their centers pivoted at the midpoints of the bonds, and require that there be no overlap of the rods (Fig. 1). Identifying the vertical and horizontal particles as species A and B, we go back to the two-component lattice gas described before with $z_A = \exp[\beta(\mu + E_v)]$, $z_B = \exp[\beta \times (\mu + E_h)]$, where μ is the chemical potential and E_v and E_h are vertical and horizontal components of the "electrical field." A phase transition in this system would correspond to a spontaneous "lining up" of the molecules parallel to each other (perhaps somewhat similar to what may happen in liquid crytals).

It is also possible to think of model 1 as the limit of an Ising spin system: We suppose that on each site of our lattice sits an Ising "spin-1" particle $S = 0, +1, -1$ and that the energy of a configuration is

$$H_3\{S\} = -J \sum_{\langle i,j\rangle} S_iS_j(1 - S_iS_j) + h \sum_i S_i - \mu \sum_i S_i^2, \tag{2.4}$$

where $\sum_{\langle i,j\rangle}$ means sum over the pairs of nearest neighbors; then, if we let $J \to +\infty$ and if we interpret $S_i = 0, +1, -1$ as meaning, respectively, that the site i is empty or occupied by an A or B particle, we realize that (2.4) defines a model equivalent to model 1 with $z_A = e^{\beta(\mu+h)}$ and $z_B = e^{\beta(\mu-h)}$. The phase transition means, in this case, that for large μ there is spontaneous magnetization when $h = 0$.

We shall define *model 3* to be the system described by the Hamiltonian in Eq. (2.4) but with $0 \le J < +\infty$. This system and some variations of it have been studied extensively by Wheeler and Widom[6] in various approximations as a model for the separation of solutes in a solution.

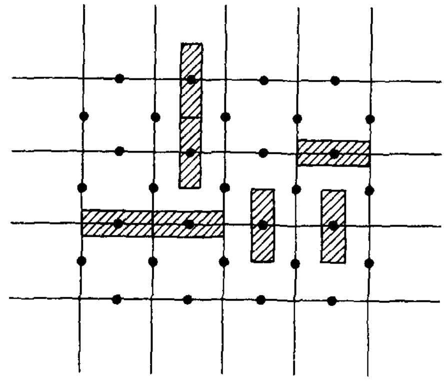

FIG. 1. An allowed configuration of orientable rods.

Model 4 will be a system similar to model 3 but with a Hamiltonian defined as

$$H_4\{S\} = -J \sum_{\langle i,j\rangle} S_iS_j + h \sum_i S_i - \mu \sum_i S_i^2. \tag{2.5}$$

This model has been studied in the literature in the mean field approximation[7] and used to interpret the magnetic properties of UO_2. It can also be interpreted as a model for an annealed alloy of magnetic and nonmagnetic atoms. The magnetic atoms have spins $S_i = \pm 1$, and μ measures their concentration. The sums in (2.5) are then interpreted as going only over sites occupied by magnetic atoms. For a quenched alloy (where the distribution of magnetic atoms is random, independent of the temperature), the existence of spontaneous magnetization at high concentrations of magnetic atoms and low temperatures has been proven previously by Griffith and Lebowitz.[8]

3. EXISTENCE OF PHASE TRANSITION IN MODELS 1 AND 2

Let $\alpha = \{x_i\}$, $i = 1, \cdots, |V|$, be a configuration in the box. As a boundary condition we shall assume that all lattice sites outside V are occupied by A particles. Each lattice site is the center of a ν-dimensional unit cube. If a lattice site x is occupied by an A particle (B particle), we shall color that cube centered on x red (black). We shall denote by $C(x, A)$ [$C(x, B)$] the union of all cubes from which B particles (A particles) are excluded by the hard core of the particle located at x. The cubes in $C(x, A)$ [$C(x, B)$] outside the cube centered at x will be colored pink (gray). The remaining cubes will be colored white. Each cube in the lattice will thus, for a permissible configuration, have one of the following colors: red, pink, black, gray, pink-gray, or white (red-pink = red, black-gray = black). The cells outside V will all be red for the boundary condition we are considering.

Without describing the shapes of the particles in detail, we shall assume (looking at a single A particle on the lattice at x) that $C(x, \mathrm{A})$ is invariant under rotations by $\pi/2$ and that its convex hull does not contain in its interior the center of any cell which is not pink, i.e., any lattice point where a black particle may be placed. We shall assume further that when the lattice spacing is unity, then there exists an integer δ such that, starting from any surface of $C(x, \mathrm{A})$, it is possible to move in a direction perpendicular to this surface into the interior of $C(x, \mathrm{A})$ for a distance δ passing through pink cells only. For our model 1, $\delta = 1$, while for "cubical" particles the side of the cube is $2\delta + 1$. To investigate the limit in which the lattice spacing $d \to 0$, we define the hard core for different d's to be the union of all the cubes whose centers lie inside the convex hull of the $C(x, \mathrm{A})$ for $d = 1$, i.e., the convex hull of $C(x, \mathrm{A})$ does not change as $d \to 0$. With this definition δ increase as d^{-1} when $d \to 0$. [A similar description holds of course also for $C(x, \mathrm{B})$].

The union of all $C(x, \mathrm{B})$, i.e., the union of all black, gray, and gray-pink cubes is separated from the rest of the lattice by a $(\nu - 1)$-dimensional surface $S(\alpha)$ which decomposes as a union of closed connected polyhedra, which we call contours. To avoid ambiguity in this decomposition when all four faces adjacent to the same edge belong to $S(\alpha)$, we may imagine the corners of the cubes clipped off.

Let G be an outer contour, i.e., it is possible to draw a path from G to the surface of V without crossing any other contour, and let $|G|$ denote the area of this contour measured in units of $d^{\nu-1}$. We have that $|G|$ is an integer. The probability of such a contour G for $z_\mathrm{A} = z_\mathrm{B} = z$ is given by

$$P(G) = \sum_{\alpha \supset G} z^{[N_\mathrm{A}(\alpha)+N_\mathrm{B}(\alpha)]} \Big/ \sum_{\alpha} z^{[N_\mathrm{A}(\alpha)+N_\mathrm{B}(\alpha)]}, \quad (3.1)$$

where $\alpha \supset G$ means a configuration in which there is a contour G. We shall now obtain an upper bound on $P(G)$ from which will follow an upper bound on the probability $\pi_\mathrm{B}(x)$ that a site x is occupied by a B particle by the standard argument that if x is occupied by a B particle it must be inside some contour G, so that

$$\pi_\mathrm{B}(x) \leq \sum_{|G|} K(|G|)\hat{P}(|G|), \quad (3.2)$$

where $\hat{P}(|G|)$ is an upper bound on $P(G)$ and

$$K(|G|) = (|G|/2\nu)^{\nu/\nu-1} 3^{|G|-\nu} \quad (3.3)$$

is the Peierls' upper bound[1–4] on the number of contours of area $|G|$ which contain a site x. It will then be seen that the density of B particles $\rho_\mathrm{B} \leq \max_x \pi_\mathrm{B}(x)$ is bounded by a decreasing function of the fugacity z for sufficiently large z. Since, however, the total density of particles $\rho_\mathrm{A} + \rho_\mathrm{B}$ is a nondecreasing function of z, being the derivative with respect to $\ln z$ of the grand canonical pressure which is a convex function of $\ln z$, there will exist a z' such that, for $z > z'$, $\rho_\mathrm{B} < \rho_\mathrm{A}$. By symmetry, the opposite will be true for a boundary condition in which all the sites outside V are occupied by B particles. This will show the nonuniqueness of the infinite volume "Gibbs state"[2–4] for $z > z'$. It follows further from the uniqueness of the state at low values of the fugacity[4] that there will be some nonanalyticity in the correlation functions for some $z < z'$. We may also deduce from the equality of the pressure (in the thermodynamic limit) for the different boundary conditions that there will be a discontinuity in the densities ρ_A and ρ_B whenever the fugacities z_A and z_B cross each other at a value of $z > z'$.

To get an upper bound on $P(G)$, we shall restrict the sum in the denominator of (4.1). Before doing that, we need the following definition: A set of lattice points x_i, $i = 1, \cdots, n$, occupied by A or B particles is said to form a cluster if, by the rules of the hard-core exclusion, these particles have to be all of the A type or all of the B type, i.e., we can label the particles in such a way that $x_i \in C(x_{i+1}, \cdot)$ for *all i*. Consider now a configuration $\alpha \supset G$. Moving from any point on G into the interior in a direction perpendicular to G, one will find δ gray or gray-pink cubes; i.e., given G, we know that these cubes cannot have any other colorings. Let G_δ be the set of all these cubes. Their number $|G_\delta| \geq |G|\,\delta/2\nu$. The pinkness of these cubes may be due to red particles exterior to G or to red particles interior to G or both. For each configuration $\alpha \supset G$ there will be another configuration $T_0(\alpha)$ in which all the B particles at positions x_j in the interior of G whose cores $C(x_j, \mathrm{B})$ contain any of the cubes in G_δ, as well as all B particles which are in the same cluster with any of these, are replaced by A particles. The transformation $\alpha \to T_0(\alpha)$ is not always a one-to-one transformation as there may be more than one $\alpha \supset G$ going into the same $T_0(\alpha)$. It is clear, however, from our definition of $C(x, \cdot)$ that there will be a bound of the form $m^{|G|}$ on the number of such α's with m independent of the lattice spacing d. [For $\nu = 2$ and $C(x, \cdot)$ a square of side $(2\delta + 1)$, there will at most 2^n of these, where n is the number of "corners" of G whose angle in the interior of G is $3\pi/2$.] It is clear that in the configuration $T_0(\alpha)$ all the cubes in G_δ will be colored pink. Let

$T_l(\alpha)$, $l = 1, \cdots, |G_\delta|$, be the configuration where there are A particles in l cubes of G_δ, i.e., $T_l(\alpha)$ is a configuration obtained from $\alpha \supset G$ by first changing α to $T_0(\alpha)$ and then putting l A particles in the region G_δ. We then have as a lower bound on the denominator in (3.1)

$$\sum_\alpha z^{[N_A(\alpha)+N_B(\alpha)]} \geq m^{-|G|} \sum_{\alpha\supset G} z^{[N_A(\alpha)+N_B(\alpha)]} \sum_{l=0} z^l \binom{|G_\delta|}{l} \geq m^{-|G|}(1+z)^{|G|\,\delta/2\nu} \sum_{\alpha\supset G} z^{[N_A(\alpha)+N_B(\alpha)]}, \quad (3.4)$$

where we have used the upper bound $|G_\delta| \geq |G|\,\delta/2\nu$. Substituting (3.4) into (3.2), we get an upper bound on the density of B particles, for the boundary condition used,

$$\rho_B \leq \sum_{k=k_{\min}}^{\infty} 3^{-\nu}\left(\frac{k}{\nu}\right)^{\nu/\nu-1} (3m)^{2k}(1+z)^{-\delta k/\nu} = \hat{\rho}_B(z). \quad (3.5)$$

Here $k = |G|/2$ is an integer and $k_{\min} = \frac{1}{2}|G_{\min}|$, where $G_{\min}$ is the surface area of $C(x, \mathrm{A})$ in units of $d^{\nu-1}$. For large values of z, $\hat{\rho}_B(z)$ is a decreasing function of z. Hence, as discussed earlier, there will exist a z' such that, for $z > z'$, $\rho_B < \rho_A$, and thus there will be some kind of phase transition for $z < z'$.

If the lattice spacing d is decreased, δ will increase as (D/d) while ρ_B and ρ_A will decrease as $(d/D)^\nu$, where D is the "diameter" of the hard cores, which remains fixed. As mentioned in the Introduction, the passage to the continuum involves the replacement of z by $z_c d^\nu$ and ρ by $\rho_c d^\nu$ so that the right side of (3.5) would not give any bound on the continuum density of B particles for any finite z_c.

4. EXISTENCE OF PHASE TRANSITION IN MODELS 3 AND 4

We now color the cubes which contain A particles red and those containing B particles black and the empty ones white (no pink or gray) and fill all the cubes outside V with A particles. For a configuration α we consider the union of all the white and black cubes and let G be an outer contour of such a region. Then all the cubes adjacent to G from the outside are colored red while the cubes adjacent to G from the inside are either black or white. Suppose that there are $l(G)$ cubes adjacent to G from the inside, $l(G) \geq |G|/2\nu$, and k of these, labeled $\xi_1, \cdots, \xi_k$, are black. The probability of a contour G with specified $\xi_1, \cdots, \xi_k$ is given by

$$P(G:\xi_1,\cdots,\xi_k) = \sum_{\alpha\supset(G:\xi_1,\cdots,\xi_k)} e^{\beta[\mu N(\alpha)-U(\alpha)]} \Big/ \sum_\alpha e^{\beta[\mu N(\alpha)-U(\alpha)]}, \quad (4.1)$$

where $N(\alpha) = N_A(\alpha) + N_B(\alpha)$ is the total number of particles in this configuration, μ is the chemical potential which is the same for the A and B particles and $U(\alpha)$ is the potential energy of this configuration. To obtain a lower bound on the denominator in (4.1), we restrict the sum there to configurations $T(\alpha)$, where $\alpha \supset (G:\xi_1, \cdots, \xi_k)$ and $T(\alpha)$ is a configuration obtained from α by interchanging all the A and B particles inside G and filling all the empty $(l-k)$ cubes adjacent to the interior of G with A particles. We then have for model 3

$$N(T(\alpha)) = N(\alpha) + (l-k) \quad (4.2)$$

and

$$U(T(\alpha)) \geq U(\alpha) - Jk + J(2\nu-1)(l-k), \quad (4.3)$$

the last term in (4.3) arising from the possibility that an empty site after being filled with an A particle may find itself surrounded on $(2\nu - 1)$ sides with B particles. This transformation $\alpha \to T(\alpha)$ is one to one since we are specifying the positions of the sites adjacent to G which contain B particles. Hence we have

$$P(G:\xi_1,\cdots,\xi_k) \leq \exp\{-\beta Jk - \beta[\mu-(2\nu-1)J](l-k)\}, \quad (4.4)$$

and thus

$$\begin{aligned} P(G) &= \sum_{k=0}^{l} \sum_{(\xi_1,\cdots,\xi_k)} P(G:\xi_1,\cdots,\xi_k) \\ &\leq [\exp(-\beta J) + \exp\{-\beta[\mu-(2\nu-1)J]\}]^l \\ &\leq [\exp(-\beta J) + \exp\{-\beta[\mu-(2\nu-1)J]\}]^{|G|/2\nu}, \end{aligned} \quad (4.5)$$

where the last inequality holds when the term in the bracket is less than unity since $l \geq |G|/2\nu$.

We can now find an upper bound on the sum of the probabilities $\pi_0(x) + \pi_B(x)$ that a lattice site x is empty or occupied by a B particle since in either case x will have to be inside some outer contour G because of our boundary conditions. Using the same bound as in Sec. 3 on the number of contours of area $|G|$ which can contain x, we have

$$\pi_0(x) + \pi_B(x) \leq \sum_{k=\nu}^{\infty} 3^{-\nu}\left(\frac{k}{\nu}\right)^{\nu/\nu-1} 3^{2k} \times [\exp(-\beta J) + \exp\{-\beta[\mu-(2\nu-1)J]\}]^{k/\nu}. \quad (4.6)$$

For a given $J > 0$ there will be a region in the (β, μ) plane bounded by some curve $\beta(\mu)$ (see Fig. 2), such that whenever β and μ are in that region the right

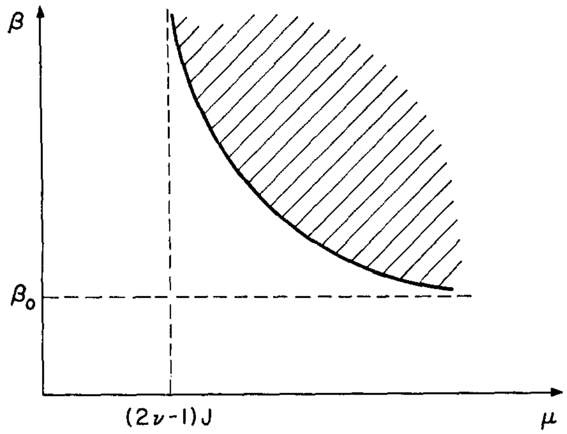

FIG. 2. The dashed area is contained in the two-phase region for model 3. The J dependence of β_0 is roughly $\propto J^{-1}$. A similar picture holds for model 4.

side of (4.6) will be less than $\frac{1}{2}$. But, since

$$\pi_A(x) = 1 - \pi_0(x) - \pi_B(x), \quad (4.7)$$

we will have

$$\pi_A(x) > \pi_B(x) \quad \text{whenever} \quad \pi_0(x) + \pi_B(x) < \tfrac{1}{2}, \quad (4.8)$$

and thus the equilibrium state will depend on the boundary conditions and not be unique. The existence of a phase transition then follows from the same arguments as in Sec. 3.

Model 4 can be treated as model 3 but (4.3) is replaced by

$$U(T(\alpha)) \leq U(\alpha) - 2Jk + J(2\nu - 1)(l - k); \quad (4.9)$$

therefore, the conclusions of model 3 can be drawn also for model 4.

ACKNOWLEDGMENT

We would like to thank Dr. E. Lieb for many valuable discussions.

* Supported in part by the U.S. Air Force Office of Scientific Research.

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[1] R. E. Peierls, Proc. Cambridge Phil. Soc. **32**, 477 (1936).

[2] R. Griffiths, Phys. Rev. **136**, 1437 (1964): R. L. Dobrushin, Teoriya Veroyatnostei i ee Primeneniya **10**, 209 (1965) [Theory Probability Appl. **10**, 209 (1965)], and *Fifth Symposium on Mathematical Statistics and Probability* (U. of California Press, Berkeley, 1967), Vol. III, p. 73; J. Ginibre, A. Grossman, and D. Ruelle, Commun. Math. Phys. **3**, 187 (1966).

[3] R. L. Dobrushin, Teoriya Veroyatnostei i ee Primeneniya **13**, 201 (1968) [Theory Probability Appl. **13**, 201 (1968)]; Functional Anal. Appl. **2**, 31, 44 (1968).

[4] The work of Dobrushin and earlier work is reviewed by J. Ginibre, in *Colloques Internationaux Du CNRS*, No. 181 (Editions du CNRS, Paris, 1970), p. 163. We follow the notation and general format of Ginibre's presentation and refer the reader to Ginibre's paper for background.

[5] M. Kac, G. E. Uhlenbeck, and P. C. Hemmer, J. Math. Phys. **4**, 216 (1963); J. L. Lebowitz and O. Penrose, *ibid.* **7**, 98 (1966).

[6] J. C. Wheeler and B. Widom, J. Chem. Phys. **52**, 5334 (1970), and references given there.

[7] R. B. Griffith, Physica **33**, 683 (1967), and references given there.

[8] R. B. Griffith and J. L. Lebowitz, J. Math. Phys. **9**, 1284 (1968).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Note on the New Symmetry of the Racah Coefficients

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(Received 8 December 1970)

It is shown that the "new symmetry" of Racah coefficients, recently derived in a paper by Minton [J. Math. Phys. **11**, 3061 (1970)], does not exist.

We wish to point out that the "new symmetry of the Racah coefficients," recently derived by Minton,[1] does not exist since it would require that $b + c - e + f + 1 = 0$, which can be shown to be violated for any b, c, e, or f of $W(abcd; ef)$ satisfying the equality (10) in Minton's article.[1]

To see this, we recall that one of the Regge symmetries[2] gives

$$W(abcd; ef) = (-)^{e+f-b-c} W(a'b'c'd'; e'f'). \quad (1)$$

We can use another one to show that

$$\begin{aligned} &W(\tfrac{1}{2}[a + c + d - b], \tfrac{1}{2}[e - f - a + d - 1], \\ &\quad \tfrac{1}{2}[e - f + a - d - 1], \tfrac{1}{2}[a + b + d - c]; \\ &\quad \tfrac{1}{2}[e + f + b + c + 1], \tfrac{1}{2}[e + f - b - c - 1]) \\ &\qquad = (-)^{2f+1} W(a'b'c'd'; e'f''). \quad (2) \end{aligned}$$

In Eqs. (1) and (2),

$$\begin{aligned} a' &= \tfrac{1}{2}(e + f + a - d), & b' &= \tfrac{1}{2}(a + d + b - c), \\ c' &= \tfrac{1}{2}(a + d - b + c), & d' &= \tfrac{1}{2}(e + f - a + d), \\ e' &= \tfrac{1}{2}(b + c + e - f), & f' &= \tfrac{1}{2}(b + c - e + f), \\ f'' &= \tfrac{1}{2}(e - f - b - c - 2). \end{aligned}$$

Clearly, if the equality claimed by Minton has to hold for any a', b', c', d', or e', then $f' = f''$ or

$$b + c - e + f + 1 = 0. \quad (3)$$

But $b + c - e + f = 2f'$ must be positive or zero. This shows that condition (3) can never be satisfied.

ACKNOWLEDGMENT

The author wishes to thank Professor A. K. Bose for having brought the article to his attention.

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[1] B. M. Minton, J. Math. Phys. **11**, 3061 (1970).
[2] T. Regge, Nuovo Cimento **11**, 116 (1959).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Remark on Minton's Symmetry for Racah Functions*

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It is shown that the symmetry relation for Racah coefficients recently given by Minton holds only for an analytical continuation of the Racah coefficients to unphysical angular momenta, and even then is valid only under unrealistically stringent conditions.

In a recent paper[1] Minton has proposed a new symmetry for the Racah coefficients. Denoting the Racah coefficient by $W(abcd; ef)$, Minton's result reads

$$\begin{aligned} &W(abcd; ef) \\ &= W(\tfrac{1}{2}[a + c + d - b], \tfrac{1}{2}[e - f - a + d - 1], \\ &\quad \tfrac{1}{2}[e - f + a - d - 1], \tfrac{1}{2}[a + b + d - c]; \\ &\quad \tfrac{1}{2}[e + f + b + c + 1], \tfrac{1}{2}[e + f - b - c - 1]). \quad (1) \end{aligned}$$

Racah[2] explicitly defined the coefficient to be nonzero only when the four triads

$$(a, b, e), (c, d, e), (a, c, f), (b, d, f) \quad (2)$$

each have an integral sum and the elements of each triad satisfy the triangle inequalities. One sees immediately that the six parameters on the right-hand side of Eq. (1) cannot obey the triangle inequalities simultaneously with the left-hand side. Moreover, it can be verified by direct substitution that we never get a "physical" Racah coefficient on the right-hand side of Eq. (1) for a "physical" $W(abcd;ef)$.

Thus, at best, Eq. (1) can have a significance only as an analytic continuation of the Racah function. In this paper, we shall show that even in this extended sense Eq. (1) is true only under further unrealistically stringent conditions.

For the sake of easy comparison we shall use the same notation as in Minton's paper.

A suitable definition for Racah coefficients, valid also in analytic continuation, is[3]

$$W(abcd;ef) = \Big\{\Delta(abe)\,\Delta(cde)\,\Delta(acf)\,\Delta(bdf) \times \Gamma\begin{bmatrix} a+b+c+d+2 \\ a+b+1-e,\, c+d+1-e,\, a+c+1-f,\, b+d+1-f \end{bmatrix} \times \Gamma\begin{bmatrix} 1 \\ e+f+1-c-b,\, e+f+1-a-d \end{bmatrix}\Big\} \times {}_4F_3[e-a-b,\, e-c-d,\, f-c-a,\, f-b-d: -a-b-c-d-1,\, e+f-a-d+1,\, e+f-b-c+1;1]. \quad (3)$$

The analytic continuation is taken by adding small imaginary parts to the parameters a, b, c, d, e, and f. We shall assume that the real parts of the parameters $a, b, \cdots, f$ are physical angular momenta and obey the usual triangle inequalities. Then the gamma functions and the ${}_4F_3$ series is always well behaved, and the ${}_4F_3$ series is still of Saalschutzian type.

Now following the approach in Minton's paper, we want to transform the ${}_4F_3$ series in Eq. (3) to another ${}_4F_3$ series by means of the theorem[4]

$${}_4F_3[A,B,C,D;E,F,G;1] = \Gamma\begin{bmatrix} E+F-A-B-D,\, E+F-A-B-C,\, F-C-D,\, F \\ E+F-A-B,\, E+F-A-B-C-D,\, F-C,\, F-D \end{bmatrix} \times {}_4F_3[E-A,\, E-B,\, C,\, D;\, E,\, E+F-A-B,\, E+G-A-B;1]. \quad (4)$$

This theorem is only valid for terminating Saalschutzian series; thus we get a condition on the analytic continuation, i.e.,

$$f-c-a = \text{real negative integer and/or} \quad f-b-d = \text{real negative integer}. \quad (5)$$

Using Eq. (4) [with the constraint (5)], we find that Eq. (3) now becomes

$$W(abcd;ef) = \{-------\} \times \Gamma\begin{bmatrix} b+f+d+2,\, a+c+f+2,\, a+d+e-f+1,\, e+f-b-c+1 \\ 2f+2,\, a+b+c+d+2,\, a+e-b+1,\, e+d-c+1 \end{bmatrix} \times {}_4F_3[b+f+1-d,\, c+f+1-a,\, f-a-c,\, f-b-d;\, e+f+1-a-d,\, 2f+2,\, f-e-a-d;1], \quad (6)$$

where $\{-------\}$ represents a similarly bracketed term in Eq. (3).

We now apply Eq. (3) to the right-hand side of Eq. (1), compare it with Eq. (6), and after some algebra obtain the following result:

$$W(\tfrac{1}{2}[a+c+d-b],\, \tfrac{1}{2}[e-f-a+d-1],\, \tfrac{1}{2}[e-f+a-d-1],\, \tfrac{1}{2}[a+b+d-c];\, \tfrac{1}{2}[e+f+b+c+1],\, \tfrac{1}{2}[e+f-b-c-1]) = \left(\frac{\csc(\pi[a+b-e])\csc(\pi[c+d-e])}{\csc(\pi[b+f-d])\csc(\pi[c+f-a])}\right) \times W(abcd;ef). \quad (7)$$

Here we have used the relation that $\Gamma(z)\Gamma(-z) = -\pi z^{-1}\csc(\pi z)$. It is particularly important to maintain considerable care in deriving Eq. (7) so as not to cancel possible infinities in expressions that may be indeterminate. For deriving Eq. (7) it was necessary to assume that $\Gamma(d-b-f)$ and $\Gamma(a-f-c)$ were finite, so that gives us additional constraints in analytic continuation that

$$c+f-a \neq \text{positive integer or zero}, \quad b+f-d \neq \text{positive integer or zero}. \quad (8)$$

It should be mentioned here that Eq. (7) is the actual result which follows from Minton's work as against Eq. (1). In the "physical" realm, the left-hand side of Eq. (7) vanishes for quantum mechanical reasons [cf. discussion around Eq. (2)] and the expression

$$\frac{\csc(\pi[a+b-e])\csc(\pi[c+d-e])}{\csc(\pi[b+f-d])\csc(\pi[c+f-a])} \tag{9}$$

on the right-hand side of Eq. (7) is indeterminate.

The result for the physical world should be the limiting value of Eq. (7) when the angular momenta approach "physical" values. Thus to obtain Minton's result, we should have, in addition to Eqs. (8) and (5), further constraints on the limiting process for the values of the six angular momenta, such that, in the limit, expression (9) is unity. In general, of course, the expression is not unity, except at some isolated points in analytic continuation.

We conclude, therefore, that the symmetry relation [Eq. (1)] proposed by Minton is valid only under the special conditions mentioned in Eqs. (5), (8), and in the last paragraph and that even then is of no help in abbreviating tabulations of the physical Racah coefficients.

ACKNOWLEDGMENT

I am indebted to Professor L. C. Biedenharn for his interest in this work.

* Supported in part by the National Science Foundation and the Army Research Office in Durham.

[1] B. M. Minton, J. Math. Phys. **11**, 3061 (1970).
[2] G. Racah, Phys. Rev. **62**, 438 (1942), reprinted in L. C. Biedenharn and H. Van Dam (eds.), *Quantum Theory of Angular Momentum* (Academic Press, New York and London, 1965), p. 146.
[3] See Ref. 1, Eqs. (3a) and (3b).
[4] See Ref. 1, Eq. (6).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Static Gravitational Fields. I. Eight Theorems*

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(Received 8 January 1971)

In a fresh look on static gravitational fields in general relativity, eight new theorems have resulted. Also in the process of deriving theorems a new solution has emerged. In the first of these theorems an invariant necessary integral condition for the existence of a solution has been derived. Physically this condition corresponds to the equilibrium of matter. In the second theorem a scalar condition has been found which implies the flatness of the static gravitational universe. In the third theorem, it has been proved that there cannot occur any group of motion along "the lines of forces." In Theorems 5 and 6, the questions of whether the spatial part of a static gravitational universe can be Einstein, projectively flat, or Stäckel are investigated. In the seventh theorem, the static gravitational field equations have been reduced to the geometrized equations in a spatial universe. In the last theorem, all conformastat gravitational universes have been found. One of these is the universe due to "an infinite plate," and this is a new solution.

1. INTRODUCTION

In the recent years the subject of static gravitational fields remained in a rather passive state while gravitational radiation carried away most of the popular enthusiasm. This area of the general relativity, being the closest to the Newtonian gravitation and classical potential theory, is far from being barren or exhausted. There remain many an intriguing problem in this field, of which a few have been mentioned in the present investigation. In the following the motivations and contents of the various theorems derived here will be elaborated.

The analog of the equations of motion in the static case are the equilibrium conditions. That the equilibrium conditions are inherent in static gravitational equations has been proved[1] exactly in the axially symmetric case. In the more general situation similar results have been proved only in the approximate techniques.[2] In the first theorem of this paper an exact invariant integral condition has been derived from the field equations, and that corresponds to the equilibrium condition.

In a four-dimensional Riemannian universe the necessary and sufficient conditions of flatness are the vanishing of the Riemann tensor, and that amounts to twenty equations. But in a static gravitational universe a single scalar condition implies the flatness. Physically this condition means that "the magnitude of gravitational force vanishes." This is the theme of the second theorem.

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In a four-dimensional Riemannian universe the necessary and sufficient conditions of flatness are the vanishing of the Riemann tensor, and that amounts to twenty equations. But in a static gravitational universe a single scalar condition implies the flatness. Physically this condition means that "the magnitude of gravitational force vanishes." This is the theme of the second theorem.

In the third theorem it has been proved that if the "lines of forces" generate a Killing vector congruence, then the gravitational universe is flat. Physically it means that "the equipotential surface cannot be rigidly transported along the lines of forces."

The fourth theorem contains two parts. In the first part, for subsequent application, Synge's[3] result that the curvature invariant of the spatial part of a static gravitational universe vanishes has been stated. In the second part it has been proved that the constancy of the curvature invariant of a 3-space conformal to the spatial universe implies that the "lines of forces" constitute a geodesic congruence in the 3-space.

In his first attempt to geometrize electromagnetism, Einstein equated the energy–momentum–stress tensor to $R_{ij} - \frac{1}{4}g_{ij}R$ (observe the group-theoretic overtone). Outside matter, then, $R_{ij} = \frac{1}{4}g_{ij}R$. The generalization of this property to any finite-dimensional Riemannian space introduces the concept of Einstein space. In Riemannian geometry there may exist spaces with different Riemann curvatures which have identical geodesics (which may well be straight lines). Weyl[4] discovered the projective curvature tensor which remains invariant under geodesic-preserving mappings. The vanishing of this tensor is the criterion of projective flatness. The definition of a space of constant Riemannian curvature is well known. In the fifth theorem it has been proved that if the spatial part, or the 3-space conformal to it, is Einstein, or projectively flat, or of constant curvature, then the static gravitational space–time universe is flat.

The physical and geometrical implications of these theorems are the following: The spatial part of a nonflat static gravitational universe cannot have straight lines for geodesics. Also the spatial part does not have as much symmetry as the Euclidean 3-space in the sense of allowing a six-parameter group of motion.

Eisenhart[5] and Robertson[6] have shown that the Riemannian spaces where the Hamilton–Jacobi and Schrödinger equations allow solutions with variables separated are Stäckel spaces.[7] It is also known that in the Euclidean 3-space the metric forms in the usual orthogonal curvilinear systems constitute Stäckel space. It is pertinent then to enquire about static gravitational universes with the spatial part being Stäckel. In the sixth theorem this question has been partially answered.

Following the pursuit of Rainich[8], Misner and Wheeler[9] completely geometrized electro-gravitational equations. Subsequently, combined scalar-gravitational equations have been geometrized.[10] From the analogy of static gravitational equations and the combined scalar-gravitational equations (the only difference between the two systems is in the dimensions of the Riemannian spaces involved), the former has been geometrized in a 3-space. Theorem 7 tackles this.

Brinkman[11] proved the nonexistence of conformally flat purely gravitational universes. On the other hand, there exist important classes of static gravitational universes containing other fields which have for their spatial parts a conformally flat 3-space.[12] For such a universe, Synge[13] has coined the word "conformastat" in his well-known book on general relativity. He obtained some interesting results for the purely gravitational conformastat universes and concluded the topic with the following remarks: ". . . the determination of a vacuum conformastat field looks rather hopeless . . . ." By utilizing Schouten's[14] criterion of the conformal flatness of a 3-space, this problem has been solved in the eighth theorem. It turns out that the static gravitational universe due to "an infinite plate," the Schwarzschild universe, and the pseudo-Schwarzschild universe constitute this class. Each of these universes allows a four-parameter group of motion.

In the concluding section a classification scheme for the static gravitational universe has been suggested. The classification turns out to be very simple but structureless. Next a cosmological model has been arrived at from the universe of the infinite plate by interchange of a space and time variables. It has also been suggested how to generate combined scalar-gravitational, electro-gravitational, and magneto-gravitational universes due to "an infinite charged plate" from the purely gravitational case. Before conclusion, two open problems have been suggested which are both intriguing but unyielding.

2. DEFINITIONS AND NOTATIONS

Definition 1: V_4 denotes a four-dimensional Riemannian manifold and physically represents the space–time universe of events. A point $x \in V_4$ has the real coordinates x^i, where i and other Latin indices take the values $1, 2, 3, 4$. V_3 denotes an x^4-constant submanifold of V_4 and represents a spatial universe. A point $\mathbf{x} \in V_3$ has the real coordinates x^α, where α and other Greek indices take the values 1, 2, 3.

Definition 2: V_4 has the index of inertia -2, i.e., the metric form $\Phi \overset{\text{DEF}}{=} g_{ab}(x)\, dx^a\, dx^b$ is reducible at any regular point to $\Phi = -(dX^1)^2 - (dX^1)^2 - (dX^3)^2 + (dX^4)^2$. Here and subsequently, the summation convention is followed unless otherwise mentioned.

Definition 3: The Einstein tensor which represents the energy–momentum–stress density is defined by

$$G_{ij} \overset{\text{DEF}}{=} R_{ij} - \tfrac{1}{2}g_{ij}R,$$

where R_{ij} and R stand for the Ricci tensor and the curvature invariant.

Definition 4: A V_4 is called purely gravitational iff

$$G_{ij} = 0 \Leftrightarrow R_{ij} = 0.$$

It is also known as a special Einstein space.

Definition 5: The metric form of a static V_4 is given by $\Phi = -\bar{e}^{w(\mathbf{x})}\bar{g}_{\alpha\beta}(\mathbf{x})\, dx^\alpha\, dx^\beta + e^{w(\mathbf{x})}(dx^4)^2$. Such a V_4 admits group of motions along x^4 lines. The x^4-constant V_3 is a totally geodesic hypersurface[15] of V_4.

The metric form $\bar{\Phi} = \bar{g}_{\alpha\beta}(\mathbf{x})\, dx^\alpha\, dx^\beta$ defines a positive-definite Riemannian manifold $\bar{V}_3$.

Remark: The topology assumed for V_4 is the product topology $E^1 \times E^1 \times E^1 \times E^1$ and that for V_3 or $\bar{V}_3$ is $E^1 \times E^1 \times E^1$, where E^1 is the real number system.

3. THEOREMS ON STATIC GRAVITATIONAL FIELDS

Lemma 1: Let V_4 be a static universe such that w and $\bar{g}_{\alpha\beta}$ are in C^2 and $\det \bar{g}_{\alpha\beta} > 0$ in a domain $\mathbf{D} \subset V_3$. If the domain $\mathbf{D}$ is both static and gravitational, then

$$\textbf{(F)}: \quad \begin{aligned} \tilde{\sigma}_{\alpha\beta} &\overset{\text{DEF}}{=} \bar{R}_{\alpha\beta} + \tfrac{1}{2}w_{,\alpha}w_{,\beta} = 0, \\ 2\rho &\overset{\text{DEF}}{=} \bar{\Delta}_2 w = 0, \end{aligned} \tag{3.1}$$

where $\bar{R}_{\alpha\beta}$ and $\bar{\Delta}_2$ are the Ricci tensor and invariant Laplacian in $\bar{V}_3$ and subscript, α stands for the partial differentiation with respect to x^α.

The proof is straightforward with the use of $R_{ij} = 0$.

Remark: The static gravitational field equations **(F)** are derivable from a variational principle.

If three coordinate conditions $C_\alpha(\bar{g}_{\mu\nu}) = 0$ are added to **(F)**, then the resulting system is a determinate system of coupled nonlinear partial differential equations. This is so because of the identities $\sigma_{\alpha\cdot\|\beta}^{\ \beta} = \tfrac{1}{2}\rho w_{,\alpha}$ where $\sigma^{\alpha\beta} \overset{\text{DEF}}{=} \tilde{\sigma}^{\alpha\beta} - \tfrac{1}{2}\bar{g}^{\alpha\beta}\tilde{\sigma}^{\mu}{}_{\mu}$, the double stroke denotes covariant differentiation in $\bar{V}_3$, and indices have been raised with $\bar{g}_{\alpha\beta}$. The existence of the identities hinges on the assumptions of differentiability,

$$w \in C^2(\mathbf{D}), \quad \bar{g}_{\alpha\beta} \in C^3(\mathbf{D}), \quad \det(\bar{g}_{\alpha\beta}) > 0, \tag{3.2}$$

where $\mathbf{D}$ is a domain of $\bar{V}_3$.

Definition 6: The interior of a regular body in a static gravitational universe is a bounded domain where (3.1) does not hold but (3.2) does. Moreover, in the neighboring exterior points of the body, **(F)** must hold.

Theorem 1: Let the interior of a regular body $\mathbf{D}_B$ be simply connected and have the piecewise smooth, orientable boundary $\partial(\mathbf{D}_B)$. Let there exist a Killing vector ξ^α in $\mathbf{D}_B$. If, moreover, $\sigma_{\alpha\beta}n^\beta$, where n^β is the unit outer normal to $\partial(\mathbf{D}_B)$, is continuous across the boundary $\partial(\mathbf{D}_B)$, then

$$\int_{\mathbf{D}_B} \rho w_{,\alpha}\xi^\alpha d_3v = 0, \tag{3.3}$$

where d_3v is the invariant volume element in $\bar{V}_3$.

Proof: Now $\sigma_{\alpha\beta} = 0$ by **(F)** in the neighboring exterior points of the body. From the assumption of the continuity it follows then that $\sigma_{\alpha\beta}n^\beta = 0$ on $\partial(D_B)$. Applying the divergence theorem to convert a surface integral into a volume integral, one obtains

$$\begin{aligned} 0 &= \int_{\partial(\mathbf{D}_B)} \sigma_{\alpha\beta}\xi^\alpha n^\beta d_2s = \int_{\mathbf{D}_B} (\sigma_{\alpha\cdot}^{\ \beta}\xi^\alpha)_{\|\beta} d_3v \\ &= \int_{\mathbf{D}_B} \sigma_{\alpha\cdot\|\beta}^{\ \beta}\xi^\alpha d_3v = \int_{\mathbf{D}_B} \rho w_{,\alpha}\xi^\alpha d_3v, \end{aligned}$$

where d_2s is the invariant surface element of $\partial(D_B)$. In the proof above the Killing equation $\xi_{\alpha\|\beta} + \xi_{\beta\|\alpha} = 0$ and the contracted Bianchi's identity

$$(\bar{R}_{\alpha\cdot}^{\ \beta} - \tfrac{1}{2}\delta_{\alpha\cdot}^{\ \beta}\bar{R}^{\gamma}_{\cdot\gamma})_{\|\beta} = 0$$

have been used.

As for the physical interpretation it may be mentioned that in the Newtonian gravitation the integral condition (3.3) would have implied the vanishing of the total force and the total torque on the body.

Theorem 2: Let the field equations **(F)** and the conditions (3.2) be satisfied in a domain $\mathbf{D} \subset \bar{V}_3$. Then the vanishing of curvature invariant $\bar{R}$ in $\mathbf{D}$ implies that the corresponding open cylinder in V_4 is flat.

Proof: The vanishing of $\bar{R}$ implies by virtue of **(F)** that

$$\bar{\Delta}_1 w \overset{\text{DEF}}{=} \bar{g}^{\alpha\beta}w_{,\alpha}w_{,\beta} = 0 \tag{3.4}$$

in $\mathbf{D}$. From the positive definiteness of the above expression, it follows that $w_{,\alpha} = 0 \Rightarrow w = c$, a constant. Therefore, from **(F)** it follows that $\bar{R}_{\alpha\beta} = 0 \Rightarrow \mathbf{D} \subset V_3$ is a domain of Euclidean space. Using the Cartesian coordinates in $\mathbf{D}$, the metric form of the corresponding open cylinder in V_4 becomes

$$\Phi = -\bar{e}^c[(dx^1)^2 + (dx^2)^2 + (dx^3)^2] + e^c(dx^4)^2.$$

This is obviously a flat metric.

Physically this result means that the vanishing of the magnitude of "the gravitational force" $\bar{g}^{\alpha\beta}w_{,\alpha}w_{,\beta}$ implies the flatness of the space–time. The converse theorem is not true.

For the statement and proof of the next theorem the metric form of the static V_4 will be expressed as

$$\Phi = g_{\alpha\beta}(\mathbf{x})\, dx^\alpha\, dx^\beta + e^{w(\mathbf{x})}(dx^4)^2.$$

The metric of the x^4-constant hypersurface V_3 is

$$\mathbf{\Phi} = g_{\alpha\beta}\, dx^\alpha\, dx^\beta.$$

The field equations (F) and the differentiability conditions (3.2) go over to

$$\mathbf{R}_{\alpha\beta} + \bar{e}^{w/2}(e^{w/2})_{|\alpha\beta} = 0, \quad \mathbf{\Delta}_2(e^{w/2}) = 0, \qquad (3.5)$$

$$w \in C^2(\mathbf{D}), \quad g_{\alpha\beta} \in C^3(\mathbf{D}), \quad \det(g_{\alpha\beta}) < 0, \quad (3.6)$$

where $\mathbf{R}_{\alpha\beta}$ and $\mathbf{\Delta}_2$ are the Ricci tensor and the Laplacian in V_3 and the bold stroke denotes the covariant differentiation in V_3.

Theorem 3: Let the field equations (3.5) and the conditions (3.6) be valid in a domain $\mathbf{D} \subset V_3$. If $(e^{w/2})_{,\alpha}$ is a Killing vector in $\mathbf{D}$, then the corresponding open cylinder in V_4 is flat.

Proof: If $(e^{w/2})_{,\alpha}$ is a Killing vector in $\mathbf{D} \subset V_3$, then

$$(e^{w/2})_{|\alpha\beta} + (e^{w/2})_{\beta\alpha} = 2(e^{w/2})_{|\alpha\beta} = 0. \qquad (3.7)$$

Therefore, (3.5) gives

$$\mathbf{R}_{\alpha\beta} = 0 \Leftrightarrow \mathbf{R}_{\alpha\beta\gamma\delta} = 0 \qquad (3.8)$$

in $\mathbf{D} \subset V_3$. But the Riemann tensor of the corresponding open cylinder of V_4 is[16]

$$R_{\alpha\beta\gamma\delta} = \mathbf{R}_{\alpha\beta\gamma\delta}, \quad R_{\alpha\beta\gamma 4} = 0, \quad R_{\alpha 44\beta} = -e^{w/2}(e^{w/2})_{\alpha\beta}. \qquad (3.9)$$

By (3.7), (3.8), and (3.9) it follows that the cylinder is flat.

The physical meaning of this result is that an "equipotential surface cannot be rigidly transported along the lines of forces."

Theorem 4: (i) If static gravitational field equations (3.5) together with the conditions (3.6) hold in a domain $\mathbf{D} \subset V_3$, then the curvature invariant $\mathbf{R}$ must vanish in $\mathbf{D}$.

(ii) Let the field equations (F) and the differentiability conditions (3.2) hold in a domain $\mathbf{D} \subset \bar{V}_3$. If, moreover, the curvature invariant $\bar{R}$ is a nonzero constant in $\mathbf{D}$, then $w_{,\alpha}/(\Delta_1 w)^{\frac{1}{2}}$ constitute a geodesic congruence there.

Proof: (i) From (3.5) it follows that

$$\mathbf{R} = g^{\alpha\beta}\mathbf{R}_{\alpha\beta} = -\bar{e}^{w/2}\mathbf{\Delta}_2(e^{w/2}) = 0.$$

(ii) From (F) it follows that

$$\bar{R} = -\tfrac{1}{2}\bar{\Delta}_1 w \le 0.$$

If $\bar{R}$ is a nonzero constant, it has to be a negative constant and in that case

$$0 = \bar{R}_{,\alpha} = -\tfrac{1}{2}(\bar{\Delta}_1 w)_{,\alpha} = -\bar{g}^{\beta\gamma}w_{,\gamma}w_{\|\alpha\beta}. \quad (3.10)$$

Let the unit tangent vector field be introduced by

$$u_\alpha \overset{\text{DEF}}{=} w_{,\alpha}/(\Delta_1 w)^{\frac{1}{2}} = w_{,\alpha}/(-2\bar{R})^{\frac{1}{2}} = cw_{,\alpha}, \quad (3.11)$$

where c is a constant. From (3.10) and (3.11) it follows that $u^\beta u_{\alpha\|\beta} = 0$, i.e., the u_α constitute a geodesic congruence.

Definition 7: V_3 is an Einstein space iff $R_{\alpha\beta} = \frac{1}{3}g_{\alpha\beta}R$.

Definition 8: V_3 is of constant Riemannian curvature K iff $R_{\alpha\beta\gamma\delta} = K(g_{\alpha\gamma}g_{\beta\delta} - g_{\alpha\delta}g_{\beta\gamma})$.

Definition 9: V_3 is projectively flat iff

$$W^{\alpha}_{\cdot\beta\gamma\delta} \overset{\text{DEF}}{=} R^{\alpha}_{\cdot\beta\gamma\delta} - \tfrac{1}{2}(\delta^{\alpha}_{\cdot\delta}R_{\beta\gamma} - \delta^{\alpha}_{\cdot\gamma}R_{\beta\delta}) = 0.$$

Lemma 2: (i) V_3 is an Einstein space iff it is of constant Riemannian curvature.

(ii) If V_3 is projectively flat, then it is of constant Riemannian curvature.

For the proof of part (i) see Schouten and Struik[17] and for part (ii) see Weyl.[4]

Theorem 5: (i) Let the field equations (3.5) and conditions (3.6) hold in a domain $\mathbf{D} \subset V_3$. If, moreover, V_3 is Einstein or projectively flat, then the open cylinder in V_4 corresponding to $\mathbf{D}$ is flat.

(ii) If the field equations (3.5), conditions (3.6), and V_3 in the previous part are replaced by (F), (3.2), and $\bar{V}_3$, respectively, then the resulting statement is true.

Proof: (i) By Lemma 2, V_3 is of constant curvature. Therefore, by Definition 8, the curvature invariant $\mathbf{R} = -6K$, a constant. But, by Theorem 4(i), $\mathbf{R} = 0 \Rightarrow K = 0 \Rightarrow V_3$ is flat. Via (3.8), (3.5), and (3.9) the theorem is proved.

(ii) By Lemma 2, $\bar{V}_3$ is of constant curvature. Therefore, the curvature invariant $\bar{R} = -6K$, a constant.

Now, from (F), $\bar{R} \leq 0$. This implies that $0 \leq K$. In case $0 < K$, by Lemma 2 and (F) one obtains

$$\bar{R}_{\alpha\beta} = \tfrac{1}{3}\bar{g}_{\alpha\beta}\bar{R} = -2K\bar{g}_{\alpha\beta} = -\tfrac{1}{2}w_{,\alpha}w_{,\beta},$$
$$\bar{g}_{\alpha\beta} = \tfrac{1}{4}K^{-1}w_{,\alpha}w_{,\beta} \Rightarrow \det(\bar{g}_{\alpha\beta}) = 0.$$

The last equation contradicts conditions (3.2). Therefore, $K = 0 \Rightarrow \bar{V}_3$ is flat. By Theorem 2 the completion of the proof follows.

Definition 10: $\bar{V}_3$ is a Stäckel space[7] provided that the metric has the normal form $\bar{\Phi} = H_1^2(dx^1)^2 + H_2^2(dx^2)^2 + H_3^2(dx^3)^2$, and

$$(\ln H_\alpha^2)_{,\alpha\beta} + (\ln H_\alpha^2)_{,\beta}(\ln H_\beta^2)_{,\alpha} = 0, \quad (3.12)$$

$$(\ln H_\alpha^2)_{,\beta\gamma} - (\ln H_\alpha^2)_{,\beta}(\ln H_\alpha^2)_{,\gamma} + (\ln H_\alpha^2)_{,\beta}(\ln H_\beta^2)_{,\gamma} + (\ln H_\alpha^2)_{,\gamma}(\ln H_\gamma^2)_{,\beta} = 0, \quad (3.13)$$

where indices α, β, and γ are all different. The summation convention will be temporarily suspended for the discussion of the Stäckel space.

Theorem 6: Let (F) and (3.2) hold in a domain $\mathbf{D} \subset \bar{V}_3$. If, moreover, $\bar{V}_3$ is Stäckel and $w_{,\alpha} \neq 0$ is in $\mathbf{D}$, then w is transformable to the form

$$w = W(x^1 + x^2 + x^3).$$

Proof: From (3.12) it follows that

$$[\ln(H_\alpha^2/H_\beta^2)]_{,\alpha\beta} = 0. \quad (3.14)$$

By virtue of (3.13)

$$\bar{R}_{\beta\alpha\alpha\gamma} = \tfrac{3}{4}H_\alpha^2(\ln H_\alpha^2)_{,\beta\gamma}. \quad (3.15)$$

If the field equations (F) are written in the Stäckel system, then half of the equations can be expressed as

$$\bar{R}_{\beta\alpha\alpha\gamma} = -\tfrac{1}{2}H_\alpha^2 w_{,\beta}w_{,\gamma}. \quad (3.16)$$

Comparing (3.15) and (3.16), one obtains

$$(\ln H_\alpha^2)_{,\beta\gamma} = -\tfrac{2}{3}w_{,\beta}w_{,\gamma}. \quad (3.17)$$

From (3.14) and (3.17) it follows that

$$[\ln(H_\alpha^2/H_\beta^2)]_{,\alpha\beta\gamma} = 0 = -\tfrac{2}{3}(w_{,\beta}w_{,\alpha\gamma} - w_{,\alpha}w_{,\beta\gamma}),$$
$$\Rightarrow w_{,\alpha}/w_{,\beta} = F^{\beta}_{.\alpha}(x^\alpha, x^\beta). \quad (3.18)$$

Permuting (3.18) cyclically and considering the resulting equations on three coordinate surfaces in $\mathbf{D}$, one can conclude that

$$F^{\beta}_{.\alpha}(x^\alpha, x^\beta) = f_\alpha(x^\alpha)/f_\beta(x^\beta), \quad f_\beta \neq 0. \quad (3.19)$$

Therefore, from (3.18) and (3.19) one arrives at the following relations:

$$w_{,1}/f_1(x^1) = w_{,2}/f_2(x^2) = w_{,3}/f_3(x^3). \quad (3.20)$$

Defining the functions

$$X_\alpha(x^\alpha) \overset{\text{DEF}}{=} \int f_\alpha(x^\alpha)\, dx^\alpha,$$

one obtains from (3.20)

$$w = W[X_1(x^1) + X_2(x^2) + X_3(x^3)]. \quad (3.21)$$

Now by making a coordinate transformation $x'^\alpha = X_\alpha(x^\alpha)$ and dropping primes subsequently, it follows from (3.21) that

$$w = W(x^1 + x^2 + x^3).$$

The next theorem can be considered as the solution of the Rainich problem for the field equations (F).

Theorem 7: Let the conditions (3.2) and $\bar{R}_{\alpha\beta} \neq 0$ be satisfied in a domain $\mathbf{D} \subset \bar{V}_3$. Consider the geometrized equations

$$(\mathbf{F}'): \quad \bar{R}_{\alpha[\beta}\bar{R}_{\mu]\nu} = 0,$$
$$\bar{R}_{\alpha\beta}\bar{R}_{\mu[\nu\|\lambda]} + \bar{R}_{\alpha\mu}\bar{R}_{\beta[\nu\|\lambda]} = \bar{R}_{\alpha[\nu}\bar{R}_{\beta\mu\|\lambda]} = 0,$$

where square brackets denote antisymmetrization and cyclic permutation. Then equations (F)$\Leftrightarrow$(F′) in $\mathbf{D}$ provided that

$$w = \pm 2^{\frac{1}{2}} \sum_{\alpha=1}^{3} \int^{\mathbf{x}} (-R_{\alpha\alpha})^{\frac{1}{2}}\, dx^\alpha.$$

For the proof, see Kuchař.[10]

4. THEOREMS ON THE CONFORMASTAT UNIVERSES

Definition 11: A static V_4 with the metric form

$$\Phi = g_{\alpha\beta}(\mathbf{x})\, dx^\alpha\, dx^\beta + e^{w(\mathbf{x})}(dx^4)^2,$$

where the metric form $\mathbf{\Phi} = g_{\alpha\beta}(\mathbf{x})\, dx^\alpha\, dx^\beta$ defines a conformally flat[18] V_3, is called a conformastat universe.[13]

Synge's Theorem[13]*:* Let D be a domain of a conformastat, gravitational universe V_4. Let the metric form of V_4 be

$$\Phi = -U^4(\mathbf{x})[(dx^1)^2 + (dx^2)^2 + (dx^3)^2] + e^{w(\mathbf{x})}(dx^4)^2$$

such that U, $w \in C^2(D)$ and $U \neq 0$ in D. Then $U(\mathbf{x})$ is a Euclidean harmonic function in $\mathbf{D}$, which is a x^4-constant subset of D.

Proof: The curvature invariant $\mathbf{R}$ of V_3, a x^4-constant hypersurface of V_4, as calculated from the conformastat metric is

$$\mathbf{R} = -8U^{-5}\nabla^2 U, \quad (4.1)$$

where ∇^2 denotes the Euclidean Laplace operator. Now, by Theorem 4(i), $\mathbf{R} = 0$, which together with (4.1) implies that U is a Euclidean harmonic function.

Schouten's Lemma: A $\bar{V}_3$ is conformally flat iff

$$\bar{R}_{\alpha\beta\gamma} \overset{\text{DEF}}{=} \bar{R}_{\alpha[\beta\|\gamma]} + \tfrac{1}{4}\bar{g}_{\alpha[\gamma}\bar{R}_{,\beta]} = 0, \tag{4.2}$$

where the square bracket denotes antisymmetrization.

For the proof, see Schouten.[14]

Theorem 8: Let V_4 be a conformastat gravitational universe with the metric form

$$\Phi = -e^{-w(\mathbf{x})}\bar{g}_{\alpha\beta}(\mathbf{x})\, dx^\alpha\, dx^\beta + e^{w(\mathbf{x})}(dx^4)^2.$$

(i) Then a w = const surface ("equipotential"!) in $\bar{V}_3$ (cf. Definition 5) is a surface of constant curvature.

(ii) Moreover, V_4 is (A) flat or due to the infinite plate, or (B) Schwarzschild, or else (C) pseudo-Schwarzschild according as the constant of curvature is (A) zero or (B) positive, or else (C) negative.

Proof: (i) From the Definition 11 it follows that for the conformastat V_4 the corresponding $\bar{V}_3$ must be conformally flat. Then by Schouten's lemma Eq. (4.2) must hold. Via the field equations (F), it is seen that Eqs. (4.2) go over to

$$w_{,[\beta}w_{\|\gamma]\alpha} + \tfrac{1}{2}\bar{g}^{\mu\nu}\bar{g}_{\alpha[\gamma}w_{\|\beta]\mu}w_{,\nu} = 0. \tag{4.3}$$

To integrate (4.3), three coordinate conditions, which one is allowed to impose, are chosen to be

$$w(\mathbf{x}) = x^1, \quad \bar{g}_{12} = \bar{g}_{13} = 0. \tag{4.4}$$

Via (4.4), Eqs. (4.3) can be integrated to obtain the metric form of $\bar{V}_3$,

$$\bar{\Phi} = U^2(x^1)(dx^1)^2 + U(x^1)[f(x^2, x^3)(dx^2)^2 + g(x^2, x^3)(dx^3)^2 + 2h(x^2, x^3)\, dx^2\, dx^3], \tag{4.5}$$

where U, f, g, and h are arbitrary functions of class C^3 with the constraint $U^4(fg - h^2) > 0$. To determine these functions, the field equations (F) have to be used. But instead of (F) the following equivalent form (F″) will be more convenient:

$$(\text{F}''){:}\ \sigma_{\mu\alpha\beta\gamma} \overset{\text{DEF}}{=} \bar{R}_{\mu\alpha\beta\gamma} + \tfrac{1}{2}(\bar{g}_{\mu[\gamma}w_{,\beta]}w_{,\alpha} + \bar{g}_{\alpha[\beta}w_{,\gamma]}w_{,\mu}) + \tfrac{1}{4}\bar{\Delta}_1 w\bar{g}_{\alpha[\gamma}\bar{g}_{\beta]\mu} = 0, \quad \rho = \bar{\Delta}_2 w = 0. \tag{4.6}$$

Plugging (4.5) and the coordinate condition $w = x^1$ into either $\sigma_{1221} = 0$ or $\sigma_{1331} = 0$, one obtains the solution

$$U(x^1) = (ae^{\frac{1}{2}x^1} - be^{-\frac{1}{2}x^1})^{-2}, \tag{4.7}$$

where a and b are constants of integration such that one of these must be different from zero. On the other hand, the equation $\sigma_{2332} = 0$ leads to

$$r_{2332} = ab(h^2 - fg), \tag{4.8}$$

where r_{2332} is the Riemann tensor of the "equipotential" surface with the metric form $\varphi = f(dx^2)^2 + g(dx^3)^2 + 2h\, dx^2\, dx^3$. Equation (4.8) denotes, by virtue of the Definition 8, a surface with the constant curvature ab.

(ii) From the trichotomy of real numbers one has to consider three cases: (A) $ab = 0$, (B) $ab > 0$, and (C) $ab < 0$.

Case (A): Now $ab = 0 \Rightarrow$ either $a = 0$ or $b = 0$ or both $a = b = 0$. The subcase $a = b = 0$ is excluded because $U(x^1)$ would be singular. In the subcase $a = 0$ it is easy to show that V_4 is flat.

In the subcase $b = 0$ the metric form of V_4 can be reduced to the following:

$$\Phi = -(1 - mx^1)^4[(dx^1)^2 + (dx^2)^2 + (dx^3)^2] + (1 - mx^1)^{-2}(dx^4)^2, \tag{4.9}$$

where m is a constant. This metric form allows four-parameter group of motions, the generators being $\partial/\partial x^2$, $\partial/\partial x^3$, $\partial/\partial x^4$, $x^2\partial/\partial x^3 - x^3\partial/\partial x^2$. From this consideration and also by observing the potential function $1 - mx^1$ (cf. Synge's theorem), we conclude that the above metric is due to an infinite plate parallel to (x^2, x^3) plane.

Case (B): In the case $ab > 0$, the so-called Riemannian metric form of the surface of constant curvature becomes

$$\varphi = \{1 + \tfrac{1}{4}ab[(x^2)^2 + (x^3)^2]\}^{-2}[(dx^2)^2 + (dx^3)^2].$$

Plugging above into (4.5), making the coordinate transformation

$$r(1 + m/2r)^2 = [1 - (a/b)e^{x^1}]^{-1},$$
$$\theta = \arctan\,[\tfrac{1}{2}ab(x^{2^2} + x^{3^2})]^{\frac{1}{2}},$$
$$\varphi = \arctan\,(x^3/x^2), \quad t = (b/a)^{\frac{1}{2}}x^4,$$

and denoting the constant $m = \frac{1}{8}(ab^{-3})^{\frac{1}{2}} > 0$, we find that the metric form of V_4 goes to Schwarzschild form

$$\Phi = -(1 + m/2r)^4[dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)] + \left(\frac{1 - m/2r}{1 + m/2r}\right)^2 dt^2.$$

Schwarzschild's V_4 obviously allows a four-parameter group of motion.

Case (C): In the case $ab < 0$ the metric form of V_4 goes to the unphysical pseudo-Schwarzschild form

$$\Phi = -(1 - m/2R)^4[dR^2 + R^2(d\Psi^2 + \sinh^2\Psi\, d\varphi^2)] + \left(\frac{1 + m/2R}{1 - m/2R}\right)^2 dt^2.$$

5. CONCLUDING REMARKS

A few words on the classification of the static gravitational V_4 should be mentioned. Instead of V_4 the subspace $\bar{V}_3$ will be considered. This is because the static gravitational V_4 can be generated by a suitably chosen $\bar{V}_3$, by Theorem 7. In $\bar{V}_3$ the Ricci tensor will be classified instead of the Riemann tensor. They are algebraically related anyway. The classification of Ricci tensor is extremely simple due to the field equations $\bar{R}_{\alpha\beta} = -\frac{1}{2}w_{,\alpha}w_{,\beta}$. It is obvious that the Ricci tensor at any regular point of $\bar{V}_3$ will have one nonpositive and two other zero eigenvalues.

The nonstatic V_4 with the metric

$$\Phi = -t^{-\frac{2}{3}}\,dx^2 - t^{\frac{4}{3}}(dy^2 + dz^2) + dt^2, \quad t > 0,$$

which is obtained from (4.9) via an "illegal" transformation, may be of some use in cosmology.

By application of the theorems of De,[19] Buchdahl,[20] Majumdar,[21] and Bonnor,[22] respectively, one can generate out of (4.9) the static combined scalar-gravitational, electro-gravitational, and magneto-gravitational fields due to an "infinite charged plate."

One of the open questions which remains to be settled is to find the class of Stäckel $\bar{V}_3$, which is a hypersurface of static gravitational V_4. The author has a conjecture which arises out of the Weyl[23] solution, Majumdar's[1] work, and the physical implication of Theorem 1. The conjecture is that, from a Newtonian potential due to matter at equilibrium, a static gravitational V_4 can be generated. This problem is a challenge to the ingenuity.

* This research has been supported by the N.R.C. Grant A-3993.

1 S. D. Majumdar, Phys. Rev. **72**, 390 (1947).
2 N. Rosen, Rev. Mod. Phys. **21**, 503 (1948); H. Bondi, *ibid.* **29**, 423 (1957); A. Das, P. S. Florides, and J. L. Synge, Proc. Roy. Soc. (London) **A263**, 451 (1961).
3 J. L. Synge, *Relativity: The General Theory* (North-Holland, Amsterdam, 1960).
4 H. Weyl, Göttinger Nachr., 99 (1921).
5 L. P. Eisenhart, Ann. Math. **35**, 284 (1934).
6 H. P. Robertson, Math. Am. **98**, 749 (1927).
7 L. P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1966), p. 130.
8 G. Y. Rainich, Proc. Natl. Acad. Sci. (U.S.) **10**, 124 (1924); Bull. Am. Math. Soc. **30**, 294 (1924).
9 C. W. Misner and J. A. Wheeler, Ann. Phys. (N.Y.) **2**, 525 (1957).
10 K. Kuchař, Czech. J. Phys. **B13**, 551 (1963).
11 H. W. Brinkman, Proc. Natl. Acad. Sci. **9**, 172 (1923).
12 S. D. Majumdar, Ref. 1; A. Das, Proc. Roy. Soc. (London) **A267**, 1 (1962) and J. Math. Phys. **4**, 45 (1963); A. Das and C. V. Coffman, *ibid.* **8**, 1720 (1967); N. De, Progr. Theoret. Phys. (Kyoto) **33**, 545 (1965).
13 J. L. Synge, Ref. 3, p. 341.
14 J. A. Schouten, Math. Z. **11**, 58 (1921).
15 L. P. Eisenhart, Ref. 7, p. 183.
16 J. L. Synge, Ref. 3, p. 339.
17 J. A. Schouten and D. J. Struik, Am. J. Math. **43**, 213 (1921).
18 L. P. Eisenhart, Ref. 7, p. 89.
19 N. De, Progr. Theoret. Phys. (Kyoto) **32**, 177 (1964).
20 H. A. Buchdahl, Phys. Rev. **115**, 1325 (1959).
21 S. D. Majumdar, Proc. Phys. Soc. (London) **A79**, 657 (1962).
22 W. B. Bonnor, Proc. Phys. Soc. (London) **A67**, 225 (1954).
23 J. L. Synge, Ref. 3, p. 309.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Analytic Continuation of the Regular Solution of the Schrödinger Equation in the Complex Angular Momentum Plane*

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(Received 16 September 1970)

In this paper we develop a method of performing the analytic continuation of functions that are Stieltjes or Laplace transforms. We apply the method to find the regular solution and its asymptotic behavior in the left half-plane. The irregular solution and the S matrix are briefly discussed.

INTRODUCTION

One of the basic questions in potential scattering[1] is the nature of the solutions, partial waves, of

$$\left(\frac{d^2}{dr^2} + 1 - V(r) - \frac{\lambda^2 - \frac{1}{4}}{r^2}\right)\Phi_\lambda(r) = 0, \qquad (1)$$

where $0 \le r < \infty$, λ is a complex parameter, and the potential $V(r)$ satisfies the conditions that for some $0 < c$

$$\int_0^c rV(r)\,dr < \infty \quad \text{and} \quad \int_c^\infty r^2V(r)\,dr < \infty. \qquad (2)$$

It is convenient to define three, of course, not linearly independent solutions of (1). Two are defined by boundary conditions at infinity, the irregular solutions

$$\lim_{r\to\infty} e^{ir}f_\lambda^\pm(r) = 1, \qquad (3)$$

and the third is defined by boundary conditions at the origin, the regular solution

$$\lim_{r\to 0} \pi^{-\frac{1}{2}}(\tfrac{1}{2}r)^{-\lambda-\frac{1}{2}}\Gamma(1+\lambda)\varphi_\lambda(r) = 0, \quad \operatorname{Re}\lambda \ge 0, \qquad (4)$$

where $\Gamma(z)$ is the gamma function.[2]

5. CONCLUDING REMARKS

A few words on the classification of the static gravitational V_4 should be mentioned. Instead of V_4 the subspace $\bar{V}_3$ will be considered. This is because the static gravitational V_4 can be generated by a suitably chosen $\bar{V}_3$, by Theorem 7. In $\bar{V}_3$ the Ricci tensor will be classified instead of the Riemann tensor. They are algebraically related anyway. The classification of Ricci tensor is extremely simple due to the field equations $\bar{R}_{\alpha\beta} = -\frac{1}{2}w_{,\alpha}w_{,\beta}$. It is obvious that the Ricci tensor at any regular point of $\bar{V}_3$ will have one nonpositive and two other zero eigenvalues.

The nonstatic V_4 with the metric

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which is obtained from (4.9) via an "illegal" transformation, may be of some use in cosmology.

By application of the theorems of De,[19] Buchdahl,[20] Majumdar,[21] and Bonnor,[22] respectively, one can generate out of (4.9) the static combined scalar-gravitational, electro-gravitational, and magneto-gravitational fields due to an "infinite charged plate."

One of the open questions which remains to be settled is to find the class of Stäckel $\bar{V}_3$, which is a hypersurface of static gravitational V_4. The author has a conjecture which arises out of the Weyl[23] solution, Majumdar's[1] work, and the physical implication of Theorem 1. The conjecture is that, from a Newtonian potential due to matter at equilibrium, a static gravitational V_4 can be generated. This problem is a challenge to the ingenuity.

* This research has been supported by the N.R.C. Grant A-3993.

[1] S. D. Majumdar, Phys. Rev. **72**, 390 (1947).
[2] N. Rosen, Rev. Mod. Phys. **21**, 503 (1948); H. Bondi, *ibid.* **29**, 423 (1957); A. Das, P. S. Florides, and J. L. Synge, Proc. Roy. Soc. (London) **A263**, 451 (1961).
[3] J. L. Synge, *Relativity: The General Theory* (North-Holland, Amsterdam, 1960).
[4] H. Weyl, Göttinger Nachr., 99 (1921).
[5] L. P. Eisenhart, Ann. Math. **35**, 284 (1934).
[6] H. P. Robertson, Math. Am. **98**, 749 (1927).
[7] L. P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1966), p. 130.
[8] G. Y. Rainich, Proc. Natl. Acad. Sci. (U.S.) **10**, 124 (1924); Bull. Am. Math. Soc. **30**, 294 (1924).
[9] C. W. Misner and J. A. Wheeler, Ann. Phys. (N.Y.) **2**, 525 (1957).
[10] K. Kuchař, Czech. J. Phys. **B13**, 551 (1963).
[11] H. W. Brinkman, Proc. Natl. Acad. Sci. **9**, 172 (1923).
[12] S. D. Majumdar, Ref. 1; A. Das, Proc. Roy. Soc. (London) **A267**, 1 (1962) and J. Math. Phys. **4**, 45 (1963); A. Das and C. V. Coffman, *ibid.* **8**, 1720 (1967); N. De, Progr. Theoret. Phys. (Kyoto) **33**, 545 (1965).
[13] J. L. Synge, Ref. 3, p. 341.
[14] J. A. Schouten, Math. Z. **11**, 58 (1921).
[15] L. P. Eisenhart, Ref. 7, p. 183.
[16] J. L. Synge, Ref. 3, p. 339.
[17] J. A. Schouten and D. J. Struik, Am. J. Math. **43**, 213 (1921).
[18] L. P. Eisenhart, Ref. 7, p. 89.
[19] N. De, Progr. Theoret. Phys. (Kyoto) **32**, 177 (1964).
[20] H. A. Buchdahl, Phys. Rev. **115**, 1325 (1959).
[21] S. D. Majumdar, Proc. Phys. Soc. (London) **A79**, 657 (1962).
[22] W. B. Bonnor, Proc. Phys. Soc. (London) **A67**, 225 (1954).
[23] J. L. Synge, Ref. 3, p. 309.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Analytic Continuation of the Regular Solution of the Schrödinger Equation in the Complex Angular Momentum Plane*

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(Received 16 September 1970)

In this paper we develop a method of performing the analytic continuation of functions that are Stieltjes or Laplace transforms. We apply the method to find the regular solution and its asymptotic behavior in the left half-plane. The irregular solution and the S matrix are briefly discussed.

INTRODUCTION

One of the basic questions in potential scattering[1] is the nature of the solutions, partial waves, of

$$\left(\frac{d^2}{dr^2} + 1 - V(r) - \frac{\lambda^2 - \frac{1}{4}}{r^2}\right)\Phi_\lambda(r) = 0, \quad (1)$$

where $0 \leq r < \infty$, λ is a complex parameter, and the potential $V(r)$ satisfies the conditions that for some $0 < c$

$$\int_0^c rV(r)\,dr < \infty \quad \text{and} \quad \int_c^\infty r^2V(r)\,dr < \infty. \quad (2)$$

It is convenient to define three, of course, not linearly independent solutions of (1). Two are defined by boundary conditions at infinity, the irregular solutions

$$\lim_{r\to\infty} e^{ir} f_\lambda^{\pm}(r) = 1, \quad (3)$$

and the third is defined by boundary conditions at the origin, the regular solution

$$\lim_{r\to 0} \pi^{-\frac{1}{2}}(\tfrac{1}{2}r)^{-\lambda-\frac{1}{2}}\Gamma(1 + \lambda)\varphi_\lambda(r) = 0, \quad \operatorname{Re}\lambda \geq 0, \quad (4)$$

where $\Gamma(z)$ is the gamma function.[2]

Since (3) does not depend on λ and (1) depends on λ^2, only the irregular solutions are even functions of λ. But (4) depends on an odd power of λ; therefore, the regular solution in general will not be an even function of λ. One needs to find the analytic continuation of $\varphi_\lambda(r)$ from the domain $\mathrm{Re}\,\lambda \geq 0$ into $\mathrm{Re}\,\lambda < 0$.[3]

The boundary conditions were chosen so that

$$\varphi_\lambda(r) = (2i)^{-1}W(\varphi_\lambda(r), f_\lambda^+(r))f_\lambda^-(r) - (2i)^{-1}W(\varphi_\lambda(r), f_\lambda^-(r))f_\lambda^+(r)$$

is the decomposition of the solution of (1) into the sum of incoming and outgoing waves. Using this decomposition, we define the S matrix by

$$S_\lambda = e^{i\pi(\lambda+\frac{1}{2})}W(\varphi_\lambda(r), f_\lambda^+(r))/W(\varphi_\lambda(r), f_\lambda^-(r)).$$

The purpose of this paper is to describe a method which was designed to perform the analytic continuation of the regular solution $\varphi_\lambda(x)$. While it seems that no other restrictions on the potential than (2) is needed, to show this requires a major effort. It will be shown that this method is applicable to a more restrictive class, which includes most potentials that are used in physics. Other, more pathological potentials, at the present, must be investigated individually.

The numerous efforts to find analytic continuations made direct use of (1) or some equivalent integral equations. While the theory of differential and integral equations aided these efforts, it also limited them. It limited the admissable potentials essentially to the class of analytic potentials. Some of these efforts are described when the present results are compared to the previous ones. Others are found in Refs. 1 and 3.

The method of this paper differs basically from the previous ones. To continue $\varphi_\lambda(r)$ for a fixed $r = r_0$ with the previous methods, one needs to continue $\varphi_\lambda(r)$ for all r in the closed interval $[0, r_0]$. The present method finds the analytic continuation only for $r = r_0$; thus it avoids the critical point $r = 0$. Moreover, knowing the analytic continuation of $\varphi_\lambda(r)$ for an interval (R_1, R_2), one can find the analytic continuation for $r < R_1$ and $r > R_2$ by joining the general solution of (1) to $\varphi_\lambda(r)$ at the points R_1 and R_2, requiring that the logarithmic derivatives be continuous there.

The method of this paper uses the integral representation[4]

$$\varphi_\lambda(r) = \varphi_\lambda^c(r) - \int_0^r s^{-2}K(r, s)\varphi_\lambda^c(s)\,ds \qquad (5)$$

of the regular solution of (1), where $\varphi_\lambda^c(r)$ is the exact regular solution for some comparison potential $V^c(r)$. To find $K(r, s)$, one needs to substitute Eq. (5) into (1). The result is that $K(r, s)$ is the solution of

$$r^2\left(\frac{\partial^2}{\partial r^2} + 1 - V(r) + V^c(r)\right)K(r, s) = s^2\left(\frac{\partial^2}{\partial s^2} + 1 + V^c(s)\right)K(r, s), \quad (6)$$

$$V(r) - V^c(r) = -2r^{-1}\frac{d}{dr}[r^{-1}K(r, r)],$$

$\lim_{s\to 0} K(r, s) = 0$ uniformly in r in the domain $r \geq s$.

A detailed derivation of the equation for the kernel of the identical representation of the irregular solutions is given in Appendix A. The origins of (6) are found in that section.

When $V^c(r)$ is selected such that the analytic properties of $\varphi_\lambda^c(r)$ are known for all λ, it only remains to find the analytic continuation of the integral $\int_0^r s^{-2}K(r, s)\varphi_\lambda^c(s)\,ds$. From the existence of $\varphi_\lambda(r)$ for $\mathrm{Re}\,\lambda \geq 0$, it follows that this integral will be finite for $\mathrm{Re}\,\lambda \geq 0$. But in general there will be a positive number p, such that when $\mathrm{Re}\,\lambda \leq -p$, this integral will diverge. When we choose $V^c(r) = -1$, then $\varphi_\lambda^c(r) = (\frac{1}{2}\pi)^{\frac{1}{2}-\lambda}\Gamma^{-1}(\lambda + 1)r^{\lambda+\frac{1}{2}}$; thus the mathematical problem can be formulated as follows: Given $f(x)$ such that, for $\mathrm{Re}\,\lambda \geq 0$, $g(\lambda) = \int_0^1 f(x)x^\lambda\,dx$ is an analytic function, find the largest domain in the complex λ plane onto which $g(\lambda)$ can be analytically continued, and determine the nature of the singularities at the boundaries.

Section 1 contains the method for performing the analytic continuation of functions that are Stieltjes or Laplace or other more general transforms. Section 2 uses this method for the regular solution and its asymptotic behavior in the left half-plane.

There are three applications given. The first one shows that, for most potentials that are presently used, the regular solution is an analytic function in the complex angular momentum plane cut from $-\infty$ to 0. The second application finds that the S matrix is a meromorphic function in the same domain. For cutoff potentials we also find the asymptotic behavior of the S matrix. In the final application we find new integral representations and bounds for the Bessel and gamma functions.

In Appendix A we give a new integral representation of the irregular solution. In Appendix B we discuss the integral representation of the regular solution.

1. MATHEMATICAL TOOLS

In this section two proofs are given. Lemma 1 is the key to the analytic continuation of the regular solution. Lemma 2 is a useful variant of Lemma 1.

Lemma 1: Let

(i) $f(t)\ln(t)$ be a continuous function of the real variable t at $t = 0$,

(ii) $f(e^{-w})$, $w = u + iv$, be an analytic function of w in the domain $u > 0$ and continuous at $u = 0$,

(iii) $f(e^{-w})$ be polynomially bounded in the domain, and define $g(\lambda)$ by

$$g(\lambda) = \int_0^1 f(t)t^\lambda\, dt, \quad \mu \geq 0, \quad \lambda = \mu + i\nu;$$

then $g(\lambda)$ is an analytic function of λ in the domain $\mu \geq 0$, and its analytic continuation to the domain $\mu < 0$ can have singularities only on the negative real axis and at infinity.

Proof: By (ii), $f(e^{-u})$ is continuous in $0 \leq u < \infty$, i.e., $f(t)$ is continuous in $0 < t \leq 1$. Combining this with (i), we have that, in $0 < t \leq 1$, $f(t)t^\lambda$ and $\partial f(t)t^\lambda/\partial\lambda = f(t)\ln(t)t^\lambda$ are continuous functions of t and the continuity of $\partial f(t)t^\lambda/\partial\lambda$ *qua* function of λ in the domain $\mu \geq 0$ is uniform with respect to the variable t. Hence $g(\lambda)$ is an analytic function of λ in the domain $\mu \geq 0$.[5] Perform the transformation $t = e^{-w}$ to get

$$g(\lambda) = \int_0^\infty f(e^{-w})e^{-(\lambda+1)w}\, dw.$$

By (ii), $f(e^{-w})e^{-(\lambda+1)w}$ is an analytic function of w in the domain $u > 0$ and continuous at $u = 0$. We apply Cauchy's theorem to the function $f(e^{-w})e^{-(\lambda+1)w}$. Consider two cases.

Case 1: $\nu < 0$: The closed contour is the positive real axis, a circular arc connecting it to the positive imaginary axis and the positive imaginary axis. We have

$$\lim_{\substack{|w|\to\infty \\ u\geq 0, v\geq 0}} [|wf(e^{-w})e^{-(\lambda+1)w}|]$$
$$= \lim_{\substack{|w|\to\infty \\ u\geq 0, v\geq 0}} [|f(e^{-w})e^{-\frac{1}{2}u+\frac{1}{2}\nu v}|\, |u^2 + v^2|^{\frac{1}{2}}\, e^{-(\mu+\frac{1}{2})u+\frac{1}{2}\nu v}] = 0.$$

Therefore, the integral over the circular arc vanishes as the radius of the arc goes to infinity. Thus,

$$\text{(A)} \quad g(\lambda) = i\int_0^\infty f(e^{-iv})e^{\nu v - i(\mu+1)v}\, dv, \quad \mu \geq 0, \quad \nu < 0.$$

The integral and the integrand are uniformly bounded in $\nu \leq \nu_0 < 0$ and $-\infty < \mu < \infty$. Hence the analytic continuation can be accomplished under the integral sign, and (A) defines $g(\lambda)$ in the lower half of the λ plane.

Case 2: $\nu > 0$: The closed contour consists of the negative imaginary axis, a large circular arc connecting it to the positive real axis and the positive real axis. We have

$$\lim_{\substack{|w|\to\infty \\ u\geq 0, v\leq 0}} [|wf(e^{-w})e^{-(\lambda+1)w}|] = 0.$$

Hence the integral over the circular arc goes to zero as the radius of the arc goes to infinity, and

$$\text{(B)} \qquad g(\lambda) = -i\int_0^\infty f(e^{iv})e^{-\nu v+i(\mu+1)v}\, dv,$$
$$\mu \geq 0, \quad \nu > 0.$$

Again the integral and the integrand are uniformly bounded in $\nu \geq \nu_0 > 0$ and $-\infty < \mu < \infty$, and (B) is the analytic continuation of $g(\lambda)$ to the upper half of the λ plane.

This shows that there are no singularities in the λ plane except maybe on the negative real axis and at infinity. To find the singularities, one needs to evaluate the integrals (A) and (B) and let $\nu \to 0$. Where these two functions become infinite or where they do not match, there is a singularity. This proves the lemma.

Remarks:

(1) The conditions of the lemma, for example, are satisfied by the functions which are analytic in the domain $|t| \leq 1$, by $t\ln(t)$, by the Bessel function $J_p(t)$, and by t^p when p is any positive real number.

(2) The function $f(t) = t^{a+ib} + t^{a-ic}$, $a > 0$, $b > 0$, and $c > 0$ does not satisfy (iii). But, when $\nu > b$ and when $\nu < -c$, the integrals over the circular arcs vanish as the radii of the arcs go to infinity. Hence with the above method one can find the analytic continuation to $\mu < 0$ excluding the strip $-c \leq \nu \leq b$. However, one can write $f(t) = f_1(t) + f_2(t)$, where $f_1(t) = t^{a+ib}$ and $f_2(t) = t^{a-ic}$ and continue $f_1(t)$ and $f_2(t)$ individually. First let $\tau = \lambda + ib$; then

$$g_1(\lambda) \equiv \int_0^1 f_1(t)t^\lambda\, dt = \int_0^1 t^{a+ib+\lambda}\, dt = \int_0^\infty e^{-(a+\tau+1)w}\, dw.$$

When $\operatorname{Im}\tau < 0$, then

$$g_1(\lambda) = i\int_0^\infty e^{-i(a+\tau+1)v}\, dv = -(a + \tau + 1)^{-1}.$$

When $\operatorname{Im}\tau > 0$, then

$$g_1(\lambda) = -i\int_0^\infty e^{i(a+\tau+1)v}\, dv = -(a + \tau + 1)^{-1}.$$

As $\operatorname{Im}\tau \to 0$, the two functions match everywhere and there is only a polar singularity at $\tau = -a - 1$, i.e., at $\lambda_1 = -a - 1 - ib$. Next let $\tau = \lambda - ic$; the same procedure gives that $f_2(t)$ has only a polar singularity at $\lambda_2 = -a - 1 + ic$. Thus $g(\lambda)$ is a meromorphic function with poles at λ_1 and at λ_2.

(3) As an example, let $f(t) = \sin \pi t$; then

$$g(\lambda) = \int_0^1 x^\lambda \sin \pi x \, dx,$$

and so by Lemma 1, when $\lambda = \mu \pm i|\nu|$ and $|\nu| > 0$,

$$g(\lambda) = \pm i \int_0^\infty e^{\pm i(\lambda+1)v} \sin(\pi e^{\pm iv}) \, dv,$$

$$g(\lambda) = \pm i \sum_{n=0}^{\infty} \int_0^{2\pi} e^{\pm i(\lambda+1)2\pi n} e^{\pm i(\lambda+1)x} \sin(\pi e^{\pm ix}) \, dx.$$

Interchanging the summation and integration is permitted since $|\nu| > 0$. We have

$$\begin{aligned} g(\lambda) &= \left(\pm i \int_0^{2\pi} e^{\pm i(\lambda+1)x} \sin(\pi e^{\pm ix}) \, dx\right) \sum_{n=0}^{\infty} e^{\pm 2\pi i n(\lambda+1)} \\ &= \pm i(1 - e^{\pm 2\pi i(\lambda+1)})^{-1} \int_0^{2\pi} e^{\pm i(\lambda+1)x} \sin(\pi e^{\pm ix}) \, dx \\ &= \pm i(1 - e^{\pm 2\pi i(\lambda+1)})^{-1} \left(\int_0^\pi + \int_\pi^{2\pi}\right) \\ &= \pm i(1 - e^{\pm 2\pi i(\lambda+1)})^{-1}(1 - e^{\pm i\pi(\lambda+1)}) \\ &\quad \times \int_0^\pi e^{\pm ix(\lambda+1)} \sin(\pi e^{\pm ix}) \, dx. \end{aligned}$$

The analytic continuation and its asymptotic form is clear. To see what happens when $|\nu| \to 0$, write $u = e^{\pm ix}$; then

$$g(\lambda) = (1 - e^{\pm 2\pi i(\lambda+1)})^{-1}(1 - e^{\pm i(\lambda+1)}) \int_{-1}^1 u \sin \pi u \, du.$$

(a) When $\lambda = 2m + 1 \pm i|\nu|$, $\pm m = 0, 1, 2, \cdots$, as $|\nu| \to 0$, the factor $(1 - e^{\pm i\pi(\lambda+1)}) \to 0$ and cancels the singularity of $(1 - e^{\pm 2\pi i(\lambda+1)})^{-1}$.

(b) When $\lambda = 2m \pm i|\nu|$, $m = 0, 1, 2, \cdots$, as $|\nu| \to 0$,

$$\int_{-1}^1 u^\lambda \sin \pi u \, du \to 0$$

and cancels the singularity of $(1 - e^{+2\pi i(\lambda+1)})^{-1}$.

(c) When $\lambda = -2m \pm i|\nu|$, $m = 1, 2, \cdots$, there is a polar singularity.

Note that the two halves match everywhere on the real axis.

Lemma 2: Let $f(t)$ be as in Lemma 1, and define $g(\lambda)$ by

$$g(\lambda) \equiv \int_0^1 f(t) J_\lambda(t) \, dt, \quad \mu \geq 0, \quad \lambda = \mu + i\nu,$$

where $J_\lambda(t)$ is the Bessel function. Then $g(\lambda)$ is an analytic function and its continuation to the domain $\mu < 0$ can have singularities only on the negative real axis and at infinity.

Proof: An identical proof to that of Lemma 1 shows that $g(\lambda)$ is analytic. To find the analytic continuation to the domain $\mu < 0$, we again employ Cauchy's theorem and transfer the integration to the imaginary axis.

Case 1: $\nu < 0$: The closed contour consists of the following lines: $v = 0, 0 \leq u \leq c$, $u = c, 0 \leq v \leq c$; $v = c, 0 \leq u \leq c$; and $u = 0, 0 \leq v \leq c$. Here $c > 0$ is a constant. The identity[6] $J_\lambda(ze^{im\pi}) = e^{im\pi\lambda} J_\lambda(z)$ shows that when $\nu < 0$, m and n are integers, and $m > n$, then

$$|J_\lambda(ze^{-2im\pi})| < |J_\lambda(ze^{-2in\pi})|.$$

Therefore,

$$\begin{aligned} \sup_{\substack{0 \leq v \\ c > 0}} |J_\lambda(e^{-c-iv})| &= \sup_{\substack{0 \leq v \leq 2\pi \\ c > 0}} |J_\lambda(e^{-c-iv})| \\ &= \sup_{\substack{0 \leq v \leq 2\pi \\ 0 \leq r < 1}} |J_\lambda(re^{-iv})| = M. \end{aligned}$$

Thus,

$$\begin{aligned} &\lim_{c \to \infty} (c\,|f(e^{-c-iv}) e^{-c-iv} J_\lambda(e^{-c-iv})|) \\ &\qquad = \lim_{c \to \infty} (Mce^{-c}\,|f(e^{-c-iv})|) = 0, \end{aligned}$$

and

$$\begin{aligned} &\lim_{c \to \infty} (c\,|f(e^{u-ic}) e^{-u-ic} J_\lambda(e^{-u-ic})|) \\ &\qquad \leq \lim_{c \to \infty} (Mce^{-c}\,|f(e^{-u-ic})|\, e^{N\pi\lambda}) = 0, \end{aligned}$$

where N is the greatest integer less than or equal to $c/2\pi$. Hence the integrals over the lines $u = c, 0 \leq v \leq c$, and $v = c$, $0 \leq u \leq c$, vanish as $c \to \infty$, and

$$g(\lambda) = i \int_0^\infty f(e^{-iv}) e^{-iv} J_\lambda(e^{-iv}) \, dv.$$

Since the integral and the integrand are uniformly bounded in $-\infty < \mu < \infty$ and $\nu \leq \nu_0 < 0$, the analytic continuation is accomplished under the integral sign.

Case 2: $\nu > 0$: The closed contour consists of the following lines: $u = 0$, $0 \geq v \geq -c$; $0 \leq u \leq c$, $v = -c$; $u = c$, $-c \leq v \leq 0$; and $v = 0$, $c \geq v \geq 0$. Here $c > 0$ is a constant. Henceforth the proof is the same as in Case 1, and the conclusion follows as in Lemma 1.

Remark: We have used only certain analytic properties of the Bessel functions. The extension of the lemma to functions with similar behavior is immediate.

2. THE ANALYTIC CONTINUATION OF $\varphi_\lambda(r)$ AND ITS BEHAVIOR FOR LARGE $|\lambda|$

We continue $\varphi_\lambda(r)$, the regular solution of (1), using the integral representation

$$\varphi_\lambda(r) = \varphi_\lambda^c(r) - \int_0^r s^{-2} K(r, s) \varphi_\lambda^c(s) \, ds,$$

where $K(r, s)$ satisfies (6) and $\varphi_\lambda^c(r)$ is the comparison wavefunction. The two most convenient comparison wavefunctions with the corresponding comparison potentials are

$$\text{(i)}\quad \varphi_\lambda^c(r) = (\tfrac{1}{2}\pi)^{\frac{1}{2}} 2^{-\lambda}\Gamma^{-1}(\lambda+1) r^{\lambda+\frac{1}{2}} \quad \text{and} \quad V^c(r) = -1,$$

$$\text{(ii)}\quad \varphi_\lambda^c(r) = (\tfrac{1}{2}\pi)^{\frac{1}{2}} r^{\frac{1}{2}} J_\lambda(r) \quad \text{and} \quad V^c(r) = 0.$$

Theorem 1 gives the analytic continuation when $V^c(r) = -1$ is used as the comparison potential. The proof of the theorem when $V^c(r) = 0$ uses Lemma 2 instead of Lemma 1. Theorem 2 gives the behavior of $\varphi_\lambda(r)$ for large $|\lambda|$.

As stated in the Introduction, the exact requirements on the potential are unknown. It is convenient to set the conditions on $K(r, s)$ directly. Appendix B shows that these conditions are satisfied when a rather large class of potentials is used to determine $K(r, s)$.

Theorem 1: Let $K(r, s)$ have the following properties for a fixed $r > 0$:

(i) $s^{-\frac{3}{2}}K(r, s) \ln s$, as a function of the real variable s, is continuous at $s = 0$;

(ii) $K(r, re^{-w})$, $w = u + iv$, is an analytic function of w, regular in the domain $u > 0$ and continuous at $u = 0$;

(iii) $K(r, re^{-w})$, as a function of the variable w, is polynomially bounded in the domain $u \geq 0$. Then,

$$\varphi_\lambda(r) = (\tfrac{1}{2}\pi)^{\frac{1}{2}} 2^{-\lambda}\Gamma^{-1}(\lambda+1) \times \left(r^{\lambda+\frac{1}{2}} - \int_0^r s^{-2} K(r, s) s^{\lambda+\frac{1}{2}}\, ds\right), \quad \mu \geq 0,$$

and $\lambda = \mu + iv$ is an analytic function of λ and has an analytic continuation to the domain $\mu < 0$ with singularities, if any, on the negative real axis and at infinity.

Proof: Write $s = rt$; then

$$\varphi_\lambda(r) = (\tfrac{1}{2}\pi)^{\frac{1}{2}} 2^{-\lambda}\Gamma^{-1}(\lambda+1) r^{\lambda+\frac{1}{2}} \times \left(1 - r^{-1}\int_0^1 K(r, rt) t^{-\frac{3}{2}}\, dt\right).$$

The functions $2^{-\lambda}$, $\Gamma^{-1}(\lambda + 1)$, and $r^{\lambda+\frac{1}{2}}$ are entire functions of λ. The conditions on $K(r, s)$ were selected such that $t^{-\frac{3}{2}}K(r, rt) \equiv f(t)$ satisfies the conditions of Lemma 1. Hence the analytic properties of

$$\int_0^1 K(r, rt) t^{\lambda-\frac{3}{2}}\, dt$$

are given by Lemma 1, and the conclusions of the theorem follow.

Remark: Plemelj's method[7] provides a way to lessen the restrictions on $K(r, s)$. Assume that $H(x)$ is differentiable in $0 < x < 1$, continuous at $x = 0$ and at $x = 1$, and that $H(0) = H(1) = 0$. Define

$$G(z) \equiv \int_0^1 \frac{H(x)\, dx}{x - z},$$

$$G^+(x) \equiv \lim_{\substack{z\to x \\ \operatorname{Im} z > 0}} G(z) \quad \text{and} \quad G^-(x) \equiv \lim_{\substack{z\to x \\ \operatorname{Im} z < 0}} G(z).$$

Then, $G(z)$ is an analytic function in the z plane cut from 0 to 1, and $H(x) = G^+(x) - G^-(x)$ for $0 \leq x \leq 1$.

Claim: If the solutions of (6), $K(r, s) = \tilde{K}(r, s) + H(r, s)$, where $\tilde{K}(r, s)$ satisfies the conditions of Theorem 1,

$$\lim_{s\to 0} s^{-\frac{3}{2}} H(r, s) = H(r, r) = 0,$$

and $s^{-\frac{3}{2}}H(r, s)$, lead to a $G(r, z)$ with the property that $G(r, -rt)$ satisfies the conditions of Theorem 1, then the conclusions of Theorem 1 hold.

Proof: We only need to investigate the analytic properties of

$$I(\lambda, r) \equiv \int_0^r H(r, s) s^{\lambda-\frac{3}{2}}\, ds.$$

The differentiability and continuity conditions needed to apply Plemelj's method are satisfied because $K(r, s)$ is the solution of (6) and $\tilde{K}(r, s)$ satisfies the conditions of Theorem 1. Thus

$$\begin{aligned} I(\lambda, r) &= r^{\lambda-\frac{1}{2}} \int_0^1 H(r, rt) t^{\lambda-\frac{3}{2}}\, dt \\ &= r^{\lambda-\frac{1}{2}} \int_0^1 (G^+(r, rt) - G^-(r, rt)) t^{\lambda-\frac{3}{2}}\, dt \\ &= r^{\lambda-\frac{1}{2}} \lim_{\epsilon\to 0} \left(\int_{0+i\epsilon}^{1+i\epsilon} G(r, rz) z^{\lambda-\frac{3}{2}}\, dz - e^{-2\pi i(\lambda-\frac{1}{2})} \int_{0-i\epsilon}^{1-i\epsilon} G(r, rz) z^{-\frac{3}{2}}\, dz \right). \end{aligned}$$

Interchanging the order of limit and integration is justified because continuity on a closed interval implies uniform continuity. We then apply Cauchy's theorem[8] to $G(r, rz)z^{-\frac{3}{2}}$, using the contour shown in Fig. 1, and get

$$\begin{aligned} I(\lambda, r) = {} & ir^{-\frac{1}{2}}(e^{-2i(\lambda-\frac{1}{2})} - 1) \int_{-1}^0 G(r, rz) z^{\lambda-\frac{3}{2}}\, dz \\ & - ir^{\lambda-\frac{1}{2}} \int_0^\pi G(r, re^{i\theta}) e^{i(\lambda-\frac{1}{2})\theta}\, d\theta \\ & - ir^{\lambda-\frac{1}{2}} e^{-2\pi i(\lambda-\frac{1}{2})} \int_\pi^{2\pi} G(r, re^{i\theta}) e^{i(\lambda-\frac{1}{2})\theta}\, d\theta. \end{aligned}$$

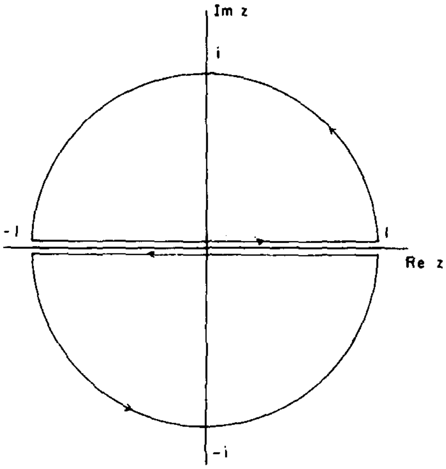

FIG. 1. The contour C in the application of Plemelj's method.

With a change of variable we get

$$I(\lambda, r) = 2\sin\pi\lambda\int_0^1 G(r, -rt)t^{\lambda-\frac{3}{2}}\,dt - ir^{\lambda-\frac{1}{2}}\int_0^\pi (G(r, re^{i\theta}) + e^{-i\pi(\lambda-\frac{1}{2})}G(r, re^{i(\pi+\theta)}))e^{i(\lambda-\frac{1}{2})\theta}\,d\theta.$$

$G(r, -rt)$ was assumed to satisfy the conditions of Theorem 1. The second integrand and integral are uniformly bounded in $-\infty < \mu < \infty$ for any fixed $\nu = \nu_0 \neq 0$. Therefore, the analytic continuation of the second integral is accomplished by continuing the integrand.

But this is not the most general form for $K(r, s)$. The derivation of (6) in Appendix A shows that (5) may be a valid representation of $\varphi_\lambda(r)$ even when $K(r, s)$ is a solution of (6) only in the distributional sense. Plemelj's method is also applicable to certain distributions.[9]

Theorem 2:

Let $\varphi_\lambda(r)$ be defined as in Theorem 1. Then

(i) for $\mu = \mu_0$ as $|\nu| \to \infty$, $\varphi_\lambda(r) = \pi^{\frac{1}{2}}\Gamma^{-1}(1 + \lambda)(\frac{1}{2}r)^{\lambda+\frac{1}{2}}[1 + o(1)]$,

(ii) for $\nu = \nu_0 \neq 0$ as $|\mu| \to \infty$ $\varphi_\lambda(r) = \pi^{\frac{1}{2}}\Gamma^{-1}(1 + \lambda)(\frac{1}{2}r)^{\lambda+\frac{1}{2}}[1 + o(1)]$, where $f(z) = o(g(z))$ as $z \to \infty$ means that $|f(z)/g(z)| \to 0$ as $z \to \infty$.

Proof: We have

$$\varphi_\lambda(r) = \pi^{\frac{1}{2}}2^{-\lambda-\frac{1}{2}}\Gamma^{-1}(1 + \lambda) \times \left(r^{\lambda+\frac{1}{2}} - \int_0^r K(r, s)s^{\lambda-\frac{3}{2}}\,ds\right), \quad \mu \geq 0, \quad \lambda = \mu + i\nu.$$

Using Theorem 1, we obtain

$$\varphi_\lambda(r) = \pi^{\frac{1}{2}}\Gamma^{-1}(1 + \lambda)(\tfrac{1}{2}r)^{\lambda+\frac{1}{2}} \times \left(1 \pm ir^{-1}\int_0^\infty K(r, re^{\pm iv})e^{\pm i(\mu-\frac{1}{2})v-|\nu|v}\,dv\right), \quad -\infty < \mu < \infty \quad |\nu| \neq 0.$$

The plus or minus sign is chosen to be opposite of the sign of ν. Thus (ii) is a consequence of the Riemann–Lebesgue lemma.[10] To prove (i), we recall that $K(r, re^{\pm iv})$ is continuous and polynomially bounded in $|v|$; thus we write

$$C(r, \lambda) = \left|\int_0^\infty K(r, re^{\pm iv})e^{\pm i(\mu-\frac{1}{2})v-|\nu|v}\,dv\right| \leq \int_0^\infty |K(r, re^{\pm iv})e^{-\frac{1}{2}|\nu|v}|\, e^{-\frac{1}{2}|\nu|v}\,dv \leq M\int_0^\infty e^{-\frac{1}{2}|\nu|v}\,dv = \frac{2M}{|\nu|} \to 0 \quad \text{as} \quad |\nu| \to \infty.$$

This proves the theorem.

3. APPLICATIONS

A. Analytic Properties of $\varphi_\lambda(r)$

We now show that the method of this paper is applicable to many often used potentials. The potential $V(r)$ is said to belong to class $\mathcal{V}(R)$ if

(i) $V(z)$ is an analytic function of $z = re^{i\theta}$ in $0 < r < R < \infty$ and $-\infty < \theta < \infty$ and continuous at $r = R$,

(ii) there exists a $\gamma > 0$ such that $r^{2-2\gamma}V(re^{i\theta}) \to 0$ as $r \to 0$ and θ is fixed, and

(iii) there exists a k, $\frac{1}{2} > k > 0$, such that $V(re^{i\theta})\theta^{-k} \to 0$ as $|\theta| \to \infty$ and r is fixed.

This class contains, for example, $V(r) = J_p(cr)$, where $p > 0$ and c is any complex number, $V(r) = (\log r)^{\frac{1}{3}}$, and the combination of such potentials.

Appendix B shows that if $V(r) \in \mathcal{V}(R)$, then the corresponding $K(r, s)$ satisfies conditions (i) and (ii) of Theorem 1. Condition (iii) of Theorem 1 was given to ensure that the integrals over the circular arcs will vanish as the radii of the arcs go to infinity. The bounds we have in (B5) will serve the same purpose, since

$$|t|\,(1 + |\mathrm{Im}\, t|)^{\frac{3}{2}k+\frac{1}{2}} \times \exp\,[c(1 + |\mathrm{Im}\, t|^{k+\frac{1}{2}})e^{-|\nu\,\mathrm{Im}\,t|-\mathrm{Re}\,t}] \to 0$$

for $c > 0$, $|\nu| > 0$, as $|t| \to \infty$ and $\mathrm{Re}\, t \geq 0$. Therefore, the conclusion of Theorem 1 does hold, and $\varphi_\lambda(r)$ has an analytic continuation onto the entire λ plane with singularities, if any, on the negative real axis and at infinity.

This result agrees with the result of Cheng.[11] He uses the fact that

$$(2\lambda)^{-1}\int_0^r (r^{\lambda+\frac{1}{2}}x^{-\lambda+\frac{1}{2}} - x^{\lambda+\frac{1}{2}}r^{-\lambda+\frac{1}{2}})x^p\,dx = r^{p+2}(p+\lambda+\tfrac{3}{2})^{-1}(p-\lambda+\tfrac{3}{2})^{-1},$$

p any complex number, when the integral exists. He used the right-hand side to define the integral for all λ. To find the analytic continuation of $\varphi_\lambda(r)$ in the λ plane, he solves the integral equation

$$\varphi_\lambda(r) = \pi^{\frac{1}{2}}2^{-\lambda-\frac{1}{2}}\Gamma^{-1}(1+\lambda) \times \left(r^{\lambda+\frac{1}{2}} - (2\lambda)^{-1}\int_0^r (r^{\lambda+\frac{1}{2}}x^{-\lambda+\frac{1}{2}} - x^{\lambda+\frac{1}{2}}r^{-\lambda+\frac{1}{2}})\right) \times V(x)\varphi_\lambda(x)\,dx,$$

using the above definition for the integral, by iteration. He needs to restrict the potentials to those which can be written $V(r) = \sum_j a_j r^{b_j}$, $\operatorname{Re} b_j > -2 + 2\gamma$ for all j and some $\gamma > 0$, the sum being absolutely and uniformly convergent. He finds that $\varphi_\lambda(r)$ is a meromorphic function of λ. The location of the poles are determined by the b_j. When all the b_j are real, the poles are on the negative real axis.

His potentials with the b_j real are in the class $\mathcal{V}(R)$, and thus the singularities of $\varphi_\lambda(r)$ have to be on the negative real axis of the λ plane. It can be seen from the remark following Lemma 1 that the method of this paper is applicable to the case where the b_j are not real, but the analysis is more complicated than Cheng's method.

Mandelstam[12] considers potentials that can be represented by

$$V(r) = r^{-1}\sum_{k=0}^{\infty} v_k r^k,$$

and writes the solution of Eq. (1) in the form

$$\varphi_\lambda(r) = e^{ir}\sum_{k=0}^{\infty} a_k r^{k+s}.$$

From the recurrence relations for the a_k, his conclusions about the positions of the possible singularities are the same as ours. Having made such a strong assumption on the potential, he is able to find the behavior of the residues. While in theory one could reproduce his results with the method of this paper, in practice it would involve a great amount of labor.

B. Asymptotic Behavior of the S Matrix and the Jost Function

In this section the asymptotic behavior of the S matrix and the Jost function will be investigated for a restricted class of potentials in the domains

$$D^+ = \{\lambda \mid 0 < |\theta| < \tfrac{1}{2}\pi\},$$
$$D^- = \{\lambda \mid 0 < |\pi - \theta| < \tfrac{1}{2}\pi, \theta = \arg\lambda\}.$$

These four sectors were selected because in there we can use Stirling's asymptotic formula for the gamma function[13] to find that $\Gamma(1-\lambda)/\Gamma(1+\lambda)$ goes either to zero or to infinity as $|\lambda| \to \infty$. Let $V(r) \in \mathcal{V}(R)$ and let it have the additional property that $V(R) \neq 0$ and $V(r) = 0$ for $R < r$. Then in the open interval $(0, R)$ the regular solution of Eq. (1) has the representation

$$\varphi_\lambda(r) = \pi^{\frac{1}{2}}\Gamma^{-1}(1+\lambda)2^{-\lambda-\frac{1}{2}}\left(r^{\lambda+\frac{1}{2}} - \int_0^r K(r,s)s^{\lambda-\frac{3}{2}}\,ds\right),$$

and in the interval (R, ∞) the irregular solutions of (1) are

$$f_\lambda^{0\pm}(r) = -ie^{-i\pi\frac{1}{2}(\lambda-\frac{1}{2})}(\tfrac{1}{2}r)^{\frac{1}{2}}H_\lambda^{\pm}(r),$$

where

$$H_\lambda^-(r) = H_\lambda^{(1)}(r) \quad\text{and}\quad H^+(r) = H_\lambda^{(2)}(r)$$

are the Hankel functions.[2]

Since the regular solution, the irregular solution, and their derivatives are continuous, the Jost function $F^\pm(\lambda) \equiv W(\varphi_\lambda(r), f_\lambda^{0\pm}(r))$ is determined most conveniently by evaluating the Wronskian at $r = R$. With the aid of the identity

$$H^\pm(r) = \pm i\csc\pi\lambda[J_{-\lambda}(r) - e^{\pm i\pi\lambda}J_\lambda(r)],$$

we find

$$F^\pm(\lambda) = \pm e^{\frac{1}{2}i\pi(\lambda-\frac{1}{2})}[g_1(\lambda) - e^{\pm i\pi\lambda}g_2(\lambda)],$$

where

$$g_1(\lambda) = \csc\pi\lambda W(\varphi_\lambda(R), J_{-\lambda}(R))$$

and

$$g_2(\lambda) = \csc\pi\lambda W(\varphi_\lambda(R), J_\lambda(R)).$$

Next we rewrite the representation of $\varphi_\lambda(r)$. We define $U(rs, rs^{-1}) = (rs)^{-\frac{1}{2}}K(r,s)$ and let $s = re^{-w}$. Then

$$\varphi_\lambda(r) = \pi^{\frac{1}{2}}\Gamma^{-1}(1+\lambda)(\tfrac{1}{2}r)^{\lambda+\frac{1}{2}} \times \left(1 - \int_0^\infty U(r^2e^{-w}, e^w)e^{-w}\,dw\right),$$

$$\frac{d\varphi_\lambda(r)}{dr} = \pi^{\frac{1}{2}}\Gamma^{-1}(1+\lambda)(\tfrac{1}{2}r)^{\lambda-\frac{1}{2}} \times \left((\tfrac{1}{2}\lambda + \tfrac{1}{4})\left(1 - \int_0^\infty U(r^2e^{-w}, e^w)e^{-w}\,dw\right) - r^2\int_0^\infty U_1(r^2e^{-w}, e^w)e^{-(\lambda+1)w}\,dw.\right.$$

The subscripts 1 and 2 denote differentiation with respect to the first (r^2e^{-w}) and second (e^w) arguments, respectively. The differentiation under the integral sign is justified in Appendix B. Finally, using the identities $\Gamma(1+z) = z\Gamma(z)$ and $\Gamma(z)\Gamma(1-z) = \csc\pi z$ and the series expansion

$$J_p(z) = \left(\frac{z}{2}\right)^p \sum_{k=0}^{\infty}\frac{(-1)^k z^{2k}2^{-2k}}{2!\,\Gamma(1+\lambda+k)},$$

we find that

$$g_1(\lambda) = \lambda^{-1}\sum_{k=0}^{\infty}\frac{(-1)^k z^{2k}2^{-2k}}{k!\,(1-\lambda)_k} \times \{(k+\lambda)[1 - I(R,0)] - R^2 I_1(R,1)\},$$

where we used the notation $(a)_0 = 1$ and $(a)_k = a(1+a)(2+a)\cdots(k-1+a)$ for $k = 1, 2, \cdots$ and

$$I_{i\cdots j}(R, n) = \int_0^\infty U_{i\cdots j}(R^2e^{-w}, e^w)e^{-(\lambda+n)w}\,dw.$$

Using the results of Appendix B, we analytically continue $I(R, 0)$ and $I_1(R, 0)$ to $\mu < 0$ by transferring the integration to the imaginary axis. Moreover, from the bounds given in Appendix B for U and U_1 it follows that $I(R, 0)$ and $I_1(R, 1)$ are both $o(1)$ as $|\lambda| \to \infty$ in $D^\pm$. Therefore, when $|\lambda|$ is large enough to make $\gamma > 1$, for $n = 1, 2, \cdots$,

$$\left|\lambda^{-1}\sum_{k=n}^{\infty}\frac{(-1)^k z^{2k}2^{-2k}}{k!\,(1-\lambda)_k} \times \{(k+\lambda)[1 - I(R,0)] - R^2 I_1(R,1)\}\right| \le |1 + 2k\lambda^{-1}|\,\frac{\exp(\frac{1}{4}R^2)}{(1-\lambda)_n} = o(\lambda^{-n+1})$$

as $|\lambda|$ goes to infinity; hence $g_1(\lambda) = 1 + o(1)$ as $|\lambda| \to \infty$ in $D^\pm$. Similarly,

$$g_2(\lambda) = \lambda^{-1}\Gamma(1-\lambda)\Gamma^{-1}(1+\lambda)\sum_{k=0}^{\infty}\frac{(-1)^k z^{2k}2^{-2k}}{k!\,(1+\lambda)_k}\left(\frac{R}{2}\right)^2 \times \{k[1 - I(R,0)] - R^2 I_1(R,1)\}.$$

Thus

$$g_2(\lambda) = -\lambda^{-1}\Gamma(1-\lambda)\Gamma^{-1}(1+\lambda)(R/2)^{2\lambda+2} \times [(1+\lambda)^{-1} + 4I_1(R,1) + o(\lambda^{-1})].$$

Integrating $I_1(R, 1)$ by parts, we obtain

$$\begin{aligned} I_1(R,1) &= -(1+\lambda)^{-1}[-U(R^2,1) + R^2 I_{11}(R,2) - I_{12}(R,0)] \\ &= (1+\lambda)^{-1}U(R^2,1) + o(\lambda^{-1}) \\ &= -\tfrac{1}{4}[V(R) + 1] + o(\lambda^{-1}) \quad \text{as} \quad |\lambda| \to \infty. \end{aligned}$$

Therefore, $g_2(\lambda) = \Gamma(1-\lambda)\Gamma^{-1}(1+\lambda)V(R)\lambda^{-1}(1+\lambda)^{-1}(R/2)^{2\lambda+2}[1 + o(1)]$ as $|\lambda| \to \infty$. Because of the factor $\Gamma(1-\lambda)\Gamma^{-1}(1+\lambda)$ when $\lambda \in D^\pm$ as $|\lambda| \to \infty$, we have

(i) for $\mu > 0$, $g_2(\lambda) = o(g_1(\lambda))$, i.e., $F^\pm(\lambda) = \pm e^{\mp\frac{1}{2}i(\lambda-\frac{1}{2})}[1 + o(1)]$,

(ii) for $\mu < 0$, $g_1(\lambda) = o(g_2(\lambda))$, i.e.,

$$F^\pm(\lambda) = \mp e^{\pm\frac{1}{2}i\pi(\lambda+\frac{1}{2})}\Gamma(1-\lambda)\Gamma^{-1}(1+\lambda) \times V(R)\lambda^{-1}(1+\lambda)^{-1}(R/2)^{2\lambda+2}[1 + o(1)]$$

and hence

$$S_\lambda(1) = e^{i\pi(\lambda+\frac{1}{2})}\frac{F^+(\lambda)}{F^-(\lambda)} = \begin{cases} 1 + o(1), & \operatorname{Re}\lambda > 0 \\ \exp(2\pi i\lambda)[1 + o(1)], & \operatorname{Re}\lambda < 0 \end{cases}$$

as $|\lambda| \to \infty$.

If $V(R) = 0$, the only complication that arises is that one needs to evaluate higher-order terms of $g_2(\lambda)$. Removing the restriction that $V(r) = 0$ for $r > R$ remains as an unsolved problem. To see the difficulties, assume that the potential allows the representation

$$f_\lambda^\pm(r) = f_\lambda^{0\pm}(r) - \int_r^\infty s^{-\frac{3}{2}}K(r,s)f_\lambda^{0\pm}(s)\,ds$$

for the irregular solutions of (1). Appendix A shows that there are such potentials. The first term is proportional to $r^{\frac{1}{2}}H_\lambda^\pm(r)$. The argument of $H_\lambda^\pm(s)$ is integrated from R to ∞. Its order is neither small nor large nor equal to its argument.

It is thought that, for $\operatorname{Re}\lambda > 0$,

$$h_1(\lambda) \equiv \int_R^\infty s^{-\frac{3}{2}}K(R,s)J_{-\lambda}(s)\,ds$$

dominates

$$h_2(\lambda) \equiv \int_R^\infty s^{-\frac{3}{2}}K(R,s)J_\lambda(s)\,ds \quad \text{as} \quad |\lambda| \to \infty,$$

and the same statement holds for their derivatives with respect to r. It is equally likely that $h_2(\lambda + 1)$ is an order of λ smaller than $h_2(\lambda)$. Assuming the above to be true, using the identity

$$J(z) = \frac{z}{\lambda}\left(J_{\lambda+1}(z) + \frac{d}{dz}J_\lambda(z)\right),$$

and integrating by parts, one can see a certain pattern. We write

$$\begin{aligned} F^\pm(\lambda) &= W\left(\varphi_\lambda(R), f_\lambda^{0\pm}(R) - \int_R^\infty s^{-\frac{3}{2}}K(R,s)f_\lambda^{0\pm}(s)\,ds\right) \\ &= \exp[\pm\tfrac{1}{2}i\pi(\lambda - \tfrac{1}{2})] \\ &\quad \times [g_1(\lambda) - h_1(\lambda) + \exp(\pm i\pi\lambda)] \\ &\quad \times [g_2(\lambda) - h_2(\lambda)]. \end{aligned}$$

We find that $h_1(\lambda) = o(g_1(\lambda))$ as $|\lambda| \to \infty$, and there is no such relation between $h_2(\lambda)$ and $g_2(\lambda)$. But, since it was assumed that, for $\lambda \in D^\pm$, $\operatorname{Re}\lambda > 0$, and $|\lambda| \to \infty$, $h_1(\lambda)$ dominates $h_2(\lambda)$, we can conclude that $S_\lambda \to 1$.

The cancellations between $g_2(\lambda)$ and $h_2(\lambda)$ will determine the behavior of the S matrix in the left half-plane. Assume that the potential has derivatives of all order in the interval (R, ∞). This enables us to take any number of derivatives of $K(r, s)$ and therefore integrate by parts any number of times. If $V(R)$ is continuous at $R = r$, then the first-order terms of $g_2(\lambda)$ and $h_2(\lambda)$ cancel each other. The second-order term of $g_2(\lambda)$ depends on $\lim (\frac{1}{2}r)^{2\lambda+2}\, dV(r)/dr$ as $r \to R$. It is also cancelled by the second-order term of $h_2(\lambda)$ if the derivative of the potentials is continuous. As the powers of λ^{-1} in $g_2(\lambda)$ increase, so do the powers of $\frac{1}{4}R^2$. If the potential is analytic on $(0, \infty)$, then the value of the Jost function should not depend on R. It seems that $g_2(\lambda) - h_2(\lambda)$ should be zero. This is certainly the case when $V(r) = 0$. In that case $S_\lambda \to 1$ as $|\lambda| \to \infty$ in any direction inside $D^\pm$. However, if any derivative of $V(R)$ is not zero, then $S_\lambda \to e^{2\pi i\lambda}$ as $|\lambda| \to \infty$, $\operatorname{Re} \lambda < 0$, $\lambda \in D^\pm$.

C. New Integral Representation of $J_\lambda(z)$ and $\Gamma(\lambda)$

As a last application, we derive a known integral representation of $J_\lambda(r)$ in the domain $\mu > 0$, $\lambda = \mu + i\nu$, and analytically continue it to the domain $\mu \le 0$, getting a new integral representation and a new bound that is valid for all λ and r. We also find a new representation and bound for $\Gamma(\lambda)$ in the domain $\mu < 0$.

The equation

$$\left(\frac{d^2}{dr^2} + 1 - (\lambda^2 - \tfrac{1}{4})r^{-2}\right)\varphi_\lambda(r) = 0 \qquad (7)$$

is Eq. (1) with $k^2 = 0$ and $V(r) = -1$. Hence for $\mu > 0$

$$\varphi_{\lambda-\frac{1}{2}}(r) = \pi^{\frac{1}{2}} 2^{-\lambda-\frac{1}{2}} \Gamma^{-1}(1+\lambda) \times \left(r^{\lambda+\frac{1}{2}} - \int_0^r K(r,s) s^{\lambda-\frac{3}{2}}\, ds\right),$$

where $K(r, s)$ is the solution of (6) with $V^c(r) = -1$, i.e., $K(r,s) = 2^{-\frac{1}{2}} r s^{-\frac{1}{2}} (r-s)^{-\frac{1}{2}} J_1([r(r-s)]^{\frac{1}{2}})$. Therefore,

$$\varphi_{\lambda-\frac{1}{2}}(r) = \pi^{\frac{1}{2}} \Gamma^{-1}(1+\lambda)\left(\frac{r}{2}\right)^{\lambda+\frac{1}{2}} \left(1 - r\int_0^1 (1-t^2)^\lambda J_1(rt)\, dt\right).$$

Integrating by parts, we obtain

$$\varphi_{\lambda-\frac{1}{2}}(r) = 2\pi^{\frac{1}{2}} \Gamma^{-1}(1+\lambda)\left(\frac{r}{2}\right)^{\lambda+\frac{1}{2}} \times \int_0^1 (1-t^2)^{\lambda-1} t J_0(rt)\, dt. \qquad (8)$$

But (7) has the solution $\varphi_{\lambda-\frac{1}{2}}(r) = \pi^{\frac{1}{2}} 2^{-\frac{1}{2}} r^{\frac{1}{2}} J_\lambda(r)$. Comparing it with (8), we get the known representation

$$J_\lambda(r) = \left(\frac{r}{2}\right)^\lambda \Gamma^{-1}(\lambda) \int_0^1 (1-t^2)^{\lambda-1} t J_0(rt)\, dt$$

or

$$J_\lambda(r) = \left(\frac{r}{2}\right)^\lambda \Gamma^{-1}(\lambda) \int_0^1 J_0(r(1-s)^{\frac{1}{2}}) s^{\lambda-1}\, ds.$$

Using the method of this paper and Lemma 1, we find

$$\begin{aligned} J_\lambda(r) &= i\left(\frac{r}{2}\right)^\lambda \Gamma^{-1}(\lambda) \int_0^\infty J_0(r[1-\exp(-iv)]^{\frac{1}{2}}) e^{-i\lambda v}\, dv \\ &= i\left(\frac{r}{2}\right)^\lambda \Gamma^{-1}(\lambda) \sum_{n=0}^\infty e^{-i2\pi\lambda n} \times \int_0^{2\pi} J_0(r[1-\exp(-iv)]^{\frac{1}{2}}) e^{-i\lambda v}\, dv \\ &= i\left(\frac{r}{2}\right)^\lambda \Gamma^{-1}(\lambda)(1-e^{-i2\pi\lambda})^{-1} \times \int_0^{2\pi} J_0(r[1-\exp(-iv)]^{\frac{1}{2}}) e^{-i\lambda v}\, dv \end{aligned}$$

for $-\infty < \mu < \infty$ and $\nu \le \nu_0 < 0$. Similarly, for $\nu \ge \nu_0 > 0$, we find

$$J_\lambda(r) = -i\left(\frac{r}{2}\right)^\lambda \Gamma^{-1}(\lambda)(1-e^{i2\pi\lambda})^{-1} \times \int_0^{2\pi} J_0(r[1-\exp(iv)]^{\frac{1}{2}}) e^{i\lambda v}\, dv.$$

One can show that, as $\nu \to 0$, the two halves match everywhere and are finite.

Using[14]

$$|J_0(r[1-\exp(\pm iv)]^{\frac{1}{2}})| \le \exp(\operatorname{Im}\{r[1-\exp(\pm iv)]^{\frac{1}{2}}\}) \le \exp(2^{\frac{1}{2}} r),$$

we find that for $-\infty < \mu < \infty$ and $|\nu| \ge \nu_0 > 0$

$$\begin{aligned} |J_\lambda(r)| &\le (\tfrac{1}{2}r)^\mu |\Gamma^{-1}(\lambda)| \times \exp(2^{\frac{1}{2}} r)\, |1 - \exp[-i2\pi(\pm\mu - i|\nu|)^{-1}]| \times \int_0^{2\pi} e^{-|\nu| v}\, dv \\ &\le (\tfrac{1}{2}r)^\mu |\Gamma^{-1}(\lambda)| \exp(2^{\frac{1}{2}} r)\, |\nu_0|^{-1}. \end{aligned}$$

For the gamma function write, for $\mu > 0$,

$$\Gamma(\lambda) = \int_0^\infty e^{-z} z^{\lambda-1}\, dz = I_1 + I_2,$$

where

$$I_1 = \int_0^1 e^{-z} z^{\lambda-1}\, dz \quad \text{and} \quad I_2 = \int_1^\infty e^{-z} z^{\lambda-1}\, dz.$$

We use Lemma 1 to continue I_1, i.e., repeat the steps used in the analytic continuation of $J_\lambda(r)$. We find that, for $|\nu| \ge \nu_0 > 0$ and $-\infty < \mu < \infty$,

$$I_1 = \mp i\{1 - \exp[-i2\pi(\pm\mu - i|\nu|)]\}^{-1} \times \int_0^{2\pi} \exp(-\cos v \pm i \sin v \mp i\mu v - |\nu|\, v)\, dv.$$

Thus $|I_1| \le e\, |\nu_0|^{-1}$. The analytic continuation of I_2 is accomplished by letting μ become negative under the integral sign.

Note that this representation enables one to find the asymptotic behavior of the gamma function for $|\arg \lambda| = \pi$.

These examples show that with the method of this paper one can continue those functions that are Stieltjes or Laplace transforms of well-behaved functions.

CONCLUSIONS

We have demonstrated that when mild restrictions are imposed on the potential at the origin, the regular solution of the Schrödinger equation has an integral representation. We also showed that with severe restrictions on the potential at infinity the irregular solution also has similar integral representation. The analytic continuation of the regular solution then depends on finding the analytic continuation of a function defined by an integral. We devised a method that performs the analytic continuation of a rather large class of functions. Thus we are able to continue the regular solutions that corresponds to a rather large class of potentials.

ACKNOWLEDGMENTS

I wish to thank Professor R. G. Newton for guiding me, for suggesting the problem, and for the integral prepresentation that leads to the solution. I owe thanks to Professor R. P. Gilbert and to Mr. M. A. Hooshyar for our many discussions.

APPENDIX A

We are looking for a representation of the irregular solutions

$$f^{\pm}_{\lambda}(r) = f^{c\pm}_{\lambda}(r) - \int_r^\infty s^{-2}K(r, s) f^{c\pm}_{\lambda}(r), \qquad \text{(A1)}$$

where

$$^{\pm}_{\lambda}(r) = e^{-i\frac{1}{2}\pi(\lambda+\frac{1}{2})}(\tfrac{1}{2}r)^{\frac{1}{2}}H^{\pm}_{\lambda}(r).$$

Substituting (A1) into (1), the natural way to proceed is to use Liebnitz's rule[15] to differentiate under the integral sign. For this we need that the continuity of $\partial K(r, s)/\partial r$ and $\partial^2 K(r, s)/\partial r^2$ as functions of r be uniform with respect to the variable s in the region $0 < R \leq r < s$ (Condition 1). The inverse scattering problem suggests making $K(r, s)$ satisfy

$$r^2\left(\frac{\partial^2}{\partial r^2} + 1 - V(r)\right)K(r, s) = s^2\left(\frac{\partial^2}{\partial s^2} + 1\right)K(r, s), \qquad \text{(A2)}$$

$$\frac{2}{r}\frac{d}{dr}\frac{K(r, r)}{r} = V(r) \quad \text{and} \quad \lim_{s\to\infty} K(r, s) = 0$$

uniformly in r. Using (A2) and integrating by parts, we find that (A1) is indeed a representation of the irregular solution provided that we also require that

$$\lim_{s\to\infty} \frac{\partial}{\partial s} K(r, s) = 0$$

uniformly in r (Condition 2). It must be emphasized that Conditions 1 and 2 are sufficient but not necessary conditions. It is probably sufficient that $K(r, s)$ be a weak solution of (A2) to make (A1) a valid representation of $f^{\pm}_{\lambda}(r)$.

Now we proceed to convert (A2) into an equivalent integral equation. Introduce the change of variables $r = x^{-\frac{1}{2}}y^{-\frac{1}{2}}$ and $s = x^{-\frac{1}{2}}y^{\frac{1}{2}}$. This transformation is one to one except for the line at infinity. (See Fig. 2.) Also introducing the new function $x^{-\frac{1}{2}}U(x, y) = K(r, s)$, we see that (A2) becomes

$$\frac{\partial^2}{\partial x \partial y} U(x, y) + \frac{1}{4x^2y^2}[1 - y^2 - V(x^{-\frac{1}{2}}y^{-\frac{1}{2}})]U(x, y) = 0,$$

$$-4x^2 \frac{d}{dx} U(x, 1) = V(x^{-\frac{1}{2}}) \qquad \text{(A3)}$$

and

$$\lim_{x\to 0} x^{-\frac{1}{2}}U(x, y) = 0 \quad \text{uniformly in } y,$$

which can be integrated to give

$$U(x, y) = -\tfrac{1}{4}\int_0^x ds \int_1^y dt\, s^{-2}t^{-2}[1 - t^2 - V(s^{-\frac{1}{2}}t^{-\frac{1}{2}})]U(s, t) - \tfrac{1}{4}\int_0^x s^{-2}V(s^{-\frac{1}{2}})\, ds. \qquad \text{(A4)}$$

The most general condition on $V(r)$ for which this integral equation has a solution is not known. But if we make the assumptions that $e^{kr^2}V(r)$, $e^{kr^2}\,dV(r)/dr$, and $e^{kr^2}\,d^2V(r)/dr^2$ remain bounded as $r \to \infty$ for some $k > 0$ and that $d^2V(r)/dr^2$ is continuous,[16] then (A4)

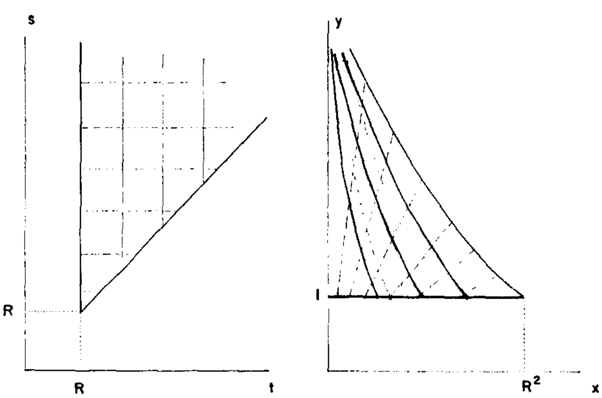

FIG. 2. The transformation in Appendix A: $r = x^{-\frac{1}{2}}y^{-\frac{1}{2}}$ and $s = x^{-\frac{1}{2}}y^{\frac{1}{2}}$. The line $r = r_0 =$ const goes into $y = r_0^{-2}x^{-1}$ and the line $s = s_0 =$ const goes into $y = s_0^2 x$.

does have a solution satisfying Conditions 1 and 2. To show that we solve (A4) by iteration, define

(i) $U(x, y) = \sum_{n=0}^{\infty} U_n(x, y)$,

(ii) $U_n(x, y) = -\frac{1}{4}\int_0^x ds \times \int_1^y dt\, s^{-2}t^{-2}[1 - t^2 - V(s^{-\frac{1}{2}}t^{-\frac{1}{2}})]U_{n-1}(s, t)$ for $n \geq 1$,

(iii) $U_0(x, y) = -\frac{1}{4}\int_0^x s^{-2}V(s^{-\frac{1}{2}})\, ds$,

(iv) $M = \max\left\{\exp(kr^2)\,|V(r)|, \exp(kr^2)\left|\frac{dV(r)}{dr}\right|, \exp(kr^2)\left|\frac{d^2V(r)}{dr^2}\right|\right\}$,

then

$$\begin{aligned}|U_0(x, y)| &\leq \tfrac{1}{4}\int_0^x ds\, s^{-2}\,|V(s^{-\frac{1}{2}})| \\ &\leq \tfrac{1}{4}M\int_0^x ds\, s^{-2}\exp\left(-\frac{k}{s}\right) \\ &= \tfrac{1}{4}Mk^{-1}\exp\left(-\frac{k}{x}\right),\end{aligned}$$

$$\begin{aligned}|U_n(x, y)| &\leq \tfrac{1}{4}\int_0^x ds\int_1^y dt\, s^{-2}t^{-2}\,|1 - t^2 - V(s^{-\frac{1}{2}}t^{-\frac{1}{2}})| \\ &\quad \times |U_{n-1}(s, t)| \\ &\leq \tfrac{1}{4}\int_0^x ds\, s^{-2}\int_1^y dt(M + 2)\,|U_{n-1}(s, t)| \\ &\leq [\tfrac{1}{4}(M + 2)]^n\int_0^x dx_{n-1}x_{n-1}^{-2} \\ &\quad \times \int_1^y dy_{n-1}\cdots\int_1^y dy_0\,\frac{1}{4}\frac{M}{k}\exp\left(-\frac{k}{x_0}\right) \\ &\leq \frac{1}{4}\frac{M}{k}\left(\frac{M + 2}{4k}\right)^n\exp\left(-\frac{k}{x}\right)\frac{(y - 1)^n}{n!}.\end{aligned}$$

Thus

$$\begin{aligned}|U(x, y)| &\leq \sum_{n=0}^{\infty}|U_n(x, y)| \\ &\leq \frac{1}{4}\frac{M}{k}\exp\left(-\frac{k}{x}\right)\sum_0^{\infty}\left(\frac{M + 2}{4k}\right)^n\frac{(y - 1)^n}{n!} \\ &= \frac{1}{4}\frac{M}{k}\exp\left(-\frac{k}{x} + \frac{M + 2}{4k}(y - 1)\right) \\ &< \frac{1}{4}\frac{M}{k}\exp\left(-\frac{k}{x} + \frac{M + 2}{4k}y\right). \qquad \text{(A5)}\end{aligned}$$

Therefore, (A4) has a unique solution for this class of potentials. Note that the bound on $U(x, y)$ says that

$$\begin{aligned}|K(r, s)| &\leq (rs)^{\frac{1}{2}}\frac{1}{4}\frac{M}{k}\exp\left(-krs + \frac{M + 2}{4k}\frac{s}{r}\right) \\ &\leq \frac{1}{4}\frac{M}{k}s\exp\left[-s\left(kr - \frac{M + 2}{4kr}\right)\right], \qquad \text{(A6)}\end{aligned}$$

so that for a given k there always is an R such that for $r \geq R$ $\lim K(r, s) = 0$ uniformly in r as $s \to \infty$.

To see that Conditions 1 and 2 are satisfied, observe that when $s = \text{const}$, then $r = s^{-1}x^{-1}$ and $y = s^2x$ and $\partial/\partial r = -x^2s\, d/dx$. Thus

$$\begin{aligned}&\frac{\partial}{\partial t}K(t, s)\big|_{t=r} \\ &= -x^2s\frac{d}{dx}[x^{-\frac{1}{2}}U(x, s^2x)]\big|_{x=r^{-1}s^{-1}} \\ &= \tfrac{1}{2}r^{-\frac{1}{2}}s^{\frac{1}{2}}U(r^{-1}s^{-1}, r^{-1}s) \\ &\quad + \tfrac{1}{4}r^{\frac{1}{2}}s^{\frac{3}{2}}\int_1^{r^{-1}s}dt[1 - t^2 - V(r^{\frac{1}{2}}s^{\frac{1}{2}}t^{-\frac{1}{2}})]t^{-2}U(r^{-1}s^{-1}, t) \\ &\quad + \tfrac{1}{4}r^{\frac{1}{2}}s^{-\frac{1}{2}}\int_0^{r^{-1}s^{-1}}t^{-2}[1 - r^{-2}s^2 - V(r^{\frac{1}{2}}s^{-\frac{1}{2}}t^{-\frac{1}{2}})] \\ &\quad \times U(t, r^{-1}s) + \tfrac{1}{4}r^{\frac{1}{2}}s^{\frac{3}{2}}V(r^{\frac{1}{2}}s^{\frac{1}{2}}). \qquad \text{(A7)}\end{aligned}$$

$\partial K(r, s)/\partial r$ and $\partial^2K(r, s)/\partial r^2$ are evaluated from (A7) by differentiation. Then, using (A5) and the bounds on the derivatives of the potential, we easily show that

$$\left|\frac{\partial^n}{\partial r^n}K(r, s)\right| < L_n < \infty, \quad n = 1, 2, 3, \cdots.$$

Now

$$\begin{aligned}L_n\delta &\geq \int_r^{r+\delta}\left|\frac{\partial^n}{\partial r^n}K(r, s)\right| dr \\ &\geq \left|\int_r^{r+\delta}\frac{\partial^n}{\partial r^n}K(r, s)\, dr\right| \\ &= \left|\frac{\partial^{n-1}}{\partial r^{n-1}}[K(r + \delta, s) - K(r, s)]\right|\end{aligned}$$

and thus the continuity of $K(r, s)$, $\partial K(r, s)/\partial r$, and $\partial^2K(r, s)/\partial r^2$ in r is uniform with respect to s. This proves that Condition 1 is satisfied. To show that Condition 2 is satisfied, observe that when $r = \text{const}$, then $s = ry$, $x = r^{-2}y^{-1}$, and $\partial/\partial s = r^{-1}\, d/dy$. Therefore,

$$\begin{aligned}&\frac{\partial}{\partial s}K(r, s) \\ &= \frac{1}{r}\frac{d}{dy}[ry^{\frac{1}{2}}U(r^{-2}y^{-1}, y)]\big|_{y=sr^{-1}} \\ &= \tfrac{1}{2}y^{-\frac{1}{2}}U(r^{-2}y^{-1}, y) + y^{\frac{1}{2}}\frac{d}{dy}U(r^{-2}y^{-1}, y)\big|_{y=sr^{-1}} \\ &= (2s)^{-1}K(r, s) \\ &\quad + \tfrac{1}{4}r^{\frac{3}{2}}s^{\frac{1}{2}}\int_1^{sr^{-1}}dt\, t^{-2}[1 - t^2 - V(s^{\frac{1}{2}}r^{\frac{1}{2}}t^{-\frac{1}{2}})U(s^{-1}r^{-1}, t)] \\ &\quad - \tfrac{1}{4}\int_0^{s^{-1}r^{-1}}dt\, t^{-2}r^2s^{-2}[1 - r^{-2}s^2 - V(r^{\frac{1}{2}}s^{-\frac{1}{2}}t^{-\frac{1}{2}})] \\ &\quad \times U(t, r^{-1}s) - \tfrac{1}{4}r^2V(r^{\frac{1}{2}}s^{\frac{1}{2}}),\end{aligned}$$

$$\left|\frac{\partial}{\partial s} K(r, s)\right|$$
$$\leq (2s)^{-1} |K(r, s)| + \frac{M+2}{16k} s^{\frac{1}{2}} r^{\frac{3}{2}} \exp\left[-s\left(kr - \frac{M+2}{4kr}\right)\right] + \frac{M}{16k}\frac{r^2}{s^2}\left(\frac{s^2}{r^2} + 1 + M\right)\exp\left(\frac{M+2}{4kr}\right) \times \int_0^{s^{-1}r^{-1}} dt\, t^{-2}\exp\left(-\frac{k}{t}\right) + \tfrac{1}{4}r^2 |V(r^{\frac{1}{2}}s^{\frac{1}{2}})|$$
$$< \left(\frac{1}{2s} + \frac{(M+2)M}{16k}s^2 + \frac{M}{16k^2}(2+M)\right) \times \exp\left(-s\left(kr - \frac{M+2}{4kr}\right)\right) + \tfrac{1}{4}Ms^2e^{-krs},$$

which vanishes as $s \to \infty$ uniformly in r for $r \geq R$. This shows that Condition 2 is also satisfied.

APPENDIX B

Consider (6) with $V^c(r) = -1$, i.e.,

$$r^2\left(\frac{\partial^2}{\partial r^2} - V(r)\right)K(r, s) = s^2\frac{\partial^2}{\partial s^2}K(r, s),$$
$$-\frac{2}{r}\frac{d}{dr}[r^{-1}K(r, r)] = V(r) + 1, \qquad \text{(B1)}$$

$\lim_{s\to 0} K(r, s) = 0$ uniformly in r, in the region $0 \leq s \leq r < R$.

Introduce the change of variables $r = x^{\frac{1}{2}}y^{\frac{1}{2}}$ and $s = x^{\frac{1}{2}}y^{-\frac{1}{2}}$. This transformation is one to one except for the point $r = 0$. This transformation leads to the differential equation for $U(x, y) = r^{-\frac{1}{2}}s^{-\frac{1}{2}}K(r, s)$,

$$\frac{\partial^2}{\partial x \partial y}U(x, y) - \tfrac{1}{4}V(x^{\frac{1}{2}}y^{\frac{1}{2}})U(x, y) = 0,$$
$$-4\frac{d}{dx}U(x, 1) = V(x^{\frac{1}{2}}) + 1 \qquad \text{(B2)}$$

and

$$\lim_{x\to 0} U(x, y) = 0 \quad \text{uniformly in } y,$$

which can be integrated to give

$$U(x, y) = \tfrac{1}{4}\int_0^x ds\int_1^y dt V(s^{\frac{1}{2}}t^{\frac{1}{2}})U(s, t) - \tfrac{1}{4}\int_0^x [1 + V(s^{\frac{1}{2}})]\, ds. \qquad \text{(B3)}$$

We will be interested in $K(r, s)$ after the transformation $s = re^{-w}$. Therefore, we will proceed directly. Let $x = e^{-z}$ and $y = e^{-w}$; then, retaining the notation $U(z, w)$ for the new function, we obtain

$$U(z, w) = \tfrac{1}{4}\int_z^\infty ds\int_0^w dt e^{t-s}V(e^{\frac{1}{2}t-\frac{1}{2}s})U(s, t) - \tfrac{1}{4}\int_z^\infty e^{-s}[V(e^{-\frac{1}{2}s}) + 1]\, ds. \qquad \text{(B4)}$$

Again the most general conditions on $V(r)$ for which (B4) has a solution with the properties that $\lim K(r, s) = 0$ uniformly in r as $s \to 0$ and that the continuity of $\partial K(r, s)/\partial r$ and $\partial^2 K(r, s)/\partial r^2$ in r is uniform with respect to s is unknown. However, sufficient conditions are

(i) $V(x)$ is an analytic function of $z = re^{i\theta}$ in $-\infty < \theta < \infty$, $0 < r < R < \infty$ and continuous at $r = R$,

(ii) there exists a $\gamma > 0$ such that $r^{2(1-\gamma)}V(re^{i\theta}) \to 0$ as $r \to 0$ and θ is fixed,

(iii) there exists a $k < \frac{1}{2}$ such that $V(re^{i\theta})\theta^{-k} \to 0$ as $|\theta| \to \infty$ and r is fixed.

The last two conditions imply that $|V(re^{i\theta})| < Mr^{2\gamma-2}(1 + |\theta|)^k$.

We solve (B4) by iteration and at the same time continue $U(z, w)$ to complex z and w by letting them become complex in the integral equation. Let $w = u + iv$ and $z = x + iy$, $x - u \geq -\ln R$; and

(1) $U(z, w) = \sum_{n=0}^{\infty} U_n(z, w)$,

(2) $U_n(z, w) = \frac{1}{4}\int_z^{\infty+i0} ds\int_0^w dt e^{t-s}V(e^{\frac{1}{2}t-\frac{1}{2}s})U_{n-1}(s, t)$

for $n \geq 1$ and the contours of integrations lie in the domain of analyticity of $U_{n-1}(s, t)$,

(3) $U_0(z, w) = -\frac{1}{4}\int_z^{\infty+i0} ds e^{-s}[V(e^{-\frac{1}{2}s}) + 1]$

and the contour lies in the domain $\operatorname{Re} s > \ln R$.

To find $U_0(z, w)$, we select the contour shown in Fig. 3, i.e.,

$$U_0(z, w) = -\tfrac{1}{4}\int_x^c e^{-s-iy}(1 + V(e^{-\frac{1}{2}s+\frac{1}{2}iy})\, ds - \frac{i}{4}\int_y^0 e^{-c-is}[1 + V(e^{-\frac{1}{2}c+\frac{1}{2}is})]\, ds - \tfrac{1}{4}\int_c^\infty e^{-s}[1 + V(e^{-\frac{1}{2}s})]\, ds.$$

Because of (ii) and (iii) the last two integrals vanish as $c \to \infty$, and

$$|U_0(z, w)| \leq \tfrac{1}{4}\int_x^\infty e^{-s}|1 + V(e^{-\frac{1}{2}s+\frac{1}{2}iy})|\, ds$$
$$\leq \tfrac{1}{4}\int_x^\infty e^{-s}[1 + Me^{(1-\gamma)s}(1 + |y|)^k]\, ds$$
$$\leq (4\gamma)^{-1}(1 + M)(1 + |y|)^k e^{-\gamma x}.$$

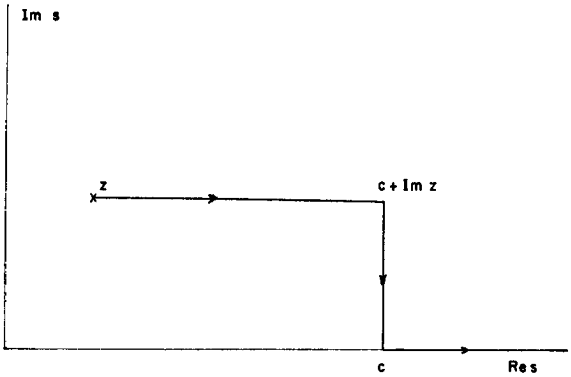

FIG. 3. The contour of integration in Appendix B.

Thus $U_0(z, w)$ is an analytic function of z in the domain $x > -\ln R$, $|y| \le Y < \infty$. To find $U_1(z, w)$, we use the contour shown in Fig. 3 for the s integration and a portion of the real axis and a line parallel to the imaginary axis for the t integration. Again we let $c \to \infty$, and use

$$|1 + \mathrm{Im}\,(s - t)| \le 1 + |\mathrm{Im}\,t| + |\mathrm{Im}\,s| \le (1 + |\mathrm{Im}\,t|)(1 + |\mathrm{Im}\,s|)$$

to find

$$\begin{aligned} |U_1(z, w)| &= \tfrac14 \left| \int_z^{\infty+i0} ds \int_0^w dt\, e^{t-s} V(e^{\frac12 t - \frac12 s}) U_0(s, t) \right| \\ &\le \frac{M(M+1)}{16\gamma^2 2!} e^{-2\gamma x}(1 + |y|)^k \times \left(\int_0^u e^t\, dt + e^u \int_0^{|v|} (1 + t)^k\, dt \right) \\ &\le \frac{M(M+1)}{(4\gamma)^2 2!} e^{-2\gamma x}(1 + |y|)^{2k} \times \left(\frac{1}{\gamma}(e^u - 1) + e^u \frac{(1 + |v|)^k - 1}{k + 1} \right) \\ &\le \frac{M(M+1)}{(4\gamma)^2 2!} e^{-2\gamma x}(1 + |y|)^{2k} e^u \left(\frac{1}{\gamma} + (1 + |v|)^{k+1} \right). \end{aligned}$$

Thus $U_1(z, w)$ is an analytic function in the domain $x - u > -\ln R$, $u > 0$, with u, $|y|$, $|v|$ bounded. Similarly

$$|U_n(z, w)| \le \frac{(M+1)}{4\gamma}\left(\frac{M}{4\gamma}\right)^n \frac{1}{(n+1)!} \times e^{-(n+1)\gamma x}(1 + |y|)^{(n+1)k} \frac{1}{n!} e^{n\gamma u} \times \left[\left(\frac{|v| + 1}{\gamma} \right)^n + (|v| + 1)^{n(k+1)} \right],$$

and analytic in the domain where $U_1(z, w)$ is analytic. Thus

$$\begin{aligned} |U(z, w)| &\le \sum_{n=0}^{\infty} |U_n(z, w)| \\ &\le \sum_{n=0}^{\infty} \left(\frac{M+1}{4\gamma}\right)\left(\frac{M}{4\gamma}\right)^n \frac{1}{(n+1)!\, n!} \times e^{-(n+1)\gamma x} e^{n\gamma u}(1 + |y|)^{(n+1)k} \times \left(\frac{2}{\gamma}\right)^n (1 + |v|)^{n(k+1)} \\ &\le (1 + |y|)^k \frac{M+1}{4} R^\gamma \sum_{n=0}^{\infty} \left(\frac{M}{2\gamma^2}\right)^n \frac{1}{n!\,(n+1)!} \times (1 + |y|)^{nk}(1 + |v|)^{n(k+1)} R^{n\gamma} \\ &< (1 + |y|)^{\frac12 k} \frac{M+1}{2\gamma(2M)^{\frac12}} R^{\frac12 \gamma} \times J_1\left(i \frac{(2M)^{\frac12}}{\gamma} \right) [1 + |y|^{\frac12 k}(1 + |v|)^{\frac12 k + \frac12} R^{\frac12 \gamma}]. \end{aligned}$$

Hence, by the Weierstrass theorem,[17] $U(z, w)$ is an analytic solution of (B4) in the domain of analyticity of $U_1(z, w)$. The bounds on u, $|y|$, and $|v|$ were arbitrary in the definition of $U_1(z, w)$. Therefore, $U(z, w)$ is analytic in the domain $u \ge 0$ and $x - u > -\ln R$.

Having these bounds on $U(z, w) = (rs)^{-\frac12} K(r, s)$, using (B4) and the method of Appendix A, it is straightforward for us to show that differentiating under the integral sign and integrating by parts were justified and therefore (5) is indeed a solution of (1).

To find bounds on $K(r, s) = K(r, re^{-t})$, notice that $r = (xy)^{\frac12} = e^{\frac12 w - \frac12 z}$ is real and therefore $\mathrm{Im}\, z = \mathrm{Im}\, w$. Then[14]

$$\begin{aligned} |K(r, re^{-t})| &= |e^{-\frac12 z} U(z, w)| \\ &\le (1 + |\mathrm{Im}\,t|)^{\frac12 k}(M + 1)2^{-\frac32} M^{-\frac12} R^{\frac12 \gamma} \times |J_1(i 2^{\frac12} M^{\frac12} \gamma^{-1}(1 + |\mathrm{Im}\,t|)^{k + \frac12} R^{\frac12 \gamma})| \\ &< (M + 1)\gamma^{-1} R^{\frac32}(1 + |\mathrm{Im}\,t|)^{\frac32 k + \frac12} \times \exp(2^{\frac12} M^{\frac12} \gamma^{-1} R^{\frac12 \gamma}(1 + |\mathrm{Im}\,t|)^{k + \frac12}). \end{aligned} \quad \text{(B5)}$$

* Work supported in part by NASA and the U.S. Army Office of Research.

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[1] For an authoritative treatment of scattering theory, see R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[2] For the properties of all special functions used in this thesis see Whittaker and Watson, *A Course of Modern Analysis* (Cambridge Press, Cambridge, 1965).

[3] For more detail see R. G. Newton, *The Complex j-Plane* (Benjamin, New York, 1964).

[4] The form $s^{-2}K(r, s)$ was suggested by the inverse scattering problem. For details see text referenced in footnote 1.

[5] See Ref. 2, p. 92.

[6] R. G. Watson, *Theory of Bessel Functions* (Cambridge Press, Cambridge, pp. 75.

[7] N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff, N. V-Groningen, Holland, 1946), pp. 38 and 43.
[8] See Ref. 2, p. 85.
[9] H. Bremmerman, *Distributions, Complex Variables, and Fourier Transforms* (Addison-Wesley, Reading, Mass., 1965).
[10] See Ref. 2, p. 172.
[11] H. Cheng, Phys. Rev. **127**, 647 (1962).
[12] S. Mandelstam, Ann. Phys. (N.Y.) **19**, 254 (1962).
[13] See Ref. 2, p. 279.
[14] The bound we used on $J_\lambda(z)$ is found on p. 49 of Ref. 6.
[15] See Ref. 2, p. 67.
[16] These conditions can be weakened, as it will be seen from the proof.
[17] Reference 2, p. 49.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Prolate-Spheroidal Expansions of the Spin-Orbit, Spin-Spin, and Orbit-Orbit Operators

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(Received 28 October 1970)

Prolate-spheroidal expansions of the spin-orbit, spin-spin, and orbit-orbit operators are derived. These expansions are analogs of the Neumann expansion for $1/r_{12}$ and can be used to study the corresponding exchange interactions in diatomic molecules.

I. INTRODUCTION

An important contribution to the multiplet splitting of molecular energy states is attributable to two-body interactions involving magnetic fields associated with electron spin and orbital angular momenta. A first-order approximation to this splitting is obtained by calculating the expectation values of the well-known two-electron spin-orbit and spin-spin operators. In the multicenter orbital approximation, these expectation values reduce to sums of Coulomb, hybrid, and exchange integrals.

In recent articles,[1] formulas were derived for computing one- and two-center spin-orbit, spin-spin, and orbit-orbit integrals containing arbitrary combinations of Slater-type basis orbitals. In particular, the two-center exchange integrals were evaluated by using partial integration to relate them to electron-repulsion integrals, following the approach suggested by Schrader[2a] and by Hall and Hardisson.[2b] An alternate method of evaluating these integrals is to employ prolate-spheroidal expansions of the three operators. This allows the integrals to be reduced from six to two dimensions. The remaining integrations can then be performed either numerically or analytically by means of suitable recursion formulas. The expansions required for this purpose are derived in the present paper.

It is useful to note that one- and two-center expansions in terms of spherical polar coordinates have been reported previously. In particular, Fontana and Meath[3] have derived such expansions for the Breit-Pauli Hamiltonian. Closely related are the two-center expansions of $(r_{12})^{-n}$ of Sack.[4] Additional expansions have been reported by Pitzer, Kern, and Lipscomb,[5] by Chiu,[6] by Nozawa,[7] and by Kay, Todd, and Silverstone.[8]

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The two-electron spin-(other)-orbit operator in the Pauli approximation to the Breit Hamiltonian[9] has the

[7] N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff, N. V-Groningen, Holland, 1946), pp. 38 and 43.
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Spin-Orbit Expansion

The two-electron spin-(other)-orbit operator in the Pauli approximation to the Breit Hamiltonian[9] has the form

$$\mathcal{H}_{so} = -\tfrac{1}{2}[(\mathbf{r}_{12}/r_{12}^3) \times \mathbf{p}_1] \cdot (\mathbf{s}_1 + 2\mathbf{s}_2). \quad (1)$$

In spherical-tensor notation[10] this reduces to[11]

$$\mathcal{H}_{so} = \tfrac{1}{2} \sum_{\mu} (-)^{\mu} \mathcal{H}_{so}^{\mu} (s_1 + 2s_2)^{-\mu}, \quad (2)$$

where

$$\mathcal{H}_{so}^{\mu} = [\nabla_1(1/r_{12}) \times \mathbf{p}_1]^{\mu}. \quad (3)$$

This can be further reduced to

$$\mathcal{H}_{so}^{\mu} = (-)^{\mu}(\sqrt{6}) \sum_{\beta\beta'} \begin{pmatrix} 1 & 1 & 1 \\ \beta & -\beta' & \mu \end{pmatrix} \mathcal{H}_{so}^{\mu}(\beta, \beta'), \quad (4)$$

where

$$\mathcal{H}_{so}^{\mu}(\beta, \beta') = \nabla_1^{-\beta}(1/r_{12}) \nabla_1^{\beta'}. \quad (5)$$

Each of the sums in Eqs. (2) and (4) ranges between $+1$ and -1.

An expansion for $\mathcal{H}_{so}^{\mu}(\beta, \beta')$ is obtained in the following way. As a first step, the Neumann expansion[12] of $1/r_{12}$ in prolate-spheroidal coordinates,

$$\frac{1}{r_{12}} = \frac{16\pi}{R} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{(2l+1)} \times \hat{\mathfrak{I}}_l^m(\xi_<) \hat{Q}_l^{-m}(\xi_>) Y_l^m(\eta_1, \phi_1) Y_l^{-m}(\eta_2, \phi_2), \quad (6)$$

is substituted into Eq. (5), giving

$$\mathcal{H}_{so}^{\mu}(\beta, \beta') = (16\pi/R) \sum_{lm} (2l+1)^{-1} \times [\nabla_1^{-\beta} \hat{\mathfrak{I}}_l^m(\xi_1) Y_l^m(\eta_1, \phi_1)] \times \hat{Q}_l^{-m}(\xi_2) Y_l^{-m}(\eta_2, \phi_2) \nabla_1^{\beta'} \quad (7)$$

for $\xi_1 < \xi_2$. For convenience in notation, we have defined[13]

$$\hat{\mathfrak{I}}_l^m(\xi) = [\tfrac{1}{2}(2l+1)(l-m)!/(l+m)!]^{\frac{1}{2}} \hat{P}_l^m(\xi) \quad (8)$$

and

$$\hat{Q}_l^{-m}(\xi) = [\tfrac{1}{2}(2l+1)(l-m)!/(l+m)!]^{\frac{1}{2}} Q_l^m(\xi), \quad (9)$$

where $\hat{P}_l^m(\xi)$ and $Q_l^m(\xi)$ are, respectively, Legendre polynomials of the first and second kind. In the Appendix it is shown that

$$\nabla^{\alpha} \hat{\mathfrak{I}}_l^m(\xi) Y_l^m(\eta, \phi) = g^{\alpha} \frac{(2l+1)}{R} \sum_{n=|m+\alpha|\,(2)}^{l-1} \hat{\mathfrak{I}}_n^{m+\alpha}(\xi) Y_n^{m+\alpha}(\eta, \phi). \quad (10)$$

Substitution of this expansion into Eq. (7) yields

$$\mathcal{H}_{so}^{\mu}(\beta, \beta') = g^{\beta}(16\pi/R^2) \sum_{lmn} \hat{\mathfrak{I}}_n^{m-\beta}(\xi_1) Y_n^{m-\beta}(\eta_1, \phi_1) \times \hat{Q}_l^{-m}(\xi_2) Y_l^{-m}(\eta_2, \phi_2) \nabla_1^{\beta'}. \quad (11)$$

It is easily verified that, for the case $\xi_1 > \xi_2$,

$$\mathcal{H}_{so}^{\mu}(\beta, \beta') = -g^{\beta}(16\pi/R^2) \sum_{lmn} \hat{\mathfrak{I}}_n^{m-\beta}(\xi_2) Y_n^{m-\beta}(\eta_2, \phi_2) \times \hat{Q}_l^{-m}(\xi_1) Y_l^{-m}(\eta_1, \phi_1) \nabla_1^{\beta'}. \quad (12)$$

In Eqs. (11) and (12), the lower limit on n is $|m - \beta|$, where the parity restrictions given in the Appendix must be observed.

Spin–Spin Expansion

The spin–spin operator has the form

$$\mathcal{H}_{ss} = [r_{12}^2(\mathbf{s}_1 \cdot \mathbf{s}_2) - 3(\mathbf{r}_{12} \cdot \mathbf{s}_1)(\mathbf{r}_{12} \cdot \mathbf{s}_2)]/r_{12}^5 \quad (13)$$

or

$$\mathcal{H}_{ss} = (\mathbf{s}_1 \cdot \nabla_1)(\mathbf{s}_2 \cdot \nabla_2)(1/r_{12}). \quad (14)$$

This reduces, in spherical-tensor notation, to

$$\mathcal{H}_{ss} = \sum_{\alpha\alpha'} (-)^{\alpha+\alpha'} \mathcal{H}_{ss}^{-\alpha\alpha'} s_1^{\alpha} s_2^{-\alpha'}, \quad (15)$$

where

$$\mathcal{H}_{ss}^{-\alpha\alpha'} = \nabla_1^{-\alpha} \nabla_2^{\alpha'}(1/r_{12}). \quad (16)$$

The indices α and α' each take on the values 0 and ± 1.

As a first step in obtaining an expansion of $\mathcal{H}_{ss}^{-\alpha\alpha'}$, Eq. (6) is substituted into Eq. (16), yielding

$$\mathcal{H}_{ss}^{-\alpha\alpha'} = (16\pi/R) \sum_{lm} (2l+1)^{-1} \times [\nabla_1^{-\alpha} \hat{\mathfrak{I}}_l^m(\xi_1) Y_l^m(\eta_1, \phi_1)] \times [\nabla_2^{\alpha'} \hat{Q}_l^{-m}(\xi_2) Y_l^{-m}(\eta_2, \phi_2)] \quad (17)$$

for $\xi_1 < \xi_2$. It is shown in the Appendix that

$$\nabla^{\alpha} \hat{Q}_l^m(\xi) Y_l^m(\eta, \phi) = -g^{\alpha} \frac{(2l+1)}{R} \sum_{n=l+1(2)}^{\infty} \hat{Q}_n^{m+\alpha}(\xi) Y_n^{m+\alpha}(\eta, \phi). \quad (18)$$

Using this result and Eq. (10), it is found, after a manipulation of the sums, that

$$\mathcal{H}_{ss}^{-\alpha\alpha'} = -g^{\alpha} g^{\alpha'} \frac{16\pi}{R^3} \sum_{n=0}^{\infty} \sum_{m=-n+\alpha}^{n+\alpha} \sum_{l=n+1(2)}^{\infty} \hat{\mathfrak{I}}_n^{m-\alpha}(\xi_1) \times Y_n^{m-\alpha}(\eta_1, \phi_1) f_l^{-m+\alpha'}(\xi_2, \eta_2, \phi_2), \quad (19)$$

where

$$f_l^{-m+\alpha'}(\xi, \eta, \phi) = (2l+1) \sum_{k=l+1(2)}^{\infty} \hat{Q}_k^{-m+\alpha'}(\xi) Y_k^{-m+\alpha'}(\eta, \phi). \quad (20)$$

The sum over l in Eq. (19) can be simplified by observing that

$$\sum_{l=n+1(2)}^{\infty} f_l^{-m+\alpha'}(\xi, \eta, \phi) = \tfrac{1}{2} \sum_{k=n+2(2)}^{\infty} (k-n)(k+n+1) \times \hat{Q}_k^{-m+\alpha'}(\xi) Y_k^{-m+\alpha'}(\eta, \phi). \quad (21)$$

If Eq. (21) is substituted into Eq. (19) and n is replaced by $(l-1)$ and k by $(\lambda+1)$, there results

$$\mathcal{H}_{ss}^{-\alpha\alpha'} = -g^{\alpha} g^{\alpha'} (8\pi/R^3) \times \sum_{lm\lambda} (\lambda - l + 2)(\lambda + l + 1) \hat{\mathfrak{I}}_{l-1}^{m-\alpha}(\xi_1) \times Y_{l-1}^{m-\alpha}(\eta_1, \phi_1) \hat{Q}_{\lambda+1}^{-m+\alpha'}(\xi_2) Y_{\lambda+1}^{-m+\alpha'}(\eta_2, \phi_2), \quad (22)$$

where $1 \leq l \leq \infty$, $-l + \alpha + 1 \leq m \leq l + \alpha - 1$, and $l \leq \lambda \leq \infty$. The sum over λ proceeds in steps of 2. For the case $\xi_1 > \xi_2$, it is merely necessary to interchange electrons 1 and 2 everywhere they appear on the rhs of Eq. (22).

It is important to notice that the use of this expansion to calculate spin–spin integrals requires that a delta-function term[14] be added to $\langle \mathcal{H}_{ss}^{-\alpha\alpha'} \rangle$ in order to account for the exclusion of an infinitesimal volume (in this case a prolate spheroid) about $r_{12} = 0$.

Orbit–Orbit Expansion

The orbit–orbit operator has the form

$$\mathcal{H}_{oo} = -\tfrac{1}{2}\{[(\mathbf{p}_1 \cdot \mathbf{p}_2)/r_{12}] + \mathbf{r}_{12} \cdot [(\mathbf{r}_{12}/r_{12}^3) \cdot \mathbf{p}_1] \cdot \mathbf{p}_2\} \tag{23}$$

and may be written in spherical-tensor notation as

$$\mathcal{H}_{oo} = \tfrac{1}{2} \sum_{\alpha\alpha'} (-)^{\alpha} \mathcal{H}_{oo}^{-\alpha\alpha'} \nabla_1^{-\alpha'} \nabla_2^{\alpha}, \tag{24}$$

where

$$\mathcal{H}_{oo}^{-\alpha\alpha'} = (1/r_{12})\delta(\alpha, \alpha') + (-)^{\alpha'+1} r_{12}^{-\alpha} \nabla_1^{\alpha'}(1/r_{12}). \tag{25}$$

If Eqs. (6) and (10) are now substituted into Eq. (25), we find ($\xi_1 < \xi_2$)

$$\begin{aligned}\mathcal{H}_{oo}^{-\alpha\alpha'} = {} & (16\pi/R) \\ & \times \Big(\delta(\alpha, \alpha') \sum_{lm} (2l + 1)^{-1} \hat{\mathfrak{I}}_l^m(\xi_1) Y_l^m(\eta_1, \phi_1) \\ & \times \hat{Q}_l^{-m}(\xi_2) Y_l^{-m}(\eta_2, \phi_2) + (-)^{\alpha'+1} g^{\alpha'}(r_{12}^{-\alpha}/R) \\ & \times \sum_{lmn} \hat{\mathfrak{I}}_n^{m+\alpha'}(\xi_1) Y_n^{m+\alpha'}(\eta_1, \phi_1) \\ & \times \hat{Q}_l^{-m}(\xi_2) Y_l^{-m}(\eta_2, \phi_2)\Big).\end{aligned} \tag{26}$$

The results for $\xi_1 > \xi_2$ are obtained from Eq. (26) by simply interchanging electrons 1 and 2. The expansion

$$r_{12}^{-\alpha} = \frac{8\pi R}{3g^{\alpha}} \sum_{L=0}^{1} (-)^{L+\alpha} \hat{\mathfrak{I}}_{1-L}^{-\alpha_0}(\xi_1) Y_{1-L}^{-\alpha_0}(\eta_1, \phi_1) \times \hat{\mathfrak{I}}_L^{-\alpha_1}(\xi_2) Y_L^{-\alpha_1}(\eta_2, \phi_2), \tag{27}$$

where $\alpha_0 = \alpha\delta(0, L)$ and $\alpha_1 = \alpha\delta(1, L)$, can now be used to obtain a final expression for $\mathcal{H}_{oo}^{-\alpha\alpha'}$ in prolate-spheroidal coordinates. Since the substitution is a simple one and the resulting expression is rather cumbersome, we will not write out the final form.

Equations (11), (22), and (26) are analogs of the Neumann expansion for $1/r_{12}$. As a check on the results, it can be demonstrated[15] that each expansion reduces to its proper one-center limit as R goes to zero. One application of these expansions is in the evaluation of two-center exchange integrals. The advantages and disadvantages of this approach relative to the method of Ref. 1 are being investigated.

ACKNOWLEDGMENTS

The advice and encouragement of Professor R. M. Pitzer are gratefully acknowledged. One of us (R. L. M.) gratefully acknowledges support by the Welch Foundation through Grant No. E-397 and by the Battelle Memorial Institute.

APPENDIX: EXPANSIONS OF $\nabla^{\alpha}\hat{\mathfrak{I}}_l^m Y_l^m$ AND $\nabla^{\alpha}\hat{Q}_l^m Y_l^m$

In the following, we obtain, respectively, series expansions of $\nabla^{\alpha}\hat{\mathfrak{I}}_l^m Y_l^m$ and $\nabla^{\alpha}\hat{Q}_l^m Y_l^m$ in terms of the product functions $\hat{\mathfrak{I}}_\lambda^\mu Y_\lambda^\mu$ and $\hat{Q}_\lambda^\mu Y_\lambda^\mu$. We begin by considering the former for the special case $\alpha = 0$. In prolate-spheroidal coordinates,

$$\begin{aligned}W_l^m &\equiv \nabla^0 \hat{P}_l^m(\xi) P_l^m(\eta) e^{im\phi} \\ &= \frac{2}{R(\xi^2 - \eta^2)}\left(\eta(\xi^2 - 1)\frac{\partial}{\partial\xi} + \xi(1 - \eta^2)\frac{\partial}{\partial\eta}\right) \\ &\quad \times \hat{P}_l^m(\xi) P_l^m(\eta) e^{im\phi}.\end{aligned} \tag{A1}$$

Introducing the relationship

$$(1 - \eta^2)\frac{d}{d\eta} P_l^m(\eta) = -l\eta P_l^m(\eta) + (l + m) P_{l-1}^m(\eta) \tag{A2}$$

and a corresponding expression for $\hat{P}_l^m$ into Eq. (A1) leads to

$$\begin{aligned}W_l^m = {} & (2/R)[(l + m)/(\xi^2 - \eta^2)] \\ & \times e^{im\phi}[\xi \hat{P}_l^m(\xi) P_{l-1}^m(\eta) - \eta \hat{P}_{l-1}^m(\xi) P_l^m(\eta)].\end{aligned} \tag{A3}$$

Rearrangement of W_l^m then gives us

$$W_l^m = [2(l + m)/R(\xi^2 - \eta^2)] e^{im\phi}[(\xi + \eta) U_l^m + V_l^m], \tag{A4}$$

where

$$U_l^m = \hat{P}_l^m(\xi) P_{l-1}^m(\eta) - \hat{P}_{l-1}^m(\xi) P_l^m(\eta) \tag{A5}$$

and

$$V_l^m = \xi \hat{P}_{l-1}^m(\xi) P_l^m(\eta) - \eta \hat{P}_l^m(\xi) P_{l-1}^m(\eta). \tag{A6}$$

To reduce U_l^m, we apply recursion formulas of the type

$$(2l + 1)\eta P_l^m(\eta) = (l - m + 1) P_{l+1}^m(\eta) + (l + m) P_{l-1}^m(\eta), \tag{A7}$$

and obtain

$$U_l^m = [(2l - 1)/(l - m)](\xi - \eta) \hat{P}_{l-1}^m(\xi) P_{l-1}^m(\eta) + [(l + m - 1)/(l - m)] U_{l-1}^m. \tag{A8}$$

By induction,

$$U_l^m = \frac{(l + m - 1)!}{(l - m)!}(\xi - \eta) \times \sum_{n=|m|}^{l-1} \frac{(2n + 1)(n - m)!}{(n + m)!} \hat{P}_n^m(\xi) P_n^m(\eta). \tag{A9}$$

Using Eq. (A4), we can rewrite V_l^m in the form

$$V_l^m = -[(l+m-1)/(l-m)] \times [\xi \hat{P}_{l-1}^m(\xi)P_{l-2}^m(\eta) - \eta \hat{P}_{l-2}^m(\xi)P_{l-1}^m(\eta)]. \quad (A10)$$

Comparing Eqs. (A10) and (A3), substituting Eq. (A9) and (A10) into Eq. (A4), and then using W_{l-1}^m, we find

$$W_l^m = \frac{2}{R}\frac{(l+m)}{(l-m)}(2l-1)\hat{P}_{l-1}^m(\xi)P_{l-1}^m(\eta) + \frac{(l+m)(l+m-1)}{(l-m)(l-m-1)}W_{l-2}^m. \quad (A11)$$

By induction, it follows that

$$\nabla^0 \hat{P}_l^m(\xi)P_l^m(\eta)e^{im\phi} = \frac{2}{R}\frac{(l+m)!}{(l-m)!}\sum_{n=|m|\,(2)}^{l-1}\frac{(2n+1)(n-m)!}{(n+m)!} \times \hat{P}_n^m(\xi)P_n^m(\eta)e^{im\phi}. \quad (A12)$$

The sum over n proceeds in steps of two, so that the lower limit must have the same parity as $(l-1)$; if $|m|$ is not of the same parity, then the sum begins at $n = |m| + 1$.

We next consider the case $\alpha = 1$, for which

$$\nabla^1 \hat{P}_l^m(\xi)P_l^m(\eta)e^{im\phi} = -\frac{2}{\sqrt{2}}\frac{1}{R(\xi^2-\eta^2)}e^{i(m+1)\phi} \times \left([(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}}\left(\xi\frac{\partial}{\partial\xi} - \eta\frac{\partial}{\partial\eta}\right) - \frac{m(\xi^2-\eta^2)}{[(\xi^2-1)(1-\eta^2)]^{\frac{1}{2}}}\right) \times \hat{P}_l^m(\xi)P_l^m(\eta). \quad (A13)$$

By a suitable manipulation of recurrence formulas, Eq. (A13) can be expressed in the form

$$\nabla^1 \hat{P}_l^m(\xi)P_l^m(\eta)e^{im\phi} = -(2/\sqrt{2})e^{i(m+1)\phi}/R(\xi^2-\eta^2)(l-m) \times [\xi \hat{P}_l^{m+1}(\xi)P_{l-1}^{m+1}(\eta) - \eta \hat{P}_{l-1}^{m+1}(\xi)P_l^{m+1}(\eta)]. \quad (A14)$$

Comparing Eqs. (A14), (A3), and (A12), we find that

$$\nabla^1 \hat{P}_l^m(\xi)P_l^m(\eta)e^{im\phi} = -\frac{2}{\sqrt{2}}\frac{(l+m)!}{R(l-m)!}e^{i(m+1)\phi} \times \sum_{n=|m+1|\,(2)}^{l-1}\frac{(2n+1)(n-m-1)!}{(n+m+1)!} \times \hat{P}_n^{m+1}(\xi)P_n^{m+1}(\eta). \quad (A15)$$

As in Eq. (A12), the lower limit of n must be increased by one when it is not of the same parity as $l-1$.

For the case $\alpha = -1$, we simply change the sign of m in Eq. (A15) and take the complex conjugate of both sides, giving

$$\nabla^{-1} \hat{P}_l^m(\xi)P_l^m(\eta)e^{im\phi} = -\frac{2}{\sqrt{2}}\frac{(l+m)!}{R(l-m)!}e^{i(m-1)\phi} \times \sum_{n=|m-1|\,(2)}^{l-1}\frac{(2n+1)(n-m+1)!}{(n+m-1)!} \times \hat{P}_n^{m-1}(\xi)P_n^{m-1}(\eta), \quad (A16)$$

where the same parity considerations for the lower limit of n hold. In general, then,

$$\nabla^\alpha \hat{P}_l^m(\xi)P_l^m(\eta)e^{im\phi} = (-)^\alpha \frac{2(l+m)!}{2^{|\alpha|/2}R(l-m)!} \times \sum_{n=|m+\alpha|\,(2)}^{l-1}\frac{(2n+1)(n-m-\alpha)!}{(n+m+\alpha)!} \times \hat{P}_n^{m+\alpha}(\xi)P_n^{m+\alpha}(\eta)e^{i(m+\alpha)\phi} \quad (A17)$$

or

$$\nabla^\alpha \hat{\mathfrak{J}}_l^m(\xi)Y_l^m(\eta,\phi) = g^\alpha \frac{(2l+1)}{R}\sum_{n=|m+\alpha|\,(2)}^{l-1}\hat{\mathfrak{J}}_n^{m+\alpha}(\xi)Y_n^{m+\alpha}(\eta,\phi), \quad (A18)$$

where $g^\alpha = 2(-)^\alpha/2^{|\alpha|/2} = 2$ when $\alpha = 0$ and $-\sqrt{2}$ when $\alpha = \pm 1$. The lower limit of n must have the same parity as $(l-1)$.

To determine the corresponding expansion of $\nabla^\alpha \hat{Q}_l^m Y_l^m$, we make use of the fact that

$$\nabla_1^\alpha(1/r_{12}) = -\nabla_2^\alpha(1/r_{12}). \quad (A19)$$

Substituting from Eq. (6) for $1/r_{12}$ and using Eqs. (A18) and (A19), we find $(\xi_1 < \xi_2)$

$$\nabla_2^\alpha(1/r_{12}) = -(16\pi/R)\sum_{lm}(2l+1)^{-1} \times [\nabla_1^\alpha \hat{\mathfrak{J}}_l^m(\xi_1)Y_l^m(\eta_1,\phi_1)] \times \hat{Q}_l^{-m}(\xi_2)Y_l^{-m}(\eta_2,\phi_2)$$
$$= -g^\alpha(16\pi/R^2)\sum_{lmn}\hat{\mathfrak{J}}_n^{m+\alpha}(\xi_1)Y_n^{m+\alpha}(\eta_1,\phi_1) \times \hat{Q}_l^{-m}(\xi_2)Y_l^{-m}(\eta_2,\phi_2). \quad (A20)$$

We now rearrange the summation indices in the following manner:

$$\sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=|m+\alpha|\,(2)}^{l-1} \to \sum_{n=0}^{\infty}\sum_{m=-n-\alpha}^{n-\alpha}\sum_{l=n+1(2)}^{\infty}. \quad (A21)$$

After setting $\bar{m} = m + \alpha$, we find that

$$\nabla_2^\alpha\left(\frac{1}{r_{12}}\right) = -g^\alpha\frac{16\pi}{R^2}\sum_{n=0}^{\infty}\sum_{\bar{m}=-n}^{n}\hat{\mathfrak{J}}_n^{\bar{m}}(\xi_1)Y_n^{\bar{m}}(\eta_1,\phi_1) \times \sum_{l=n+1(2)}^{\infty}\hat{Q}_l^{-\bar{m}+\alpha}(\xi_2)Y_l^{-\bar{m}+\alpha}(\eta_2,\phi_2). \quad (A22)$$

If we compare Eq. (A22) with the intermediate result

$$\nabla_2^\alpha(1/r_{12}) = (16\pi/R)\sum_{lm}(2l+1)^{-1}\hat{\mathcal{P}}_l^m(\xi_1)Y_l^m(\eta_1,\phi_1) \times [\nabla_2^\alpha\hat{Q}_l^{-m}(\xi_2)Y_l^{-m}(\eta_2,\phi_2)], \quad \text{(A23)}$$

obtained in deriving Eq. (A20), it becomes apparent that

$$\nabla^\alpha\hat{Q}_l^m(\xi)Y_l^m(\eta,\phi) = -g^\alpha\frac{(2l+1)}{R}\sum_{n=l+1(2)}^{\infty}\hat{Q}_n^{m+\alpha}(\xi)Y_n^{m+\alpha}(\eta,\phi). \quad \text{(A24)}$$

This is the expansion we require.

[1] (a) R. L. Matcha, C. W. Kern, and D. M. Schrader, J. Chem. Phys. **51**, 2152 (1969); (b) R. L. Matcha and C. W. Kern, *ibid.* **51**, 3434 (1969); see also (c) R. L. Matcha, D. J. Kouri, and C. W. Kern, *ibid.* **53**, 1052 (1970), for a treatment of other Breit-Pauli operators.

[2] (a) D. M. Schrader, J. Chem. Phys. **41**, 3266 (1964); (b) G. G. Hall and A. Hardisson, Proc. Roy. Soc. (London) **A278**, 129 (1964).

[3] P. R. Fontana and W. J. Meath, J. Math. Phys. **9**, 1357 (1968).

[4] R. A. Sack, J. Math. Phys. **5**, 245, 252 (1964).

[5] R. M. Pitzer, C. W. Kern, and W. N. Lipscomb, J. Chem. Phys. **37**, 267 (1962).

[6] Y.-N. Chiu, J. Math. Phys. **5**, 283 (1964).

[7] R. Nozawa, J. Math. Phys. **7**, 1841 (1966).

[8] K. G. Kay, H. D. Todd, and H. J. Silverstone, J. Chem. Phys. **51**, 2363 (1969).

[9] J. O. Hirschfelder, C. F. Curtiss, and R. K. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954), p. 1044.

[10] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U.P., Princeton, N.J., 1957).

[11] The factor $(-)^\mu$ in Eq. (2) represents a correction to Eq. (35) of Ref. 1a.

[12] For a derivation, see K. Ruedenberg, J. Chem. Phys. **19**, 1459 (1951). The original derivation, due to J. Neumann, is given in Crelles J. Reine Angew. Math. **37**, 21 (1848).

[13] The definitions of Legendre polynomials employed here are those of A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. I, pp. 120–81.

[14] R. M. Pitzer, J. Chem. Phys. **51**, 3191 (1969); see also R. M. Pitzer, Ohio State University, Theoretical Chemistry Group, Report No. 11, 1969.

[15] R. L. Matcha, R. H. Pritchard, and C. W. Kern, BMI-OSU Theoretical Chemistry Group, Report No. 7, 1970.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Effect of Electromagnetic Radiation on the Secular Stability of a Homogeneous, Charged, Rotating Drop*

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(Received 4 January 1971)

It is shown that electromagnetic radiation induces a secular instability in a homogeneous rotating charged drop, held together by surface tension, at the point of bifurcation at which a triaxial sequence of equilibrium figures branches from the axially symmetric figures.

1. INTRODUCTION

In the theory of self-gravitating, rotating bodies, it has recently been shown by Chandrasekhar[1] that axisymmetric figures of equilibrium, the Maclaurin spheroids, become unstable when energy and angular momenta are dissipated through gravitational radiation. The instability occurs at the point at which a triaxial sequence of equilibrium figures, the Jacobi ellipsoids, branches off from the Maclaurin sequence. A peculiarity is that the mode of oscillation which is made unstable by gravitational radiation is different from the one that is made secularly unstable by viscous dissipation.

Rosenkilde[2] has shown that there exists a point of bifurcation where a triaxial sequence of equilibrium figures branches off from a spheroidal sequence of homogeneous, rotating, charged drops held together by surface tension. The question arises as to whether or not electromagnetic radiation can engender secular instability in the manner of gravitational radiation.

In order to answer this question, we will first determine in Sec. 2 the radiation reaction terms in the equation of motion and their contribution to the second-order virial equations. (For an explanation of virial methods in equilibrium and stability investigations, see Chandrasekhar.[3]) In Sec. 3 we will evaluate the effect of the radiation on the modes that do become unstable. It will be shown that electromagnetic radiation induces secular instability in the charged, spheroidal drop in precisely the same way that gravitational radiation induces instability in the Maclaurin spheroids.

2. RADIATION REACTION AND THE SECOND-ORDER VIRIAL EQUATION

Our principal goal will be to show that the frequency of a specific second harmonic mode of oscillation of the rotating drop becomes imaginary in a way

If we compare Eq. (A22) with the intermediate result

$$\nabla_2^\alpha(1/r_{12}) = (16\pi/R)\sum_{lm}(2l+1)^{-1}\hat{\mathcal{S}}_l^m(\xi_1)Y_l^m(\eta_1,\phi_1) \times [\nabla_2^\alpha\hat{Q}_l^{-m}(\xi_2)Y_l^{-m}(\eta_2,\phi_2)], \quad (A23)$$

obtained in deriving Eq. (A20), it becomes apparent that

$$\nabla^\alpha\hat{Q}_l^m(\xi)Y_l^m(\eta,\phi) = -g^\alpha\frac{(2l+1)}{R}\sum_{n=l+1(2)}^{\infty}\hat{Q}_n^{m+\alpha}(\xi)Y_n^{m+\alpha}(\eta,\phi). \quad (A24)$$

This is the expansion we require.

[1] (a) R. L. Matcha, C. W. Kern, and D. M. Schrader, J. Chem. Phys. **51**, 2152 (1969); (b) R. L. Matcha and C. W. Kern, *ibid.* **51**, 3434 (1969); see also (c) R. L. Matcha, D. J. Kouri, and C. W. Kern, *ibid.* **53**, 1052 (1970), for a treatment of other Breit-Pauli operators.

[2] (a) D. M. Schrader, J. Chem. Phys. **41**, 3266 (1964); (b) G. G. Hall and A. Hardisson, Proc. Roy. Soc. (London) **A278**, 129 (1964).

[3] P. R. Fontana and W. J. Meath, J. Math. Phys. **9**, 1357 (1968).

[4] R. A. Sack, J. Math. Phys. **5**, 245, 252 (1964).

[5] R. M. Pitzer, C. W. Kern, and W. N. Lipscomb, J. Chem. Phys. **37**, 267 (1962).

[6] Y.-N. Chiu, J. Math. Phys. **5**, 283 (1964).

[7] R. Nozawa, J. Math. Phys. **7**, 1841 (1966).

[8] K. G. Kay, H. D. Todd, and H. J. Silverstone, J. Chem. Phys. **51**, 2363 (1969).

[9] J. O. Hirschfelder, C. F. Curtiss, and R. K. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954), p. 1044.

[10] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U.P., Princeton, N.J., 1957).

[11] The factor $(-)^\mu$ in Eq. (2) represents a correction to Eq. (35) of Ref. 1a.

[12] For a derivation, see K. Ruedenberg, J. Chem. Phys. **19**, 1459 (1951). The original derivation, due to J. Neumann, is given in Crelles J. Reine Angew. Math. **37**, 21 (1848).

[13] The definitions of Legendre polynomials employed here are those of A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. I, pp. 120–81.

[14] R. M. Pitzer, J. Chem. Phys. **51**, 3191 (1969); see also R. M. Pitzer, Ohio State University, Theoretical Chemistry Group, Report No. 11, 1969.

[15] R. L. Matcha, R. H. Pritchard, and C. W. Kern, BMI-OSU Theoretical Chemistry Group, Report No. 7, 1970.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Effect of Electromagnetic Radiation on the Secular Stability of a Homogeneous, Charged, Rotating Drop*

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(Received 4 January 1971)

It is shown that electromagnetic radiation induces a secular instability in a homogeneous rotating charged drop, held together by surface tension, at the point of bifurcation at which a triaxial sequence of equilibrium figures branches from the axially symmetric figures.

1. INTRODUCTION

In the theory of self-gravitating, rotating bodies, it has recently been shown by Chandrasekhar[1] that axisymmetric figures of equilibrium, the Maclaurin spheroids, become unstable when energy and angular momenta are dissipated through gravitational radiation. The instability occurs at the point at which a triaxial sequence of equilibrium figures, the Jacobi ellipsoids, branches off from the Maclaurin sequence. A peculiarity is that the mode of oscillation which is made unstable by gravitational radiation is different from the one that is made secularly unstable by viscous dissipation.

Rosenkilde[2] has shown that there exists a point of bifurcation where a triaxial sequence of equilibrium figures branches off from a spheroidal sequence of homogeneous, rotating, charged drops held together by surface tension. The question arises as to whether or not electromagnetic radiation can engender secular instability in the manner of gravitational radiation.

In order to answer this question, we will first determine in Sec. 2 the radiation reaction terms in the equation of motion and their contribution to the second-order virial equations. (For an explanation of virial methods in equilibrium and stability investigations, see Chandrasekhar.[3]) In Sec. 3 we will evaluate the effect of the radiation on the modes that do become unstable. It will be shown that electromagnetic radiation induces secular instability in the charged, spheroidal drop in precisely the same way that gravitational radiation induces instability in the Maclaurin spheroids.

2. RADIATION REACTION AND THE SECOND-ORDER VIRIAL EQUATION

Our principal goal will be to show that the frequency of a specific second harmonic mode of oscillation of the rotating drop becomes imaginary in a way that leads to instability when quadrupole radiation of the system is taken into account. To study the effect of radiation on the second harmonic modes of oscillation, it is necessary to know the contribution of the electromagnetic field to the second-order virial equations. This contribution is found by multiplying the α component (in this paper all indices take the values 1, 2, or 3) of the force caused by the electromagnetic field F_α by the coordinate x_γ and integrating the resulting expression over the volume of the fluid. The force, in terms of the potentials of the field, is given by the Lorentz law:

$$F_\alpha = (\sigma/c)[v_\beta(A_{\beta,\alpha} - A_{\alpha,\beta}) - A_{\alpha,t} - c\phi_{,\alpha}], \quad (1)$$

where $\mathbf{A}$ and ϕ are the vector and scalar potentials, respectively, σ is the charge density, and v_β is the β component of the fluid velocity; also the comma preceding the subscripts, such as α and t in Eq. (1), denotes differentiation with respect to x_α or t. Accordingly, the contributions to the virial equations, $L_{\gamma\alpha}$, from the electromagnetic field are

$$L_{\gamma\alpha} = c^{-1}\int \sigma x_\gamma[v_\beta(A_{\beta,\alpha} - A_{\alpha,\beta}) - A_{\alpha,t} - c\phi_{,\alpha}]\, d^3x, \quad (2)$$

The Coulomb portion of the electromagnetic field is a necessary consideration in Rosenkilde's[2] virial analysis of the homogeneous drop. Our purpose will be to consider effects of the radiation field as small corrections to a particular set of his equations. To this end, we suppose that an expansion of the retarded solutions of Maxwell's equations in powers of c^{-1} correctly describes the electromagnetic field (see Jackson, Ref. 4, p. 586, for a description of the expansion). Furthermore, we assume that it is sufficient to consider only the lowest-order contributions in c^{-1}, to the virial equation from the radiation. Although it might appear that both an $O(c^{-3})$ dipole-moment term and an $O(c^{-5})$ quadrupole-moment term are relevant, it is easy to see that the dipole term does not contribute to the virial equation analysis, by noting the coincidence of the center of charge with the center of mass; indeed, both the charge and mass densities are assumed uniform. Since the center of mass is taken as the origin of the coordinates and is not subject to variation, the conclusion is manifest.

In order to compute the $O(c^{-5})$ contributions to the virial equation, it is sufficient to consider the partial derivatives of the $O(c^{-4})$ term in the expansion of the vector potential and the $O(c^{-5})$ term in the expansion of the scalar potential. These potential terms are

$$A_\beta = -\frac{1}{c^4}\frac{1}{3!}\frac{\partial^3}{\partial t^3}\int \sigma v_\beta\, |\mathbf{x} - \mathbf{x}'|^2\, d^3x' \quad (3)$$

and

$$\phi = -\frac{1}{c^5}\frac{1}{5!}\frac{\partial^5}{\partial t^5}\int \sigma\, |\mathbf{x} - \mathbf{x}'|^4\, d^3x', \quad (4)$$

where in the preceding equations it is understood that A_β and ϕ represent only specific terms in a series expansion of the potentials A_β and ϕ. To facilitate further calculations, the following definitions are useful:

$$I_{\alpha\beta} = \int \sigma x_\alpha x_\beta d^3x \quad (5)$$

and

$$\mathfrak{C}_{\alpha;\beta} = \int \sigma v_\alpha x_\beta d^3x. \quad (6)$$

Taking the derivatives of expressions (3) and (4) necessary for a subsequent substitution into Eq. (2) while including in that calculation the usual mathematical statement of charge conservation along with a zero value for the dipole moment, we obtain

$$L_{\gamma\alpha} = \frac{1}{3}\frac{1}{c^5}\left(\frac{1}{5}I_{\gamma\mu}\frac{d^5}{dt^5}I_{\alpha\mu} + \frac{1}{10}I_{\gamma\alpha}\frac{d^5}{dt^5}I_{\mu\mu} - I_{\mu\gamma}\frac{d^4}{dt^4}\mathfrak{C}_{\alpha;\mu}\right). \quad (7)$$

We can further reduce Eq. (7) by expressing $\mathfrak{C}_{\alpha;\mu}$ in terms of $I_{\alpha\mu}$ with the aid of the equation expressing the conservation of angular momentum to $O(c^0)$; this equation is

$$\frac{d}{dt}\int \rho v_\alpha x_\beta d^3x = \frac{d}{dt}\int \rho v_\beta x_\alpha d^3x, \quad (8)$$

where ρ is the mass density. In view of Eq. (8), it is easily verified that

$$\frac{d}{dt}\int \rho x_\alpha x_\beta d^3x = 2\int \rho v_\alpha x_\beta d^3x. \quad (9)$$

Since both σ and ρ are assumed to be constant throughout the fluid, we can suppress ρ in Eq. (9) while multiplying both sides by σ. The expression then becomes

$$\frac{d}{dt}I_{\alpha\beta} = 2\mathfrak{C}_{\alpha;\beta}. \quad (10)$$

By virtue of Eq. (10) we may rewrite Eq. (7) as

$$L_{\gamma\alpha} = \frac{1}{10}\frac{1}{c^5}\left(\frac{1}{3}I_{\gamma\alpha}\frac{d^5}{dt^5}I_{\mu\mu} - I_{\gamma\mu}\frac{d^5}{dt^5}I_{\gamma\mu}\right), \quad (11)$$

which is the required contribution to the second-order virial equation from the electromagnetic radiation.

3. VARIATION OF THE VIRIAL EQUATIONS AND STABILITY CONSIDERATIONS

Stability of our fluid system to second harmonic mode perturbations can be investigated by considering variations of the second-order virial equations when the perturbation is described by an infinitesimal Lagrangian displacement (in the rotating frame) of the form

$$e^{\lambda t}\boldsymbol{\zeta}(x).$$

The parameter λ determines the characteristic values of the modes of vibration. In an analysis employing the virial equations, the characteristic value equations are most easily obtained by describing the variation in terms of the quantities

$$v_{\alpha\beta} = \int(\zeta_\alpha x_\beta + \zeta_\beta x_\alpha)\rho\, d^3x.$$

If the axis of rotation of the spheroidal drop is oriented along the x_3 direction, then for the particular modes we are interested in—the toroidal modes—the only nonvanishing contributions to $V_{\alpha\beta}$ are (see Chandrasekhar[3])

$$V_{11},\quad V_{22},\quad \text{and}\quad V_{12};$$

moreover,

$$V_{11} = -V_{22}. \tag{12}$$

To be in a position to add our radiational terms to Eqs. (57) and (58) of Rosenkilde,[2] which describes the toroidal modes to $O(c^0)$, we must express the variation of Eq. (11), transformed to a frame of reference rotating with the drop, in terms of the foregoing $V_{\alpha\beta}$. A solution of the amended equations will then yield the effect of radiation on the characteristic values of these modes. The variation of Eq. (11) is

$$\delta L_{\gamma\alpha} = \frac{1}{10}\frac{1}{c^5}\left[\frac{1}{3}\left(\delta I_{\gamma\alpha}\frac{d^5}{dt^5}I_{\mu\mu} + I_{\gamma\alpha}\delta\frac{d^5}{dt^5}I_{\mu\mu}\right) - \left(\delta I_{\gamma\mu}\frac{d^5}{dt^5}I_{\alpha\mu} + I_{\gamma\mu}\delta\frac{d^5}{dt^5}I_{\alpha\mu}\right)\right]. \tag{13}$$

Because of the axial symmetry an inertial observer does not see changes in the unperturbed values of $I_{\alpha\beta}$ with time: thus the relation which must subsequently be transformed to the rotating frame of the drop is

$$\delta L_{\gamma\alpha} = \frac{1}{10}\frac{1}{c^5}\left(\frac{1}{3}I_{\gamma\alpha}\delta\frac{d^5}{dt^5}I_{\mu\mu} - I_{\gamma\mu}\delta\frac{d^5}{dt^5}I_{\alpha\mu}\right). \tag{14}$$

To carry out the transformation of Eq. (14), time derivatives of the inertial frame moments $I_{\alpha\beta}$ must first be transformed to the rotating frame of the drop and then expressed in terms of moments in the rotating frame. Variation of these transformed, time-differentiated, inertial frame moments is then expressible in terms of the Lagrangian displacements or $V_{\alpha\beta}$. An account of how one performs these computations accompanied with formulas applying specifically to the toroidal modes is given in Chandrasekhar[1]; Eq. (28) given therein is relevant to our purpose. If that equation is multiplied by the factor σ/ρ to convert it from a mass to an electric moment formula, we obtain

$$\left[\delta\frac{d^5}{dt^5}I_{\alpha\beta}\right]^{(R)} = \frac{\sigma}{\rho}[\lambda^5 V_{\alpha\beta} - 20\lambda\Omega^2(\lambda^2 - 2\Omega^2)(V_{\alpha\beta} + \sigma_{\alpha\gamma}V_{\gamma\mu}\sigma_{\mu\beta}) + \Omega(5\lambda^4 - 40\lambda^2\Omega^2 + 16\Omega^4)(V_{\alpha\gamma}\sigma_{\gamma\beta} - \sigma_{\alpha\gamma}V_{\alpha\beta})], \tag{15}$$

where Ω is the angular velocity of the rotating drop and the superscript (R) over the bracket means that the inertial quantity inside is referred to the rotating system; $\sigma_{\alpha\beta}$ is a 2×2 matrix defined by

$$\sigma_{\gamma\beta} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{16}$$

With the aid of Eq. (15) it may be verified that the variation of $L_{\gamma\alpha}$ referred to the rotating frame is just

$$[\delta L_{\gamma\alpha}]^{(R)} = -D\left[\lambda^5\begin{pmatrix} V_{11} & V_{12} \\ V_{12} & V_{22}\end{pmatrix} - 20\lambda\Omega^2(\lambda^2 - 2\Omega^2) \times \begin{pmatrix} V_{11} - V_{22} & 2V_{12} \\ 2V_{12} & V_{22} - V_{11}\end{pmatrix} + \Omega(5\lambda^4 - 40\lambda^2\Omega^2 + 16\Omega^4) \times \begin{pmatrix} -2V_{12} & V_{11} - V_{22} \\ V_{11} - V_{22} & 2V_{12}\end{pmatrix}\right], \tag{17}$$

where D is defined as

$$D \equiv \tfrac{1}{10}(1/c^5)(\sigma/\rho)I_{11}; \tag{18}$$

I_{11} is the constant electric quadrupole moment (measured perpendicular to the axis of rotation) of the unperturbed body in the rotating frame. Finally, appending Eq. (17) onto Eqs. (57) and (58) given by Rosenkilde,[2] we obtain the virial equations for the toroidal modes modified by radiation reaction:

$$[\lambda^2 + 2(p - \Omega^2)]V_{12} + \lambda\Omega(V_{11} - V_{22}) = -2D\{[\lambda^5 - 40\lambda\Omega^2(\lambda^2 - 2\Omega^2)]V_{12} + \Omega(5\lambda^4 - 40\lambda^2\Omega^2 + 16\Omega^4)(V_{11} - V_{22})\}; \tag{19}$$

$$[\lambda^2 + 2(p - \Omega^2)](V_{11} - V_{22}) - 4\lambda\Omega V_{12} = -2D\{[\lambda^5 - 40\lambda\Omega^2(\lambda^2 - 2\Omega^2)](V_{11} - V_{22}) - 4\Omega(5\lambda^4 - 40\lambda^2\Omega^2 + 16\Omega^4)V_{12}\}. \tag{20}$$

If we define the quantity ω by

$$\lambda \equiv i\omega, \tag{21}$$

then the modified characteristic value equation, to the first order in D and in terms of ω, is

$$\omega^2 - 2(p - \Omega^2) - 2\omega\Omega - 2DA = 0, \tag{22}$$

where

$$\begin{aligned} A &= i(\omega^5 + 40\omega^3\Omega^2 + 80\omega\Omega^4 - 10\Omega\omega^4 \\ &\quad - 80\omega^2\Omega^3 - 32\Omega^5) \\ &= i(\omega - 2\Omega)^5. \end{aligned} \tag{23}$$

If ω_0 is a root of the unmodified characteristic value equation [Eq. (22) with $D = 0$], then it is convenient to express the corresponding root of Eq. (22) by the relation

$$\omega = \omega_0 + \delta, \tag{24}$$

where δ is a small quantity of the first order in D. By use of Eqs. (22) and (24), it may be verified that

$$i\delta = +D(2\Omega - \omega_0)^5/(\omega_0 - \Omega). \tag{25}$$

The two values ω_0 may take are

$$\omega_0^1 = \Omega - (2p - \Omega^2)^{\frac{1}{2}} \tag{26}$$

and

$$\omega_0^2 = \Omega + (2p - \Omega^2)^{\frac{1}{2}}. \tag{27}$$

The corresponding values of $i\delta$ are then

$$i\delta^1 = -D[\Omega + (2p - \Omega^2)^{\frac{1}{2}}]^5/(2p - \Omega^2)^{\frac{1}{2}}, \tag{28}$$

and

$$i\delta^2 = D[\Omega - (2p - \Omega^2)^{\frac{1}{2}}]^5/(2p - \Omega^2)^{\frac{1}{2}}. \tag{29}$$

Instability ensues when $i\delta$ is greater than zero. Radiational damping of the ω_0^1 mode therefore results in the entire range of possible angular velocities [the upper limit on Ω is seen to be $\Omega = (2p)^{\frac{1}{2}}$ from Eq. (26)]. On the other hand, the ω_0^2 mode is damped prior to the point of bifurcation [again from Eq. (26) it is evident that a neutral point exists at $p = \Omega^2$] and is amplified by the radiation in the range $2p > \Omega^2 > p$.

4. CONCLUDING REMARKS

The principal result of this investigation is that electromagnetic radiation reaction begins to produce instabilities in a rotating, spheroidal, charged drop, by virtue of toroidal perturbations, beyond the point at which an ellipsoidal sequence of equilibrium figures branches off from the original spheroidal sequence.

* The research reported in this paper has in part been supported by the National Science Foundation under Contract GP-15973 with the University of Chicago. This work will be presented as a part of a thesis to the Department of Physics, University of Chicago, in partial fulfillment of the requirements for the Ph.D. degree.

[1] S. Chandrasekhar, Astrophys. J. **161**, 561 (1970).
[2] C. E. Rosenkilde, J. Math. Phys. **8**, 98 (1967).
[3] S. Chandrasekhar, *Ellipsoidal Figures of Equilibrium* (Yale U.P., New Haven, Conn., 1969).
[4] J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

T Matrix for the Exponential Potential

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(Received 30 October 1970)

An analytic expression for the s-wave part of the exponential potential T matrix is obtained. The separability of the residue of the T matrix at bound state or virtual state poles is demonstrated explicitly.

1. INTRODUCTION

Recent interest in the two-particle T matrix has been stimulated mainly by the discovery of the Faddeev equations.[1] In the Faddeev scheme a three-particle system is described by a set of coupled integral equations, the kernels of which are simply related to the two-particle T matrix. In general, the T matrix is obtained as the solution of a singular integral equation in momentum space.[2] Except for the case of separable potentials,[3] it appears that analytic solutions to this equation cannot easily be obtained. An alternative to the integral equation approach to the T matrix has been given by Van Leeuwen and Reiner,[4] who have shown that the T matrix can be obtained from the solution of a differential equation. Their approach is a generalization of the well-known result that the half-off shell T matrix can be obtained from the solution of the Schrödinger equation.[5] Their differential equation is closely related to the Bethe–Goldstone equation.[6] They give explicit solutions for the square well potential and for the hard-core square well potential. The differential equation approach has been applied to a potential consisting of an exponential function outside of a hard core by Laughlin and Scott.[7] They solved the differential equation numerically.

In this paper we show that it is possible to obtain an analytic expression for the s-wave part of the exponential potential T matrix by using the differential equation approach of Van Leeuwen and Reiner.[4] In particular, we show that the differential equation which arises in the case of the exponential potential can be transformed into an inhomogeneous Bessel differential equation, whose particular integral is a Lommel function. The transformation used is the one introduced by Bethe and Bacher.[8] Half-off the energy shell, the solution of the differential equation becomes the well-known solution of the s-wave Schrödinger equation with the exponential potential.[9] The final formula for the T matrix involves Bessel functions, Lommel functions, and generalized hypergeometric functions. The infinite series representations for these functions converge for all values of the argument. We demonstrate explicitly the separability of the residue of the exponential potential T matrix at bound state or virtual state poles.

2. THE T MATRIX FOR THE EXPONENTIAL POTENTIAL

The two-particle T matrix is the solution of either of the equations

$$T(s) = V + VG_0(s)T(s), \tag{2.1}$$

$$T(s) = V + T(s)G_0(s)V, \tag{2.2}$$

where V is the two-particle potential, s is a complex parameter, and $G_0(s)$, the free particle resolvent, is defined formally in terms of the kinetic energy operator H_0 by

$$G_0(s) = (s - H_0)^{-1}. \tag{2.3}$$

Unless stated otherwise, we will assume that s has a small positive imaginary part, thereby guaranteeing the correct outgoing wave boundary condition; i.e.,

$$s = E + i\epsilon, \quad 0 < \epsilon \ll 1. \tag{2.4}$$

Following Van Leeuwen and Reiner,[4] we define

$$\Omega(s) = 1 + G_0(s)T(s). \tag{2.5}$$

Using (2.1) and (2.3), we obtain

$$T(s) = V\Omega(s), \tag{2.6}$$

and

$$(s - H_0 - V)\Omega(s) = s - H_0, \tag{2.7}$$

which we write out in a mixed representation; i.e.,

$$[s + \nabla^2 - V(r)]\, \langle \mathbf{r}|\, \Omega(s)\, |qlm\rangle = (s - q^2)\langle \mathbf{r} \mid qlm\rangle, \tag{2.8}$$

where

$$\langle \mathbf{r} \mid qlm\rangle = (2\pi^2)^{-\frac{1}{2}} j_l(qr)\, Y_{lm}(\hat{r}). \tag{2.9}$$

$j_l(qr)$ is the usual spherical Bessel function and $Y_{lm}(\hat{r})$ is a spherical harmonic. We are working in units in which $\hbar^2/2\mu$ is one. Since the potential is central, we can write

$$\langle \mathbf{r}|\, \Omega(s)\, |qlm\rangle = u_l(r, q; s)\, Y_{lm}(\hat{r})/qr(2\pi^2)^{\frac{1}{2}}, \tag{2.10}$$

which upon substitution into (2.8) gives us

$$\left(s + \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - V(r)\right)u_l(r, q; s) = (s - q^2)qrj_l(qr). \quad (2.11)$$

From now on we consider only $l = 0$, since even the ordinary Schrödinger equation for the exponential potential cannot be solved for $l \neq 0$. We write the exponential potential in the form

$$V(r) = -(z_0^2/4a^2)\exp(-r/a). \quad (2.12)$$

If we substitute (2.12) into (2.11) with $l = 0$ and make the transformation

$$z = z_0 e^{-r/2a}, \quad (2.13)$$

we obtain, dropping the subscript on u,

$$\left(z\frac{d}{dz}z\frac{d}{dz} + (z^2 + 4k^2a^2)\right)u = -4a^2(k^2 - q^2)\,\mathrm{Im}\left(\frac{z}{z_0}\right)^{2iqa}, \quad s = k^2. \quad (2.14)$$

This is an inhomogeneous Bessel differential equation, the solution of which is simply related to the solution of the equation

$$\left(z\frac{d}{dz}z\frac{d}{dz} + (z^2 - \nu^2)\right)w = z^{\mu+1}. \quad (2.15)$$

A particular integral of (2.15) is the Lommel function $s_{\mu,\nu}(z)$,[10] which is given by

$$s_{\mu,\nu}(z) = [z^{\mu+1}/(\mu - \nu + 1)(\mu + \nu + 1)] \times {}_1F_2(1; \tfrac{1}{2}\mu - \tfrac{1}{2}\nu + \tfrac{3}{2}; \tfrac{1}{2}\mu + \tfrac{1}{2}\nu + \tfrac{3}{2}; -\tfrac{1}{4}z^2). \quad (2.16)$$

The generalized hypergeometric function in (2.16) is a special case of

$$_mF_n(\alpha_1, \alpha_2, \cdots, \alpha_m; \beta_1, \beta_2, \cdots, \beta_n; z) = \sum_{k=0}^{\infty} \frac{(\alpha_1)_k(\alpha_2)_k \cdots (\alpha_m)_k}{(\beta_1)_k(\beta_2)_k \cdots (\beta_n)_k}\frac{z^k}{k!}. \quad (2.17)$$

Using the relation[10]

$$s_{\mu+2,\nu}(z) = z^{\mu+1} - [(\mu + 1)^2 - \nu^2]s_{\mu,\nu}(z), \quad (2.18)$$

we can easily show that the well-behaved solution of (2.14) is

$$u(r, q; s) = \frac{1}{J_{-2ika}(z_0)}\left[-J_{-2ika}(z)\,\mathrm{Im}\left(\frac{s_{1+2iqa,2ika}(z_0)}{z_0^{2iqa}}\right) + J_{-2ika}(z_0)\,\mathrm{Im}\left(\frac{s_{1+2iqa,2ika}(z)}{z_0^{2iqa}} - \left(\frac{z}{z_0}\right)^{2iqa}\right)\right]. \quad (2.19)$$

The function given by (2.19) vanishes at $r = 0$, and one can show by using (2.13) and the power series for the Lommel function and the Bessel function that for large r we have

$$u(r, q; s) \underset{r\to\infty}{\sim} -\frac{(2/z_0)^{2ika}}{\Gamma(1 - 2ika)J_{-2ika}(z_0)} \times \mathrm{Im}\left(\frac{s_{1+2iqa,2ika}(z_0)}{z_0^{2iqa}}\right)e^{ikr} + \sin(qr), \quad k^2 = s. \quad (2.20)$$

The exponential e^{ikr} in (2.20) is consistent with approaching the positive k axis from above. We are assuming that the upper half of the k plane corresponds to the physical energy sheet. It follows from (2.11) that when $s = k^2 = q^2$, $u(r, q; s)$ should become the ordinary Schrödinger wavefunction. It is easy to show that $u(r, q; s)$ does this by using (2.19) with $q = k$ and the relation

$$s_{1+\nu,\nu}(z) = z^\nu - 2^\nu\Gamma(1 + \nu)J_\nu(z), \quad (2.21)$$

which follows directly from (2.16), (2.17), and the power series for $J_\nu(z)$. The s-wave S matrix for the exponential potential can be obtained directly from (2.20) with $q = k$, and is given by the relations

$$e^{2i\delta(k)} = f(-k)/f(k), \quad (2.22)$$

$$f(k) = (z_0/2)^{2ika}\Gamma(1 - 2ika)J_{-2ika}(z_0). \quad (2.23)$$

In order to find the T matrix in momentum space, we combine (2.6), (2.9), and (2.10) to obtain

$$\langle plm|\, T(s)\,|qlm\rangle = (2\pi^2 q)^{-1}\int_0^\infty j_l(pr)V(r)u_l(r, q; s)r\,dr. \quad (2.24)$$

For $l = 0$, with $V(r)$ given by (2.12), this becomes via (2.13)

$$T(p, q; s) \equiv \langle p00|\, T(s)\,|q00\rangle = \frac{z_0}{8\pi^2 pqia}\int_0^{z_0}\left[\left(\frac{z}{z_0}\right)^{1+2ipa} - \left(\frac{z}{z_0}\right)^{1-2ipa}\right] \times u(r, q; s)\,dz. \quad (2.25)$$

Fortunately, the integrals that arise when (2.19) is inserted in (2.25) can be related to tabulated integrals. Using Eq. 6.862.1 of Ref. 11 or Eq. 92 on p. 199 of

Ref. 12, we can easily show with the help of (2.18) that

$$X(p, q, k) \equiv \int_0^{z_0} \left(\frac{z}{z_0}\right)^{1+\lambda} \left[\left(\frac{z}{z_0}\right)^{\mu} - \frac{s_{1+\mu,\nu}(z)}{z_0^{\mu}}\right] \frac{dz}{z_0}$$

$$= \frac{1}{(\lambda + \mu + 2)} \times {}_2F_3\left(1, \frac{\lambda + \mu + 2}{2}; \frac{\mu - \nu + 2}{2}, \frac{\mu + \nu + 2}{2}, \frac{\lambda + \mu + 4}{2}; -\frac{z_0^2}{4}\right), \quad (2.26)$$

where

$$\lambda = 2ipa, \quad \mu = 2iqa, \quad \nu = 2ika. \quad (2.27)$$

From (2.21) and (2.26), it follows that

$$Y(p, k) \equiv \int_0^{z_0} \left(\frac{z}{z_0}\right)^{1+\lambda} J_{-\nu}(z) \frac{dz}{z_0}$$

$$= \frac{(2/z_0)^{\nu}}{\Gamma(1 - \nu)(\lambda - \nu + 2)} \times {}_1F_2\left(\frac{\lambda - \nu + 2}{2}; 1 - \nu, \frac{\lambda - \nu + 4}{2}; -\frac{z_0^2}{4}\right), \quad (2.28)$$

where λ and ν are given by (2.27). Another form of $Y(p, k)$ can be obtained by using Eq. 6.561.13 of Ref. 11 or Eq. (8) on p. 22 of Ref. 12. The result is

$$Y(p, k) = z_0^{-\lambda-2}\Big((\lambda - \nu) z_0 J_{-\nu}(z_0) S_{\lambda,-1-\nu}(z_0) - z_0 J_{-1-\nu}(z_0) S_{\lambda+1,-\nu}(z_0) + 2^{\lambda+1} \frac{\Gamma(\frac{1}{2}\lambda - \frac{1}{2}\nu + 1)}{\Gamma(-\frac{1}{2}\lambda - \frac{1}{2}\nu)}\Big). \quad (2.29)$$

The Lommel function $S_{\mu,\nu}(z)$ differs from the Lommel function given by (2.16) and (2.17) by a linear combination of Bessel functions. Explicit formulas and general properties are given in Ref. 10. The relation between Lommel functions, Bessel functions, and the generalized hypergeometric function ${}_1F_2$ implied by (2.28) and (2.29) does not appear to have been noted before.

Inserting (2.19) into (2.25) and using (2.26) and (2.28) or (2.29), we obtain the expression for the s-wave part of the exponential potential T matrix:

$$T(p, q; s) = [(-)z_0^2/8\pi^2 pqia J_{-2ika}(z_0)] \times \{\mathrm{Im}\,[z_0^{-2iqa} s_{1+2iqa,2ika}(z_0)] \times [Y(p, k) - Y(-p, k)] + [J_{-2ika}(z_0)/2i] \times [X(p, q, k) - X(-p, q, k) - X(p, -q, -k) + X(-p, -q, -k)]\}. \quad (2.30)$$

A useful check on (2.30) is to see if it has the right on-shell limit; i.e., when $p = q = k$, we should have

$$T(k, k; s) = -(2\pi^2 k)^{-1} e^{i\delta(k)} \sin \delta(k), \quad (2.31)$$

where $\delta(k)$, the phase shift, is given by (2.22) and (2.23). Taking the on-shell limit of $Y(p, k) - Y(-p, k)$ is most easily done by using (2.29) and the fact that[10]

$$S_{1\pm\sigma,\sigma}(z) = z^{\pm\sigma}. \quad (2.32)$$

We find

$$Y(k, k) - Y(-k, k) = \frac{4ika}{z_0^2}\left(J_{-2ika}(z_0) - \frac{(2/z_0)^{2ika}}{\Gamma(1 - 2ika)}\right). \quad (2.33)$$

From (2.17), (2.26), and (2.28) it follows that

$$X(k, k, k) - X(-k, k, k) = \Gamma(1 + 2ika)(2/z_0)^{2ika}[Y(k, -k) - Y(-k, -k)]. \quad (2.34)$$

Combining (2.21), (2.33), and (2.34) with (2.30), one easily checks that $T(p, q; s)$ has the correct on-shell limit.

It is by now well known[13] that the residue of the T matrix is separable at bound state or resonance energies. The poles of (2.30) occur when

$$J_{-2ik_0a}(z_0) = 0, \quad (2.35)$$

where we have distinguished the solutions of (2.35) by the symbol k_0. It is immediately obvious from (2.35) that the residue of (2.30) is separable in p and q; however, it is not clear that the residue is the product of a function of p times the *same* function of q. That this is so follows from the relation[10]

$$s_{\mu,\nu}(z) = \frac{\pi}{2 \sin \nu\pi}\left(J_\nu(z)\int_0^z z^\mu J_{-\nu}(z)\, dz - J_{-\nu}(z)\int_0^z z^\mu J_\nu(z)\, dz\right). \quad (2.36)$$

Combining (2.28), (2.30), (2.35), and (2.36), we find

$$T(p, q; s) J_{-2ika}(z_0) \xrightarrow[k \to k_0]{} \{z_0^4 J_{2ik_0a}(z_0)/[32\pi pqa \sin(2ik_0a\pi)]\} \times [Y(p, k_0) - Y(-p, k_0)] \times [Y(q, k_0) - Y(-q, k_0)]. \quad (2.37)$$

We conclude by noting that the infinite series representations for all of the functions that appear in (2.30) have infinite radii of convergence; thus one should be able to evaluate (2.30) numerically and use it as a check on programs which attempt to solve (2.1) and (2.2) directly. It should be possible to sum the series on a computer, since very fast programs for computing gamma functions now exist. Furthermore, for all of the series that arise, the nth term for large n becomes $(-\frac{1}{4}z_0^2)^n/(n!)^2$; thus the series converge rapidly for $\frac{1}{4}z_0^2$ of order 1.

[1] L. D. Faddeev, Zh. Eksp. Teor. Fiz. **39**, 1459 (1960) [Sov. Phys. JETP **12**, 1014 (1961)].
[2] For general discussions of the T matrix, see any of the following: T. Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Englewood Cliffs, N.J., 1962); M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964); R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).
[3] Y. Yamaguchi, Phys. Rev. **95**, 1628 (1954).
[4] J. M. J. Van Leeuwen and A. S. Reiner, Physica **27**, 99 (1961).
[5] C. Moller, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd., **23**, 1 (1945); T. Ikebe, Arch. Ratl. Mech. Anal. **5**, 1 (1960).
[6] H. A. Bethe and J. Goldstone, Proc. Roy. Soc. (London) **A238**, 551 (1957).
[7] R. Laughlin and B. L. Scott, Phys. Rev. **171**, 1196 (1968).
[8] H. A. Bethe and R. Bacher, Rev. Mod. Phys. **8**, 82 (1936).
[9] See, for example, P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. II, p. 1687.
[10] G. N. Watson, *Theory of Bessel Functions* (Cambridge U.P. London, 1944); A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 2.
[11] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals Series and Products* (Academic, New York, 1965). There are misprints in Eq. 6.862.1.
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[13] C. Lovelace, Phys. Rev. **135**, B 1225 (1964); J. Nuttal, J. Math. Phys. **8**, 873 (1967); M. G. Fuda, Phys. Rev. C **1**, 1910 (1970).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Construction of Relativistic Potentials When the Energy Is Fixed

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(Received 14 December 1970)

We use generalized translation operators for solving the relativistic inverse problem at fixed energy and study the extension of Newton's method. Both the Klein–Gordon equation and the Dirac equation are considered. The determination of the so-called coefficients of interpolation remains a crucial point of the solution. In the case of the Klein–Gordon equation, these coefficients are obtained by the same system of equations as the system obtained for nonrelativistic spinless particles. Therefore, the same singular problem is encountered whether the spinless particles are relativistic or not. In the case of the Dirac equation, the problem with two potentials differs from the problem where only one potential is present. When there are two potentials, a generalized translation operator exists, and the inverse problem can be solved by inverting a singular matrix equation for the coefficients of interpolation. When only one potential is present, the solution of the inverse problem is restricted by a compatibility requirement.

I. INTRODUCTION

In 1962 Newton[1] developed a method for determining a nonrelativistic potential at fixed energy. He was able to reconstruct a potential which produces a certain set of asymptotic phase shifts from the knowledge of these phase shifts at one fixed energy. The resulting potential was expressed by an expansion whose coefficients (the coefficients of interpolation[2]) were the unknown quantities of the problem. They were obtained by solving an infinite system of linear equations. Newton showed that the solution of the problem was not unique and, in particular, that there exists a nontrivial central potential which leads to zero phase shift at all energies; for this reason it was called "transparent potential." In a recent paper[3] we generalized Newton's method to complex and Coulomb phase shifts and naturally met again the transparent potentials. In the course of the paper we show that a powerful mathematical tool was used in the construction of the potential, namely the theory of the generalized translation operator (GTO).[3] When a GTO does exist between two equations (more exactly between two operators), one unknown and the second known, one can write explicitly an integral representation of the solution of the unknown equation in terms of the solution of the known one. Newton's equation results by some appropriate manipulation from this representation without any explicit recourse to an underlying Gel'fand–Levitan equation.[4] To fix the notations, we recall that in any inverse problem one for all of the series that arise, the nth term for large n becomes $(-\frac{1}{4}z_0^2)^n/(n!)^2$; thus the series converge rapidly for $\frac{1}{4}z_0^2$ of order 1.

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Construction of Relativistic Potentials When the Energy Is Fixed

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We use generalized translation operators for solving the relativistic inverse problem at fixed energy and study the extension of Newton's method. Both the Klein–Gordon equation and the Dirac equation are considered. The determination of the so-called coefficients of interpolation remains a crucial point of the solution. In the case of the Klein–Gordon equation, these coefficients are obtained by the same system of equations as the system obtained for nonrelativistic spinless particles. Therefore, the same singular problem is encountered whether the spinless particles are relativistic or not. In the case of the Dirac equation, the problem with two potentials differs from the problem where only one potential is present. When there are two potentials, a generalized translation operator exists, and the inverse problem can be solved by inverting a singular matrix equation for the coefficients of interpolation. When only one potential is present, the solution of the inverse problem is restricted by a compatibility requirement.

I. INTRODUCTION

In 1962 Newton[1] developed a method for determining a nonrelativistic potential at fixed energy. He was able to reconstruct a potential which produces a certain set of asymptotic phase shifts from the knowledge of these phase shifts at one fixed energy. The resulting potential was expressed by an expansion whose coefficients (the coefficients of interpolation[2]) were the unknown quantities of the problem. They were obtained by solving an infinite system of linear equations. Newton showed that the solution of the problem was not unique and, in particular, that there exists a nontrivial central potential which leads to zero phase shift at all energies; for this reason it was called "transparent potential." In a recent paper[3] we generalized Newton's method to complex and Coulomb phase shifts and naturally met again the transparent potentials. In the course of the paper we show that a powerful mathematical tool was used in the construction of the potential, namely the theory of the generalized translation operator (GTO).[3] When a GTO does exist between two equations (more exactly between two operators), one unknown and the second known, one can write explicitly an integral representation of the solution of the unknown equation in terms of the solution of the known one. Newton's equation results by some appropriate manipulation from this representation without any explicit recourse to an underlying Gel'fand–Levitan equation.[4] To fix the notations, we recall that in any inverse problem one starts from some known potential, which is called hereafter the reference potential, and one tries to determine the functional dependence of some unknown potential.

The question which comes to mind is whether the same method of GTO exists in relativistic situations so that Newton's method has an extension for solving relativistic inverse problems at fixed energy. In a recent paper[3] we answered affirmatively, limiting ourselves to sketching the method. This paper is devoted to the full treatment of the problem.

When relativistic particles are considered, it must be specified whether they are spinless or not. Here we will be concerned with spinless particles and spin-$\frac{1}{2}$ particles. The former are dependent on the Klein–Gordon equation while the latter depend on the Dirac equation. Both instances are considered, and the method for determining a potential is developed in both cases.

In Sec. II, we examine spinless particles and the Klein–Gordon equation. The first problem we are concerned with is the existence of a GTO. Two Klein–Gordon equations are considered simultaneously, one containing some potential V_0, the second a potential V. We show that a GTO exists which transforms the operator containing V_0 into the operator containing V. The only difference between the Schrödinger case and Klein–Gordon (KG) case lies in the statement of the Cauchy problem which specifies the GTO. This arises naturally from the introduction of the potentials through a quadratic form in the KG equation. Taking potential V_0 as the reference potential, we move on to the problem of finding V through the integral representation of the solutions relative to the potential V. The asymptotic method of Newton applies, and an equation identical to the one obtained in Ref. 1 gives the interpolation coefficients. Most of the results that Newton obtained in the nonrelativistic case remain valid. Since the same equation is obtained for the interpolation coefficients, the same singular matrix has to be inverted. As in the nonrelativistic case, from the reference potential V_0 and the asymptotic phase shifts one obtains a one-parameter family of potentials V. The only difference between the cases is the way the potentials V_0 and V are introduced in the wave equation; thus Newton's result on the first moment of the difference between V_0 and V has to be slightly modified: For relativistic spinless particles it is found that if the interpolation coefficients decrease fast enough when l goes to infinity, and this is the case when finite expansions are considered, one has

$$\int_0^\infty r(V - V_0)(V + V_0 + 2E)\, dr = 0 \qquad (1)$$

instead of

$$\int_0^\infty r(V - V_0)\, dr = 0 \qquad (2)$$

obtained for the Schrödinger case.

The Dirac equation is studied in Sec. III. The same order is followed. Does a GTO exist between two different Dirac equations? If so, can one derive an extension of Newton's method for the inverse problem? The Dirac equation is somewhat different from both the Schrödinger and the Klein–Gordon equation. This is due to the fact that it is a system of coupled first-order equations and therefore must be handled as a matrix equation. The method for finding a GTO introduces then some specific algebra and leads to somewhat different consequences. Two cases are distinguished according to whether the Dirac equation contains one or two central potentials. When two potentials are present in two different Dirac equations, a GTO exists, and a kind of Gel'fand–Levitan equation, which we will call the Gel'fand–Levitan–Regge–Newton[5] equation can be derived for the matrix integral kernel which represents the solution of the unknown equation in terms of the solution of the equation chosen as reference. Newton's method is applied by inserting the asymptotic phase shifts; the interpolation coefficients, which are numbers and not matrices, are obtained by solving a set of linear algebraic equations. They are different from the one obtained previously by Newton. Although different, the matrix to be inverted is singular. We are able to give an explicit form for a left and right inverse of this matrix and for a vector annihilated by it. Transparent potentials will still occur in the solution of this inverse problem. Two main differences are found between the Schrödinger and the Dirac case with two potentials: One, there is no result analogous to that which concerns the first moment of the difference between the potentials and, two, the singularities of the Jost functions in the Dirac case are due exclusively to the choice of the reference potentials. The Dirac equation with one potential creates an additional special problem: Although a GTO may exist since the equations for the GTO are almost the same at fixed energy as at fixed angular momentum, a compatibility condition limits the solution of the inverse problem. When Newton's method is used for the interpolation coefficients, it is necessary to verify the compatibility condition before obtaining the unknown potential.

II. THE KLEIN–GORDON EQUATION

We consider here spinless particles, for instance, mesons. The wave equation follows readily from the equality

$$E = p^2 + \mu^2. \tag{3}$$

It is a scalar equation which reads

$$-\frac{\partial^2\psi}{\partial t^2} = -\Delta\psi + \mu^2\psi \tag{4}$$

with $\hbar = c = 1$. In Eqs. (3) and (4) μ is the rest mass of the particle.

In the presence of an external electromagnetic field, $\mathbf{p}$ and E must be replaced respectively by $\mathbf{p} - e\mathbf{A}$ and $E - e\phi$ in Eq. (3), where $\mathbf{A}$ and ϕ are, respectively, the vector and the scalar potential, while e is the charge of the particle. Therefore, Eq. (4) becomes

$$\left(i\frac{\partial}{\partial t} - e\phi\right)^2\psi = \left[\left(\frac{\nabla}{i} - e\mathbf{A}\right) + \mu^2\right]\psi. \tag{5}$$

If now we make the assumption that $\mathbf{A} = 0$ and that a central static $V(r)$ describes the motion of the Klein–Gordon particle, Eq. (5) reduces to

$$\left(i\frac{\partial}{\partial t} - V(r)\right)^2\psi = (\mu^2 - \Delta)\psi. \tag{6}$$

We will limit our interest in this paper to Eq. (6). Looking for a stationary solution, we set

$$\psi(\mathbf{r}, t) = \phi(\mathbf{r})e^{-iEt}.$$

The equation for $\phi(\mathbf{r})$ is

$$[E - V(r)]^2\phi(\mathbf{r}) = [\mu^2 - \Delta]\phi(\mathbf{r}). \tag{7}$$

As for the Schrödinger equation, we use a partial wave expansion in Eq. (7),

$$\phi(\mathbf{r}) = \sum_l [\phi_l(r)/r]Y_l^0(\theta, \varphi),$$

to obtain the radial equation

$$[E - V(r)]^2\phi_l(r) = \left(\mu^2 + \frac{l(l+1)}{r^2} - \frac{\partial^2}{\partial r^2}\right)\phi_l(r). \tag{8}$$

At fixed energy E, a set of differential equations is obtained in this way for each value of the angular momentum l.

Existence of GTO and Newton's Method

To study the existence of a GTO[3,6] at fixed energy, two equations of the form (8) are considered, one containing a potential V and the second a potential V_0:

$$\begin{aligned} A_l &\equiv r^2\left([E - V(r)]^2 - \mu^2 + \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2}\right), \\ B_l &\equiv r^2\left([E - V_0(r)]^2 - \mu^2 + \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2}\right). \end{aligned} \tag{9}$$

These operators A_l and B_l being defined, the method for a GTO applies in a straightforward manner (see Ref. 3).

One can notice that Eq. (8) is identical with the nonrelativistic Schrödinger equation once V in the latter is replaced by $V(2E - V)$. Since E is fixed here, everything done in Refs. 1 and 2 carries over, and one may make the same substitution in the results.

We limit ourselves to some particular aspects and define

$$V^{\mathrm{NR}} - V_0^{\mathrm{NR}} = -\frac{2}{r}\frac{d}{dr}\frac{K(r, r)}{r},$$

where NR stands for nonrelativistic. V_{NR} is a one-parameter family of potentials which will be obtained in the nonrelativistic case by the same set of phase shifts. It is real if the phase shifts are themselves real. More precisely, we have

$$V^2 - V_0^2 - 2E(V - V_0) = V^{\mathrm{NR}} - V_0^{\mathrm{NR}}. \tag{10}$$

We assume that $V^{\mathrm{NR}} - V_0^{\mathrm{NR}}$ is a negative quantity; then

$$V = -EV_0 \pm [V_0^2(E^2 + 1) + V_0^{\mathrm{NR}} - V^{\mathrm{NR}}]^{\frac{1}{2}}$$

is a real potential.

The result of Newton in Ref. 2 on the first moment of the potential has to be modified to take into consideration Eq. (10).

What one obtains here is simply that the first moment of the difference $V^{\mathrm{NR}} - V_0^{\mathrm{NR}}$ has to vanish when the interpolation coefficients vanish rapidly as $l \to \infty$.

Therefore, the first moment which must vanish in the relativistic case is the first moment of the quantity $(V - V_0)(V + V_0 - 2E)$.

Another result needs some change: It is that of Sabatier[2] concerning the asymptotic behavior of the potential, since it is related to the asymptotic behavior of $V^{\mathrm{NR}} - V_0^{\mathrm{NR}}$. Applying Sabatier's result, we can determine the unique parameter which specifies the family of potentials so that the solution of the problem becomes unique.

If the parameter is selected in order that

$$V^{\mathrm{NR}} - V_0^{\mathrm{NR}} = O(r^{-\frac{3}{2}}),$$

then

$$(V - V_0)(V + V_0 + 2E) = O(r^{-\frac{3}{2}}).$$

It results that $V \to V_0$ when $r \to \infty$ as $r^{-\frac{3}{2}} \to 0$.

Equations being the same for spinless particles in both the relativistic and the nonrelativistic case, the singularities of the Jost functions will depend on both cases on the choice of the contour C as well as that of the reference potential.

According to all that precedes, the problems are substantially identical for the Klein–Gordon and the Schrödinger equations; the situation will change when the Dirac equation is considered. This is the topic of the following section.

III. DIRAC EQUATION

When a Dirac field interacts with some other fields, the Dirac equation reads[7–9]

$$\frac{i\partial}{\partial t}\Phi(\mathbf{r}, t) = [\boldsymbol{\alpha}\cdot(\mathbf{p} - e\mathbf{A}) + V(r) + \beta(m + g_s\phi_s) + \rho_2 g_p\phi_p]\Phi(\mathbf{r}, t). \quad (11)$$

In Eq. (11) $\mathbf{p} = -i\boldsymbol{\nabla}$ and m are, respectively, the three-component momentum and the reduced mass of the particle. The 4×4 matrices α_k, β, and ρ are given by

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \rho_2 = i\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$

with 0 and I being the 2×2 matrices zero and unity and with the Pauli matrices being

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad i\sigma_2 = \omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (12)$$

In addition, $A = (\mathbf{A}, iV)$ is a quadrivector potential and the subscripts p and s stand for pseudoscalar and scalar.

A special case of interest is that of a spin-$\frac{1}{2}$ particle subjected to a diagonal matrix central potential $V(r)$ such that

$$V(r) = \begin{pmatrix} V_1(r)I & 0 \\ 0 & V_2(r)I \end{pmatrix}$$

so that the Dirac equation reduces to

$$[\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m + V(r)]\Phi(\mathbf{r}, t) = \frac{i\partial}{\partial t}\Phi(\mathbf{r}, t). \quad (13)$$

Defining

$$V_1(r) = V(r) + W(r), \quad V_2(r) = V(r) - W(r), \quad (14)$$

we find that Eq. (13) becomes

$$\{\boldsymbol{\alpha}\cdot\mathbf{p} + \beta[m + W(r)] + V(r)\}\Phi(\mathbf{r}, t) = \frac{i\partial}{\partial t}\Phi(\mathbf{r}, t). \quad (15)$$

When Eq. (14) is compared to the general equation (11), it is seen that the case where $V(r)$ is a diagonal matrix corresponds to

$$\mathbf{A} = (\mathbf{0}, iV), \quad g_s\phi_s = W(r), \quad g_r\phi_r = 0.$$

From the definition of α_k and β, the following identities hold:

$$\alpha_k\alpha_l + \alpha_l\alpha_k = 2\delta_{kl}, \quad \alpha_k\beta + \beta\alpha_k = 0, \quad \alpha_k^2 = \beta^2 = 1.$$

The solution $\Phi(\mathbf{r}, t)$ of Eq. (15) is therefore a four-component vector. We look for a stationary solution and write

$$\Phi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-iEt}; \quad (16)$$

via the definition (16), Eq. (15) becomes

$$\{\boldsymbol{\alpha}\cdot\mathbf{p} + \beta[m + W(r)] + V(r)\}\psi(\mathbf{r}) = E\psi(r). \quad (17)$$

When $V(r)$ and $W(r)$ are central potentials, the angular momentum $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ does not commute with the Hamiltonian H (it is not a good quantum number). To obtain operators which do commute with H, the total angular momentum

$$\mathbf{J} = \mathbf{l} + \mathbf{s}$$

is introduced. Now spherical harmonics are used for a partial wave expansion:

$$y_{Jl}^m(\theta, \phi) = \sum_{m_s=\pm\frac{1}{2}} \langle l\tfrac{1}{2}M - m_s m_s \mid JM\rangle Y_l^{M-m_s}(\theta, \phi)X_{m_s}^{\frac{1}{2}}. \quad (18)$$

In the definition (18) the $X_{m_s}^{\frac{1}{2}}$ are the normalized spin functions, the $Y_l^{M-m_s}$ the spherical harmonics, and the $\langle l\frac{1}{2}M - m_s m_s \mid JM\rangle$ the coupling coefficients.

Another operator K which commutes with H is defined by

$$K = \beta(\boldsymbol{\sigma}\cdot\mathbf{l} + 1).$$

One can prove the equality $K^2 = \mathbf{J}^2 + \frac{1}{4}$.[9] Therefore, the eigenfunctions of J are eigenfunctions of K with eigenvalue $\pm(J + \frac{1}{2})$. The eigenfunctions of H can be specified with the help of the eigenfunctions of J and K. Their common eigenfunctions form a complete set[10,11]; thus any solution $\psi(\mathbf{r})$ of Eq. (16) can be expanded as

$$\psi(\mathbf{r}) \equiv \psi(r, \theta, \phi) = \sum_{\lambda M} v_\lambda(r)f^{\lambda M}(\theta, \phi), \quad (19)$$

where λ and the normalized spinors $f^{\lambda M}(\theta, \phi)$ are defined by

$$Kf^{\lambda M}(\theta, \phi) = -\lambda f^{\lambda M}(\theta, \phi).$$

From its definition, λ is an integer different from zero (see Table I).

To solve the Dirac equation it is sufficient to determine the spinors $v_\lambda(r)$. If one sets[12]

$$v_\lambda(r) = G_\lambda(r)\tfrac{1}{2}(1 + \beta) + F_\lambda(r)\tfrac{1}{2}(1 - \beta), \quad (20)$$

Eq. (17) separates into a set of coupled equations. The problem is then reduced to that of finding the scalar functions $G_\lambda(r)$, $F_\lambda(r)$.

TABLE I.

	$f^{\lambda M}$
$\lambda = J + \frac{1}{2}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} y^M_{J,J+\frac{1}{2}}(\theta,\phi) \\ -iy^M_{J,J-\frac{1}{2}}(\theta,\phi)\end{pmatrix}$
$\lambda = -(J + \frac{1}{2})$	$\frac{1}{\sqrt{2}}\begin{pmatrix} iy^M_{J,J-\frac{1}{2}}(\theta,\phi) \\ y^M_{J,J+\frac{1}{2}}(\theta,\phi)\end{pmatrix}$

Inserting (19) and (20) into (16), one obtains the equations[13] for $G_\lambda(r)$ and $F_\lambda(r)$:

$$\begin{aligned}&[E - V - (m + W)]G_\lambda(r) + \left(\frac{d}{dr} + \frac{1-\lambda}{r}\right)F_\lambda(r) = 0,\\ &[E - V + (m + W)]F_\lambda(r) - \left(\frac{d}{dr} + \frac{1+\lambda}{r}\right)G_\lambda(r) = 0.\end{aligned} \tag{21}$$

Defining $rG_\lambda(r) = g_\lambda(r)$ and $rF_\lambda(r) = f_\lambda(r)$, one obtains the new set of equations

$$\begin{aligned}&[E - V - (m + W)]g_\lambda(r) + \left(\frac{d}{dr} - \frac{\lambda}{r}\right)f_\lambda(r) = 0,\\ &[E - V + (m + W)]f_\lambda(r) - \left(\frac{d}{dr} + \frac{\lambda}{r}\right)g_\lambda(r) = 0.\end{aligned} \tag{22}$$

If one defines

$$\phi_\lambda(r) = \begin{pmatrix} f_\lambda(r) \\ g_\lambda(r)\end{pmatrix},$$

Eq. (22) takes a matrix form

$$\left(\frac{d}{dr} - \frac{\lambda}{r}\sigma_3 + (E - V)\omega - (m + W)\sigma_1\right)\phi_\lambda(r) = 0. \tag{23}$$

Another equivalent expression can be given:

$$\left(\omega\frac{d}{dr} - (m + W)\sigma_3 - \frac{\lambda}{r}\sigma_1 + [V(r) - E]\right)\phi_\lambda(r) = 0.$$

The equation satisfied by

$$\sigma_1\phi_\lambda(r) = \begin{pmatrix} g_\lambda(r) \\ f_\lambda(r)\end{pmatrix}$$

will be needed in the following and is easily derived from Eq. (22).

A. Existence of a GTO

We are concerned here with the inverse problem at fixed energy, but it can be recalled that the problem at fixed l has been solved by Gasimov and Levitan.[14,15] As in Sec. II we study the problem of the existence of a GTO prior to its application to the inverse problem.

Let us define the two families of operators

$$\begin{aligned}\bar{A}_\lambda &= \frac{d}{dr} - \frac{\lambda}{r}\sigma_3 + (E - V)\omega - (m + W)\sigma_1,\\ \bar{B}_\lambda &= \frac{d}{dr} - \frac{\lambda}{r}\sigma_3 + (E - V_0)\omega - (m + W_0)\sigma_1,\end{aligned} \tag{24}$$

where V, W, V_0, and W_0 are four scalar potentials. Since λ is the parameter specifying the members of each family and since we want a GTO valid for the family as such, it is preferable[3] to consider the two following families rather than $\bar{A}_\lambda$ and $\bar{B}_\lambda$:

$$A_\lambda = r\sigma_3^{-1}\bar{A}_\lambda, \quad B_\lambda = r\sigma_3^{-1}\bar{B}_\lambda.$$

Explicitly we have

$$A_\lambda = +r\left(\sigma_3\frac{d}{dr} - \frac{\lambda}{r} + (E - V)\sigma_1 - (m + W)\omega\right). \tag{25}$$

In addition, we consider the set $\mathcal{E}$ of twice-differentiable vector functions ϕ, which satisfy the condition

$$\lim_{r\to 0}\phi_\lambda(r) = r^\lambda\begin{pmatrix}[(2\lambda - 1)!!]^{-1} \\ 0\end{pmatrix}.$$

We ask for a translation operator X defined by

$$A_\lambda X\phi = XB_\lambda\phi \tag{26}$$

for any ϕ in the set $\mathcal{E}$.

The explicit form which is required for X is

$$X\phi = M(r)\phi - \int_0^r \frac{K(r,s)}{s}\phi(s)\,ds. \tag{27}$$

In Eq. (27), $M(r)$ and $K(r, s)$ are two unknown matrices to be defined by Eq. (26).

With the help of the two following identities,

$$\frac{\partial}{\partial r}\int_0^r K(r,s)\frac{\phi(s)}{s}\,ds = \frac{K(r,r)}{r}\phi(r) + \int_0^r \frac{\partial}{\partial r}K(r,s)\frac{\phi(s)}{s}\,ds,$$

$$\int_0^r K(r,s)\sigma_3\frac{\partial}{\partial s}\phi(s)\,ds = K(r,r)\sigma_3\phi(r) - \int_0^r \frac{\partial}{\partial s}K(r,s)\sigma_3\phi(s)\,ds,$$

one obtains $A_\lambda X\phi$ and $XB_\lambda\phi$:

$$
\begin{aligned}
A_\lambda X\phi = r\Big(&\sigma_3 M'(r)\phi + \sigma_3 M(r)\phi' - \frac{\lambda}{r}M(r)\phi \\
&+ (E - V)\sigma_1 M(r)\phi - (m + W)\omega M(r)\phi \\
&- \sigma_3 \frac{K(r, r)}{r}\phi(r) - \sigma_3 \int_0^r \frac{\partial}{\partial r}K(r, s)\frac{\phi(s)}{s}\,ds \\
&+ \frac{\lambda}{r}\int_0^r \frac{K(r, s)}{s}\phi(s)\,ds \\
&- (E - V)\sigma_1 \int_0^r \frac{K(r, s)}{s}\phi(s)\,ds \\
&+ (m + W)\omega \int_0^r \frac{K(r, s)}{s}\phi(s)\,ds\Big), \qquad (28)
\end{aligned}
$$

$$
\begin{aligned}
XB_\lambda\phi = {} & M(r)r\sigma_3\phi' - M(r)\lambda\phi(r) \\
&+ M(r)r(E - V_0)\sigma_1\phi \\
&- M(r)(m + W_0)r\omega\phi(r) - K(r, r)\sigma_3\phi(r) \\
&+ \int_0^r \frac{\partial}{\partial s}K(r,s)\sigma_3\phi(s)\,ds + \lambda\int_0^r \frac{K(r, s)}{s}\phi(s)\,ds \\
&- \int_0^r K(r, s)[E - V_0(s)]\sigma_1\phi(s)\,ds \\
&+ \int_0^r K(r, s)[m + W_0(s)]\omega\phi(s)\,ds. \qquad (29)
\end{aligned}
$$

Since $\phi(r)$ is an arbitrary element of $\mathcal{E}$, Eq. (26) separates. One has

$$\sigma_3 M(r) - M(r)\sigma_3 = 0, \qquad (30)$$

$$
\begin{aligned}
r\sigma_3 M' + {} & r(E - V)\sigma_1 M(r) \\
&- r(m + W)\omega M(r) - \sigma_3 K(r, r) \\
&= M(r)r(E - V_0)\sigma_1 - rM(r)(m + W_0)\omega \\
&\quad - K(r, r)\sigma_3, \qquad (31)
\end{aligned}
$$

$$
\begin{aligned}
r\Big(&-\sigma_3 \frac{\partial}{\partial r}K(r, s) - [E - V(r)]\sigma_1 K(r, s) \\
&+ [m + W]\omega K(r, s)\Big) \\
&= s\Big(\frac{\partial}{\partial s}K(r, s)\sigma_3 - K(r, s)[E - V_0(s)]\sigma_1 \\
&\quad + K(r, s)(m + W_0)\omega\Big). \qquad (32)
\end{aligned}
$$

Equation (30) tells that $M(r)$ is a diagonal matrix

$$M(r) = \begin{pmatrix} M_{11} & 0 \\ 0 & M_{22} \end{pmatrix}.$$

Writing Eq. (31) explicitly, one obtains

$$M'_{11} = M'_{22} = 0,$$

so that M is a constant matrix. With this in mind, Eq. (31) becomes

$$
\begin{aligned}
&[E - V(r)]M_{22} - [m + W(r)]M_{22} - [E - V_0(r)]M_{11} \\
&\qquad + [m + W_0(r)]M_{11} = +2K_{12}(r, r)/r, \qquad (33) \\
&[E - V(r)]M_{11} + [m + W(r)]M_{11} - [E - V_0(r)]M_{22} \\
&\qquad - [m + W_0]M_{22} = -2K_{21}(r, r)/r,
\end{aligned}
$$

if $K(r, s)$ is written

$$K(r, s) = \begin{pmatrix} K_{11}(r, s) & K_{12}(r, s) \\ K_{21}(r, s) & K_{22}(r, s) \end{pmatrix}. \qquad (34)$$

If one asks that $\phi \in \mathcal{E}$ implies $X\phi \in \mathcal{E}$ in order to get an integral representation of solutions with the same boundary conditions through the kernel $K(r, s)$, then M_{11} must be equal to 1. The same value 1 will be the value of M_{22} if the behavior of the β component of $X\phi$ has to be the same as that of ϕ. When Newton's method is used, it will be shown that $M_{11} = M_{22} = 1$; then Eqs. (33) reduce to

$$
\begin{aligned}
V_0(r) - V(r) - W(r) + W_0(r) &= 2K_{12}/r, \\
V_0(r) - V(r) + W(r) - W_0(r) &= -2K_{21}/r.
\end{aligned} \qquad (35)
$$

In addition to Eqs. (33), we have the partial differential equation (32) to be satisfied. When it is rendered explicit, we have

$$
r\begin{Bmatrix} -\dfrac{\partial K_{11}}{\partial r} + [m + W + V - E]K_{21}, & -\dfrac{\partial K_{12}}{\partial r} + [m + W + V - E]K_{22} \\ \dfrac{\partial K_{21}}{\partial r} + [-m - W + V - E]K_{11}, & \dfrac{\partial K_{22}}{\partial r} + [-m - W + V - E]K_{12} \end{Bmatrix}
$$

$$
= s\begin{Bmatrix} \dfrac{\partial K_{11}}{\partial s} + [-m - W_0 + V_0 - E]K_{12}, & -\dfrac{\partial K_{12}}{\partial s} + [m + W_0 + V_0 - E]K_{11} \\ \dfrac{\partial K_{21}}{\partial s} + [-m - W_0 + V_0 - E]K_{22}, & -\dfrac{\partial K_{22}}{\partial s} + [m + W_0 + V_0 - E]K_{21} \end{Bmatrix}. \qquad (36)
$$

In Eq. (36) V and W depend on r while V_0 and W_0 depend on s.

The system (36) together with the boundary conditions (35) may not be sufficient to define a unique GTO. However, it shows that such an operator exists, and therefore an integral representation can be obtained for the regular solution of one Dirac equation in terms of the regular solution of a second Dirac equation.

Namely, if $A\phi = 0$ and $B\phi^0 = 0$ (ϕ and ϕ^0, regular solutions), there exists a kernel such that

$$\phi_\lambda(r) = M\phi_\lambda^0(r) - \int_0^r K(r,s)\phi_\lambda^0(s)s^{-1}\,ds. \quad (37)$$

Investigation of Eq. (36) shows that one must set

$$K_{\alpha\beta}(r,s) = \int_C dh(\lambda)[\phi_\lambda(r)]_\alpha[\sigma_1\phi_\lambda^0(s)]_\beta,$$

where $[\phi_\lambda]_\beta$ means the β component of the column vector ϕ.

The contour C and the measure $h(\lambda)$ must be chosen so that the conditions (35) are satisfied.

B. The Inverse Problem

Following the example of Newton, we reduce the contour C to the sets of integer numbers and write

$$K_{\alpha\beta}(r,s) = \sum_\lambda c_\lambda[\Phi_\lambda(r)]_\alpha[\sigma_1\Phi^0(s)]_\beta. \quad (38)$$

When the Dirac equation is concerned, there is no reason to restrict the summation to the positive values of λ. In fact, the change λ into $-\lambda$ does not give the same solution. Precisely, one has

$$\Phi(-\lambda, E, V, W) = \sigma_1\Phi(\lambda, -E, -V, W).$$

So the development will contain positive and negative values of λ.

A Gel'fand–Levitan–Regge–Newton equation can be obtained to define the kernel K.

For this purpose we introduce the matrix

$$P_{\alpha\beta}(r,s) = \sum_\lambda c_\lambda[\Phi^0(r)]_\alpha[\sigma_1\Phi^0(s)]_\beta \quad (39)$$

and use the integral representation (37) for Φ_λ:

$$[\Phi_\lambda]_\alpha(r) = M_{\alpha\alpha}[\Phi_\lambda^0(r)]_\alpha - \int_0^r \sum_\gamma K_{\alpha\gamma}(r,t)[\Phi_\lambda^0(t)]_\gamma \frac{dt}{t}. \quad (40)$$

Equation (40) is multiplied by $c_\lambda[\sigma_1\Phi_\lambda(s)]_\beta$ from the left and the summation over λ is performed, so that one obtains

$$K_{\alpha\beta}(r,s) = M_{\alpha\alpha}P_{\alpha\beta}(r,s) - \int_0^r \sum_\gamma K_{\alpha\gamma}(r,t)P_{\gamma\beta}(t,s)\frac{dt}{t} \quad (41)$$

or in matrix notation

$$K(r,s) = MP(r,s) - \int_0^r K(r,t)P(t,s)\frac{dt}{t}. \quad (42)$$

The set of constants c_λ has to be calculated to solve the inverse problem. For this purpose r is allowed to go to infinity in Eq. (40), and the asymptotic behavior of each solution is incorporated into the equation.

As was done previously, we write

$$[\Phi_\lambda(r)]_\alpha = M_{\alpha\alpha}[\phi_\lambda^0(r)]_\alpha - \sum_\mu c_\mu L_{\lambda\mu}(r)[\phi_\mu(r)]_\alpha \quad (43)$$

and the similar equation for $[\Phi_\lambda(r)]_\beta$. In Eq. (43) one has

$$L_{\lambda\mu}(r) = \int_0^r \sum_\beta \frac{ds}{s}[\sigma_1\Phi_\mu^0(s)]_\beta[\phi_\lambda^0(s)]_\beta. \quad (44)$$

This last equation can be rewritten as

$$L_{\lambda\mu}(r) = \int_0^r \frac{ds}{s}[\sigma_1\Phi_\mu^0(s)]^{\mathrm{T}}\Phi_\lambda^0(s), \quad (45)$$

with the symbol T standing for

$$[\Phi^0(s)]^{\mathrm{T}} = (f_\mu^0(s), g_\mu^0(s)). \quad (46)$$

Therefore, $L_{\lambda\mu}(r)$ is a scalar which can be evaluated by considering the equations for Φ_λ and $[\sigma_1\Phi_\mu^0]^{\mathrm{T}}$.

We have

$$\left(-\sigma_3\frac{d}{dr} + (m+W_0)\omega + \frac{\lambda}{r} + \sigma_1[V_0(r) - E]\right)\Phi_\lambda^0(r) = 0, \quad (47)$$

$$[\sigma_1\Phi_\mu^0(r)]^{\mathrm{T}}\left(\sigma_3\frac{\overleftarrow{d}}{dr} + (m+W_0)\omega + \frac{\mu}{r} + \sigma_1[V_0 - E]\right) = 0. \quad (48)$$

Left multiplication of Eq. (38) by $[\sigma_1\Phi_\mu^0(r)]^{\mathrm{T}}$ and right multiplication of Eq. (37) by $\Phi_\lambda^0(r)$ yields, after subtractions,

$$\frac{d}{dr}\{[\sigma_1\Phi_\mu^0(r)]^{\mathrm{T}}\sigma_3\Phi_\lambda^0(r)\} - \frac{\lambda-\mu}{r}[\sigma_1\Phi_\mu^0(r)]^{\mathrm{T}}\Phi_\lambda^0(r) = 0. \quad (49)$$

Therefore, integration from zero to r gives

$$L_{\lambda\mu}(r) = (\lambda-\mu)^{-1}[\sigma_1\Phi_\mu^0(r)]^{\mathrm{T}}\sigma_3\Phi_\lambda^0(r). \quad (50)$$

If λ goes to μ, Eq. (49) is still valid, so that one has

$$L_{\lambda\lambda}(r) = \lim_{\mu\to\lambda} L_{\lambda\mu}(r).$$

When r goes to infinity, Eqs. (33) become

$$\Phi_\lambda(\infty) = M\Phi_\lambda^0(\infty) - \sum_\mu c_\mu L_{\lambda\mu}(\infty)\Phi_\mu(\infty). \quad (51)$$

We adopt the following normalizations:

$$\Phi_\lambda(\infty) = \frac{A_\lambda}{k^\lambda}\begin{pmatrix}\cos(kr - \frac{1}{2}\lambda\pi + \eta_\lambda) \\ [k/(E-m)]\sin(kr - \frac{1}{2}\lambda\pi + \eta_\lambda)\end{pmatrix} = \frac{A_\lambda}{k^\lambda}\begin{pmatrix}C_\lambda \\ S_\lambda\end{pmatrix}, \quad (52)$$

$$\Phi_\lambda^0(\infty) = \frac{B_\lambda}{k^\lambda}\begin{pmatrix}\cos(kr - \frac{1}{2}\lambda\pi + \eta_\lambda^0) \\ [k/(E-M)]\sin(kr - \frac{1}{2}\lambda\pi + \eta_\lambda^0)\end{pmatrix} = \frac{B_\lambda}{k^\lambda}\begin{pmatrix}C_\lambda^0 \\ S_\lambda^0\end{pmatrix}. \quad (53)$$

Since the dependence on k in the real quantities A_λ, B_λ, η_λ, and η_λ^0 is evident, it has been omitted in Eqs. (52) and (53).

We get

$$L_{\lambda\mu}(\infty) = \frac{1}{\lambda-\mu} B_\lambda B_\mu \frac{k^{1-\mu-\lambda}}{E-m} \times \sin[(\lambda-\mu)\tfrac{1}{2}\pi + \eta_\mu^0 - \eta_\lambda^0], \quad (54)$$

$$L_{\lambda\lambda}(\infty) = +B_\lambda^2 \frac{k^{1-2\lambda}}{E-m}\left(\frac{\pi}{2} - \frac{d\eta_\lambda^0}{d\lambda}\right). \quad (55)$$

Inserting (52) and (53) into (51) gives

$$A_\lambda\begin{pmatrix}C_\lambda \\ S_\lambda\end{pmatrix} = B_\lambda\begin{pmatrix}C_\lambda^0 \\ M_{22}S_\lambda^0\end{pmatrix} - \sum_\mu c_\mu L_{\lambda\mu}(\infty) A_\mu \begin{pmatrix}C_\mu \\ S_\mu\end{pmatrix} k^{\lambda-\mu}. \quad (56)$$

The linear independence of e^{ikr} and e^{-ikr} separates Eq. (56) into two sets of equations, one set being the complex conjugate of the other, and shows that necessarily $M_{22} = 1$. Since the matrix M reduces to unity, Eqs. (37) and (42) become now

$$\Phi_\lambda(r) = \Phi_\lambda^0(r) - \int_0^r \frac{K(r,s)\Phi_\lambda^0(s)}{s}\, ds, \quad (37')$$

$$K(r,s) = P(r,s) - \int_0^r \frac{K(r,t)P(t,s)}{t}\, dt, \quad (42')$$

and one has

$$A_\lambda \exp(i\eta_\lambda)\left[1 + c_\lambda B_\lambda^2 \frac{k^{1-2\lambda}}{E-m}\left(\frac{\pi}{2} - \frac{d\eta_\lambda^0}{d\lambda}\right)\right] = B_\lambda\Big(\exp(i\eta_\lambda^0) - \sum_{\lambda\neq\mu} i^{\lambda-\mu} \frac{c_\mu B_\mu A_\mu}{\lambda-\mu}\frac{k^{1-2\mu}}{E-m} \times \sin[\tfrac{1}{2}(\lambda-\mu)\pi + \eta_\mu^0 - \eta_\lambda^0]\exp(i\eta_\mu)\Big) \quad (57)$$

and its complex conjugate.

The two sets of equations (57) are nonlinear in the unknown quantities A_λ and c_λ; they can be linearized by defining

$$D_\lambda = c_\lambda A_\lambda B_\lambda k^{1-2\lambda}(E-m)^{-1} \quad (58)$$

to obtain

$$\frac{A_\lambda}{B_\lambda} = \exp[i(\eta_\lambda^0 - \eta_\lambda)] - D_\lambda\left(\frac{\pi}{2} - \frac{d\eta_\lambda^0}{d\lambda}\right) - \sum_{\lambda\neq\mu} \frac{D_\mu}{\lambda-\mu}(i)^{\lambda-\mu}\sin[\tfrac{1}{2}(\lambda-\mu)\pi + \eta_\mu^0 - \eta_\lambda^0] \times \exp[i(\eta_\mu - \eta_\lambda)]. \quad (59)$$

Since j is an integer, the parity of $\lambda - \mu$ may be considered; this has an effect of separating the sum over (59) into two terms:

$$-\sum_{\substack{\mu\neq\lambda \\ (\mu-\lambda)\text{even}}} [D_\mu/(\lambda-\mu)]\sin(\eta_\mu^0 - \eta_\lambda^0)\exp[i(\eta_\mu - \eta_\lambda)] + i^{-1}\sum_{(\mu-\lambda)\text{odd}} [D_\mu/(\lambda-\mu)]\cos(\eta_\mu^0 - \eta_\lambda^0) \times \exp[i(\eta_\mu - \eta_\lambda)].$$

Finally, we can separate the real and the imaginary part of Eq. (59) and obtain the linear equation for D_λ:

$$0 = \sin(\eta_\lambda^0 - \eta_\lambda) - \sum_{(\lambda-\mu)\text{odd}} [D_\mu/(\lambda-\mu)]\cos(\eta_\mu^0 - \eta_\lambda^0)\cos(\eta_\mu - \eta_\lambda) - \sum_{(\lambda-\mu)\text{even}} [D_\mu/(\lambda-\mu)]\sin(\eta_\mu^0 - \eta_\lambda^0)\sin(\eta_\mu - \eta_\lambda). \quad (60)$$

The equation for A_λ will be

$$\frac{A_\lambda}{B_\lambda} = \cos(\eta_\mu^0 - \eta_\lambda^0) - D_\lambda\left(\frac{\pi}{2} - \frac{d\eta_\lambda^0}{d\lambda}\right) - \sum_{\substack{\lambda\neq\mu \\ (\lambda-\mu)\text{even}}} \frac{D_\mu}{\lambda-\mu}\sin(\eta_\mu^0 - \eta_\lambda^0)\cos(\eta_\mu - \eta_\lambda) + \sum_{(\lambda-\mu)\text{odd}} \frac{D_\mu}{\lambda-\mu}\cos(\eta_\mu^0 - \eta_\lambda^0)\sin(\eta_\mu - \eta_\lambda). \quad (61)$$

When D_λ and A_λ are obtained, using (60), one gets c_λ. Going back to Eq. (60) and using the scalar function $L_{\lambda\mu}(r)$, we can construct for each value of r the vector $\phi_\lambda(r)$ and the matrix $K_{\alpha\beta}(r,s)$. Therefore, $V(r)$ and $W(r)$ are obtained. All the calculations will require an electronic computer.

C. Discussion of the Method

To simplify the discussion, only the case where the reference potential is chosen equal to zero is considered. Then, setting all the η_λ^0 equal to zero in Eq. (50), one gets

$$0 = \sin\eta_\lambda + \sum_{(\lambda-\mu)\text{odd}} [D_\mu/(\lambda-\mu)]\cos(\eta_\mu - \eta_\lambda). \quad (62)$$

There is no restriction in considering such a case. The general case where the reference potentials are not equal to zero can be constructed in two steps.

The first step will be to construct from the given reference potentials a transparent potential. For this, η_λ is set equal to zero in Eq. (50). An equation identical to (52) is obtained with the η_λ replaced by η_λ^0. This transparent potential obtained, the final potential is constructed through solving (52). It results that (52) is used twice and that its discussion is sufficient to understand the singularity of the problem.

Restricting the attention to Eq. (52), we consider the possibility of transparent potentials, that is, potentials which produce zero phase shifts. So we set all the η_λ equal to zero in Eq. (52) and get

$$0 = \sum_{(\lambda-\mu)\,\mathrm{odd}} D_\mu/(\lambda - \mu). \tag{63}$$

Transparent potentials will exist, if there is a set of constants D_μ not equal to zero, such that the rhs of Eq. (53) vanishes. In other words, the possibility of transparent potentials depends on the matrix

$$M_{\lambda\mu} = \begin{cases} (\lambda-\mu)^{-1}, & \lambda - \mu \text{ odd} \\ 0, & \lambda - \mu \text{ even} \end{cases}, \tag{64}$$

where λ and μ are integers different from zero, being singular. If a matrix M^{-1} exists, it will be an antisymmetric matrix; it is then easy to show that

$$M^{-1}_{\lambda\mu} = 0 \quad \text{if} \quad \lambda - \mu \text{ is even.}$$

In fact, we have for a right inverse

$$\sum_p M_{2r,2p+1} M^{-1}_{2p+1,n} = \delta_{2r,n}, \tag{65}$$

$$\sum_n M_{2p+1,2n} M^{-1}_{2n,r} = \delta_{2p+1,r}. \tag{66}$$

So only the terms $M^{-1}_{2p+1,2q}$ and $M^{-1}_{2p,2q+1}$ contribute to the summation (64), (65), and we may choose

$$M^{-1}_{2p,2q} = M^{-1}_{2p+1,2q+1} = 0.$$

We show now that the antisymmetric matrix N

$$N_{2n,2r+1} = \begin{Bmatrix} -\dfrac{4}{\pi^2}\dfrac{2n}{[(2n-(2r+1)](2r+1)} \\ 0 \quad \text{otherwise} \end{Bmatrix} = -N_{2r+1,2n}$$

is a right inverse of M. In other words, $MN = 1$. Equation (66) in an explicit form is composed of two relations analogous to (64) and (65). The first one may be written

$$-\frac{4}{\pi^2}\sum_{p=-\infty}^{+\infty} \frac{2n}{(2n-2p-1)(2p+1)(2p+1-2r)} = \delta_{2r,2n}. \tag{67}$$

The infinite sum to be computed is

$$\sum_{p=-\infty}^{+\infty} \frac{1}{[2n-(2p+1)](2p+1-2r)(2p+1)}.$$

For this purpose we consider the integral

$$\int_c \frac{\pi \cot \pi z\, dz}{[2n-(2z+1)](2z+1-2r)(2z+1)} = \int_c f(z)\, dz,$$

where c is the large circle centered at the origin. When the radius of the circle c goes to infinity, the integrand vanishes; therefore the integral is equal to zero.

Inside the circle c, $f(z)$ is analytic everywhere except perhaps at the poles of $\cot \pi z$ and at the zeros of the denominator. The poles of $\cot \pi z$ happen for $z = p$, p any integer, and the zeros of the denominator for $z = -\frac{1}{2}$, $z = r - \frac{1}{2}$, and $z = n - \frac{1}{2}$. But for these zeros $\cot \pi z$ vanishes; if $r \neq n$, they are not true poles of the function $f(z)$; therefore, we get

$$\sum_{p=-\infty}^{+\infty} \frac{1}{[2n-(2p+1)](2p+1)(2p+1-2r)} = 0 \quad \text{if} \quad r \neq n.$$

Equation (67) is therefore proved if $r \neq n$.

When $r = n$, the situation is different due to the fact that the denominator has a zero of order 2. So an additional term occurs:

$$\sum_{p=-\infty}^{+\infty} \frac{1}{[2n-(2p+1)]^2[2p+1]} = \frac{\pi^2}{4(2n)};$$

therefore, Eq. (67) holds.

We prove now that the sum analogous to Eq. (65) is verified,

$$\frac{4}{\pi^2}\sum_{n=-\infty}^{+\infty} \frac{2n}{(2r+1)(2p+1-2n)(2r+1-2n)} = \delta_{rp}, \tag{68}$$

and write the lhs as

$$\frac{4}{\pi^2(2r+1)}\left(\sum_{n>0} \frac{2n}{(2p+1-2n)(2r+1-2n)} - \frac{2n}{(2p+1+2n)(2r+1+2n)}\right)$$
$$= \frac{4(p+r+1)}{\pi^2(2r+1)} \times \sum_{n>0} \frac{16n^2}{[(2p+1)^2-4n^2][(2r+1)^2-4n^2]};$$

this last sum has already been calculated by Redmond,[16] who found

$$\sum_{n=1}^{+\infty} \frac{(2n)^2}{[(2n)^2-(2p+1)^2][(2n)^2-(2r+1)^2]} = \frac{\pi}{4}\frac{(2r+1)\cot \frac{1}{2}(2r+1)\pi}{(2p+1)^2-(2r+1)^2}.$$

Since r is integer, $\cot \frac{1}{2}(2r+1)\pi$ vanishes. So, if $p \neq r$, the sum is zero. Now, if $p = r$, we have a form

0/0 to be specified. Computing

$$\lim_{x\to 2p+1}\frac{\cot\frac{1}{2}x\pi}{(2p+1)^2-x^2}=\frac{-\frac{1}{2}\pi}{-2x\sin\frac{1}{2}x\pi}\bigg|_{x=2p+1}=\frac{\pi}{4(2p+1)},$$

we obtain

$$\sum_{n=1}^{+\infty}\frac{(2n)^2}{(2n)^2-(2p+1)^2}=\frac{\pi^2}{16},$$

so that Eq. (68) holds.

Having found that N is a right inverse, we prove that it is a left inverse too. The equations to be verified are

$$-(4/\pi^2)\sum_r 2r/(2p+1-2r)\times(2r-2n-1)(2p+1)=\delta_{pn}, \quad (69)$$

$$(4/\pi^2)\sum_p 2r/(2n-2p+1)\times[2r-(2p+1)](2p+1)=\delta_{rn}, \quad (70)$$

which reduce, respectively, to (68) and (69). (More generally, it can be proved that if an antisymmetric matrix N is right inverse of an antisymmetric matrix M, it is also a right inverse and conversely.)

The inverse N is not unique, since we can introduce a vector Δ which is annihilated from the right and the left by M:

$$M\Delta=\Delta^{\mathrm{T}}M=0. \quad (71)$$

It is

$$\Delta_{2n+1}=(4/\pi^2)(2n+1)^{-1},\quad \Delta_{2n}=0.$$

The first Eq. (71) is

$$\sum_n M_{2r,2n+1}\Delta_{2n+1}=\sum_n\{[2r-(2n+1)](2n+1)\}^{-1}.$$

Introducing the function $g(z)$ defined by

$$g(z)=\pi\cot(\pi z)/[2r-(2z+1)](2z+1)$$

and its integral along a circle of infinite radius, one finds by a calculation of residues that

$$\sum_n\{[2r-(2n+1)](2n+1)\}^{-1}=0;$$

the second equality follows:

$$\sum_n\Delta_{2n+1}M_{2n+1,2r}=\sum_n[(2n+1)(2n+1-2r)]^{-1}=0.$$

So a vector exists which is annihilated by M and the two-side inverse N is not unique. This leads to the possibility of transparent potentials for the Dirac equation with two potentials.

When the Dirac equation with one potential is considered, the system of equations defining the GTO reduces to

$$r\left(-\sigma_3\frac{\partial}{\partial r}K(r,s)-[E-V(r)]\sigma_1K(r,s)+m\omega K(r,s)\right)$$
$$=s\left(\frac{\partial}{\partial s}K(r,s)\sigma_3-[E-V_0(s)]K(r,s)\sigma_1+mK(r,s)\omega\right), \quad (72)$$

$$[V_0(r)-V(r)]+m(1-M_{22})=2K_{12}(r,r)/r, \quad (73)$$

$$[V_0(r)-V(r)]M_{22}+m(1-M_{22})=-2K_{21}(r,r)/r.$$

So, in general, a GTO will exist. However, when one wants to apply the method to the inverse problem, troubles occur. The asymptotic behavior of Φ implies that $M_{22}=1$ so that the last system reduces to

$$V(r)-V_0(r)=-2K_{12}(r,r)/r=2K_{21}(r,r)/r.$$

Even if the system seems to have a solution of the form

$$K_{\alpha\beta}(r,s)-\int_c dh(\lambda)[\Phi_\lambda(r)]_\alpha[\sigma_1\phi_\lambda^0(s)]_\beta \quad (74)$$

since expansion (74) contains two unknown data, the contour C and the measure $h(\lambda)$, the fact remains that if C is fixed *a priori*, as it is in Newton's method, a strong compatibility requirement is introduced. For the method to be valid, when the matrix $K_{\alpha\beta}(r,s)$ is constructed, one needs to verify that

$$K_{12}(r,r)+K_{21}(r,r)=0.$$

As an end to this paper, it seems worthwhile to point out the two main differences between the Schrödinger–Klein–Gordon and the Dirac cases, two potentials or one potential when a solution exists.

The deduction of the potential from the kernel K is obtained without any derivative, and there is no result concerning the first moment of the difference between the potentials.

In addition, the singular matrices are, respectively,

$$M_{\mathrm{S}}=M_{\mathrm{KG}}=1/(l-m)(l+m+1),\quad l\neq m,\quad l,m>0,$$
$$M_{\mathrm{D}}=1/(l-m),\quad l\neq m,\quad l,m\gtrless 0.$$

In the first case a pole is obtained when $l=-m-1$. Therefore, the Jost function[1b] may have poles due to the reference potential and to the choice of the contour C. Specifically, there will be a pole for $l=-(C'+1)$, where C' is the part of C which does not contain the set N of integers. In the second case, the poles of the Jost function are uniquely due to the choice of the reference potential. In addition to these two main differences, a third one is also apparent.

As a function of m, we have

$$M_{\mathrm{S}} = M_{\mathrm{KG}} \sim 1/m^2.$$

So when the matrix is iterated, the order of summation can be permuted,[16] and the uniqueness of the vector annihilated by M results.

Iterating M_{D} and making the assumption that the order of summation can be permuted, we prove the uniqueness of Δ. But

$$M_{\mathrm{D}} \sim 1/m,$$

and no general theorem on the uniform convergence of a double series can be used, so that the assumption has no support. Therefore, the uniqueness of Δ remains to be proved.

APPENDIX A

Since it has been proved[15] that an integral representation exists for the regular solution of the Dirac equation with one potential, it is interesting to compare the set of equations (72), (73) to that obtained by applying the GTO method between two Dirac equations at λ constant.

Then the two families of operators to be compared are

$$A_E = \omega \frac{d}{dr} - m\sigma_3 - \frac{\lambda}{r}\sigma_1 + V(r) - E,$$

$$B_E = \omega \frac{d}{dr} - m\sigma_3 - \frac{\lambda}{r}\sigma_1 + V_0(r) - E.$$

The equation $A_E X\phi = XB_E\phi$, where

$$X\phi = M(r)\phi - \int_0^r K(r,s)\phi(s)\,ds,$$

gives

$$\omega M - M\omega = 0, \tag{A1}$$

$$\begin{aligned}\omega M' - m\sigma_3 M - \lambda r^{-1}\sigma_1 M &+ (V - E)M(r) - \omega K(r,r)\\ &= -mM\sigma_3 - \lambda r^{-1}M\sigma_1 + (V_0 - E)M - K(r,r)\omega,\end{aligned} \tag{A2}$$

$$\begin{aligned}-\omega\frac{\partial K}{\partial r} + m\sigma_3 K + \lambda r^{-1}\sigma_1 K - V(r)K\\ = \frac{\partial K}{\partial s}\omega + mK\sigma_3 + \lambda s^{-1}K\sigma_1 - KV_0(s).\end{aligned} \tag{A3}$$

Equation (A1) states that

$$M(r) = \begin{pmatrix} M_{11} & M_{12} \\ -M_{12} & M_{11}\end{pmatrix}.$$

Without loss of generality $M(r)$ can be chosen to be an orthogonal matrix; using this result in (A2), one obtains

$$\begin{aligned}\begin{pmatrix} -M'_{12} & M'_{11} \\ -M'_{11} & -M'_{12}\end{pmatrix} - 2m\begin{pmatrix} 0 & M_{12} \\ M_{12} & 0\end{pmatrix} - 2\frac{\lambda}{r}\begin{pmatrix} -M_{12} & 0 \\ 0 & M_{12}\end{pmatrix} + (V - V_0)\begin{pmatrix} M_{11} & M_{12} \\ -M_{12} & M_{11}\end{pmatrix}\\ - \begin{pmatrix} K_{21} + K_{12} & K_{22} - K_{11} \\ K_{22} - K_{11} & -K_{12} - K_{21}\end{pmatrix} = 0.\end{aligned}$$

The nondiagonal terms yield

$$\begin{aligned}M'_{11} - 2mM_{12} + (V - V_0)M_{12} - (K_{22} - K_{11}) &= 0,\\ -M'_{11} - 2mM_{12} - (V - V_0)M_{12} - (K_{22} - K_{11}) &= 0.\end{aligned} \tag{A4}$$

Therefore, one obtains

$$M'_{11} = (V_0 - V)M_{12} \quad \text{and} \quad 2M_{12}m = K_{22} - K_{11}. \tag{A5}$$

On the other hand, the diagonal terms give

$$\begin{aligned}-M'_{12} + 2\lambda r^{-1}M_{12} + (V - V_0)M_{11} - (K_{12} + K_{21}) &= 0,\\ -M'_{12} - 2\lambda r^{-1}M_{12} + (V - V_0)M_{11} + (K_{12} + K_{21}) &= 0,\end{aligned}$$

that is,

$$2\lambda M_{12} = (K_{21} + K_{12})r, \quad M'_{12} = M_{11}(V - V_0).$$

Thus a compatibility condition enters the picture, namely,

$$K_{22} - K_{11} = mr\lambda^{-1}(K_{12} + K_{21}). \tag{A6}$$

This last relation has been obtained by Prats and Toll[15] in a slightly different form. See their Eq. (48). They first set

$$K(r,t) = M(r)F(r,t)$$

with the orthogonal matrix

$$M(r) = \begin{pmatrix} \cos\Delta\mu, & \sin\Delta\mu \\ -\sin\Delta\mu, & \cos\Delta\mu\end{pmatrix}.$$

They have defined

$$\Delta\mu = \mu(r) - \mu_0(r),$$

$$\mu(r) = \int_0^r V(s)\,ds, \quad \mu_0(r)\int_0^r V_0(r)\,dr.$$

These definitions are clearly compatible with our Eqs. (A5). Next they obtain the condition for the kernel

$$\omega K(r,r) - K(r,r) - (M^{\mathrm{T}} - M)(\sigma_1\lambda r^{-1} - \sigma_3 m) = 0. \tag{A7}$$

Equations (A7) and (A4) are identical. When (A7) is made explicit, one obtains their Eq. (48) or, equivalently, the following:

$$K_{21} + K_{12} + 2\lambda r^{-1} \sin \Delta = 0, \quad K_{22} - K_{11} + 2m \sin \Delta = 0, \tag{A8}$$

which shows that condition (A6) remains valid.

In their paper Prats and Toll have shown that, given two potentials whose moments satisfy the usual conditions, there exists an integral representation of the solutions of one Dirac equation, in terms of another Dirac equation. They have shown, in addition, that when the scattering data of these two potentials are known, it is possible to *reconstruct* one of these potentials, the second being chosen as reference. However, they have not completely solved the inverse problem. Specifically they have not answered the following question: Given two sets of scattering data satisfying the usual conditions, is condition (A6) automatically verified? And if the answer is no, as it seems, for what class of scattering data is the answer yes?

APPENDIX B

We study here the uniqueness of the vector D_m,

$$0 = \sum_{\substack{m=-\infty \\ (m-l)\text{odd}}}^{+\infty} \frac{D_m}{l-m} = \sum_m M_{lm} D_m, \tag{B1}$$

and follow a method developed by Redmond in Ref. 16. This method consists of studying the secular equation for the eigenvalues of the matrix M_{lm},

$$M\mathbf{D} = \boldsymbol{\lambda} D, \tag{B2}$$

where $\mathbf{D}$ is the eigenvector with the eigenvalue λ.

Let us assume the absolute convergence of the series (B1).

Since M_{lm} vanishes when $l - m$ is even, Eq. (B1) separates into two coupled equations

$$\lambda D_{2n} = \sum_k (2n - 2k - 1)^{-1} D_{2k+1}, \quad n \neq 0$$
$$\lambda D_{2p+1} = \sum_r (2p + 1 - 2r)^{-1} D_{2r}, \quad r \neq 0. \tag{B3}$$

We can therefore eliminate D_{2k+1} in the first and D_{2r} in the second of these last equations and obtain

$$\lambda^2 D_{2n} = \sum_k \sum_r [(2n-2k-1)(2k+1-2r)]^{-1} D_{2r}, \tag{B4}$$

$$\lambda^2 D_{2p+1} = \sum_n \sum_k [(2p+1-2n)(2n-2k-1)]^{-1} D_{2k+1}. \tag{B5}$$

Because of the assumption on the convergence of (B1), these two series converge uniformly, and the order of summation can be permuted to get

$$\lambda^2 D_{2n} = \sum_r D_{2r} \sum_k [(2n - 2k - 1)(2k + 1 - 2r)]^{-1}, \tag{B6}$$

$$\lambda^2 D_{2p+1} = \sum_k D_{2k+1} \times \sum_n [(2p + 1 - 2n)(2n - 2k - 1)]^{-1}. \tag{B7}$$

A simple evaluation by the method of residues yields the following:

$$(\lambda^2 + \tfrac{1}{4}\pi^2) D_{2n} = 0, \tag{B8}$$

$$\lambda^2 D_{2p+1} = +(2p + 1)^{-1} \sum_{k \neq p} (2k + 1)^{-1} D_{2k+1} - [\tfrac{1}{4}\pi^2 - (2p + 1)^{-2}] D_{2p+1}. \tag{B9}$$

We get

$$X = \sum_k D_{2k+1}/(2k + 1) \tag{B10}$$

and get, instead of (B7),

$$(2p + 1)(\lambda^2 + \tfrac{1}{4}\pi^2) D_{2p+1} = +X.$$

Thus

$$D_{2p+1} = X/(2p + 1)(\lambda^2 + \tfrac{1}{4}\pi^2).$$

When we set $\lambda = 0$,

$$D_{2p+1}(0) = +4X/(2p + 1)\pi^2. \tag{B11}$$

Substituting (B9) into (B8) yields

$$X = \sum_p 4X/(2p + 1)^2 \pi^2$$

or

$$\tfrac{1}{4}\pi^2 = \sum_p (2p + 1)^{-2},$$

which is exact.

Therefore, the eigenvalue $\lambda = 0$ is a possible eigenvalue, and a vector $\mathbf{D}$ exists defined by

$$D_{2p} = 0, \quad D_{2p+1} = r/\pi^2(2p + 1), \tag{B12}$$

which annihilates M.

Since the assumption on the absolute convergence of (B1) is gratuitous, there is no guarantee that the order of summations can be permuted in (B4) and (B5), and a solution may exist which is annihilated by M such that the series (B1) does not converge absolutely.

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[1] R. G. Newton, J. Math. Phys. (a) **3**, 75 (1962); (b) **8**, 1566 (1967).
[2] P. C. Sabatier, J. Math. Phys. **7**, 1515, 2079 (1966); **9**, 1241 (1968).
[3] C. Coudray and M. Coz, Ann. Phys. (N.Y.) **61**, 488 (1970).
[4] I. M. Gel'fand and B. M. Levitan, Izv. Akad. Nauk SSSR, Math Ser.,**15**, 309 (1951);L.O. Faddeev J. Math. Phys. **4**, 72 (1963).

[5] T. Regge, Nuovo Cimento **14**, 1951 (1959).
[6] B. M. Levitan, *Generalized Translation Operators* (Israel Program for Scientific Translation, Jerusalem, 1966).
[7] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon, Oxford, 1962).
[8] W. Pauli, Ann. Inst. Henri Poincaré **6**, 109, 137 (1936).
[9] M. Gourdin, *Equation de Dirac* (Office National des Universités et Ecoles Françaises, Paris, 1959); G. Petiau, *Mécanique quantique generale 6* (ACES, Paris, 1960); F. Low, *Symmetries and Elementary Particles* (Gordon and Breach, New York, 1967).
[10] M. C. Barthelemy, Ann. Inst. Henri Poincaré **6**, 365 (1967); **7**, 115 (1969); Compt. Rend. **268**, 521 (1969).
[11] M. G. Gasimov and B. M. Levitan, Dokl. Akad. Nauk SSSR **167**, 967 (1966).
[12] M. C. Barthelemy, Ref. 10, can be consulted for the main properties of the phase shift method applied to the Dirac equation. Her notations are followed as much as possible. (However, x is denoted here λ.)
[13] H. Bethe and E. Salpeter, in *Handbuch der Physik* (Springer-Verlag, Berlin, 1957), Vol. XXXV, p. 151, set W equal to zero and denote F, G, and λ, respectively, by g, $-f$, and $-\lambda$. To obtain Gourdin's notation (Ref. 9) F, G, and λ have to be replaced by v, $-u$, and $-K$, with W again set equal to zero, while Petiau (Ref. 9) replaces λ by X, with W set equal to zero. (See also Ref. 12.)
[14] O. D. Corbella, J. Math. Phys. **11**, 1695 (1970), contains a bibliography of the inverse problem at fixed l.
[15] F. Prats and J. S. Toll, Phys. Rev. **113**, 363 (1959).
[16] P. J. Redmond, J. Math. Phys. **5**, 1547 (1964).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Poincaré-Irreducible Tensor Operators for Positive-Mass One-Particle States.* I

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(Received 7 July 1970)

The main objective of this article is the relativistic generalization of the ordinary $SO(3)$-irreducible spin tensor operators for particles with positive mass. Two classes of relativistic one-particle tensor operators are constructed. The tensor operators of the first class transform according to those representations of the Poincaré group that are induced by the one-valued unitary irreducible representations of the pseudo-unitary group $SU(1, 1)$ which belong to the continuous principal and the discrete principal series. These tensors are operator-valued functions of a spacelike 4-momentum transfer. The tensor operators of the second class correspond to vanishing 4-momentum transfer. They transform according to those representations of the Poincaré group that are induced by the unitary irreducible representations of the pseudo-orthogonal group $SO(3, 1)$ or its universal covering group $SL(2C)$ which belong to the principal series. Both classes of Poincaré-irreducible tensor operators are constructed in a spin helicity basis for timelike 4-momentum by means of projection operators which are continuous linear superpositions of unitary operator realizations for the groups $SU(1, 1)$ and $SL(2C)$. The Clebsch-Gordan coefficients associated with the reduction into the two classes of Poincaré-irreducible tensor operators of a dyadic product of spin-helicity basis vectors are calculated.

I. MOTIVATION AND INTRODUCTION

The usual multipole parametrization of a spin density matrix describing the polarization state of a positive-mass particle constitutes an expansion in terms of tensor operators that transform according to unitary irreducible representations of the three-dimensional rotation group. A covariant multipole parametrization can be carried out in terms of irreducible representations either of the homogeneous or of the inhomogeneous Lorentz group. Since relativistic invariance is equivalent to invariance under the *inhomogeneous* Lorentz group (Poincaré group), the correct relativistic generalization of the ordinary spin tensor operators are tensor operators transforming according to irreducible unitary representations of the (restricted) Poincaré group $ISO(3, 1)$. For the relativistic multipole expansion of a spin density matrix describing the polarization state of a positive-mass particle with sharp momentum, the relativistic multipole parametrization involves the tensor operators transforming according to those unitary irreducible representations of the Poincaré group that are induced by the homogeneous $(3 + 1)$-dimensional (restricted) Lorentz group $SO(3, 1)$. We refer to this class of tensor operators as $ISO(3, 1) \uparrow SO(3, 1)$-irreducible. An expansion into Poincaré-irreducible components of a spin density matrix corresponding to a momentum distribution, however, necessitates the construction of the tensor operators transforming according to the unitary irreducible representations of the Poincaré group that are induced by the $(2 + 1)$-dimensional (restricted) homogeneous Lorentz transformation $SO(2, 1)$. This class of tensor operators is referred to as $ISO(3, 1) \uparrow SO(2, 1)$-irreducible.

The problem of decomposing the one-particle spin-momentum projection operators (dyadics)

$$|p^s_\lambda\rangle\langle p'^{s'}_{\lambda'}|, \quad p = (p^0, \mathbf{p}), \quad s = \text{spin}, \quad \lambda = \text{helicity}, \tag{1.1}$$

[5] T. Regge, Nuovo Cimento **14**, 1951 (1959).
[6] B. M. Levitan, *Generalized Translation Operators* (Israel Program for Scientific Translation, Jerusalem, 1966).
[7] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon, Oxford, 1962).
[8] W. Pauli, Ann. Inst. Henri Poincaré **6**, 109, 137 (1936).
[9] M. Gourdin, *Equation de Dirac* (Office National des Universités et Ecoles Françaises, Paris, 1959); G. Petiau, *Mécanique quantique generale 6* (ACES, Paris, 1960); F. Low, *Symmetries and Elementary Particles* (Gordon and Breach, New York, 1967).
[10] M. C. Barthelemy, Ann. Inst. Henri Poincaré **6**, 365 (1967); **7**, 115 (1969); Compt. Rend. **268**, 521 (1969).
[11] M. G. Gasimov and B. M. Levitan, Dokl. Akad. Nauk SSSR **167**, 967 (1966).
[12] M. C. Barthelemy, Ref. 10, can be consulted for the main properties of the phase shift method applied to the Dirac equation. Her notations are followed as much as possible. (However, x is denoted here λ.)
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[16] P. J. Redmond, J. Math. Phys. **5**, 1547 (1964).

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with $[(p)^2 = (p^0)^2 - (\mathbf{p})^2]$

$$p^2 = p'^2 > 0, \quad \operatorname{sgn} p^0 = \operatorname{sgn} p'^0 = \pm 1, \quad s = 0, \tfrac{1}{2}, 1, \cdots, \tag{1.2}$$

into components that transform by unitary irreducible representations of the proper orthochronous *Poincaré group*, $ISO(3, 1)$, calls into existence two main classes of tensor operators. The two classes correspond to

$$p \neq p', Q^2 < 0, Q = p - p' \tag{1.3}$$

and

$$p = p', Q^2 = 0, Q = p - p' = (0, \mathbf{0}). \tag{1.4}$$

The construction of the Poincaré-irreducible tensor operators for $Q^2 < 0$ and $Q^2 = 0$ is based on certain unitary irreducible representations of the Lorentz groups in three and four dimensions, which are the pseudo-orthogonal groups $SO(2, 1)$ and $SO(3, 1)$. $SO(2, 1)$ is the isotropy group associated with the spacelike 4-vector Q ($Q^2 < 0$), whereas $SO(3, 1)$ is the largest subgroup of $ISO(3, 1)$ that leaves the zero 4-vector ($Q = 0$) invariant. Tensor operators of the class $Q^2 < 0$ have been introduced by Joos[1] for zero spin ($s = 0$).

In this particular case only the irreducible $SO(2, 1)$ representations belonging to the continuous principal series in the classification derived by Bargmann[2] are needed to calculate the Clebsch–Gordan coefficients associated with the decomposition into Poincaré-irreducible components of the dyadics (1.1). For $s \neq 0$, also the irreducible representations of $SO(2, 1)$ that belong to the discrete principal series have to be taken into account. More precisely, the one-valued unitary irreducible representations of the pseudo-unitary group $SU(1, 1)$ are relevant [the homomorphism from $SU(1, 1)$ to $SO(2, 1)$ is two to one].

The Poincaré-irreducible components of a dyadic belonging to the class (1.4), namely the $ISO(3, 1) \uparrow SO(3, 1)$-irreducible tensor operators, transform according to those representations of $ISO(3, 1)$ that are induced by the unitary irreducible representations of $SO(3, 1)$ [or its universal covering group $SL(2C)$] which belong to the principal series.

The entirely different problem of decomposing the projection operator (1.1) into components transforming according to irreducible representations of the *homogeneous Lorentz group* has been solved by Popov[3] by means of an integral transformation introduced by Shapiro[4] and generalized by Chou Kuang-Chao and Zastavenko.[5]

In Sec. 2 we introduce two types of spin-helicity basis vectors for a positive-mass particle. They are eigenvectors of the Pauli–Lubański operators W^0 or W^3.

Section 3 constitutes an outline of the idempotent operator method upon which hinges the construction of the two classes of Poincaré-irreducible tensor operators.

The explicit constructions according to this method of the $ISO(3, 1) \uparrow SO(2, 1)$- and the $ISO(3, 1) \uparrow SO(3, 1)$-irreducible tensor operators are carried out in Secs. 4 and 5, respectively. Both sections contain expressions for the Poincaré Clebsch–Gordan coefficients associated with the reduction of a dyadic (1.1) into either one of the two classes of tensor operators.

2. MOMENTUM-HELICITY STATE VECTORS

An element of the restricted Poincaré transformation

$$(a, \Lambda): x \to \Lambda x + a, \quad x, a \in E_{3,1}, \tag{2.1}$$

can be realized as

$$(a, \Lambda) = \exp(-ia^\mu p_\mu) \exp(-\tfrac{1}{2} i\omega^{\mu\nu} j_{\mu\nu}). \tag{2.2}$$

On the vector space $H[m, s]$ that carries the unitary irreducible $ISO(3, 1)$ representation corresponding to the orbit

$$p^\mu p_\mu = m^2 > 0 \tag{2.3}$$

and to the spin

$$s = 0, \tfrac{1}{2}, 1, \cdots, \tag{2.4}$$

the group generators p_μ and $j_{\mu\nu}$ shall be represented by the Hermitian linear operators P_μ and $J_{\mu\nu}$. The set of eigenvalue equations

$$P^\mu P_\mu |p_\lambda^s\rangle = m^2 |p_\lambda^s\rangle,$$
$$W^\mu W_\mu |p_\lambda^s\rangle = -m^2 s(s+1) |p_\lambda^s\rangle, \tag{2.5a}$$
$$W^\mu \stackrel{\text{DEF}}{=} \tfrac{1}{2}\epsilon^{\mu\nu\rho\sigma} J_{\nu\rho} P_\sigma,$$

$$\epsilon^{\mu\nu\rho\sigma} = \begin{Bmatrix} +1 \\ -1 \end{Bmatrix} \text{ if the permutation } \begin{pmatrix} 1230 \\ \mu\nu\rho\sigma \end{pmatrix} \text{ is } \begin{Bmatrix} \text{even} \\ \text{odd} \end{Bmatrix}, \tag{2.5b}$$

$$P^\mu |p_\lambda^s\rangle = p^\mu |p_\lambda^s\rangle, \tag{2.5c}$$

together with either one of the two eigenvalue equations[6]

$$W^0 |p_\lambda^s; 0\rangle = \lambda \operatorname{sgn} p^0 |\mathbf{p}| |p_\lambda^s; 0\rangle \tag{2.6}$$

or

$$W^3 |p_\lambda^s; 3\rangle = \lambda \operatorname{sgn} p^0 [(p^0)^2 - (p^1)^2 - (p^2)^2]^{\frac{1}{2}} |p_\lambda^s; 3\rangle, \tag{2.7}$$

with

$$\operatorname{sgn} p^0 = \frac{p^0}{|p^0|}, \tag{2.8}$$

defines a basis in $H[m, s]$. Corresponding to the two eigenvalue equations (2.6) and (2.7) for the *helicity* λ, we use two types of momentum–helicity vectors for a particle with positive mass m and spin s in a state characterized by the 4-momentum p and the spin projection along the line of flight λ. To the Poincaré invariant orthogonality relation

$$\Theta^{\pm}(p^0)\delta(p^2 - m^2)\langle p'^{\lambda'}_s \mid p^s_\lambda\rangle = \delta^4(p' - p)\delta^{\lambda'}{}_\lambda, \quad (2.9)$$

where

$$\Theta^{\pm}(p^0) = \tfrac{1}{2}(1 \pm p^0/|p^0|), \quad (2.10)$$

corresponds the completeness relation

$$\sum_{\lambda=-s}^{+s} \int d^4p\Theta^{\pm}(p^0)\delta(p^2 - m^2)\, |p^s_\lambda\rangle\langle p^\lambda_s| = \mathbb{1}, \quad (2.11)$$

where $\mathbb{1}$ is the unit operator on $H[m, s]$.

By virtue of the Dirac normalization (2.9), the momentum–helicity vectors form an improper basis in the Hilbert space $H[m, s]$.[7] As generalized eigenvectors (or eigendistributions) they are elements of a rigged Hilbert space.[8]

In accordance with the relation (2.9) the partial and total trace operations

$$\operatorname{tr}(|p^s_\lambda\rangle\langle p'^{\lambda'}_s|) = \langle p'^{\lambda'}_s \mid p^s_\lambda\rangle = 2\,|p^0|\,\delta^3(\mathbf{p}' - \mathbf{p})\delta^{\lambda'}{}_\lambda \quad (2.12)$$

and

$$\operatorname{Tr}(|p^s_\lambda\rangle\langle p'^{\lambda'}_s|) = \int d^4p\Theta^{\pm}(p^0)\delta(p^2 - m^2)\operatorname{tr}(|p^s_\lambda\rangle\langle p'^{\lambda'}_s| = \delta^{\lambda'}{}_\lambda \quad (2.13)$$

can be defined for the dyadic (1.1).

The momentum–helicity eigenvectors defined by Eqs. (2.5)–(2.7) transform under $(a, \Lambda) \in ISO(3, 1)$ according to the irreducible unitary representations that are characterized by the set of group invariants[9,10] $[p^2 = m^2,\ w^2 = -m^2 s(s + 1),\ \operatorname{sgn} p^0]$. The matrix realization of the transformation (a, Λ) in a momentum–helicity basis can be written as

$$D([m, s, \operatorname{sgn} p^0 = \pm 1](a, \Lambda)) = \sum_{\lambda,\lambda'=-s}^{+s} \int d^4p\Theta^{\pm}(p^0)\delta(p^2 - m^2)\, |\Lambda p^s_{\lambda'}\rangle \times \exp(-ia\cdot\Lambda p) D^s(R(\Lambda, p))^{\lambda'}{}_\lambda \langle p^\lambda_s|, \quad (2.14)$$

where $R(\Lambda, p) \in SO(3)$ is called the Wigner rotation associated with the transformation Λ and the 4-momentum p. This rotation is defined by

$$R(\Lambda, p) = \Omega^{-1}(\Lambda p)\Lambda\Omega(p), \quad (\Lambda p)^\mu = \Lambda^\mu{}_\nu p^\nu, \quad (2.15a)$$

with $\Omega(p)$ denoting the three-parameter Lorentz transformation

$$\Omega(p)^\mu{}_\nu\, {}^\circ p^\nu = p^\mu, \quad {}^\circ p = ({}^\circ p^\mu) = \pm(p^2)^{\frac{1}{2}}(1, 0, 0, 0), \quad p^2 = {}^\circ p^2 = m^2. \quad (2.15b)$$

$\Omega(p)$ is called an orbiting transformation. $D^s(R)$ realizes on the $(2s + 1)$-dimensional subspace $H[s] \subset H[m, s]$ the unitary irreducible representation of $SO(3)$ that is characterized by the group invariant

$$\mathbf{J}^2 = (J_{23})^2 + (J_{31})^2 + (J_{12})^2 = s(s + 1). \quad (2.16)$$

$SO(3)$ is the isotropy group for the timelike standard vector ${}^\circ p$. For the set of the basis vectors

$$\{|{}^\circ p^s_\lambda\rangle : -s \le \lambda \le s\}, \quad (2.17)$$

of $H[s]$, the orthogonality equation (2.9) is replaced by the orthonormality equation

$$\langle {}^\circ p^{\lambda'}_s \mid {}^\circ p^s_\lambda\rangle = 2m\delta^{\lambda'}{}_\lambda. \quad (2.18)$$

Restricted to $H[s]$, the noninvariant eigenvalue equations (2.5c) and (2.6) become

$$P^\mu\, |{}^\circ p^s_\lambda\rangle = \pm\delta^\mu{}_0 m\, |{}^\circ p^s_\lambda\rangle \quad (2.19)$$

and

$$W^0\, |{}^\circ p^s_\lambda\rangle = 0\, |{}^\circ p^s_\lambda\rangle, \quad (2.20)$$

whereas the noninvariant equations (2.7) and (2.8) are equivalent to

$$W^3\, |{}^\circ p^s_\lambda\rangle = \pm m J_{12}\, |{}^\circ p^s_\lambda\rangle = \pm m\lambda\, |{}^\circ p^s_\lambda\rangle. \quad (2.21)$$

Momentum–helicity eigenvectors satisfying the two sets of eigenvalue equations (2.5) and (2.6) or (2.5) and (2.7) can be constructed from the basis vectors (2.17) by means of the orbiting transformations[6]

$$\Omega_0(\phi, \theta, \gamma) = e^{-i\phi j_{12}} e^{-i\theta j_{31}} e^{-i\gamma j_{03}} \quad (2.22)$$

or

$$\Omega_3(\phi, \alpha, \zeta) = e^{-i\phi j_{12}} e^{-i\alpha j_{01}} e^{-i\zeta j_{03}}, \quad (2.23)$$

with the parameter domains

$$0 \le \phi < 2\pi, \quad 0 \le \theta \le \pi, \quad 0 \le \gamma < \infty, \quad 0 \le \alpha < \infty, \quad -\infty < \zeta < \infty. \quad (2.24)$$

From these orbiting transformations result the parametrizations (A6) and (A7). The constructs

$$|p^s_\lambda; 0\rangle \stackrel{\text{DEF}}{=} T(\Omega_0)\, |{}^\circ p^s_\lambda\rangle = e^{-i\phi J_{12}} e^{-i\theta J_{31}} e^{-i\gamma J_{03}}\, |{}^\circ p^s_\lambda\rangle, \quad (2.25)$$

$$|p^s_\lambda; 3\rangle \stackrel{\text{DEF}}{=} T(\Omega_3)\, |{}^\circ p^s_\lambda\rangle = e^{-i\phi J_{12}} e^{-i\alpha J_{01}} e^{-i\zeta J_{03}}\, |{}^\circ p^s_\lambda\rangle \quad (2.26)$$

are representatives of the three types of momentum–helicity eigenvectors. This is an immediate consequence of the commutation relations [see Ref. 6, Eqs. (2.75)]

$$W^0 T(\Omega_0(\phi, \theta, \gamma)) = T(\Omega_0(\phi, \theta, \gamma)) \times (W^0 \cosh\gamma - W^3 \sinh\gamma), \quad (2.27)$$

$$W^3 T(\Omega_3(\phi, \alpha, \zeta)) = T(\Omega_3(\phi, \alpha, \zeta)) \times (W^3 \cosh\zeta - W^0 \sinh\zeta). \quad (2.28)$$

The momentum–helicity eigenvectors (2.25) and (2.26) are related through the transformation (A18).

3. PRELIMINARIES ABOUT THE CONSTRUCTION OF POINCARÉ-IRREDUCIBLE TENSOR OPERATORS

The dyadic (1.1) transforms under the $ISO(3, 1)$ by the product representation

$$[p^2 = m^2, s, \operatorname{sgn} p^0 = \pm 1] \otimes [p'^2 = m^2, s, \operatorname{sgn} p'^0 = \pm 1]^\dagger. \quad (3.1)$$

The unitary irreducible representations $D[ISO(3, 1)]$ into which the product (3.1) can be decomposed fall into two classes. These are the classes induced by the unitary irreducible representations of $SO(2, 1)$ and $SO(3, 1)$, which are respectively the isotropy groups associated with a spacelike and a zero 4-momentum transfer $Q = p - p'$. The two classes will be denoted by

$$D[ISO(3, 1)] \uparrow D[SO(2, 1)], \quad Q^2 < 0, \quad (3.2)$$

and

$$D[ISO(3, 1)] \uparrow D[SO(3, 1)], \quad Q = 0. \quad (3.3)$$

The set of dyadics

$$\{|p_\lambda^s\rangle\langle p'^{\lambda'}_s| : p^2 = p'^2 = m^2, \operatorname{sgn} p^0 = \operatorname{sgn} p'^0; -s \le \lambda, \lambda' \le s\} \quad (3.4)$$

is a basis of the tensor product

$$H[m, s] \otimes H^\dagger[m, s]. \quad (3.5)$$

The complete set of irreducible tensor operators to be constructed consists of those linear combinations of the dyadics in the set (3.4) that span the irreducible vector spaces $H[Q^2, \tau]$ into which the tensor product (3.5) can be decomposed. Symbolically,

$$H[m, s] \otimes H^\dagger[m, s] = \int^{\oplus} d\mu[Q^2] \int d\mu[\tau] H[Q^2, \tau]. \quad (3.6)$$

If the measure $\mu[\tau]$ is finite, the direct integral in the decomposition (3.6) reduces to a direct sum. τ denotes the set of group invariants for $SO(2, 1)$ or $SO(3, 1)$ that characterize the unitary irreducible representation $D[SO(2, 1)]$ or $D[SO(3, 1)]$. Together with the invariant Q^2, τ therefore characterizes the induced representations (3.2) or (3.3).

An irreducible orthogonal basis in $H[Q^2, \tau]$ can be constructed by means of the projection operators[11]

$$P[\tau]^{n'}{}_n = N \int d\mu(g) D^\dagger([\tau]g)^{n'}{}_n T(g). \quad (3.7)$$

$\mu(g)$ is the invariant Haar measure on $SO(2, 1)$ or $SO(3, 1)$. $D([\tau]g)^{n'}{}_n$ is the matrix realization of the unitary linear operator $T([\tau]g)$ that represents the group element $g \in SO(2, 1)$ or $g \in SO(3, 1)$ on the carrier space $H[\tau]$ of the irreducible representations $D[SO(2, 1)]$ or $D[SO(3, 1)]$. Finally, $T(g)$ denotes a unitary linear operator representing g on the particular, generally reducible, subspace of $H[m, s] \otimes H^\dagger[m, s]$ that is spanned by the subset of the basis (3.4) for which $p - p' = (0, 0, 0, (-Q^2)^{\frac{1}{2}})$ or $p - p' = 0$. The matrix realizations of the unitary operators $T([\tau]g)$ on the irreducible spaces $H[\tau]$ fulfill the orthogonality and completeness relations[6]:

$$\int d\mu(g) D^*([\tau']g)^{n_1'}{}_{n_2'} D([\tau]g)^{n_1}{}_{n_2} = \frac{1}{\rho[\tau]} \delta(\tau', \tau) \delta_{n_1' n_1} \delta_{n_2' n_2}, \quad (3.8)$$

$$\sum_{n_1 n_2} \int d\mu[\tau] D([\tau]g)^{n_1}{}_{n_2} D^*([\tau]g')^{n_1}{}_{n_2} = \frac{1}{\rho(g)} \delta(g - g'),$$

$$d\mu(g) = \rho(g)\, dg, \quad d\mu[\tau] = \rho[\tau]\, d\tau. \quad (3.9)$$

$\mu[\tau]$ denotes the Plancherel measure on the Borel structure of the group invariant τ. Depending on whether the set τ is continuous or discrete, $\delta(\tau', \tau)$ symbolizes Dirac distributions or Kronecker deltas. If the density function $\rho[\tau]$ replaces the normalization factor N in the definition (3.7),

$$N = \rho[\tau], \quad (3.10)$$

the property

$$P[\tau_1]^{n_1'}{}_{n_1} P[\tau_2]^{n_2'}{}_{n_2} = \delta(\tau_1, \tau_2) \delta^{n_1'}{}_{n_2} P[\tau_2]^{n_2'}{}_{n_1} \quad (3.11)$$

is a consequence of the orthogonality relation (3.8) and the invariance of the Haar measure $\mu(g)$. Equation (3.10) implies that the operators (3.7) are idempotent. From the invariance of $\mu(g)$ it is immediate that

$$T(g) P[\tau]^{n'}{}_n = \sum_m P[\tau]^{n'}{}_m D([\tau]g)^m{}_n. \quad (3.12)$$

This property enables the operators (3.7) to project out of a given dyadic (1.1) those components that transform irreducibly under $ISO(3, 1)$, and which therefore constitute an (improper) basis for $H[Q^2, \tau]$.

4. $ISO(3, 1) \uparrow SO(2, 1)$-IRREDUCIBLE TENSOR OPERATORS

According to Bargmann,[2] all the unitary irreducible representations of $SO(2, 1)$ that are the one-valued unitary irreducible representations of $SU(1, 1)$ can be realized by the matrices[6,12,13]

$$D([\tau], g)^{\lambda'}{}_\lambda = D^\tau(\phi, \alpha, \psi)^{\lambda'}{}_\lambda = \langle \tau\lambda'| e^{-i\phi J_{12}} e^{-i\alpha J_{01}} e^{-i\psi J_{12}} |\tau\lambda\rangle,$$

$$J_{12} |\tau\lambda\rangle = \lambda |\tau\lambda\rangle, \quad 0 \le \phi, \psi < 2\pi, \quad 0 \le \alpha < \infty,$$

$$D([\tau], g)^{\lambda'}{}_\lambda = e^{-i\phi\lambda'} d^\tau(\alpha)^{\lambda'}{}_\lambda e^{-i\psi\lambda}, \quad (4.1)$$

where we have the following:

(a) $\tau = (\epsilon, l)$: $l = -\frac{1}{2} + i\sigma, \quad -\infty < \sigma < \infty;$

$\epsilon = 0$: $\lambda = 0, \pm 1, \pm 2, \cdots;$

$\epsilon = \frac{1}{2}$: $\lambda = \pm\frac{1}{2}, \pm\frac{3}{2}, \cdots;$

$$d^{-\frac{1}{2}-i\sigma}(\alpha)^{\lambda'}{}_{\lambda} = d^{-\frac{1}{2}+i\sigma}(\alpha)^{\lambda'}{}_{\lambda},$$

$$d^{-\frac{1}{2}+i\sigma}(\alpha)^{\lambda'}{}_{\lambda} = d^{-\frac{1}{2}+i\sigma}(\alpha)^{-\lambda}{}_{-\lambda'} = (-1)^{\lambda'-\lambda} d^{-\frac{1}{2}+i\sigma}(\alpha)^{\lambda}{}_{\lambda'};$$

(b) $\tau = k^{\pm}$: $k = \frac{1}{2}, 1, \frac{3}{2}, \cdots;$ (4.2)

k^{+}: $\lambda = k, k+1, k+2, \cdots;$

k^{-}: $\lambda = -k, -(k+1), -(k+2), \cdots;$

$$d^{k-}(\alpha)^{\lambda'}{}_{\lambda} = d^{k+}(\alpha)^{-\lambda}{}_{-\lambda'};$$

$$d^{k+}(\alpha)^{\lambda'}{}_{\lambda} = (-1)^{\lambda'-\lambda} d^{k+}(\alpha)^{\lambda}{}_{\lambda'},$$

(c) $\tau = l$: $-\frac{1}{2} < l < 0, \quad \lambda = 0, \pm 1, \pm 2, \cdots;$

(d) $\tau = l = 0, \quad \lambda = 0.$

The representation classes (a), (b), (c), and (d) are called the principal continous series, the principal discrete series, the supplementary series, and the trivial or scalar representation, respectively. The functions $d^{\tau}(\alpha)^{\lambda'}{}_{\lambda}$ are real. Their symmetry properties (4.2a) and (4.2b) correspond to those given in Eqs. (4.32) and (4.33) of Ref. 6.

For the matrix realizations (4.1), the orthogonality and completeness relations (3.8) and (3.9) are[6]

$$\frac{1}{8\pi^2}\int_0^{2\pi} d\phi \int_0^{\infty} \sinh\alpha\, d\alpha \times \int_0^{2\pi} d\psi D^{-\frac{1}{2}+i\sigma'}(\phi,\alpha,\psi)^{*\lambda'}{}_{\mu'} D^{-\frac{1}{2}+i\sigma}(\phi,\alpha,\psi)^{\lambda}{}_{\mu} = i^{-1}\sigma^{-1}\tan\pi(i\sigma - \tfrac{1}{2} - \epsilon)\delta(\sigma'-\sigma)\delta^{\lambda'\lambda}\delta_{\mu'\mu}, \quad (4.3a)$$

$$\frac{1}{8\pi^2}\int_0^{2\pi} d\phi \int_0^{\infty} \sinh\alpha\, d\alpha \times \int_0^{2\pi} d\psi D^{k'\pm}(\phi,\alpha,\psi)^{*\lambda'}{}_{\mu'} D^{k\pm}(\phi,\alpha,\psi)^{\lambda}{}_{\mu} = (2k-1)^{-1}\delta_{k'k}\delta^{\lambda'\lambda}\delta_{\mu'\mu}, \quad k > \tfrac{1}{2} \quad (4.3b)$$

$$\sum_{\lambda,\lambda'=-\infty}^{\infty} i\int_{-\infty}^{\infty} \sigma\, d\sigma \cot\pi(i\sigma - \tfrac{1}{2} - \epsilon) \times D^{-\frac{1}{2}+i\sigma}(\phi,\alpha,\psi)^{\lambda'}{}_{\lambda} D^{-\frac{1}{2}+i\sigma}(\phi',\alpha',\psi')^{*\lambda'}{}_{\lambda} + \sum_{\eta=+,-}\sum_{k=1+\epsilon}^{\infty}(2k-1) \times \sum_{\mu,\mu'=\eta n}\sum_{n=k}^{\infty} D^{k,\eta}(\phi,\alpha,\psi)^{\mu'}{}_{\mu} D^{k,\eta}(\phi',\alpha',\psi')^{*\mu'}{}_{\mu} = 8\pi^2\delta(\phi-\phi')\delta(\cosh\alpha - \cosh\alpha')\delta(\psi-\psi'). \quad (4.4)$$

The matrix realizations corresponding to the representation classes (c), (d) and to the representation $k = \frac{1}{2}$ of class (b) do not appear in the above relations since the associated Plancherel measures vanish.[2]

The idempotent operators (3.7), (3.10) for the classes (a) and (b) are therefore

$$P[\epsilon,\sigma]^{\lambda'}{}_{\lambda} = i\cot\pi(i\sigma - \tfrac{1}{2} - \epsilon)\frac{\sigma}{8\pi^2} \times \int_0^{2\pi} d\phi \int_0^{\infty}\sinh\alpha\, d\alpha \times \int_0^{2\pi} d\psi D^{-\frac{1}{2}+i\sigma}(\phi,\alpha,\psi)^{\dagger\lambda'}{}_{\lambda} T(\phi,\alpha,\psi) \quad (4.5)$$

and

$$P[k^{\pm}]^{\lambda'}{}_{\lambda} = \frac{2k-1}{8\pi^2}\int_0^{2\pi} d\phi \int_0^{\infty}\sinh\alpha\, d\alpha \times \int_0^{2\pi} d\psi D^{k\pm}(\phi,\alpha,\psi)^{\dagger\lambda'}{}_{\lambda} T(\phi,\alpha,\psi), \quad (4.6)$$

with

$$T(\phi,\alpha,\psi) = e^{-i\phi J_{12}} e^{-i\alpha J_{01}} e^{-i\psi J_{12}}. \quad (4.7)$$

The transformation relations corresponding to (3.12), namely

$$T(\phi,\alpha,\psi)P[\epsilon,\sigma]^{\lambda'}{}_{\lambda} = P[\epsilon,\sigma]^{\lambda'}{}_{\mu} D^{-\frac{1}{2}+i\sigma}(\phi,\alpha,\psi)^{\mu}{}_{\lambda} \quad (4.8)$$

(repeated indices which are eigenvalues of the angular momentum operator J_{12} are summed over)

and

$$T(\phi,\alpha,\psi)P[k^{\pm}]^{\lambda'}{}_{\lambda} = P[k^{\pm}]^{\lambda'}{}_{\mu} D^{k\pm}(\phi,\alpha,\psi)^{\mu}{}_{\lambda}, \quad (4.9)$$

ensure that the operators (which act on $H[m,s]$)

$$({}^\circ Q,\sigma)^{\tilde{\kappa}}{}_{\kappa} = P[\epsilon = 0,\sigma]^{\tilde{\kappa}}{}_{\kappa}\, |q^{s}_{\nu}\rangle\langle q'^{\nu'}_{s}| \quad (4.10)$$

and

$$({}^\circ Q,k^{\pm})^{\tilde{\kappa}}{}_{\kappa} = P[k^{\pm}]^{\tilde{\kappa}}{}_{\kappa}\, |q^{s}_{\nu}\rangle\langle q'^{\nu'}_{s}|, \quad (4.11)$$

where

$$q = (q^0,0,0,q^3), \quad q' = (q^0,0,0,-q^3), \quad {}^\circ Q = (0,0,0,(-Q^2)^{\frac{1}{2}}), \quad (4.12)$$

transform under $ISO(3,1)$ by the unitary irreducible representations (3, 2). Since

$$T(\phi,\alpha,\psi)\,|q^{s}_{\nu}\rangle\langle q'^{\nu'}_{s}| = T(\phi,\alpha,0)e^{-i\psi(\nu-\nu')}\,|q^{s}_{\nu}\rangle\langle q'^{\nu'}_{s}|, \quad (4.13)$$

the integrations with respect to the angular parameter ψ in the projections (4.10) and (4.11) imply that

$$\tilde{\kappa} = \nu - \nu'; \quad (4.14)$$

$\tilde{\kappa}$ is obviously an integer, which justifies the restriction to the case $\epsilon = 0$ in (4.10). The first of the eigenvalue equations

$$(P^{\mu}, W^0)\begin{Bmatrix}({}^\circ Q,\sigma)^{\tilde{\kappa}}{}_{\kappa}\\ ({}^\circ Q,k^{\pm})^{\tilde{\kappa}}{}_{\kappa}\end{Bmatrix} = (-Q^2)^{\frac{1}{2}}(\delta^{\mu}{}_{3},\kappa)\begin{Bmatrix}({}^\circ Q,\sigma)^{\tilde{\kappa}}{}_{\kappa}\\ ({}^\circ Q,k^{\pm})^{\tilde{\kappa}}{}_{\kappa}\end{Bmatrix} \quad (4.15)$$

follows from the commutation relations

$$[J^{\mu\nu}, P^\sigma] = i(g^{\nu\sigma}P^\mu - g^{\mu\sigma}P^\nu),$$

and the second results from the restriction of the isotropy group generators

$$W^\mu = \tfrac{1}{2}\epsilon^\mu{}_{\nu\rho\sigma}J^{\nu\rho}P^\sigma$$

to the standard spacelike 4-momentum $^\circ Q = (0, 0, 0, (Q^2))^{\frac{1}{2}}$:

$$W^\mu(^\circ Q) = \tfrac{1}{2}\epsilon^\mu{}_{\nu\rho\sigma}J^{\nu\rho}\,{}^\circ Q^\sigma = (-Q^2)^{\frac{1}{2}}(J_{12}, J_{20}, J_{01}, 0), \tag{4.16}$$

in conjunction with the transformation properties (4.8) and (4.9). From the definition (2.12) of the partial trace and the orthogonality relations (4.3a), (4.3b) follows:

$$\begin{aligned}\operatorname{tr}\,&[(^\circ Q, \sigma)^{\tilde\kappa}{}_\kappa(^\circ Q', \sigma')^{\dagger\tilde\kappa'}{}_{\kappa'}]\\ &= \frac{2}{\pi}\,\sigma\tanh\pi\sigma\left(\frac{-Q^2}{4m^2 - Q^2}\right)^{\frac{1}{2}}\\ &\quad\times\delta^4(^\circ Q - {}^\circ Q')\delta(\sigma - \sigma')\delta_{\kappa\kappa'}\delta^{\tilde\kappa\tilde\kappa'},\end{aligned} \tag{4.17}$$

$$\begin{aligned}\operatorname{tr}\,&[(^\circ Q, k^\pm)^{\tilde\kappa}{}_\kappa(^\circ Q', k'^\pm)^{\dagger\tilde\kappa'}{}_{\kappa'}]\\ &= \frac{2}{\pi}(2k - 1)\left(\frac{-Q^2}{4m^2 - Q^2}\right)^{\frac{1}{2}}\\ &\quad\times\delta^4(^\circ Q - {}^\circ Q')\delta(\sigma - \sigma')\delta_{\kappa\kappa'}\delta^{\tilde\kappa\tilde\kappa'}.\end{aligned} \tag{4.18}$$

The derivation of (4.17) and (4.18) hinges on the easily established relation

$$\begin{aligned}2\,&|p_1^0|\,2\,|p_2^0|\,\delta^3(\mathbf{p}_1' - \mathbf{p}_1)\delta^3(\mathbf{p}_2' - \mathbf{p}_2)\\ &= 8\left(\frac{-Q^2}{4m^2 - Q^2}\right)^{\frac{1}{2}}\\ &\quad\times\delta^4(Q' - Q)\delta(\cosh\alpha' - \cosh\alpha)\delta(\phi' - \phi),\end{aligned} \tag{4.19}$$

with the parametrization (A7) for p_1 and p_2 and with $Q = p_1 - p_2$, $p_1^2 = p_2^2 = m^2$.

Let $\Omega(Q)$ denote an orbiting transformation such that

$$\Omega(Q)^\mu{}_3 = [-Q^2]^{-\frac{1}{2}}Q^\mu, \tag{4.20}$$

and let $T(\Omega(Q))$ denote its operator representative on the invariant subspaces

$$H[Q^2, \sigma, \epsilon = 0] \subset H[m, s] \otimes H^\dagger[m, s] \tag{4.21}$$

and

$$H[Q^2, k^\pm] \subset H[m, s] \otimes H^\dagger[m, s]. \tag{4.22}$$

Let Ω_0 and Ω_3 denote the specific orbiting transformations defined by the identities (2.22), and (2.23). Their representatives $T(\Omega_0(Q))$ and $T(\Omega_3(Q))$ then satisfy respectively the commutation relations (2.27) and (2.28) and the transforms of the operators (4.10) and (4.11)

$$(Q, \sigma; \omega)^{\tilde\kappa}{}_\kappa \overset{\text{DEF}}{=} T(\Omega_\omega(Q))(^\circ Q, \sigma)^{\tilde\kappa}{}_\kappa, \quad \omega = 0, 3, \tag{4.23}$$

and

$$(Q, k^\pm; \omega)^{\tilde\kappa}{}_\kappa \overset{\text{DEF}}{=} T(\Omega_\omega(Q))(^\circ Q, k^\pm)^{\tilde\kappa}{}_\kappa, \quad \omega = 0, 3, \tag{4.24}$$

satisfy as vectors of the invariant subspaces (4.21) and (4.22) the eigenvalue equations

$$(P^\mu, P^\mu P_\mu)\begin{Bmatrix}(Q, \sigma; \omega)^{\tilde\kappa}{}_\kappa\\ (Q, k^\pm; \omega)^{\tilde\kappa}{}_\kappa\end{Bmatrix} = (Q^\mu, Q^2)\begin{Bmatrix}(Q, \sigma; \omega)^{\tilde\kappa}{}_\kappa\\ (Q, k^\pm; \omega)^{\tilde\kappa}{}_\kappa\end{Bmatrix}, \tag{4.25}$$

$$W^\mu W_\mu\begin{Bmatrix}(Q, \sigma; \omega)^{\tilde\kappa}{}_\kappa\\ (Q, k^\pm; \omega)^{\tilde\kappa}{}_\kappa\end{Bmatrix} = Q^2\begin{Bmatrix}(\sigma^2 + \frac{1}{4})\ \ (Q, \sigma; \omega)^{\tilde\kappa}{}_\kappa\\ k(1 - k)\ (Q, k^\pm; \omega)^{\tilde\kappa}{}_\kappa\end{Bmatrix}, \tag{4.26}$$

$$W^0\begin{Bmatrix}(Q, \sigma; 0)^{\tilde\kappa}{}_\kappa\\ (Q, k^\pm; 0)^{\tilde\kappa}{}_\kappa\end{Bmatrix} = \kappa\,|\mathbf{Q}|\begin{Bmatrix}(Q, \sigma; 0)^{\tilde\kappa}{}_\kappa\\ (Q, k^\pm; 0)^{\tilde\kappa}{}_\kappa\end{Bmatrix}, \tag{4.27}$$

$$\begin{aligned}W^3\begin{Bmatrix}(Q, \sigma; 3)^{\tilde\kappa}{}_\kappa\\ (Q, k^\pm; 3)^{\tilde\kappa}{}_\kappa\end{Bmatrix} &= \kappa[(Q^0)^2 - (Q^1)^2 - (Q^2)^2]^{\frac{1}{2}}\\ &\quad\times\begin{Bmatrix}(Q, \sigma; 3)^{\tilde\kappa}{}_\kappa\\ (Q, k^\pm; 3)^{\tilde\kappa}{}_\kappa\end{Bmatrix}.\end{aligned} \tag{4.28}$$

Let $D(a, \Lambda[Q^2, \sigma, \epsilon])$ and $D(a, \Lambda[Q^2, k^\pm])$ denote the unitary linear operators that irreducibly represent the Poincaré transformation (a, Λ) on the spaces (4.21) and (4.22). The relations (4.8) and (4.9), together with the 4-momentum eigenvalue equation in (4.25) then entail the transformation relations

$$\begin{aligned}D(a, \Lambda\,&[Q^2, \sigma, \epsilon = 0])(Q, \sigma; \omega)^{\tilde\kappa}{}_\kappa\\ &= \exp(-ia\cdot\Lambda Q)(\Lambda Q, \sigma; \omega)^{\tilde\kappa}{}_{\kappa'}D^{-\frac{1}{2}+i\sigma}(L_\omega(\Lambda, Q))^{\kappa'}{}_\kappa\end{aligned} \tag{4.29}$$

and

$$\begin{aligned}D(a, \Lambda&[Q^2, k^\pm])(Q, k^\pm, \omega)^{\tilde\kappa}{}_\kappa\\ &= \exp(-ia\cdot\Lambda Q)(\Lambda Q, k^\pm; \omega)^{\tilde\kappa}{}_{\kappa''}D^{k^\pm}(L_\omega(\Lambda, Q))^{\kappa''}{}_\kappa,\end{aligned} \tag{4.30}$$

where

$$L_\omega(\Lambda, Q) = \Omega_\omega^{-1}(\Lambda Q)\Lambda\Omega_\omega(Q), \quad L_\omega(\Lambda, Q) \in SO(2, 1),$$
$$(\Lambda Q)^\mu = \Lambda^\mu{}_\nu Q^\nu. \tag{4.31}$$

According to (4.2), the summations on κ' and κ'' extend over the domains

$$[\sigma, \epsilon = 0]\colon \kappa' = 0, \pm 1, \pm 2, \cdots, \tag{4.32}$$

$$[k^+]\colon \kappa'' = k, k + 1, k + 2, \cdots, \quad \text{if } \tilde\kappa > 0, \tag{4.33}$$

$$[k^-]\colon \kappa'' = -k, -(k + 1), -(k + 2), \cdots, \quad \text{if } \tilde\kappa < 0. \tag{4.34}$$

With the two orbiting transformations Ω_ω, Eqs. (4.20) define the parametrizations (A10) and (A11) (Appendix). The transformation relations (A22) and (A23) state the connections between the two types ($\omega = 0$) and ($\omega = 3$) of the tensor operators defined by Eqs. (4.23) or (4.24). For the standard irreducible tensor operators (4.10) and (4.11), the relations (4.29), (4.30), and (4.31) are replaced by

$$D(a, \Lambda[Q^2, \sigma])(°Q, \sigma)^{\tilde{\kappa}}{}_{\kappa} = \exp(-ia\cdot\Lambda\,°Q)(\Lambda\,°Q, \sigma; \omega)^{\tilde{\kappa}}{}_{\kappa'} D^{-\frac{1}{2}+i\sigma}(L_\omega(\Lambda, °Q))^{\kappa'}{}_{\kappa}, \tag{4.29'}$$

$$D(a, \Lambda[Q^2, k^\pm])(°Q, k^\pm)^{\tilde{\kappa}}{}_{\kappa} = \exp(-ia\cdot\Lambda\,°Q)(\Lambda\,°Q, k^\pm; \omega)^{\tilde{\kappa}}{}_{\kappa''} D^{k^\pm}(L_\omega(\Lambda, °Q))^{\kappa''}{}_{\kappa}, \tag{4.30'}$$

and

$$L_\omega(\Lambda, °Q) = \Omega_\omega^{-1}(\Lambda\,°Q)\Lambda, \quad (\Lambda\,°Q)^\mu = \Lambda^\mu{}_3(-Q^2)^{\frac{1}{2}}, \tag{4.31'}$$

where ω is now determined by the parametrization of the Lorentz transformation Λ.

By virtue of the relations (2.26), (4.7), (4.13), (4.14), the definitions (4.10) and (4.11) are equivalent to

$$(°Q, \sigma)^{\nu-\nu'}{}_{\kappa} = \frac{\sigma}{4\pi}\tanh\pi\sigma\int_0^{2\pi}d\phi\int_0^\infty \sinh\alpha\, d\alpha \times D^{-\frac{1}{2}+i\sigma}(\phi, \alpha, 0)^{\dagger\nu-\nu'}{}_{\kappa}\,|p^s_\nu; 3\rangle\langle\tilde{p}^{\nu'}_s; 3|,$$

$$(°Q, k^\pm)^{\nu-\nu'}{}_{\kappa} = \frac{2k-1}{4\pi}\int_0^{2\pi}d\phi\int_0^\infty \sinh\alpha\, d\alpha \times D^{k^\pm}(\phi, \alpha, 0)^{\dagger\nu-\nu'}{}_{\kappa}\,|p^s_\nu; 3\rangle\langle\tilde{p}^{\nu'}_s; 3|, \tag{4.35}$$

where

$$\tilde{p}^0 = p^0, \quad \tilde{p}^1 = p^1, \quad \tilde{p}^2 = p^2, \quad \tilde{p}^3 = -p^3. \tag{4.36}$$

The definitions (4.23) and (4.24) of the general $ISO(3, 1) \uparrow SO(2, 1)$-irreducible tensor operators can therefore be replaced by the expressions

$$(Q, \sigma; \omega)^{\nu-\nu'}{}_{\kappa} = \frac{\sigma}{4\pi}\tanh\pi\sigma\int_0^{2\pi}d\phi\int_0^\infty \sinh\alpha\, d\alpha \times D^{-\frac{1}{2}+i\sigma}(\phi, \alpha, 0)^{\dagger\nu-\nu'}{}_{\kappa}\,|p^s_\lambda; 3\rangle \times D^s[R(p, \Omega_\omega(Q))]^\lambda{}_\nu \times D^s[R(p', \Omega_\omega(Q))]^{\dagger\nu'}{}_{\lambda'}\langle p'^{\lambda'}_s; 3|, \tag{4.37}$$

$$(Q, k^\pm; \omega)^{\nu-\nu'}{}_{\kappa} = \frac{2k-1}{4\pi}\int_0^{2\pi}d\phi\int_0^\infty \sinh\alpha\, d\alpha \times D^{k^\pm}(\phi, \alpha, 0)^{\dagger\nu-\nu'}{}_{\kappa}\,|p^s_\lambda; 3\rangle \times D^s[R(p, \Omega_\omega(Q))]^\lambda{}_\nu \times D^s[R(p', \Omega_\omega(Q))]^{\dagger\nu'}{}_{\lambda'}\langle p'^{\lambda'}_s; 3|. \tag{4.38}$$

The Euler angles determining the Wigner rotation $R(p, \Omega_\omega(Q))$ can be obtained from the matrix equation [see Eq. (2.15a), Ref. 14]

$$R(p, \Omega_\omega(Q)) = \Omega_3^{-1}(p)\Omega_\omega(Q)\Omega_3(\Omega_\omega^{-1}(Q)p). \tag{4.39}$$

The Hermitian conjugates of the tensor operators (4.23) and (4.24) can be expressed as

$$(Q, \sigma; \omega)^{\dagger\tilde{\kappa}}{}_{\kappa} = (-1)^{\tilde{\kappa}-\kappa}(Q, \sigma; \omega)^{-\tilde{\kappa}}{}_{-\kappa} \tag{4.40}$$

and

$$(Q, k^\pm; \omega)^{\dagger\tilde{\kappa}}{}_{\kappa} = (-1)^{\tilde{\kappa}-\kappa}(Q, k^\mp; \omega)^{-\tilde{\kappa}}{}_{-\kappa}. \tag{4.41}$$

These relations are immediate consequences of the index symmetries for the functions $d^\tau(\alpha)^{\lambda'}{}_\lambda$, which are given in (4.2).

From Eqs. (4.3a), (4.3b), and (4.4) it follows that the renormalized tensor operators

$$(Q, \sigma; \omega; \tilde{\kappa})_\kappa = (4\pi/\sigma\tanh\pi\sigma)^{\frac{1}{2}}(Q, \sigma; \omega)^{\tilde{\kappa}}{}_{\kappa} \tag{4.42}$$

and

$$(Q, k^\pm; \omega; \tilde{\kappa})_\kappa = [4\pi/(2k-1)]^{\frac{1}{2}}(Q, k^\pm; \omega)^{\tilde{\kappa}}{}_{\kappa} \tag{4.43}$$

satisfy the completeness and orthogonality relations

$$\sum_{\kappa=0,\pm1,\pm2,\cdots}\int_{-\infty}^\infty d\sigma(Q', \sigma; \omega; \tilde{\kappa}')_\kappa(Q, \sigma; \omega; \tilde{\kappa})^\dagger{}_\kappa + \sum_{k=1}^{|\tilde{\kappa}|}\sum_{\kappa_1=\eta k, \eta(k+1),\cdots}(Q', k\eta; \omega; \tilde{\kappa}')_{\kappa_1}(Q, k\eta; \omega; \tilde{\kappa})^{\dagger\kappa_1} = 8[-Q^2/(4m^2-Q^2)]^{\frac{1}{2}}\delta^4(Q'-Q)\delta_{\tilde{\kappa}'}{}^{\tilde{\kappa}},$$
$$\tilde{\kappa} = \nu - \nu', \quad \eta = \operatorname{sgn}\tilde{\kappa}, \tag{4.44}$$

and

$$\operatorname{tr}[(Q, \sigma; \omega; \tilde{\kappa})_\kappa(Q', \sigma'; \omega; \tilde{\kappa}')^\dagger{}_{\kappa'}] = 8[-Q^2/(4m^2-Q^2)]^{\frac{1}{2}}\delta^4(Q-Q')\delta(\sigma-\sigma')\delta_\kappa{}^{\kappa'}\delta_{\tilde{\kappa}}{}^{\tilde{\kappa}'}, \tag{4.45}$$

$$\operatorname{tr}[(Q, k\eta; \omega; \tilde{\kappa})_\kappa(Q', k'\eta'; \tilde{\kappa}')^\dagger{}_{\kappa'}] = 8[-Q^2/(4m^2-Q^2)]^{\frac{1}{2}}\delta^4(Q-Q')\delta_{kk'}\delta_{\eta\eta'}\delta_\kappa{}^{\kappa'}\delta_{\tilde{\kappa}}{}^{\tilde{\kappa}'}. \tag{4.46}$$

By virtue of the relations (4.44)–(4.46), the decomposition of the spin-momentum operator

$$\rho([ms]p, p'; \omega) = \sum_{\lambda,\lambda'=-s}^{s}|p^s_\lambda; \omega\rangle\, a(p, p')^\lambda{}_{\lambda'}\langle p^{\lambda'}_s; \omega|$$
$$p^2 = p'^2 = m^2 > 0, \quad \operatorname{sgn}p^0 = \operatorname{sgn}p'^0 = \pm1, \quad (p-p') < 0 \tag{4.47}$$

[which is identical with the dyadic (1.1) if $a^\lambda{}_{\lambda'} = \delta^\lambda{}_{\lambda'}$], into its Poincaré-irreducible components can be written as

$$\rho([ms]p, p'; \omega) = \frac{1}{8}\left(\frac{4m^2 - Q^2}{-Q^2}\right)^{\frac{1}{2}} \sum_{\tilde{\kappa}\geq -2s}^{\tilde{\kappa}\leq 2s} \int d^4Q \left(\int_{-\infty}^{\infty} d\sigma \sum_{\kappa=0,\pm1,\pm2,\cdots} (Q, \sigma; \omega'; \tilde{\kappa})_\kappa \operatorname{tr}[(Q, \sigma; \omega'; \tilde{\kappa})^{\dagger}{}_{\kappa}\rho([ms]p, p'; \omega)] \right.$$
$$\left. + (1 - \delta_{\tilde{\kappa}0}) \sum_{k=1}^{|\tilde{\kappa}|} \sum_{\eta=\operatorname{sgn}\tilde{\kappa}} \sum_{\kappa_1=\eta n} \sum_{n=k}^{\infty} (Q, k\eta; \omega'; \tilde{\kappa})_{\kappa_1} \operatorname{tr}[(Q, k\eta; \omega'; \tilde{\kappa})^{\dagger}_{\kappa_1}\rho([ms]p, p'; \omega)] \right). \quad (4.48)$$

The evaluation of the traces is based on the definition (2.12), the helicity rearrangement transformations discussed in the Appendix, the relations (4.8), (4.9), (4.37), (4.38), and the invariance of the volume element in the space of the $SO(2, 1)$ group parameters (ϕ, α, ψ) (invariance of the Haar measure):

$$\operatorname{tr}[(Q, \sigma; \omega'; \tilde{\kappa} = \nu - \nu')^{\dagger}{}_{\kappa}\rho([ms]p, p'; \omega)] = 2\sqrt{2}\left(\frac{-Q^2}{4m^2 - Q^2}\right)^{\frac{1}{4}} \langle Q, {}^{\kappa}_{\sigma}; \omega'; \tilde{\kappa} = \nu - \nu' \mid p^{s}_{\lambda}, -p'^{\lambda'}_{s}; \omega\rangle a^{\lambda}{}_{\lambda'}, \quad (4.49)$$

$$\operatorname{tr}[(Q, k\eta; \omega'; \tilde{\kappa} = \nu - \nu')^{\dagger}{}_{\kappa}\rho([ms]p, p'; \omega)] = 2\sqrt{2}\left(\frac{-Q^2}{4m^2 - Q^2}\right)^{\frac{1}{4}} \langle Q, {}^{\kappa}_{k\eta}; \omega'; \tilde{\kappa} = \nu - \nu' \mid p^{s}_{\lambda}, -p'^{\lambda'}_{s}; \omega\rangle a^{\lambda}{}_{\lambda'}, \quad (4.50)$$

where

$$\langle Q, {}^{\kappa}_{\sigma}; \omega'; \tilde{\kappa} = \nu - \nu' \mid p^{s}_{\lambda}, -p'^{\lambda'}_{s}; \omega\rangle = \delta^4(Q - p' + p) D^{-\frac{1}{2}+i\sigma}(\phi, \alpha, 0)^{\kappa}{}_{\tilde{\kappa}} \left[\frac{2\sigma}{\pi} \tanh \pi\sigma \sqrt{\frac{-Q^2}{4m^2 - Q^2}}\right]^{\frac{1}{2}}$$
$$\times D^s[R^{-1}(p, \Omega_{\omega'}(Q))R_{\omega 3}(p)]^{\nu}{}_{\lambda} D^s[R^{-1}_{\omega 3}(p')R(p', \Omega_{\omega'}(Q))]^{\lambda'}{}_{\nu'}, \quad (4.51)$$

$$\langle Q, {}^{\kappa}_{k\eta}; \omega'; \tilde{\kappa} = \nu - \nu' \mid p^{s}_{\lambda}, -p'^{\lambda'}_{s}; \omega\rangle = \delta^4(Q - p' + p) D^{k\eta}(\phi, \alpha, 0)^{\kappa}{}_{\tilde{\kappa}} \left[\frac{2}{\pi}(2k - 1)\sqrt{\frac{-Q^2}{4m^2 - Q^2}}\right]^{\frac{1}{2}}$$
$$\times D^s[R^{-1}(p, \Omega_{\omega'}(Q))R_{\omega 3}(p)]^{\nu}{}_{\lambda} D^s[R^{-1}_{\omega 3}(p')R(p', \Omega_{\omega'}(Q))]^{\lambda'}{}_{\nu'}. \quad (4.52)$$

The parameters ϕ and α are determined by the relations

$$\tan \phi = \Omega^{-1}_{\omega'}(Q)^2{}_{\nu}p^{\nu}[\Omega^{-1}_{\omega'}(Q)^1{}_{\nu}p^{\nu}]^{-1}$$

and

$$\cosh \alpha = \Omega^{-1}_{\omega'}(Q)^0{}_{\nu}p^{\nu}[p^2 + (\Omega^{-1}_{\omega'}(Q)^3{}_{\nu}p^{\nu})^2]^{-\frac{1}{2}}. \quad (4.53)$$

The completeness relation

$$\sum_{\tilde{\kappa}\geq -2s}^{\tilde{\kappa}\leq 2s} \int d^4Q \left\{ \int_{-\infty}^{\infty} d\sigma \sum_{\kappa=0,\pm1,\pm2,\cdots} \langle p_1{}^{\lambda_1}_{s}, -p'_1{}^{s}_{\lambda_1'}; \omega \mid Q, {}^{\sigma}_{\kappa}; \tilde{\kappa}\rangle \right.$$
$$\times \langle Q, {}^{\kappa}_{\sigma}; \tilde{\kappa} \mid p_2{}^{s}_{\lambda_2}, -p'_2{}^{\lambda_2'}_{s}; \omega\rangle$$
$$+ \sum_{k=1}^{|\tilde{\kappa}|} \sum_{\kappa_1=\eta k, \eta(k+1),\cdots} \langle p_1{}^{\lambda_1}_{s}, -p'_1{}^{s}_{\lambda_1'}; \omega \mid Q, {}^{k\eta}_{\kappa_1}; \tilde{\kappa}\rangle$$
$$\left. \times \langle Q, {}^{\kappa_1}_{k\eta}; \tilde{\kappa} \mid p_2{}^{s}_{\lambda_2}, -p'_2{}^{\lambda_2'}_{s}; \omega\rangle \right\}$$
$$= 2\,|p'^0_1|\, 2\,|p^0_1|\, \delta^3(\mathbf{p}'_2 - \mathbf{p}'_1)\delta^3(\mathbf{p}_2 - \mathbf{p}_1)\delta^{\lambda'}{}_{\lambda_1'}\delta^{\lambda_1}{}_{\lambda_2}, \quad \eta = \operatorname{sgn}\tilde{\kappa}, \quad (4.54)$$

and the orthogonality relations

$$\sum_{\lambda,\lambda'=-s}^{s} \int \frac{d^3\mathbf{p}}{2\,|p^0|} \int \frac{d^3\mathbf{p}'}{2\,|p'^0|} \langle Q', {}^{\kappa'}_{\sigma}; \tilde{\kappa}' \mid p^{s}_{\lambda}; -p'^{\lambda'}_{s}; \omega\rangle$$
$$\times \langle p^{\lambda}_{s}, -p'^{s}_{\lambda'}; \omega \mid Q, {}^{\sigma}_{\kappa}; \tilde{\kappa}\rangle$$
$$= \delta^4(Q' - Q)\delta(\sigma' - \sigma)\delta^{\kappa'}{}_{\kappa}\delta^{\tilde{\kappa}'}{}_{\tilde{\kappa}}, \quad (4.55)$$

$$\sum_{\lambda,\lambda'=-s}^{s} \int \frac{d^3\mathbf{p}}{2\,|p^0|} \int \frac{d^3\mathbf{p}'}{2\,|p'^0|} \langle Q', {}^{\kappa'}_{k'\eta'}; \tilde{\kappa} \mid p^{s}_{\lambda}, -p'^{\lambda'}_{s}; \omega\rangle$$
$$\times \langle p^{\lambda}_{s}, -p'^{s}_{\lambda'}; \omega \mid Q, {}^{k\eta}_{\kappa}; \tilde{\kappa}\rangle$$
$$= \delta^4(Q' - Q)\delta_{k'k}\delta_{\eta'\eta}\delta^{\kappa'}{}_{\kappa}\delta^{\tilde{\kappa}'}{}_{\tilde{\kappa}} \quad (4.56)$$

follow from the corresponding Eqs. (4.4) and (4.3a), (4.3b) for the matrix representations.

An important application of the relations (4.48)–(4.53) is the reduction into its Poincaré-irreducible components of a product of field operators (i.e., current operators).[1] Such a reduction can be used to facilitate the evaluation of vertex functions, particularly if fields or particles with spins larger than $\frac{1}{2}$ are involved.

5. $ISO(3, 1) \uparrow SO(3, 1)$-IRREDUCIBLE TENSOR OPERATORS

The irreducible representations of $SO(3, 1)$ are characterized by the Casimir invariants[10,15,16]

$$\tfrac{1}{2}J_{\mu\nu}J^{\mu\nu} = j_0{}^2 + j^2 - 1, \quad \tfrac{1}{4}\epsilon^{\mu\nu\rho\sigma}J_{\mu\nu}J_{\rho\sigma} = -ij_0j. \quad (5.1)$$

The nontrivial irreducible representations $D([j_0j]\Lambda)$ are unitary if:

I. (a) $j_0 = \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots$ and $\operatorname{Re} j = 0$, $-\infty < \operatorname{Im} j < \infty$;

(b) $j_0 = 0$ and $\operatorname{Re} j = 0$, $0 \leq \operatorname{Im} j < \infty$;

II. $j_0 = 0$ and $0 < \operatorname{Re} j < 1$, $\operatorname{Im} j = 0$. (5.2)

The cases I and II are referred to as principal and supplementary series, respectively. Only the class I representations are used for the construction of the $ISO(3,1)\uparrow SO(3,1)$-irreducible tensor operators, since these representations form a complete orthogonal set by themselves.[17] The elements of $D([j_0 j]\Lambda)$ are labeled by the eigenvalues j and λ of the angular momentum operators $\mathbf{J}^2$ and J_{12}, where $\mathbf{J} = (J_{23}, J_{31}, J_{12})$. For the principal series, j and λ assume the values

$$j = j_0, j_0+1, j_0+2, \cdots, \lambda = -j, -j+1, \cdots, j. \tag{5.3}$$

The parametrization

$$\Lambda = R(\phi,\theta,\psi)B(\gamma)\hat{R}(0,\hat{\theta},\hat{\varphi}),\ B(\gamma) = \exp(-i\gamma j_{03}),$$
$$R(\phi,\theta,\psi) = \exp(-i\phi j_{12})\exp(-i\theta j_{31})\exp(-i\psi j_{12}),$$
$$0 \le \phi, \psi, \hat{\varphi} < 2\pi,\ 0 \le \theta, \hat{\theta} \le \pi,\ 0 \le \gamma < \infty, \tag{5.4}$$

implies the matrix decomposition

$$D([j_0 \mathbf{j}]\Lambda)^{j'\mu'}{}_{j\mu} = \sum_{\nu=-\min(j',j)}^{\min(j',j)} D([j']R)^{\mu'}{}_\nu d_\nu([j_0\mathbf{j}]B)^{j'}{}_j D([j]\hat{R})^\nu{}_\mu. \tag{5.5}$$

For the rotation functions $D([j]R)^\lambda{}_\mu$ the orthogonality and completeness relations are

$$\int d\mu(R) D([j']R)^{*\lambda'}{}_{\mu'} D([j]R)^\lambda{}_\mu = \frac{1}{\rho[j]}\delta_{j'j}\delta^{\lambda'\lambda}\delta_{\mu'\mu},$$
$$\rho[j] = 2j+1,\quad d\mu(R) = (d\phi/2\pi)(\sin\theta\, d\theta/2)(d\psi/2\pi), \tag{5.6}$$

and

$$\sum_{\substack{j=0,1,2\cdots \text{ or}\\ j=\frac12,\frac32,\cdots}} \rho[j] \sum_{\lambda,\mu=-j}^{j} D([j]R)^\lambda{}_\mu D([j]R')^{*\lambda}{}_\mu = [1/\rho(R)]\delta(R-R'),$$
$$\rho(R) = (1/8\pi^2)\sin\theta,\quad \delta(R-R') = \delta(\phi-\phi') \times \delta(\theta-\theta')\delta(\psi-\psi'). \tag{5.7}$$

For the boost functions[18–20]

$$d_\nu([j_0\mathbf{j}]B(\gamma))^{j'}{}_j = \left\langle \begin{matrix} j'\nu \\ j_0\mathbf{j}\end{matrix}\right| e^{-i\gamma J_{03}} \left|\begin{matrix} j_0\mathbf{j} \\ j\nu\end{matrix}\right\rangle,$$
$$d_\nu([j_0\mathbf{j}]B(0))^{j'}{}_j = \delta^{j'}{}_j, \tag{5.8}$$

orthogonality and completeness can be stated as

$$\sum_{\nu=-\min(j'j)}^{\min(j'j)} \int d\mu(B) d_\nu([j_0\mathbf{j}]B)^{*j'}{}_j d_\nu([j_0'\mathbf{j}']B)^{j'}{}_j = \frac{1}{\rho_{j'j}[j_0\mathbf{j}]}\delta_{j_0j_0'}\delta(i\mathbf{j}-i\mathbf{j}')$$

(if $j_0 = 0, \pm1, \pm2, \cdots$, or $j_0 = \pm\frac12, \pm\frac32, \cdots$, and $0 \le (1/i)\mathbf{j} < \infty$),

$$\rho_{j'j}[j_0\mathbf{j}] = \frac{4}{\pi}\frac{(j_0^2 - \mathbf{j}^2)}{(2j'+1)(2j+1)},$$
$$d\mu(B) = \tfrac12 \sinh^2\gamma\, d\gamma \tag{5.9}$$

and as

$$\sum_{j_0=-\min(j'j)}^{\min(j'j)} \int_0^{i\infty} \frac{1}{i} d\mathbf{j}\rho_{j'j}[j_0\mathbf{j}] d_\nu([j_0,\mathbf{j}]B)^{j'}{}_j d_\nu([j_0\mathbf{j}]B')^{j'}{}_j = \frac{1}{\rho(B)}\delta(B-B'),$$
$$\rho(B) = \tfrac12\sinh^2\gamma,\quad \delta(B-B') = \delta(\gamma-\gamma'). \tag{5.10}$$

The change of the domains for j_0 and $\mathbf{j}$

from $j_0 = 0, \frac12, 1, \frac32 \cdots$ and $-\infty < (1/i)\mathbf{j} < \infty$
to $j_0 = 0, \pm\frac12, \pm1, \pm\frac32, \cdots$ and $0 \le (1/i)\mathbf{j} < \infty$

is justified by the fact that the boost functions satisfy the (weak equivalence) relation[6]

$$d_\nu([-j_0, -\mathbf{j}]B)^{j'}{}_j = \frac{\Gamma(j'+\mathbf{j}+1)}{\Gamma(j'-\mathbf{j}+1)} d_\nu([j_0\mathbf{j}]B)^{j'}{}_j \frac{\Gamma(j-\mathbf{j}+1)}{\Gamma(j+\mathbf{j}+1)}, \tag{5.11}$$

and the relation (which follows from unitarity)

$$d_\nu([j_0\mathbf{j}]B)^{*j'}{}_j = d_\nu([j_0, -\mathbf{j}]B)^{j'}{}_j. \tag{5.12}$$

The orthogonality and completeness relations for the matrix realizations (5.5) are therefore

$$\int d\mu(\Lambda) D([j_0\mathbf{j}]\Lambda)^{j_1'\lambda_1'}{}_{j_1\lambda_1} D([j_0'\mathbf{j}']\Lambda)^{*j_2'\lambda_2'}{}_{j_2\lambda_2} = \frac{1}{\rho[j_0\mathbf{j}]}\delta_{j_0j_0'}\delta(i\mathbf{j}-i\mathbf{j}')\delta^{j_1'j_2'}\delta^{\lambda_1'\lambda_2'}\delta_{j_1j_2}\delta_{\lambda_2\lambda_2},$$
$$d\mu(\Lambda) = \frac{d\phi}{2\pi}\frac{\sin\theta\, d\theta}{2}\frac{d\psi}{2\pi}\frac{\sinh^2\gamma\, d\gamma}{2}\frac{\sin\hat{\theta}\, d\hat{\theta}}{2}\frac{d\hat{\varphi}}{2\pi},$$
$$\rho[j_0\mathbf{j}] = \frac{4}{\pi}(j_0^2 - \mathbf{j}^2) \tag{5.13}$$

and

$$\sum_{\substack{j,j'=0 \text{ or}\\ j,j'=\frac12}}^{\infty}\sum_{\lambda'=-j'}^{j'}\sum_{\lambda=-j}^{j}\sum_{j_0=-\min(jj')}^{\min(jj')} \times \int_0^{i\infty}\frac{1}{i}d\mathbf{j}\,\rho[j_0\mathbf{j}] D([j_0\mathbf{j}]\Lambda)^{j'\lambda'}{}_{j\lambda} D([j_0\mathbf{j}]\Lambda')^{*j'\lambda'}{}_{j\lambda} = \frac{1}{\rho(\Lambda)}\delta(\Lambda-\Lambda'), \tag{5.14}$$

$$\rho(\Lambda) = \frac{1}{(4\pi)^3}\sin\theta\sinh^2\gamma\sin\hat{\theta},$$
$$\delta(\Lambda-\Lambda') = \delta(\phi-\phi')\delta(\theta-\theta')\delta(\psi-\psi') \times \delta(\gamma-\gamma')\delta(\hat{\theta}-\hat{\theta}')\delta(\hat{\varphi}-\hat{\varphi}').$$

For

$$\hat{\Lambda} = R(\phi,\theta,\psi)B(\gamma) \tag{5.15}$$

and for

$$D([j_0\mathbf{j}]\hat{\Lambda})^{j'\mu'}{}_{j\mu} = D([j']R)^{\mu'}{}_\mu d_\mu([j_0\mathbf{j}]B)^{j'}{}_j, \tag{5.16}$$

the orthogonality and completeness relations are

$$\sum_{\mu,\lambda=-\min(j'j)}^{\min(j'j)} \int d\mu(\hat\Lambda) D([j_0 j]\hat\Lambda)^{j_1'\mu'}{}_{j\mu} D([j_0', j']\hat\Lambda)^{*j'\lambda'}{}_{j\lambda} = \frac{1}{\rho_j[j_0 j]} \delta_{j_0 j_0'} \delta(ij - ij') \delta^{j_1' j'} \delta^{\mu'\lambda'},$$
$$d\mu(\hat\Lambda) = \frac{d\phi}{2\pi} \frac{\sin\theta\, d\theta}{2} \frac{d\psi}{2\pi} \frac{\sinh^2\gamma\, d\gamma}{2}, \tag{5.17}$$
$$\rho_j[j_0 j] = \frac{4}{\pi} \frac{j_0^2 - j^2}{2j+1},$$

$$\sum_{j'=|\lambda|}^{\infty} \sum_{\mu'=-j'}^{j'} \sum_{j_0=-\min(j,j')}^{\min(j,j')} \times \int_0^{i\infty} \frac{1}{i} dj\, \rho_j[j_0 j] D([j_0 j]\hat\Lambda)^{j'\mu'}{}_{j\mu} D([j_0 j]\hat\Lambda')^{*j'\mu'}{}_{j\lambda} = \frac{1}{(\rho\hat\Lambda)} \delta(\hat\Lambda - \hat\Lambda')\delta_{\mu\lambda},$$
$$\rho(\hat\Lambda) = \frac{1}{(4\pi)^2} \sin\theta \sinh^2\gamma, \tag{5.18}$$
$$\delta(\hat\Lambda - \hat\Lambda') = \delta(\phi - \phi')\delta(\theta - \theta') \times \delta(\psi - \psi')\delta(\gamma - \gamma').$$

In order to construct by the idempotent operator method outlined in Sec. 3, the tensor operators that transform according to the $SO(3, 1)$-induced unitary irreducible representations of the Poincaré group [which are also the unitary irreducible representations of the $(3 + 1)$-dimensional homogeneous Lorentz group], we define the set of (projection) operators

$$P[j_0 j]^{j'\mu'}{}_{j\mu} \stackrel{\text{DEF}}{=} \rho[j_0 j] \int d\mu(\Lambda) D([j_0 j]\Lambda)^{\dagger j'\mu'}{}_{j\mu} T(\Lambda), \tag{5.19}$$

with

$$T(\Lambda)^\dagger = T(\Lambda)^{-1} = T(\Lambda^{-1}), \quad \Lambda \in SO(3,1),$$
$$T(\Lambda) = e^{-i\phi J_{12}} e^{-i\theta J_{31}} e^{-i\psi J_{12}} e^{-i\gamma J_{03}} e^{-i\hat\theta J_{31}} e^{-i\hat\psi J_{12}}. \tag{5.20}$$

The operators (5.19) transform under $SO(3, 1)$ according to the unitary irreducible representation characterized by $[j_0 j]$:

$$T(\Lambda) P[j_0 j]^{j'\mu'}{}_{j\mu} = \sum_{j''\mu''} P[j_0 j]^{j'\mu'}{}_{j''\mu''} D([j_0 j])^{j''\mu''}{}_{j\mu}. \tag{5.21}$$

This relation follows from the invariance of the Haar measure $d\mu(\Lambda)$ and the unitarity of the representation $[j_0 j]$, namely

$$D([j_0 j]\Lambda)^\dagger = D([j_0 j]\Lambda^{-1}).$$

The orthogonality (2.13), together with the invariance of $d\mu(\Lambda)$, entails the property

$$P[j_0 j]^{j_1'\mu_1'}{}_{j_1\mu_1} P[j_0' j']^{j_2'\mu_2'}{}_{j_2\mu_2} = \delta_{j_0 j_0'} \delta(ij - ij') \delta^{j_1'}{}_{j_2} \delta^{\mu_1'}{}_{\mu_2} P[j_0' j']^{j_2'\mu_2'}{}_{j_1\mu_1}. \tag{5.22}$$

This relation implies that the operators (5.19) are idempotent.

We then apply these projection operators to the ordinary spin tensor operators in the rest frame of a positive-mass ($p^2 > 0$) particle with spin s, namely to the $SO(3)$-irreducible tensor operators[21–23]

$$({}^\circ p, s)_{\sigma\mu} = |{}^\circ p^s_{\lambda'}\rangle \left\langle \begin{matrix} \lambda' & s \\ s & \lambda \end{matrix} \middle| \begin{matrix} \sigma \\ \mu \end{matrix} \right\rangle \langle {}^\circ p^\lambda_s|, \tag{5.23}$$

where

$${}^\circ p = \pm(p^2)^{\frac12}(1, 0, 0, 0), \quad p^2 = p^\mu p_\mu > 0 \tag{5.24}$$

and where

$$\left\langle \begin{matrix} \lambda' & s \\ s & \lambda \end{matrix} \middle| \begin{matrix} \sigma \\ \mu \end{matrix} \right\rangle = (-1)^{s-\lambda} \left\langle \begin{matrix} \lambda', & -\lambda \\ s & s \end{matrix} \middle| \begin{matrix} \sigma \\ \mu \end{matrix} \right\rangle \tag{5.25}$$

are the $SO(3)$ Clebsch–Gordan coefficients for the reduction

$$D([s]R)^\mu{}_\lambda D([s]R)^{\dagger\lambda'}{}_{\mu'} = \sum_{\bar s=0}^{2s} \left\langle \begin{matrix} \mu & s \\ s & \mu' \end{matrix} \middle| \begin{matrix} \bar s \\ \bar\mu \end{matrix} \right\rangle D([\bar s]R)^{\bar\mu}{}_{\bar\lambda} \left\langle \begin{matrix} \bar\lambda \\ \bar s \end{matrix} \middle| \begin{matrix} s & \lambda' \\ \lambda & s \end{matrix} \right\rangle. \tag{5.26}$$

The basis vectors

$$\{|{}^\circ p^s_\lambda\rangle: -s \le \lambda \le s\}$$

are defined by the eigenvalue equations (2.19), (2.20), and (2.21) and by the orthonormality relation (2.18):

$$\langle {}^\circ p^{\lambda'}_s \mid {}^\circ p^s_\lambda\rangle = \pm 2(p^2)^{\frac12} \delta^{\lambda'}{}_\lambda.$$

In the expression

$$P[j_0 j]^{\sigma\kappa}{}_{j\mu}({}^\circ ps)_{\sigma'\kappa'} \tag{5.27}$$

the integration over the group parameter space can partially be carried out by means of the transformation property [which is a consequence of Eq. (5.26)]

$$T(\Lambda)({}^\circ ps)_{\sigma'\kappa'} = T(\hat\Lambda)({}^\circ ps)_{\sigma'\kappa''} D([\sigma']\hat R)^{\kappa''}{}_{\kappa'}, \tag{5.28}$$
$$T(\Lambda) = T(\hat\Lambda) T(\hat R) \tag{5.29}$$

and by virtue of the matrix decomposition (5.5) and the orthogonality relation (5.6) for the rotation functions; after the integration on $\hat R$ the expression (5.27) is

$$P[j_0 j]^{\sigma\kappa}{}_{j\mu}({}^\circ ps)_{\sigma'\kappa'} = \delta^\sigma{}_{\sigma'} \delta^\kappa{}_{\kappa'} (j_0 j[ms])^\sigma{}_{j\mu}, \tag{5.30}$$

where

$$(j_0 j[ms])^\sigma{}_{j\mu} = \rho_\sigma[j_0 j] \sum_{\nu=-\min(\sigma,j)}^{\min(\sigma,j)} \int d\mu(\hat\Lambda) D([j_0 j]\hat\Lambda)^{\dagger\sigma\nu}{}_{j\mu} T(\hat\Lambda)({}^\circ ps)_{\sigma\nu}. \tag{5.31}$$

The integration with respect to the angular parameter ψ can be carried out immediately [see parametrization

(5.4) and Eq. (5.15)], since

$$T(\hat{\Lambda})({}^\circ ps)_{\sigma\nu} = e^{-i\nu\psi}T(\Omega_0(\phi,\theta,\gamma))({}^\circ ps)_{\sigma\nu}$$
$$= e^{-i\nu\psi}([p^2s]\phi,\theta,\gamma)_{\sigma\nu}, \quad (5.32)$$

where

$$T(\Omega_0(\phi,\theta,\gamma)) = e^{-i\phi J_{12}}e^{-i\theta J_{31}}e^{-i\gamma J_{03}}$$

is the unitary operator realization of the orbiting transformation introduced in Eq. (2.22) and where

$$([ms]p;0)_{\sigma\nu} = ([p^2s]\phi,\theta,\psi)_{\sigma\nu}$$
$$= |p^s_{\lambda'};0\rangle\left\langle\begin{matrix}\lambda' & s\\ s & \lambda\end{matrix}\middle|\begin{matrix}\sigma\\ \nu\end{matrix}\right\rangle\langle p^\lambda_s;0|$$
$$|p^s_\lambda;0\rangle \overset{\text{DEF}}{=} T(\Omega_0(\phi,\theta,\gamma))\,|{}^\circ p^s_\lambda\rangle. \quad (5.33)$$

Equation (5.31) can now be written as

$$(j_0 j[ms])^\sigma{}_{j\mu} = \rho_s[j_0 j]\sum_{\nu=-\min(\sigma,j)}^{\min(\sigma,j)} \times \int d\mu(\phi,\theta,\gamma)D([j_0 j]\phi,\theta,\gamma)^{\dagger\sigma\nu}{}_{j\mu}([p^2s]\phi\theta\gamma)_{\sigma\nu},$$

$$d\mu(\phi,\theta,\gamma) = \frac{d\phi}{2\pi}\frac{\sin\theta\, d\theta}{2}\frac{\sinh^2\gamma\, d\gamma}{2}, \quad (5.34)$$

where in accordance with the relation (5.16) we define

$$D([j_0 j]\phi,\theta,\gamma)^{j'\mu'}{}_{j\mu} = D([j']R(\phi,\theta,0))^{\mu'}{}_\mu d_\mu([j_0 j]B(\gamma))^{j'}{}_j. \quad (5.35)$$

From the relations (5.21), (5.30), (5.34), and (5.36) it is immediate that the operators defined by Eq. (5.31) transform according to the unitary irreducible representations of the Poincaré group that are induced by the (3 + 1)-dimensional Lorentz group, namely according to

$$D(a,\Lambda[j_0 j])(j_0 j[ms])^\sigma{}_{j\mu} = \sum_{j'\mu'}(j_0 j[ms])^\sigma{}_{j'\mu'}D([j_0 j]\Lambda)^{j'\mu'}{}_{j\mu}, \quad (5.36)$$

and are therefore the $ISO(3,1)\uparrow SO(3,1)$-irreducible tensor operators in an angular momentum basis which are associated with a particle characterized by $[p^2 > 0, s]$. In contrast, the tensor operators (5.33) transform under the Poincaré group according to reducible, nonfaithful, unitary representations. If $U(a,\Lambda)$ denotes the unitary operator realization (on $H[m,s]\otimes H^\dagger[ms]$) of the Poincaré transformation (a,Λ), then

$$U(a,\Lambda)([ms]p;0)_{\sigma\nu} = ([ms]\Lambda p;0)_{\sigma\nu'}D([\sigma]R(\Lambda,p))^{\nu'}{}_\nu. \quad (5.37)$$

The notation Λp and the Wigner rotation $R(\Lambda,p)$ are defined by (2.15a). The transformation (5.37) is a consequence of the relations (2.14) and (5.26).

With the trace operation (2.13) the orthogonality of the tensor operators (5.33) can be expressed as

$$\mathrm{Tr}\,[([p^2s]\phi\theta\gamma)_{\sigma\nu}([p^2s]\phi'\theta'\gamma')^\dagger{}_{\sigma'\nu'}] = \frac{2}{p^2}\frac{1}{\sinh^2\gamma}\frac{1}{\sin\theta}\delta(\gamma-\gamma')\delta(\phi-\phi')\delta(\theta-\theta')\delta_{\sigma\sigma'}\delta_{\nu\nu'}. \quad (5.38)$$

Together with (5.34) and (5.17) this implies that the Poincaré-irreducible tensor operators defined by (5.31) satisfy the orthogonality relation

$$\mathrm{Tr}\,[(j_0 j[ms])^\sigma{}_{j\mu}(j_0' j'[ms])^{\dagger\sigma'}{}_{j'\mu'}] = \frac{1}{4\pi m^2}\rho_\sigma[j_0 j]\delta_{j_0 j_0'}\delta(ij-ij')\delta_{jj'}\delta_{\mu\mu'}\delta^{\sigma\sigma'}. \quad (5.39)$$

The inverse of the relation (5.34), namely

$$([p^2s]\phi\theta\gamma)_{\sigma\nu} = \sum_{j=|\nu|}^{\infty}\sum_{\mu=-j}^{j}\sum_{j_0=-\min(\sigma,j)}^{\min(\sigma,j)}\int_0^{i\infty}\left(\frac{1}{i}\,dj D([j_0 j]\phi\theta\gamma)^{j\mu}{}_{\sigma\nu} \times (j_0 j[ms])^\sigma{}_{j\mu}\right), \quad (5.40)$$

is an immediate consequence of the completeness relation (5.18) provided that the substitutions

$$\rho(\hat{\Lambda}) \to \rho(\phi\theta\gamma) = 2\pi\rho(\hat{\Lambda}),$$
$$\delta(\hat{\Lambda}-\hat{\Lambda}') \to \delta[(\phi\theta\gamma)-(\phi'\theta'\gamma')] = \delta(\phi-\phi') \times \delta(\theta-\theta')\delta(\gamma-\gamma') \quad (5.41)$$

are made. By means of the partial trace (2.12), the completeness of the tensor operators (5.33) can be expressed as

$$\sum_{\sigma=0}^{2s}\sum_{\nu=-\sigma}^{\sigma}\int d\mu(\phi\theta\gamma) \times \mathrm{tr}\,[([p^2s]\phi\theta\gamma)_{\sigma\nu}([p^2s]\phi\theta\gamma)^\dagger{}_{\sigma\nu}] = \frac{1}{4\pi m^2}. \quad (5.42)$$

By virtue of the relations (5.17) and (5.42), it follows from (5.40) that the tensor operators (5.31) satisfy the relation

$$\sum_{\sigma=0}^{2s}\sum_{j_0=-\sigma}^{\sigma}\sum_{j=|j_0|}^{\infty}\sum_{\mu=-j}^{j}\int_0^{i\infty}\frac{1}{i}\,dj\,(\rho_\sigma[j_0 j])^{-1} \times \mathrm{tr}\,[(j_0 j[ms])^\sigma{}_{j\mu}(j_0 j[ms])^{\dagger\sigma}{}_{j\mu}] = \frac{1}{4\pi m^2}. \quad (5.43)$$

The connections between the tensor operators (5.31) and their Hermitian adjoints are

$$(j_0 j[ms])^{\dagger\sigma}{}_{j\mu} = (-1)^\mu(-j_0,-j[ms])^\sigma{}_{j,-\mu}. \quad (5.44)$$

This follows from (5.34) in conjunction with the easily established relation

$$([p^2, s]\phi\theta\gamma)^{\dagger}{}_{\sigma\nu} = (-1)^{\nu}([p^2, s]\phi\theta\gamma)_{\sigma,-\nu} \quad (5.45)$$

and the property

$$D([j_0 j]\hat{\Lambda})^{j\mu}{}_{\sigma\nu} = (-1)^{\mu-\nu} D([-j_0, -j]\hat{\Lambda})^{*j,-\mu}{}_{\sigma,-\nu} \quad (5.46)$$

for the matrix realization (5.16). Equation (5.46) is derived from (5.12) together with the index symmetry[6]

$$d_\nu([j_0 j]B(\gamma))^j{}_\sigma = d_{-\nu}([-j_0 j]B(\gamma))^j{}_\sigma \quad (5.47)$$

and the well-known relation

$$D([j]R)^{*\mu}{}_\nu = (-1)^{\mu-\nu} D([j]R)^{-\mu}{}_{-\nu}. \quad (5.48)$$

At this juncture, we return to the orbiting transformations (2.22) and (2.23) in order to generalize the definition (5.33) to

$$([ms]p;\omega)_{\sigma\nu} = |p^s_{\lambda'};\omega\rangle \left\langle \begin{matrix} \lambda' s \\ s\,\lambda \end{matrix} \middle| \begin{matrix} \sigma \\ \nu \end{matrix} \right\rangle \langle p^s_\lambda;\omega|,$$

$$|p^s_\lambda;\omega\rangle = T(\Omega_\omega(p))\,|{}^\circ p^s_\lambda\rangle, \quad \omega = 0, 3. \quad (5.49)$$

The helicity rearrangement transformations (A18) together with the reduction (5.26) yield the connections

$$([ms]p;\omega')_{\sigma\nu} = ([ms]p;\omega)_{\sigma\lambda} D([\sigma]R_{\omega'\omega})^\lambda{}_\nu, \quad (5.50)$$

where the rotation $R_{\omega'\omega}$ is determined by Eq. (A21). The expansion (5.40) can now be generalized to

$$([ms]p;\omega)_{\sigma\kappa} = \sum_{j_0=-\sigma}^{\sigma} \sum_{j=|j_0|}^{\infty} \sum_{\mu=-j}^{j} \int_0^{i\infty} \frac{1}{i}\, dj D([j_0 j]\Omega_0(p)R_{\omega 0})^{j\mu}{}_{\sigma\kappa} \times (j_0 j[ms])^\sigma{}_{j\mu},$$

where

$$D([j_0 j]\Omega_0(p)R_{\omega 0})^{j\mu}{}_{\sigma\kappa} = \sum_{\nu=-\min(\sigma,j)}^{\min(\sigma,j)} D([j_0 j]\phi\theta\gamma)^{j\mu}{}_{\sigma\nu} D([\sigma]R_{\omega 0})^\nu{}_\kappa. \quad (5.51)$$

This last equation corresponds to the decomposition (5.5), since in accordance with (5.4) and (5.15)

$$\Omega_0(p)R_{\omega 0} = \hat{\Lambda}(\phi,\theta,0,\gamma)\hat{R}(0,\theta_{\omega 0},0) = \Lambda(\phi,\theta,0,\gamma,\theta_{\omega 0},0) \quad (5.52)$$

and therefore

$$D([j_0 j]\Omega_0(p)R_{\omega 0})^{j\mu}{}_{\sigma\kappa} = D([j_0 j]\Lambda(\phi,\theta,0,\gamma,\theta_{\omega 0},0))^{j\mu}{}_{\sigma\kappa}. \quad (5.53)$$

The Poincaré-irreducible tensor operators (5.31) can then be realized by

$$(j_0 j[ms])^\sigma{}_{j\mu} = \rho_\sigma[j_0 j] \sum_{\kappa=-\min(\sigma,j)}^{\min(\sigma,j)} \int d\mu(\Omega_0(p)) \times D([j_0 j]\Omega_0(p)R_{\omega 0})^{\dagger\sigma\kappa}{}_{j\mu}([ms]p;\omega)_{\sigma\kappa},$$

$$d\mu(\Omega_0(p)) = d\mu(\phi,\theta,\gamma). \quad (5.54)$$

The (ordinary) multipole decomposition in terms of the operators (5.49) of the spin density matrix

$$\rho([ms]p;\omega) = \sum_{\lambda,\lambda=-s}^{s} |p^s_{\lambda'};\omega\rangle\, a(p)^{\lambda'}{}_\lambda \langle p^\lambda_s;\omega| \quad (5.55)$$

is

$$\rho([ms]p;\omega) = \sum_{\sigma=0}^{2s} \sum_{\nu=-\sigma}^{\sigma} \langle([ms]p;\omega)^\dagger_{\sigma\nu}\rangle([ms]p;\omega)_{\sigma\nu},$$

$$\langle([ms]p;\omega)^\dagger_{\sigma\nu}\rangle \overset{\text{DEF}}{=} \mathrm{Tr}\left(\int \frac{d^3\mathbf{p}'}{2\,|p'^0|}([ms]p;\omega)([ms]p;\omega)^\dagger_{\sigma\nu}\right) = \sum_{\lambda,\lambda'=-s}^{s} a(p)^{\lambda'}{}_\lambda \left\langle \begin{matrix} \nu \\ \sigma \end{matrix} \middle| \begin{matrix} s\,\lambda \\ \lambda' s \end{matrix} \right\rangle, \quad (5.56)$$

where the operation Tr is defined by Eq. (2.13). This result is an immediate consequence of the orthogonality relation (5.38). The corresponding relativistic multipole decomposition in terms of the Poincaré-irreducible tensor operators (5.31) is obtained by substituting the expansion (5.51) into the multipole decomposition (5.56). The result may be expressed as

$$\rho([ms]p;\omega) = \sum_{\sigma=0}^{2s} \sum_{j_0=-\sigma}^{\sigma} \sum_{j=|j_0|}^{\infty} \sum_{\mu=-j}^{j} \int_0^{i\infty} \frac{1}{i}\, dj(j_0 j[ms])^\sigma{}_{j\mu} \times \sum_{\lambda,\lambda'=-s}^{s} a(p)^{\lambda'}{}_\lambda \left\langle \begin{matrix} j\,\mu \\ j_0 j,\sigma \end{matrix} \middle| p^s_{\lambda'}; -p^\lambda_s;\omega \right\rangle, \quad (5.57)$$

with the $ISO(3, 1) \uparrow SO(3, 1)$ Clebsch–Gordan coefficient

$$\left\langle \begin{matrix} j\,\mu \\ j_0 j;\sigma \end{matrix} \middle| p^s_{\lambda'}; -p^\lambda_s;\omega \right\rangle = D([j_0 j]\Omega_0(p)R_{\omega 0})^{j\mu}{}_{\sigma,\lambda'-\lambda} \left\langle \begin{matrix} \lambda'-\lambda \\ \sigma \end{matrix} \middle| \begin{matrix} s\,\lambda \\ \lambda' s \end{matrix} \right\rangle. \quad (5.58)$$

The derivation of the orthogonality and completeness relations

$$\sum_{\lambda,\lambda'=-s}^{s} \int \frac{d^3\mathbf{p}}{2\,|p^\circ|} \left\langle \begin{matrix} j'\mu' \\ j_0'j';\sigma \end{matrix} \middle| p^s_{\lambda'}; -p^\lambda_s;\omega \right\rangle \times \left\langle p^{\lambda'}_s; -p^s_\lambda;\omega \middle| \begin{matrix} j_0 j;\sigma \\ j\,\mu \end{matrix} \right\rangle = \frac{4\pi p^2}{\rho_j[j_0 j]}\, \delta_{j_0 j_0'}\delta(ij - ij')\delta^{j'}{}_j \delta^{\mu'}{}_\mu \quad (5.59)$$

and

$$\sum_{\mathscr{s}=0}^{2s}\sum_{j=|\lambda'-\lambda|}^{\infty}\sum_{\mu=-j}^{j}\sum_{j_0=-\min(\mathscr{s},j)}^{\min(\mathscr{s},j)}\int_0^{i\infty}\frac{1}{i}\,dj\,\rho_j[j_0j]$$
$$\times\left\langle p'^{\lambda'}_{s};-p'^{s}_{\lambda};\omega\,\middle|\,\begin{matrix}j_0j;\mathscr{s}\\ j\,\mu\end{matrix}\right\rangle\left\langle\begin{matrix}j\,\mu\\ j_0j;\mathscr{s}\end{matrix}\,\middle|\,p^{s}_{\mu'};-p^{\mu}_{s};\omega\right\rangle$$
$$=(4\pi p^2)2\,|p^0|\,\delta^3(\mathbf{p}'-\mathbf{p})\delta^{\lambda'}{}_{\mu'}\delta^{\mu}{}_{\lambda}\qquad(5.60)$$

hinges on the orthogonality and completeness of the matrix realizations (5.25), on the well-known orthogonality and completeness relations for the $SO(3)$ Clebsch-Gordan coefficients, and on the unitarity of the helicity rearrangement transformation ($0\to\omega$).

6. FUTURE EFFORT

Two classes of Poincaré-irreducible tensor operators have been introduced here. In a future paper the connections will be established between these two classes and the Lorentz-irreducible tensor operators which transform by unitary irreducible representations of the pseudo-orthogonal groups $SO(3, 1)$ and $SO(2, 1)$. In that paper we also intend to discuss the decomposition into its Poincaré-irreducible components of a spin density matrix describing a statistical ensemble of wavepackets.

APPENDIX

The relations

$$\exp(\mp i\psi j_{ik})=\mathbb{1}-(j_{ik})^2[1-\cos\gamma]\mp ij_{ik}\sin\gamma,$$
$$\exp(\mp i\beta j_{0i})=\mathbb{1}-(j_{0i})^2[\cosh\beta-1]\mp ij_{0i}\sinh\beta,$$
$$i,k=1,2,3,\qquad(\text{A1})$$

establish the connections between the expressions (2.22) and (2.23) for the orbiting transformations $\Omega_0(\phi,\theta,\gamma)$ and $\Omega_3(\phi,\alpha,\zeta)$ and their matrix realizations:

$$[\Omega_0(\phi,\theta,\gamma)^{\mu}{}_{\nu}]=\begin{bmatrix}\cosh\gamma, & 0, & 0, & -\sinh\gamma\\ -\cos\phi\sin\theta\sinh\gamma, & \cos\phi\cos\theta, & -\sin\phi, & \cos\phi\sin\theta\cosh\gamma\\ -\sin\phi\sin\theta\sinh\gamma, & \sin\phi\cos\theta, & \cos\phi, & \sin\phi\sin\theta\cosh\gamma\\ -\cos\theta\sinh\gamma, & -\sin\theta, & 0, & \cos\theta\cosh\gamma\end{bmatrix},\qquad(\text{A2})$$

$$[\Omega_3(\phi,\alpha,\zeta)^{\mu}{}_{\nu}]=\begin{bmatrix}\cosh\alpha\cosh\zeta, & -\sinh\alpha, & 0, & -\cosh\alpha\sinh\zeta\\ -\cos\phi\sinh\alpha\cosh\zeta, & \cos\phi\cosh\alpha, & -\sin\phi, & \cos\phi\sinh\alpha\sinh\zeta\\ -\sin\phi\sinh\alpha\cosh\zeta, & \sin\phi\cosh\alpha, & \cos\phi, & \sin\phi\sinh\alpha\sinh\zeta\\ -\sinh\zeta, & 0, & 0, & \cosh\zeta\end{bmatrix}.\qquad(\text{A3})$$

The relations

$$p^{\mu}=\pm(p^2)^{\frac{1}{2}}\Omega_{\omega}(p)^{\mu}{}_{0},\quad\omega=0,3,\quad p^2>0,\qquad(\text{A4})$$

and

$$Q^{\mu}=(-Q^2)^{\frac{1}{2}}\Omega_{\omega}(Q)^{\mu}{}_{3},\quad\omega=0,3,\quad Q^2<0,\qquad(\text{A5})$$

then introduce the parametrizations

$$(p^{\mu}_{\omega=0})=\pm(p^2)^{\frac{1}{2}}(\cosh\gamma,-\cos\phi\sin\theta\sinh\gamma,$$
$$-\sin\phi\sin\theta\sinh\gamma,-\cos\theta\sinh\gamma),$$
$$0\le\gamma<\infty,0\le\theta\le\pi,0\le\phi<2\pi,\qquad(\text{A6})$$

and

$$(p^{\mu}_{\omega=3})=\pm(p^2)^{\frac{1}{2}}(\cosh\alpha\cosh\zeta,-\cos\phi\sinh\alpha\cosh\zeta,$$
$$-\sin\phi\sinh\alpha\cosh\zeta,-\sinh\zeta),$$
$$0\le\alpha<\infty,-\infty<\zeta<\infty,0\le\phi<2\pi,\qquad(\text{A7})$$

with the relations between the parameters

$$\cosh\gamma=\cosh\alpha\cosh\zeta,\ \tan\theta=\sinh\alpha/\tanh\zeta,\qquad(\text{A8})$$

$$\tanh\alpha=\sin\theta\tanh\gamma,\ \sinh\zeta=\cos\theta\sinh\gamma;\qquad(\text{A9})$$

they also introduce the parametrizations

$$(Q^{\mu}_{\omega=0})=(-Q^2)^{\frac{1}{2}}(-\sinh\gamma,\cos\phi\sin\theta\cosh\gamma,$$
$$\sin\phi\sin\theta\cosh\gamma,\cos\theta\cosh\gamma),$$
$$-\infty<\gamma<\infty,0\le\theta\le\pi,0\le\phi<2\pi\qquad(\text{A10})$$

and

$$(Q^{\mu}_{\omega=3})=(-Q^2)^{\frac{1}{2}}(-\cosh\alpha\sinh\zeta,\cos\phi\sinh\alpha\sinh\zeta,$$
$$\sin\phi\sinh\alpha\sinh\zeta,\cosh\zeta),$$
$$0\le\alpha<\infty,-\infty<\zeta<\infty,0\le\phi<2\pi,\qquad(\text{A11})$$

with the relations between the parameters

$$\sinh\gamma=\cosh\alpha\sinh\zeta,\ \tan\theta=\sinh\alpha\tanh\zeta,\qquad(\text{A12})$$

$$\tanh\alpha=\sin\theta\coth\gamma,\ \cosh\zeta=\cos\theta\cosh\gamma.\qquad(\text{A13})$$

From these relations it is immediate that the parametrization (A11) covers only the region of the orbit $Q^2<0$ for which $\cos\theta\ge1/\cosh\gamma$.

The relations

$$\Omega_{\omega}(p)^{\mu}{}_{0}=\Omega_{\omega'}(p)^{\mu}{}_{0}\qquad(\text{A14})$$

and

$$\Omega_\omega(Q)^\mu{}_3 = \Omega_{\omega'}(Q)^\mu{}_3, \quad \omega = 0, 3, \quad \omega' = 0, 3 \qquad \text{(A15)}$$

imply that

$$R_{\omega'\omega}(p) \overset{\text{DEF}}{=} \Omega_\omega^{-1}(p)\Omega_{\omega'}(p) \in SO(3) \qquad \text{(A16)}$$

and

$$L_{\omega'\omega}(Q) \overset{\text{DEF}}{=} \Omega_\omega^{-1}(Q)\Omega_{\omega'}(Q) \in SO(2, 1). \qquad \text{(A17)}$$

The transformation relations that connect the three types of momentum-helicity eigenvectors are then of the general form

$$|p_\lambda^s; \omega'\rangle = T(R_{\omega'\omega}(p))\,|p_\lambda^s; \omega\rangle = |p_\mu^s; \omega\rangle\, D^s(R_{\omega'\omega})^\mu{}_\lambda. \qquad \text{(A18)}$$

$D^s(R_{\omega'\omega})$ denotes the $(2s + 1)$-dimensional matrix realization of the transformation group (A16) on the subspace $H[s] \subset H[ms]$. Since the two orbiting transformations associated with a given 4-vector p contain the same ϕ rotation about the 3 axis, it is obvious that

$$D^s(R_{\omega'\omega})^\mu{}_\lambda = d^s(\theta_{\omega'\omega})^\mu{}_\lambda, \qquad \text{(A19)}$$

where

$$d^s(\theta_{\omega'\omega})^\mu{}_\lambda = \left\langle \begin{matrix}\mu\\ s\end{matrix} \right| e^{-i\theta_{\omega'\omega}J_{31}} \left| \begin{matrix}s\\ \lambda\end{matrix} \right\rangle, \quad 0 \le \theta_{\omega'\omega} \le \pi. \qquad \text{(A20)}$$

The angular variable $\theta_{\omega'\omega}$ is determined by the relation

$$e^{-i\theta_{\omega'\omega}j_{31}} = \Omega_\omega^{-1}(p)\Omega_{\omega'}(p). \qquad \text{(A21)}$$

In accordance with the relation (A17), the following transformations hold for each of the two sets of irreducible tensor operators (4.10) and (4.11):

$$(Q, \sigma; \omega')^{\tilde\kappa}{}_\kappa = (Q, \sigma; \omega)^{\tilde\kappa}{}_{\kappa'} D^{-\frac{1}{2}+i\sigma}(L_{\omega'\omega})^{\kappa'}{}_\kappa \qquad \text{(A22)}$$

and

$$(Q, k^\pm; \omega')^{\tilde\kappa}{}_\kappa = (Q, k^\pm; \omega)^{\tilde\kappa}{}_{\kappa'} D^{k^\pm}(L_{\omega'\omega})^{\kappa'}{}_\kappa. \qquad \text{(A23)}$$

The transformation matrices $D^{-\frac{1}{2}+i\sigma}(L_{\omega'\omega})$ and $D^{k^\pm}(L_{\omega'\omega})$ belong to the continuous principal and discrete principal series (4.2a) and (4.2b) of the one-valued unitary irreducible representations of $SU(1, 1)$. From (4.1), (2.22), (2.23), and (A17) it follows that

$$D^{-\frac{1}{2}+i\sigma}(L_{\omega'\omega})^{\kappa'}{}_\kappa = \left\langle \begin{matrix}\kappa'\\ \sigma\end{matrix} \right| e^{-i\xi_{\omega'\omega}J_{01}} \left| \begin{matrix}\sigma\\ \kappa\end{matrix} \right\rangle = d^{-\frac{1}{2}+i\sigma}(\xi_{\omega'\omega})^{\kappa'}{}_\kappa, \qquad \text{(A24)}$$

$$D^{k^\pm}(L_{\omega'\omega}) = \left\langle \begin{matrix}\kappa\\ k^\pm\end{matrix} \right| e^{-i\xi_{\omega'\omega}J_{01}} \left| \begin{matrix}k^\pm\\ \kappa\end{matrix} \right\rangle = d^{k^\pm}(\xi_{\omega'\omega})^{\kappa'}{}_\kappa. \qquad \text{(A25)}$$

The reduced matrix elements $d^{-\frac{1}{2}+i\sigma}(\xi)^{\kappa'}{}_\kappa$ and $d^{k^\pm}(\xi)^{\kappa'}{}_\kappa$ can be expressed in terms of hypergeometric functions: Eqs. (10.27a), (10.27b), (10.28a), (10.28b), (10.29a), (10.29b) of Ref. 2; Eqs. (4.30), (4.31), (4.32) of Ref. 6; Eqs. (3.9)–(3.16) of Ref. 12. The boost parameter $\xi_{\omega'\omega}$ is determined by the equation

$$e^{-i\xi_{\omega'\omega}j_{01}} = \Omega_\omega^{-1}(Q)\Omega_{\omega'}(Q). \qquad \text{(A26)}$$

We refer to the relations (A18), (A22), (A23) as helicity rearrangement transformations.

* This work was performed under the auspices of the U.S. Atomic Energy Commission.

[1] H. Joos, "Complex Angular Momentum and the Representations of the Poincaré Group with Space-like Momentum," *Lectures in Theoretical Physics* (Boulder, Colorado, 1964) (Gordon and Breach, New York, 1965), Vol. VIIA, pp. 132–38.

[2] V. Bargmann, Ann. Math. **48**, 568 (1947).

[3] V. S. Popov, Zh. Eksp.Teor. Fiz. **37**, 1116 (1959) [Sov. Phys. JETP **10**, 794 (1959)].

[4] I. S. Shapiro, Dokl. Akad. Nauk SSSR **106**, 647 (1956) [Sov. Phys. Doklady **1**, 91 (1956)].

[5] Chou Kuang-Chao and L. G. Zastavenko, Zh. Eksp. Teor. Fiz. **35**, 1417 (1958) [Sov. Phys. JETP **8**, 990 (1959)].

[6] J. Strathdee, J. F. Boyce, R. Delbourgo, and A. Salam, International Centre for Theoretical Physics, Trieste, Italy IC/67/9, 1967.

[7] H. Joos and R. S. Schrader, Commun. Math. Phys. **7**, 21 (1968).

[8] A. Böhm, "Rigged Hilbert Space and Mathematical Description of Physical Systems," *Lectures in Theoretical Physics* (Boulder, Colorado, 1966) (Gordon and Breach, New York, 1967), Vol. 9A, pp. 255–317.

[9] E. P. Wigner, Ann. Math. **40**, 39 (1939).

[10] H. Joos, Fortschr. Phys. **10**, 65 (1962).

[11] J. S. Lomont, J. Math. Phys. **1**, 237 (1960).

[12] A. Sciarrino and M. Toller, J. Math. Phys. **8**, 1252 (1967).

[13] L. Sertorio and M. Toller, Nuovo Cimento **33**, 413 (1964).

[14] V. I. Ritus, Zh. Eksp. Teor. Fiz. **40**, 352 (1961) [Sov. Phys. JETP **13**, 240 (1961)].

[15] Harish-Chandra, Proc. Roy. Soc. (London) **A189**, 372 (1947).

[16] M. A. Naimark, *Linear Representations of the Lorentz Group* (Pergamon, New York, 1964).

[17] W. Pauli, "Continuous Groups in Quantum Mechanics," *Springer Tracts in Modern Physics* (Springer-Verlag, Berlin, 1965), Vol. 37, pp. 85–104.

[18] S. Ström, Arkiv Fysik **29**, 467 (1965); **33**, 465 (1966).

[19] W. H. Greiman, Ph.D. thesis, Iowa State University, 1969.

[20] D. V. Duc and N. V. Hieu, Ann. Inst. Henri Poincaré **6**, 17 (1967).

[21] L. C. Biedenharn, Ann. Phys. (N.Y.) **4**, 104 (1958).

[22] M. J. Csonka, M. Moravcsik, and M. D. Scadron, Ann. Phys. (N.Y.) **40**, 100 (1966).

[23] A. D. Steiger and K. J. Fritz, Nuovo Cimento **51**, 461 (1967).

Exact Stationary States in $|\phi|^{2N}$ Field Theories*

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(Received 30 November 1970)

Exact physical solutions to the Schrödinger stationary state equation are reported for local, relativistic, real scalar theories featuring an interaction energy density of the form $g|\phi|^{2N}$, where the coupling constant g is positive and the exponent N is a constant parameter (not necessarily an integer) greater than unity. No interaction or scattering between the field quanta is manifest in the multiparticle state solutions, implying that the real scalar theories are effectively linear in the absence of mass or coupling constant renormalization.

Previous work has shown that exact physical solutions to the Schrödinger stationary state equation can be obtained for local relativistic theories featuring n real scalar fields and an interaction energy density that converges rapidly for large field magnitudes to the form representative of a linear theory.[1] In this work quantization is effected in the Schrödinger picture [with $\phi = \phi(\mathbf{x})$ and its conjugate momentum density $\pi = \pi(\mathbf{x})$ independent of time] and use is made of the "coordinate-diagonal" representation [with $\phi(\mathbf{x})$ diagonalized for all $\mathbf{x}$ and $\pi(\mathbf{x}) = -i\hbar\delta/\delta\phi(\mathbf{x})$, a functional differential operator]. Solutions to the Schrödinger stationary state eigenfunctional equation

$$\mathbf{H}U_\mu[\phi] = E_\mu U_\mu[\phi], \quad (1)$$

$$\mathbf{H} \equiv H\left[\phi(\mathbf{x}), -\frac{i\hbar\delta}{\delta\phi(\mathbf{x})}\right], \quad (2)$$

for the ϕ-dependent part of the wave functional $U_\mu[\phi]$ are obtained as

$$U_\mu[\phi] = \lim_{\epsilon\to 0+} U_\mu^{(\epsilon)}[\phi],$$

in which the positive real parameter

$$\epsilon \equiv [\delta_{(\epsilon)}(\mathbf{0})]^{-1} \quad (3)$$

is associated with a limit representation of the spatial δ function[2]:

$$\lim_{\epsilon\to 0+} \delta_{(\epsilon)}(\mathbf{x}) = \delta(\mathbf{x}).$$

Equation (1) is solved for $U_\mu^{(\epsilon)}[\phi]$ in place of $U_\mu[\phi]$, in conjunction with $\delta_{(\epsilon)}(\mathbf{x})$ in place of $\delta(\mathbf{x})$. The $\epsilon\to 0+$ limit operation is understood to be taken as the final step in all practical computations (scattering cross sections, etc.) involving $U_\mu[\phi]$.

The work reported in the present paper applies this method of solution to real scalar model field theories with Lagrangian densities of the form

$$\mathfrak{L} = \tfrac{1}{2}\dot{\phi}^2 - \tfrac{1}{2}|\nabla\phi|^2 - \tfrac{1}{2}m^2\phi^2 - \tfrac{1}{2}g|\phi|^{2N}, \quad (4)$$

where the mass constant m^2 is nonnegative, the coupling constant g is positive, and the exponent N is a constant parameter (not necessarily an integer) greater than unity. Here, both m^2 (≥ 0) and g (> 0) are regarded as fixed, finite constants with no mass or coupling constant renormalization to be prescribed. From (4) we obtain the quantum Hamiltonian (2) as the second-order functional differential operator

$$\mathbf{H} = \int \frac{1}{2}\left(-\hbar^2\frac{\delta^2}{\delta\phi(\mathbf{x})^2} + |\nabla\phi(\mathbf{x})|^2 + m^2\phi(\mathbf{x})^2 + g|\phi(\mathbf{x})|^{2N}\right)d^3x. \quad (5)$$

The positive (nodeless) vacuum-state eigenfunctional $U_0[\phi]$, associated with the energy

$$E_0 \equiv \min_\mu \{E_\mu\},$$

follows from the ansatz

$$U_0^{(\epsilon)}[\phi] = A^{(\epsilon)}\exp\left(-\hbar^{-1}\int[\tfrac{1}{2}\phi(\mathbf{x})(-\nabla^2 + m^2)^{\frac{1}{2}}\phi(\mathbf{x}) + (N+1)^{-1}g^{\frac{1}{2}}|\phi(\mathbf{x})|^{N+1}]d^3x\right), \quad (6)$$

where the real positive functional $A^{(\epsilon)} = A^{(\epsilon)}[\phi]$ is given by a formal infinite product

$$A^{(\epsilon)} \equiv \prod_{\mathbf{x}} F(\alpha^{(\epsilon)}(\mathbf{x})), \quad (7)$$

$$\alpha^{(\epsilon)}(\mathbf{x}) \equiv \epsilon\hbar^{-1}(N+1)^{-1}g^{\frac{1}{2}}|\phi(\mathbf{x})|^{N+1}. \quad (8)$$

In (7), $F(\alpha)$ is a real function to be determined by the requirement that the $\epsilon\to 0+$ limit of (6) satisfy the Schrödinger equation (1) with the enumerator index $\mu = 0$; $F(\alpha)$ must be positive for all $\alpha \geq 0$ [to foster positivity of the vacuum-state functional (6) for all $\phi(\mathbf{x})$] such that $F(0) = 1$ [to admit existence of the $\epsilon\to 0+$ limit of (7) for uniformly bounded $\phi(\mathbf{x})$]. The functional derivatives of (7) are computed directly as

$$\frac{\delta A^{(\epsilon)}}{\delta\phi(\mathbf{x})} = \hbar^{-1}g^{\frac{1}{2}}\phi(\mathbf{x})\,|\phi(\mathbf{x})|^{N-1}\,F'(\alpha^{(\epsilon)}(\mathbf{x}))\prod_{\mathbf{y}\neq\mathbf{x}}F(\alpha^{(\epsilon)}(\mathbf{y}))$$
$$= \hbar^{-1}g^{\frac{1}{2}}\phi(\mathbf{x})\,|\phi(\mathbf{x})|^{N-1}\,\frac{F'(\alpha^{(\epsilon)}(\mathbf{x}))}{F(\alpha^{(\epsilon)}(\mathbf{x}))}\,A^{(\epsilon)}, \quad (9)$$

$$\frac{\delta^2 A^{(\epsilon)}}{\delta\phi(\mathbf{x})^2} = [\epsilon^{-1}\hbar^{-1}Ng^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N-1}\,F'(\alpha^{(\epsilon)}(\mathbf{x})) + \hbar^{-2}g\,|\phi(\mathbf{x})|^{2N}\,F''(\alpha^{(\epsilon)}(\mathbf{x}))]\prod_{\mathbf{y}\neq\mathbf{x}}F(\alpha^{(\epsilon)}(\mathbf{y}))$$
$$= \epsilon^{-2}\phi(\mathbf{x})^{-2}\left((N^2+N)\alpha^{(\epsilon)}(\mathbf{x})\frac{F'(\alpha^{(\epsilon)}(\mathbf{x}))}{F(\alpha^{(\epsilon)}(\mathbf{x}))} + (N+1)^2\alpha^{(\epsilon)}(\mathbf{x})^2\frac{F''(\alpha^{(\epsilon)}(\mathbf{x}))}{F(\alpha^{(\epsilon)}(\mathbf{x}))}\right)A^{(\epsilon)}, \quad (10)$$

where use is made of the functional differentiation chain-rule and condition (3) through the relation $\delta\phi(\mathbf{x})/\delta\phi(\mathbf{x}) = \delta_{(\epsilon)}(\mathbf{0}) = \epsilon^{-1}$. By employing the latter formulas (9) and (10), we obtain the functional derivatives of (6) as

$$\frac{\delta U_0^{(\epsilon)}[\phi]}{\delta\phi(\mathbf{x})} = \hbar^{-1}[g^{\frac{1}{2}}\phi(\mathbf{x})\,|\phi(\mathbf{x})|^{N-1}\,R(\alpha^{(\epsilon)}(\mathbf{x})) - (-\nabla^2+m^2)^{\frac{1}{2}}\phi(\mathbf{x})]U_0^{(\epsilon)}[\phi], \quad (11)$$

where

$$R(\alpha) \equiv [F'(\alpha)/F(\alpha)] - 1 \quad (12)$$

and

$$\frac{\delta^2 U_0^{(\epsilon)}[\phi]}{\delta\phi(\mathbf{x})^2} = \{\epsilon^{-1}\hbar^{-1}(N+1)g^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N-1}\,S(\alpha^{(\epsilon)}(\mathbf{x})) - 2\hbar^{-2}g^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N}\,|(-\nabla^2+m^2)^{\frac{1}{2}}\phi(\mathbf{x})| \times R(\alpha^{(\epsilon)}(\mathbf{x})) + \hbar^{-2}[(-\nabla^2+m^2)^{\frac{1}{2}}\phi(\mathbf{x})]^2 + \hbar^{-2}g\,|\phi(\mathbf{x})|^{2N} - \hbar^{-1}[(-\nabla^2+m^2)^{\frac{1}{2}}\delta_{(\epsilon)}(\mathbf{x})]_{\mathbf{x}=0}\}U_0^{(\epsilon)}[\phi], \quad (13)$$

where

$$S(\alpha) \equiv \alpha[F''(\alpha)/F(\alpha)] + [(N+1)^{-1}N - 2\alpha] \times [F'(\alpha)/F(\alpha)] - (N+1)^{-1}N. \quad (14)$$

Therefore, it follows from (5) and (6) that

$$\mathbf{H}U_0^{(\epsilon)}[\phi] = \int\{-\tfrac{1}{2}\epsilon^{-1}\hbar(N+1)g^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N-1}\,S(\alpha^{(\epsilon)}(\mathbf{x})) + g^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N}\,|(-\nabla^2+m^2)^{\frac{1}{2}}\phi(\mathbf{x})|\,R(\alpha^{(\epsilon)}(\mathbf{x})) + \tfrac{1}{2}\hbar[(-\nabla^2+m^2)^{\frac{1}{2}}\delta_{(\epsilon)}(\mathbf{x})]_{\mathbf{x}=0}\}d^3x\,U_0^{(\epsilon)}[\phi]. \quad (15)$$

Hence, in order for $U_0[\phi] = \lim U_0^{(\epsilon)}[\phi]$ as $\epsilon \to 0+$ to satisfy the vacuum-state Schrödinger equation, we must have

$$E_0 = \lim_{\epsilon\to 0+}\tfrac{1}{2}\hbar[(-\nabla^2+m^2)^{\frac{1}{2}}\delta_{(\epsilon)}(\mathbf{x})]_{\mathbf{x}=0}\int d^3x, \quad (16)$$

the quantity (14) must vanish identically for all $\alpha \geq 0$, or equivalently $F(\alpha)$ must satisfy the ordinary differential equation

$$\alpha F''(\alpha) + [(N+1)^{-1}N - 2\alpha]F'(\alpha) - (N+1)^{-1} \times NF(\alpha) = 0, \quad (17)$$

and finally the quantity (12) must satisfy conditions of the form

$$|R(\alpha)| \leq 1, \quad \text{for all} \quad \alpha \geq 0, \quad (18)$$

$$\lim_{\alpha\to 0} R(\alpha) = 0. \quad (19)$$

Condition (18) guarantees that the second term in the integrand on the right side of (15) is dominated by the final three terms in the Hamiltonian integrand (5) for all $\phi(\mathbf{x})$ by virtue of the inequality

$$g^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N}\,|(-\nabla^2+m^2)^{\frac{1}{2}}\phi(\mathbf{x})| \leq [|(-\nabla^2+m^2)^{\frac{1}{2}}\phi(\mathbf{x})|^2 + g\,|\phi(\mathbf{x})|^{2N}]/\max\{2, r, r^{-1}\},$$

where

$$r \equiv |(-\nabla^2+m^2)^{\frac{1}{2}}\phi(\mathbf{x})|/g^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N},$$

while condition (19) is required for the second term in the integrand of (15) to vanish in the limit $\epsilon \to 0+$ for uniformly bounded $|\phi(\mathbf{x})|$. If a real positive $F(\alpha)$ exists as a solution to (17) and satisfies conditions (18), (19), and $F(0) = 1$, then the ansatz (6) provides the vacuum-state eigenfunctional solution to the Schrödinger equation. Such an $F(\alpha)$ is indeed found by solving (17), and we obtain

$$F(\alpha) = \Gamma(1-\nu)e^{\alpha}(\alpha/2)^{\nu}I_{-\nu}(\alpha), \quad (20)$$

in which the parameter

$$\nu \equiv [2(N+1)]^{-1} \quad (21)$$

is positive and less than $\frac{1}{4}$, $\Gamma(1-\nu)$ is standard notation for the gamma function of $(1-\nu)$, and $I_{-\nu}(\alpha) \equiv e^{i\pi\nu/2}J_{-\nu}(i\alpha)$ is the hyperbolic Bessel function with the infinite series representation[3]

$$I_{-\nu}(\alpha) = \sum_{k=0}^{\infty}\frac{1}{k!\,\Gamma(k+1-\nu)}\left(\frac{\alpha}{2}\right)^{2k-\nu} \quad (22)$$

and the asymptotic expansion for large positive α

$$I_{-\nu}(\alpha) = [e^{\alpha}/(2\pi\alpha)^{\frac{1}{2}}][1 + (\tfrac{1}{4}-\nu^2)(2\alpha)^{-1} + O(\alpha^{-2})]. \quad (23)$$

By putting expression (20) into (12), we find that

$$R(\alpha) = \nu\alpha^{-1} + [I'_{-\nu}(\alpha)/I_{-\nu}(\alpha)] = \begin{cases}[2(1-\nu)]^{-1}\alpha + O(\alpha^3) & \text{for } 0 \leq \alpha \ll 1\\ 1 - (\tfrac{1}{2}-\nu)\alpha^{-1} + O(\alpha^{-2}) & \text{for } \alpha \gg 1\end{cases}, \quad (24)$$

$$0 \leq R(\alpha) \leq 1 \quad \text{for all} \quad \alpha \geq 0, \quad (25)$$

and thus conditions (18) and (19) are satisfied. Hence, the $\epsilon \to 0+$ limit of (6) with (20) in (7) is the vacuum-state eigenfunctional solution to the Schrödinger equation (1).

Excited-state eigenfunctional solutions to (1) are conveniently expressed as[1]

$$U_\mu[\phi] = \Omega_\mu[\phi]U_0[\phi], \tag{26}$$

where

$$\Omega_\mu[\phi] = \lim_{\epsilon\to 0+} \Omega_\mu^{(\epsilon)}[\phi]$$

is obtained by solving the functional differential equation

$$\hbar^2 \int \left(-\frac{1}{2}\frac{\delta^2}{\delta\phi(\mathbf{x})^2} - \frac{\delta(\ln U_0^{(\epsilon)}[\phi])}{\delta\phi(\mathbf{x})}\frac{\delta}{\delta\phi(\mathbf{x})}\right) d^3x\, \Omega_\mu^{(\epsilon)}[\phi] = (E_\mu - E_0)\Omega_\mu^{(\epsilon)}[\phi], \tag{27}$$

which, in view of (11), becomes

$$\int \left(-\frac{\hbar^2}{2}\frac{\delta^2\Omega_\mu^{(\epsilon)}[\phi]}{\delta\phi(\mathbf{x})^2} + \hbar[\phi(\mathbf{x})(-\nabla^2 + m^2)^{\frac{1}{2}} - g^{\frac{1}{2}}\phi(\mathbf{x})\,|\phi(\mathbf{x})|^{N-1} R(\alpha^{(\epsilon)}(\mathbf{x}))]\frac{\delta\Omega_\mu^{(\epsilon)}[\phi]}{\delta\phi(\mathbf{x})}\right) d^3x = (E_\mu - E_0)\Omega_\mu^{(\epsilon)}[\phi]. \tag{28}$$

For fields which are uniformly bounded in absolute magnitude by an arbitrarily large positive constant M, the quantity (8) is small compared to unity for all $\mathbf{x}$ if we take ϵ to be sufficiently small, i.e., $\epsilon \ll \hbar(N+1)g^{-\frac{1}{2}}M^{-(N+1)}$. Then it follows from (24) that

$$R(\alpha^{(\epsilon)}(\mathbf{x})) = \epsilon\hbar^{-1}(2N+1)^{-1}g^{\frac{1}{2}}\,|\phi(\mathbf{x})|^{N+1} + O(\alpha^{(\epsilon)}(\mathbf{x})^3), \tag{29}$$

and the solutions to (28) with (29) are obtained as

$$\Omega_\mu^{(\epsilon)}[\phi] = \bar{\Omega}_\mu[\hat{\phi}] + O(\epsilon^3), \tag{30}$$

in which the "dressed" field

$$\hat{\phi} \equiv [1 - \epsilon^2\hbar^{-2}(N+1)^{-1}(2N+1)^{-1} \times (2N+3)^{-1}g\,|\phi|^{2N+2}]\phi \tag{31}$$

appears as the argument of a μth-order polynomial functional $\bar{\Omega}_\mu[\hat{\phi}]$. The latter functional $\bar{\Omega}_\mu[\hat{\phi}]$ describes a μ-particle state without interaction or scattering between the field quanta, as exemplified by the familiar one-particle form

$$\bar{\Omega}_1[\hat{\phi}] = \int \xi(\mathbf{x})\hat{\phi}(\mathbf{x})d^3x,$$

$$[\hbar(-\nabla^2 + m^2)^{\frac{1}{2}} - (E_1 - E_0)]\xi(\mathbf{x}) = 0, \tag{32}$$

where $\xi(\mathbf{x})$ is a one-particle (spin-0) relativistic scalar wavefunction, and the two-particle form

$$\bar{\Omega}_2[\hat{\phi}] = \tfrac{1}{2}\int \hat{\phi}(\mathbf{x})\zeta(\mathbf{x},\mathbf{y})\hat{\phi}(\mathbf{y})d^3x\,d^3y - \tfrac{1}{2}\hbar^2(E_2 - E_0)^{-1}\int \zeta(\mathbf{x},\mathbf{x})d^3x,$$

$$[(-\nabla_{\mathbf{x}}^2 + m^2)^{\frac{1}{2}} + (-\nabla_{\mathbf{y}}^2 + m^2)^{\frac{1}{2}} - \hbar^{-1}(E_2 - E_0)]\zeta(\mathbf{x},\mathbf{y}) = 0, \tag{33}$$

where $\zeta(\mathbf{x},\mathbf{y}) \equiv \zeta(\mathbf{y},\mathbf{x})$ is a two-particle (spin-0 boson) relativistic scalar wavefunction. To verify that the expressions (30) satisfy (28) with (29), we compute the functional derivatives[4]

$$\frac{\delta\Omega_\mu^{(\epsilon)}[\phi]}{\delta\phi(\mathbf{x})} = \frac{\delta\bar{\Omega}_\mu[\hat{\phi}]}{\delta\hat{\phi}(\mathbf{x})}[1 - \epsilon^2\hbar^{-2}(N+1)^{-1} \times (2N+1)^{-1}g\,|\phi(\mathbf{x})|^{2N+2}] + O(\epsilon^3), \tag{34}$$

$$\frac{\delta^2\Omega_\mu^{(\epsilon)}[\phi]}{\delta\phi(\mathbf{x})^2} = \frac{\delta^2\bar{\Omega}_\mu[\hat{\phi}]}{\delta\hat{\phi}(\mathbf{x})^2} - 2\epsilon\hbar^{-2}(2N+1)^{-1}g\phi(\mathbf{x}) \times |\phi(\mathbf{x})|^{2N}\frac{\delta\bar{\Omega}_\mu[\hat{\phi}]}{\delta\hat{\phi}(\mathbf{x})} + O(\epsilon^2) \tag{35}$$

and make use of the free-field functional differential equation satisfied by $\bar{\Omega}_\mu[\hat{\phi}]$,

$$\int \left(-\frac{\hbar^2}{2}\frac{\delta^2}{\delta\hat{\phi}(\mathbf{x})^2} + \hbar\hat{\phi}(\mathbf{x})(-\nabla^2 + m^2)^{\frac{1}{2}}\frac{\delta}{\delta\hat{\phi}(\mathbf{x})}\right) d^3x\,\bar{\Omega}_\mu[\hat{\phi}] = (E_\mu - E_0)\bar{\Omega}_\mu[\hat{\phi}]. \tag{36}$$

Hence, the $\epsilon \to 0+$ limit of (30) yields the prefactor $\Omega_\mu[\phi]$ on the right side of (26). Since there is no interaction or scattering between the field quanta manifest in the multiparticle state solutions (30), the real scalar field theories with Lagrangian densities of the form (4) are effectively linear in the absence of mass or coupling constant renormalization.[5]

* Work supported by a National Science Foundation grant.

[1] G. Rosen, J. Math. Phys. **11**, 536 (1970).

[2] For example, we have the wavenumber cutoff representation

$$\delta_{(\epsilon)}(\mathbf{x}) \equiv \int_{|\mathbf{k}|\le K} (\exp i\mathbf{k}\cdot\mathbf{x})d^3k/(2\pi)^3 \quad \text{with} \quad K \equiv (6\pi^2/\epsilon)^{\frac{1}{3}}.$$

[3] I. S. Gradshteyn and I. M. Ryzik, *Tables of Integrals, Series and Products* (Academic, New York, 1965), p. 961.

[4] In passing from (34) to (35), the second functional differentiation at $\mathbf{x}$ is expected to modify the $O(\epsilon^3)$ term in (34) by a factor ϵ^{-1}.

[5] To perform renormalization within the theoretical framework employed here, the mass and coupling constants are prescribed as appropriate functions of ϵ, and the latter parameter is related to a wavenumber cutoff.[2] Approximate solutions to such renormalized model scalar theories have been obtained by G. Rosen, Phys. Rev. **173**, 1680 (1968), and J. A. Okolowski, Ph.D. thesis, Drexel University, 1969.

Transmission of Electromagnetic Waves through a Conducting Plasma Slab*

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Some new approaches to the problem of transmission of electromagnetic waves through a finite conducting plasma slab, as formulated by Baraff, are presented. The two-point boundary value problem for the integro-differential equation of nonlocal wave interaction is reduced to a Cauchy system. It is pointed out that under circumstances where computational difficulties may be expected to occur with this Cauchy system a transformation to rotating coordinates will be beneficial. Consequently, a Cauchy system is derived for rotationally transformed equations also. Some alternative approaches are discussed, and an approximate perturbation formula is derived.

1. INTRODUCTION

In a recent series of papers, Baraff[1–3] has formulated and solved, by means of a Wiener–Hopf technique, the two-point boundary value problem for the transmission of electromagnetic waves through a conducting plasma slab of finite thickness subject to diffuse reflections at the boundaries. More recently, Kalaba[4] has shown how such a problem may be transformed into a Cauchy system, i.e., an initial value problem. However, the boundary conditions assumed by Kalaba were chosen for their mathematical simplicity rather than their physical realizability. It is the purpose of this paper to extend Kalaba's treatment to apply to the physical situation considered by Baraff, and also to explore some other feasible methods of treating this problem.

In Sec. 2 a mathematical statement of the two-point boundary value problem is given and transformed to a coupled pair of integro-differential equations. In Sec. 3 the equivalent Cauchy system is stated, a derivation of which follows in Sec. 4. In Sec. 5 it is pointed out that under some circumstances (such as a very dilute plasma, or very short wavelength radiation) computational difficulties with this Cauchy system may be expected to occur. To overcome this drawback, a transformation to rotating coordinates is made. In Sec. 6 the Cauchy system for the rotationally transformed problem is stated, and the derivation is given in Sec. 7. In Sec. 8, some iterative techniques are described as alternative methods for solving the rotationally transformed equation, and a useful approximate perturbation formula is derived.

In Appendices A and B, the Cauchy systems of Secs. 3 and 6, respectively, are validated. That is, it is shown that a solution to the Cauchy system must satisfy the original two-point boundary value problem.

2. STATEMENT OF BOUNDARY VALUE PROBLEM

Following Baraff[1–3] and Kalaba,[4] we imagine an infinite slab of plasma media of thickness x within which the electric field $e(t)$ is assumed to satisfy the following nonlocal reduced wave equation:

$$\ddot{e}(t) + k^2 e(t) = \int_0^x K(|t-y|)e(y)\,dy, \quad 0 \le t \le x. \quad (1)$$

Here the independent variable t, $0 \le t \le x$, specifies a position within the slab, while k is a constant such that $2\pi/k$ is the wavelength in the absence of the nonlocal interaction. With no essential loss in generality, we assume that the nonlocal-interaction kernel $K(r)$ may be represented as a linear superposition of exponentials[4]:

$$K(r) = \int_a^b e^{-r/z} w(z)\,dz, \quad r \ge 0. \quad (2)$$

We suppose that a plane wave of unit amplitude propagating toward the left is normally incident on the right face of the slab at $t = x$. The appropriate boundary conditions are then[5]

$$e(0) - i\dot{e}(0)/k = 0, \quad (3a)$$

$$e(x) + i\dot{e}(x)/k = 2. \quad (3b)$$

Equations (1), (2), and (3) then completely determine $e(t)$ within the slab.

It is advantageous to express these equations as an equivalent set of coupled first-order differential equations for quantities $u(t)$ and $v(t)$ defined by

$$u(t) \equiv e(t) - i\dot{e}(t)/k, \quad (4a)$$

$$v(t) \equiv e(t) + i\dot{e}(t)/k. \quad (4b)$$

Thus (1) and (3) become

$$\dot{u}(t) = iku(t) - i\int_0^x R(|t-y|)[u(y)+v(y)]\,dy, \quad (5a)$$

$$\dot{v}(t) = -ikv(t) + i\int_0^x R(|t-y|)[u(y)+v(y)]\,dy, \quad (5b)$$

and

$$u(0) = 0, \quad (6a)$$

$$v(0) = 2, \quad (6b)$$

where $R(|t-y|)$ is defined by

$$R(|t-y|) = (2k)^{-1}K(|t-y|). \tag{7}$$

That is, by (2), $R(r)$ is represented by

$$R(r) = \int_a^b e^{-r/z}\rho(z)\,dz, \quad r \geq 0, \tag{8}$$

where

$$\rho(z) \equiv (2k)^{-1}w(z). \tag{9}$$

Of particular interest are the transmitted wave at $t = 0$ and the reflected wave at $t = x$,

$$v(0) = e(0) + i\dot{e}(0)/k \tag{10a}$$

and

$$u(x) = e(x) - i\dot{e}(x)/k, \tag{10b}$$

respectively.

3. STATEMENT OF EQUIVALENT CAUCHY SYSTEM

In Eqs. (5) and (6) we replace $u(t)$ and $v(t)$ by $u(t, x)$ and $v(t, x)$, respectively, in order to explicitly exhibit their dependence upon the thickness of the slab x:

$$\dot{u}(t,x) = iku(t,x) - i\int_0^x R(|t-y|)[u(y,x)+v(y,x)]\,dy, \tag{11a}$$

$$\dot{v}(t,x) = -ikv(t,x) + i\int_0^x R(|t-y|)[u(y,x)+v(y,x)]\,dy, \tag{11b}$$

$$u(0,x) = 0, \tag{12a}$$

$$v(x,x) = 2. \tag{12b}$$

Then, with $R(|t-t'|)$ given by (7) or (8), it will be shown in Sec. 4 that the reflected component

$$u(x) \equiv u(x,x) \tag{13}$$

is determined by the following Cauchy system for the quantities $u(x)$, $E(x, z')$, $H(x, z, z')$, and $I(x, z)$:

$$u_x(x) = 2iku(x) - ig(x)\int_a^b \rho(z)[\tfrac{1}{2}E(x,z) + I(x,z)]\,dz, \tag{14}$$

$$u(0) = 0, \tag{15}$$

$$E_x(x,z') = [ik - (z')^{-1}]E(x,z') + g(x) - \tfrac{1}{2}iE(x,z')\int_a^b \rho(z)E(x,z)\,dz - ig(x)\int_a^b \rho(z)H(x,z,z')\,dz, \tag{16}$$

$$E(0,z') = 0, \tag{17}$$

$$H_x(x,z,z') = -[z^{-1} + (z')^{-1}]H(x,z,z') + I(x,z)\left(1 - i\int_a^b \rho(z)H(x,z,z')\,dz\right) + \tfrac{1}{2}E(x,z') \times \left(1 - i\int_a^b \rho(z')H(x,z,z')\,dz'\right), \tag{18}$$

$$H(0,z,z') = 0, \tag{19}$$

$$I_x(x,z) = (ik - z^{-1})I(x,z) - iI(x,z)\int_a^b \rho(z')I(x,z')\,dz' + \tfrac{1}{2}g(x)\left(1 - i\int_a^b \rho(z')H(x,z,z')\,dz'\right), \tag{20}$$

$$I(0,z) = 0. \tag{21}$$

Here, as well as in what follows, the subscript x denotes differentiation with respect to x. The quantity $g(x)$ appearing in Eqs. (14)–(21) is defined by

$$g(x) \equiv u(x) + 2. \tag{22}$$

With the solution to these equations known, the quantities $u(t, x)$ and $v(t, x)$ are then obtained as the solution to the following Cauchy system in x for fixed t, $0 \leq t \leq x$, in the variables $u(t, x)$, $v(t, x)$, $I(t, x, z)$, and $J(t, x, z)$:

$$u_x(t,x) = iku(t,x) - \tfrac{1}{2}iu(t,x)\int_a^b \rho(z)E(x,z)\,dz - ig(x)\int_a^b \rho(z)I(t,x,z)\,dz, \tag{23}$$

$$u(t,t) = u(t), \tag{24}$$

$$v_x(t,x) = ikv(t,x) - \tfrac{1}{2}iv(t,x)\int_a^b \rho(z)E(x,z)\,dz - ig(x)\int_a^b \rho(z)J(t,x,z)\,dz, \tag{25}$$

$$v(t,t) = 2, \tag{26}$$

$$I_x(t,x,z) = \tfrac{1}{2}u(t,x)\left(1 - i\int_a^b \rho(z')H(x,z,z')\,dz'\right) - z^{-1}I(t,x,z) - iI(x,z)\int_a^b \rho(z')I(t,x,z')\,dz', \tag{27}$$

$$I(t,t,z) = I(t,z), \tag{28}$$

$$J_x(t,x,z) = \tfrac{1}{2}v(t,x)\left(1 - i\int_a^b \rho(z')H(x,z,z')\,dz'\right) - z^{-1}J(t,x,z) - iI(x,z)\int_a^b \rho(z')J(t,x,z')\,dz', \tag{29}$$

$$J(t,t,z) = 0. \tag{30}$$

These equations have much the same structure as those of Ref. 4, and the discussion of the computational aspects given there will apply here as well. Observe that the transmitted component $v(0, x)$ may be obtained by solving (25), (26), (29), and (30) with t set equal to zero.

4. DERIVATION OF CAUCHY SYSTEM

The derivation makes much use of the principle of superposition for linear systems.

Differentiating the basic equations (9) and (10) with respect to x, one obtains

$$\dot{u}_x(t, x) = iku_x(t, x) - iR(x - t)g(x) - i\int_0^x R(|t - y|)[u_x(y, x) + v_x(y, x)]\,dy, \tag{31a}$$

$$\dot{v}_x(t, x) = -ikv_x(t, x) + iR(x - t)g(x) + i\int_0^x R(|t - y|)[u_x(y, x) + v_x(y, x)]\,dy, \tag{31b}$$

$$u_x(0, x) = 0, \tag{32a}$$

$$v_x(x, x) = -\dot{v}(x, x). \tag{32b}$$

In obtaining (31a) and (31b), we have used (12b) and definition (22) for $g(x)$. In (32b) and similar expressions which follow, $v_x(x, x)$ denotes differentiation with respect to the *second* argument in x, while $\dot{v}(x, x)$ denotes differentiation with respect to the first argument in x.

Now let $I(t, x, z)$ and $J(t, x, z)$ be solutions to the nonhomogeneous differential equations

$$\dot{I}(t, x, z) = ikI(t, x, z) + e^{-(x-t)/z} - i\int_0^x R(|t - y|)[I(y,x,z) + J(y,x,z)]\,dy, \tag{33a}$$

$$\dot{J}(t, x, z) = -ikJ(t, x, z) - e^{-(x-t)/z} + i\int_0^x R(|t - y|)[I(y,x,z) + J(y,x,z)]\,dy, \tag{33b}$$

subject to the homogeneous boundary conditions

$$I(0, x, z) = 0, \tag{34a}$$

$$J(x, x, z) = 0. \tag{34b}$$

Regarding (31) as an inhomogeneous set of linear differential equations in t for $u_x(t, x)$ and $v_x(t, x)$ subject to the inhomogeneous boundary condition (32), we see that it follows from the principle of superposition [and Eqs. (8), (11), (12), (33), and (34)] that

$$u_x(t, x) = -\tfrac{1}{2}\dot{v}(x, x)u(t, x) - ig(x)\int_a^b \rho(z)I(t, x, z)\,dz, \tag{35a}$$

$$v_x(t, x) = -\tfrac{1}{2}\dot{v}(x, x)v(t, x) - ig(x)\int_a^b \rho(z)J(t, x, z)\,dz. \tag{35b}$$

Next, differentiating (33) and (34) with respect to x, we obtain

$$\dot{I}_x(t, x, z) = ikI_x(t, x, z) - z^{-1}e^{-(x-t)/z} - iR(x - t)I(x, z) - i\int_0^x R(|t - y|) \times [I_x(y, x, z) + J_x(y, x, z)]\,dy, \tag{36a}$$

$$\dot{J}_x(t, x, z) = -ikJ_x(t, x, z) + z^{-1}e^{-(x-t)/z} + iR(x - t)I(x, z) + i\int_0^x R(|t - y|) \times [I_x(y, x, z) + J_x(y, x, z)]\,dy, \tag{36b}$$

$$I_x(0, x, z) = 0, \tag{37a}$$

$$J_x(x, x, z) = -\dot{J}(x, x, z), \tag{37b}$$

where $I(x, z)$ is defined by

$$I(x, z) \equiv I(x, x, z) \tag{38}$$

and we have used (34b).

Again employing the principle of superposition in the same way as above, one finds that $I_x(t, x, z)$ and $J_x(t, x, z)$ must satisfy

$$I_x(t, x, z) = -\tfrac{1}{2}\dot{J}(x, x, z)u(t, x) - z^{-1}I(t, x, z) - iI(x, z)\int_a^b \rho(z')I(t, x, z')\,dz', \tag{39a}$$

$$J_x(t, x, z) = -\tfrac{1}{2}\dot{J}(x, x, z)v(t, x) - z^{-1}J(t, x, z) - iI(x, z)\int_a^b \rho(z')J(t, x, z')\,dz'. \tag{39b}$$

To proceed further, we define quantities $E(x, z')$ and $H(x, z, z')$ by

$$E(x, z') \equiv \int_0^x e^{-(x-y)/z'}[u(y, x) + v(y, x)]\,dy \tag{40}$$

and

$$H(x, z, z') \equiv \int_0^x e^{-(x-y)/z'}[I(y, x, z) + J(y, x, z)]\,dy. \tag{41}$$

Then setting $t = x$ in Eqs. (11a), (11b), (33a), and (33b), and making use of (7) and (34b), we obtain the following equations for $\dot{u}(x, x)$, $\dot{v}(x, x)$, $\dot{I}(x, x, z)$, and $\dot{J}(x, x, z)$, respectively:

$$\dot{u}(x, x) = iku(x) - i\int_a^b \rho(z')E(x, z')\,dz', \tag{42a}$$

$$\dot{v}(x, x) = -2ik + i\int_a^b \rho(z')E(x, z')\,dz', \tag{42b}$$

$$\dot{I}(x, x, z) = ikI(x, z) + 1 - i\int_a^b \rho(z')H(x, z, z')\,dz', \tag{43a}$$

$$\dot{J}(x, x, z) = -1 + i\int_a^b \rho(z')H(x, z, z')\,dz'. \tag{43b}$$

We are now ready to derive the Cauchy system expressed by Eqs. (14)–(21) for the quantities $u(x)$, $E(x, z')$, $H(x, z, z')$, and $I(x, z)$.

Differentiating (13) with respect to x,

$$u_x(x) = \dot{u}(x, x) + u_x(x, x), \tag{44}$$

and using Eqs. (42), (35a), and (22), one obtains Eq. (14). The initial condition (15) for $u(x)$ follows from (12a).

Differentiating (40) with respect to x and using (22), one obtains

$$E_x(x, z') = (-z')^{-1}E(x, z') + g(x) + \int_0^x e^{-(x-y)/z'}[u_x(y, x) + v_x(y, x)]\,dy. \tag{45}$$

Substituting Eqs. (35) for $u_x(y, x)$ and $v_x(y, x)$ into the integrand of (45) and using (40), (41), and (42b), one obtains Eq. (16). The initial condition (17) for $E(x, z')$ follows from (40).

Differentiating (41) with respect to x and using Eqs. (38), one obtains

$$H_x(x, z, z') = (-z')^{-1}H(x, z, z') + I(x, z) + \int_0^x e^{-(x-y)/z'}[I_x(y, x, z) + J_x(y, x, z)]\,dy. \tag{46}$$

Substituting Eqs. (39) for $I_x(y, x, z)$ and $J_x(y, x, z)$ into the integrand of (46) and using (40), (41), and (43b), one obtains Eq. (18). The initial condition (19) for $H(x, z, z')$ follows from the definition (41).

Differentiating (38a) with respect to x,

$$I_x(x, z) = \dot{I}(x, x, z) + I_x(x, x, z), \tag{47}$$

and using Eqs. (43) and (39), one obtains Eq. (20). The initial condition (21) follows from (34a). This completes the derivation of the Cauchy system (14)–(21).

We now derive the Cauchy system (23)–(30) for the quantities $u(t, x)$, $v(t, x)$, $I(t, x, z)$, and $J(t, x, z)$. Equations (23) and (25) follow immediately from (35) and (42b). The initial conditions (24) and (26) follow from (13) and (12b), respectively. Equations (27) and (29) follow immediately from (39) and (43b). The initial conditions (28) and (30) follow from Eqs. (38) and (34b). This completes the derivation of the Cauchy system.

5. TRANSFORMATION TO ROTATING COORDINATES

Under certain circumstances, it may well happen that the second term in Eq. (11a) or (11b) will be much smaller than the first. This will be the case, for example, if the plasma is very dilute or if the wavelength ($= 2\pi/k$) is very small. [See also Eq. (17).] Under such circumstances, attempts at practical calculations using the Cauchy system we have just derived may fail owing to the small nonlocal-interaction terms being masked by computational inaccuracies in the ordinary wave terms. To cope with this situation, we make a rotating-coordinate transformation in order to effectively factor out the part of the solution not due to the nonlocal interaction.

We thus transform from the variables $u(t, x)$ and $v(t, x)$ to new variables $p(t, x)$ and $q(t, x)$ defined by

$$p(t, x) \equiv e^{-ik(x+t)}u(t, x), \tag{48a}$$

$$q(t, x) \equiv e^{-ik(x-t)}v(t, x). \tag{48b}$$

Our basic equations (11) and (12) then become

$$-e^{ikt}\dot{p}(t, x) = e^{-ikt}\dot{q}(t, x) = i\int_0^x R(|t - y|) \times [e^{iky}p(y, x) + e^{-iky}q(y, x)]\,dy, \tag{49}$$

$$p(0, x) = 0, \tag{50a}$$

$$q(x, x) = 2. \tag{50b}$$

6. STATEMENT OF EQUIVALENT CAUCHY SYSTEM

The reflected component in the transformed system,

$$p(x) \equiv p(x, x) = e^{-2ikx}u(x), \tag{51}$$

is determined by the following Cauchy system for the quantities $p(x)$, $L(x, z')$, $K(x, z, z')$, and $I(x, z)$ (here, and in succeeding sections, definitions given for various quantities in Secs. 3 and 4 no longer apply):

$$p_x(x) = -if(x)\int_a^b \rho(z')[L(x, z') + 2I(x, z')]\,dz', \tag{52}$$

$$p(0) = 0, \tag{53}$$

$$L_x(x, z') = -(1/z')L(x, z') + 2f(x) - 2if(x)\int_a^b \rho(z)K(x, z, z')\, dz - \tfrac{1}{2}ie^{ikx}L(x, z')\int_a^b \rho(z)L(x, z)\, dz, \quad (54)$$

$$L(0, z) = 0, \quad (55)$$

$$K_x(x, z, z') = \tfrac{1}{2}L(x, z') \times e^{ikx}\left(1 - i\int_a^b \rho(z')K(x, z, z')\, dz'\right) + I(x, z)e^{ikx}\left(1 - i\int_a^b \rho(z)K(x, z, z')\, dz\right) - [z^{-1} + (z')^{-1}]K(x, z, z'), \quad (56)$$

$$K(0, z, z') = 0, \quad (57)$$

$$I_x(x, z) = -z^{-1}I(x, z) - ie^{ikx}I(x, z)\int_a^b \rho(z')I(x, z')\, dz' + f(x) - if(x)\int_a^b \rho(z')K(x, z, z')\, dz', \quad (58)$$

$$I(0, z) = 0. \quad (59)$$

Here the quantity $f(x)$ is defined by

$$f(x) \equiv \tfrac{1}{2}e^{ikx}p(x) + e^{-ikx}. \quad (60)$$

With the solution to these equations known, the quantities $p(t, x)$ and $q(t, x)$ are then obtained as the solution to the following Cauchy system in x for fixed t, $0 \le t \le x$, in the variables $p(t, x)$, $q(t, x)$, $I(t, x, z)$, and $J(t, x, z)$:

$$p_x(t, x) = -2if(x)\int_a^b \rho(z')I(t, x, z')\, dz' - \tfrac{1}{2}ip(t, x)e^{ikx}\int_a^b \rho(z')L(x, z')\, dz', \quad (61)$$

$$p(t, t) = p(t), \quad (62)$$

$$q_x(t, x) = -2if(x)\int_a^b \rho(z')J(t, x, z')\, dz' - \tfrac{1}{2}iq(t, x)e^{ikx}\int_a^b \rho(z')L(x, z')\, dz', \quad (63)$$

$$q(t, t) = 2, \quad (64)$$

$$I_x(t, x, z) = -z^{-1}I(t, x, z) - ie^{ikx}I(x, z)\int_a^b \rho(z')I(t, x, z')\, dz' + \tfrac{1}{2}p(t, x) \times e^{ikx}\left(1 - i\int_a^b \rho(z')K(x, z, z')\, dz'\right), \quad (65)$$

$$I(t, t, z) = I(t, z), \quad (66)$$

$$J_x(t, x, z) = -z^{-1}J(t, x, z) - ie^{ikx}I(x, z)\int_a^b \rho(z')J(t, x, z')\, dz' + \tfrac{1}{2}q(t, x) \times e^{ikx}\left(1 - i\int_a^b \rho(z')K(x, z, z')\, dz'\right), \quad (67)$$

$$J(t, t, z) = 0. \quad (68)$$

The transmitted component in the transformed system,

$$q(0, x) = e^{-ikx}v(0, x), \quad (69)$$

may be obtained by solving Eqs. (63), (64), (67), and (68) with t set equal to zero.

7. DERIVATION OF CAUCHY SYSTEM

The derivation is similar to that given in Sec. 4 for the untransformed case. Differentiating Eqs. (49) and (50) with respect to x and using Eqs. (50b), (51), and (60), one obtains

$$-e^{ikt}p_x(t, x) = e^{-ikt}q_x(t, x) = 2if(x)R(x - t) + \int_0^x R(|t - y|) \times [e^{iky}p_x(y, x) + e^{-iky}q_x(y, x)]\, dy, \quad (70)$$

$$p_x(0, x) = 0, \quad (71a)$$

$$q_x(x, x) = -\dot{q}(x, x). \quad (71b)$$

Now let $I(t, x, z)$ and $J(t, x, z)$ be solutions to

$$-e^{ikt}I(t, x, z) = e^{-ikt}J(t, x, z) = i\int_0^x R(|y - t|) \times [e^{iky}I(y, x, z) + e^{-iky}J(y, x, z)]\, dy - e^{-(x-t)/z}, \quad (72)$$

$$I(0, x, z) = 0, \quad (73a)$$

$$J(x, x, z) = 0. \quad (73b)$$

Hence from the principle of superposition and Eqs. (49), (50), and (70)–(73), we obtain

$$p_x(t, x) = -\tfrac{1}{2}\dot{q}(x, x)p(t, x) - 2if(x)\int_a^b \rho(z')I(t, x, z')\, dz', \quad (74a)$$

$$q_x(t, x) = -\tfrac{1}{2}\dot{q}(x, x)q(t, x) - 2if(x)\int_a^b \rho(z')J(t, x, z')\, dz'. \quad (74b)$$

Differentiating Eqs. (72) and (73) with respect to x, one obtains

$$\begin{aligned} -e^{ikt}\dot{I}_x(t, x, z) &= e^{-ikt}\dot{J}_x(t, x, z) \\ &= i\int_0^x R(|y - t|) \\ &\quad\times [e^{iky}I_x(y, x, z) + e^{-iky}J_x(y, x, z)]\, dy \\ &\quad + iR(x - t)e^{ikx}I(x, z) + z^{-1}e^{-(x-t)/z}, \end{aligned} \tag{75}$$

$$I_x(0, x, z) = 0, \tag{76a}$$

$$J_x(x, x, z) = -\dot{J}(x, x, z), \tag{76b}$$

where $I(x, z)$ is defined by

$$I(x, z) = I(x, x, z) \tag{77a}$$

and

$$J(x, x, z) = 0. \tag{77b}$$

Hence, from the principle of superposition and Eqs. (49), (50), (72), (73), (75), and (76), we obtain

$$\begin{aligned} I_x(t, x, z) = &-\tfrac{1}{2}\dot{J}(x, x, z)p(t, x) - z^{-1}I(t, x, z) \\ &- ie^{ikx}I(x, z)\int_a^b \rho(z')I(t, x, z')\, dz', \end{aligned} \tag{78a}$$

$$\begin{aligned} J_x(t, x, z) = &-\tfrac{1}{2}\dot{J}(x, x, z)q(t, x) - z^{-1}J(t, x, z) \\ &- ie^{ikx}I(x, z)\int_a^b \rho(z')J(t, x, z')\, dz'. \end{aligned} \tag{78b}$$

Now define quantities $L(x, z)$ and $K(x, z, z')$ by

$$\begin{aligned} L(x, z') = \int_0^x & e^{-(x-y)/z'} \\ &\times [e^{iky}p(y, x) + e^{-iky}q(y, x)]\, dy, \end{aligned} \tag{79}$$

$$\begin{aligned} K(x, z, z') = \int_0^x & e^{-(x-y)/z'} \\ &\times [e^{iky}I(y, x, z) + e^{-iky}J(y, x, z)]\, dy. \end{aligned} \tag{80}$$

Then setting $t = x$ in Eqs. (49) and (72), we obtain

$$\begin{aligned} -e^{ikx}\dot{p}(x, x) &= e^{-ikx}\dot{q}(x, x) \\ &= i\int_a^b \rho(z')L(x, z')\, dz', \end{aligned} \tag{81}$$

$$\begin{aligned} -e^{ikx}\dot{I}(x, x, z) &= e^{-ikx}\dot{J}(x, x, z) \\ &= i\int_a^b \rho(z')K(x, z, z') - 1. \end{aligned} \tag{82}$$

We are now ready to derive the Cauchy system (52)–(59) for the quantities $p(x)$, $L(x, z')$, $K(x, z, z')$, and $I(x, z)$. Differentiating (51) with respect to x,

$$p_x(x) = \dot{p}(x, x) + p_x(x, x), \tag{83}$$

and using Eqs. (81), (74a), (77a), (51), and (60), one obtains (52). The initial condition (53) follows from (50a). Differentiating (79) with respect to x, and using Eqs. (74), (79), (80), and (81), one obtains (54). The initial condition (55) follows from (79). Differentiating (80) with respect to x and using Eqs. (78), (79), (80), and (82), one obtains (56). The initial condition (57) follows from (80). Differentiating Eq. (77a) with respect to x,

$$I_x(x, z) = \dot{I}(x, x, z) + I_x(x, x, z), \tag{84}$$

and using Eqs. (78a), (82), (51), and (50b), one obtains Eq. (58). The initial conditions (59) follows from (73a).

With these quantities known, we now derive the Cauchy system (61)–(68) for the quantities $p(t, x)$, $q(t, x)$, $I(t, x, z)$, and $J(t, x, z)$. Equations (61) and (63) readily follow from (74) and (81). The initial conditions (62) and (64) follow from (51) and (50b), respectively. Equations (65) and (67) readily follow from (78) and (82). The initial conditions (66) and (68) follow from (77a) and (77b), respectively. This completes the derivation of the Cauchy system.

8. ITERATIVE METHODS

Instead of reducing the problem to a Cauchy system, one may prefer to employ an iterative method. We discuss here briefly several possible approaches based upon the transformed equations (49) and (50), or rather their integral form,

$$\begin{aligned} p(t, x) = -i\int_0^t d\tau \int_0^x & dy e^{-ik\tau}R(|\tau - y|) \\ &\times [e^{iky}p(y, x) + e^{-iky}q(y, x)], \end{aligned} \tag{85a}$$

$$\begin{aligned} q(t, x) = 2 - i\int_t^x d\tau \int_0^x & dy e^{ik\tau}R(|\tau - y|) \\ &\times [e^{iky}p(y, x) + e^{-iky}q(y, x)]. \end{aligned} \tag{85b}$$

A perturbation expansion for Eqs. (85) can be obtained by replacing $R(|\tau - y|)$ by $\lambda R(|\tau - y|)$ and assuming that $p(t, x)$ and $q(t, x)$ can be expanded in powers of λ:

$$p(t, x) = \sum_{h=0}^{\infty} \lambda^n p_n(t, x), \tag{86a}$$

$$q(t, x) = \sum_{h=0}^{\infty} \lambda^n q_n(t, x). \tag{86b}$$

Equating powers of λ then leads to

$$p_0(t, x) = 0, \tag{87a}$$

$$q_0(t, x) = 2, \tag{87b}$$

$$\begin{aligned} p_{n+1}(t, x) = -i\int_0^t d\tau \int_0^x & dy e^{-ik\tau}R(|\tau - y|) \\ &\times [e^{iky}p_n(y, x) + e^{-iky}q_n(y, x)], \end{aligned} \tag{88a}$$

$$\begin{aligned} q_{n+1}(t, x) = -i\int_t^x d\tau \int_0^x & dy e^{ik\tau}R(|\tau - y|) \\ &\times [e^{iky}p_n(y, x) + e^{-iky}q_n(y, x)]. \end{aligned} \tag{88b}$$

Substituting (87) into (88) and using Eq. (8), one obtains

$$p_1(t, x) = -2i\int_a^b dz\rho(z)(k^2 + z^{-2})^{-1} \times [(-ikz)^{-1}(e^{-2ikt} - 1) + e^{-(ik+z^{-1})t} - 1 + e^{-(ik+z^{-1})x}(e^{-(ik-z^{-1})t} - 1)], \tag{89a}$$

$$q_1(t, x) = -2i\int_a^b dz\rho(z) \times [2(x-t)z^{-1}(k^2 + z^{-2})^{-1} + (z^{-1} - ik)^{-2}(e^{(ik-z^{-1})x} - e^{(ik-z^{-1})t}) - (z^{-1} + ik)^{-2}(1 - e^{-(ik+z^{-1})(x-t)})]. \tag{89b}$$

Higher-order calculations can, in principle, be similarly made, but, for cases where Eqs. (89) are inadequate, a numerical approach will most likely be more suitable. Note that any of the following circumstances will ensure that Eqs. (89) give a good approximation: plasma sufficiently dilute, wavelength ($2\pi/k$) sufficiently small, slab thickness x sufficiently small, maximum nonlocal-interaction decay length b sufficiently small.

Equations (85) can also be used as the basis of a successive-approximation calculation. Starting with assumed approximate functions $p(t, x)$ and $q(t, x)$, these may be inserted into the right side of (85), and the integrations carried out to obtain new approximate expressions for $p(t, x)$ and $q(t, x)$. The process is repeated as many times as is necessary to (hopefully!) achieve convergence to the desired accuracy. If the starting approximation is sufficiently close to the solution of (85), it may be shown that, under reasonable conditions, convergence is always attained. If one uses as a starting approximation $p(t, x) = 0$, $q(t, x) = 2$, then one readily sees that, owing to the linearity of Eqs. (91), this procedure leads to the same result (in principle) as the perturbation calculation (86)–(88). [A possible improvement on the calculation in practice stems from the fact that numerical approximations for $p(t, x)$ and $q(t, x)$ are not normally calculated simultaneously, but are calculated *alternately* using the *latest* previous approximations.]

For cases such that convergence does not occur with this starting approximation, a better starting approximation will be needed. This may be obtained by continuously imbedding (85) into a larger class of problems such that convergence is assured for some members of the class. One way of doing this is to introduce a "strength parameter" λ to multiply the right-hand sides of Eqs. (85). For small enough λ, we will be assured of convergence. If for some value of λ we have a sufficiently accurate solution, it will be close enough to the solution for some larger value of λ to serve as a suitable starting approximation for it. We thus work up stepwise to the desired case $\lambda = 1$. Alternatively, and in a similar manner, we may use the slab dimension X as our parameter and, by increasing x, work up stepwise from thin to thicker slabs.

A better understanding of the feasibility and relative merits of the various methods discussed in this paper will be obtained from numerical experiments.

ACKNOWLEDGMENT

The author thanks Professor R. Kalaba for bringing this problem to his attention, and for useful discussions.

APPENDIX A

Theorem: Assume that $u(x)$, $E(x, z')$, $H(x, z, z')$, and $I(x, z)$ are a solution to Eqs. (14)–(21) and $u(t, x)$, $v(t, x)$, $I(t, x, z)$, and $J(t, x, z)$ are a solution to Eqs. (23)–(30), $a \leq z, z' \leq b$, where $\rho(z)$ is given and $g(x)$ is defined by (22). Assume also that the following quantities exist:

$$E^*(x, z') \equiv \int_0^x e^{-(x-y)/z'}[u(y, x) + v(y, x)]\, dy, \tag{A1}$$

$$H^*(x, z, z') \equiv \int_0^x e^{-(x-y)/z'}[I(y, x, z) + J(y, x, z)]\, dy, \tag{A2}$$

$$u^*(x) \equiv -i\int_0^x d\tau\int_0^x dy e^{ik(x-\tau)}R(|\tau - y|) \times [u(y, x) + v(y, x)], \tag{A3}$$

$$I^*(x, z) = -i\int_0^x d\tau\int_0^x dy e^{ik(x-\tau)}R(|\tau - y|) \times [I(y, x, z) + J(y, x, z)] + \int_0^x d\tau \exp[(ik - 1/z)(x-\tau)], \tag{A4}$$

$$u^*(t, x) = -i\int_0^t d\tau\int_0^x dy e^{ik(t-\tau)}R(|\tau - y|) \times [u(y, x) + v(y, x)], \tag{A5}$$

$$v^*(t, x) = -i\int_t^x d\tau\int_0^x dy e^{-ik(t-\tau)}R(|\tau - y|) \times [u(y, x) + v(y, x)] + 2e^{ik(x-t)}, \tag{A6}$$

$$I^*(t, x, z) = -i\int_0^t d\tau\int_0^x dy e^{ik(t-\tau)}R(|\tau - y|) \times [I(y, x, z) + J(y, x, z)] + \int_0^t d\tau e^{ik(t-\tau)}e^{-(x-\tau)/z}, \tag{A7}$$

$$J^*(t, x, z) = -i\int_t^x d\tau\int_0^x dy e^{-ik(t-\tau)}R(|\tau - y|) \times [I(y, x, z) + J(y, x, z)] + \int_t^x d\tau e^{-ik(t-\tau)}e^{-(x-\tau)/z}. \tag{A8}$$

In these equations $R(|\tau - y|)$ is defined in terms of $\rho(z)$ by Eq. (8). Then $u(t, x)$ and $v(t, x)$ satisfy the two-point boundary value problem defined by (11) and (12).

Proof: Define the following quantities:

$$E^\dagger(x, z) \equiv E^*(x, z) - E(x, z), \tag{A9}$$

$$H^\dagger(x, z, z') \equiv H^*(x, z, z') - H(x, z, z'), \tag{A10}$$

$$U^\dagger(x) \equiv u^*(x) - u(x), \tag{A11}$$

$$I^\dagger(x, z) \equiv I^*(x, z) - I(x, z), \tag{A12}$$

$$u^\dagger(t, x) \equiv u^*(t, x) - u(t, x), \tag{A13}$$

$$v^\dagger(t, x) \equiv v^*(t, x) - v(t, x), \tag{A14}$$

$$I^\dagger(t, x, z) \equiv I^*(t, x, z) - I(t, x, z), \tag{A15}$$

$$J^\dagger(t, x, z) \equiv J^*(t, x, z) - J(t, x, z). \tag{A16}$$

The proof consists in obtaining differential equations for the daggered quantities which imply that they all vanish; hence the starred quantities equal the corresponding unstarred quantities. In particular,

$$u^*(t, x) = u(t, x), \tag{A17}$$

$$v^*(t, x) = v(t, x). \tag{A18}$$

From (A5), (A6), (A17), and (A18), it then easily follows that $u(t, x)$ and $v(t, x)$ satisfy Eqs. (11) and (12).

We work first with the four quantities $E^\dagger(x, z)$, $H^\dagger(x, z, z')$, $u^\dagger(x)$, and $I^\dagger(x, z)$.

Differentiating (A1) with respect to x and using (72), we obtain

$$E_x^*(x, z') = (-z')^{-1}E^*(x, z') + g(x) + \int_0^x e^{-(x-y)/z'}[u_x(y, x) + v_x(y, x)]\,dy. \tag{A19}$$

Substituting Eqs. (23) and (25) into the integrand of (A19) and using (A1), (A2), (A9), (A10), and (16), we obtain

$$E_x^\dagger(x, z') = [ik - (z')^{-1}]E^\dagger(x, z') - \tfrac{1}{2}iE^\dagger(x, z')\int_a^b \rho(z)E(x, z)\,dz - ig(x)\int_a^b \rho(z)H^\dagger(x, z, z')\,dz. \tag{A20}$$

From (A9), (A1), and (17), we obtain the initial condition

$$E^\dagger(0, z') = 0. \tag{A21}$$

Differentiating (A2) with respect to x and using (28) and (30), we obtain

$$H_x^*(x, z, z') \equiv I(x, z) - (z')^{-1}H^*(x, z, z') + \int_0^x e^{-(x-y)/z'}[I_x(y, x, z) + J_x(y, x, z)]\,dy. \tag{A22}$$

Substituting (27) and (29) into the integrand of (A22) and using (A1), (A2), (A9), (A10), and (18), we obtain

$$H_x^\dagger(x, z, z') = -[z^{-1} + (z')^{-1}]H^\dagger(x, z, z') + \tfrac{1}{2}E^\dagger(x, z') \times \left(1 - i\int_a^b \rho(z')H(x, z, z')\,dz'\right) - iI(x, z)\int_a^b \rho(z)H^\dagger(x, z, z')\,dz. \tag{A23}$$

From (A10), (A2), and (19), we obtain the initial condition

$$H^\dagger(x, z, z') = 0. \tag{A24}$$

Differentiating (A3) with respect to x and using (72), we obtain

$$u_x^*(x) = iku^*(x) - i\int_0^x dyR(x - y) \times [u(y, x) + v(y, x)] - i\int_0^x d\tau\int_0^x dye^{ik(x-y)}R(|\tau - y|) \times [u_x(y, x) + v_x(y, x)] - i\int_0^x d\tau e^{ik(x-\tau)}R(x - \tau)g(x). \tag{A25}$$

Substituting Eqs. (23) and (24) into the second integrand of (A25) and using (A3), (A4), (A11), (A12), (A9), (14), and (8), we obtain

$$u_x^\dagger(x) = -ig(x)\int_a^b \rho(z)I^\dagger(x, z)\,dz - i\int_a^b \rho(z)E^\dagger(x, z)\,dz + 2iku^\dagger(x) - \tfrac{1}{2}u^\dagger(x)\int_a^b \rho(z)E(x, z)\,dz. \tag{A26}$$

From (A11), (A3), and (15), we obtain the initial condition

$$u^\dagger(x) = 0. \tag{A27}$$

Differentiating (A4) with respect to x and using (28) and (30), we obtain

$$I_x^*(x, z) = -i\int_0^x d\tau\int_0^x dye^{ik(x-\tau)}R(|\tau - y|) \times [I_x(y, x, z) + J_x(y, x, z)] + ikI^*(x, z) + 1 - iI(x, z)\int_0^x d\tau e^{ik(x-\tau)}R(x - \tau) - i\int_0^x dyR(x - y)[I(y, x, z) + J(y, x, z)]. \tag{A28}$$

Substituting (27) and (29) into the first integrand of (A28) and using (A3), (A4), (A11), (A12), (A10), (20), and (8), we obtain

$$I_x^\dagger(x, z) = (ik - z^{-1})I^\dagger(x, z) - iI(x, z)\int_a^b \rho(z')I^\dagger(x, z')\,dz' + \tfrac{1}{2}u^\dagger(x)\left(1 - i\int_a^b \rho(z')H(x, z, z')\,dz'\right) - i\int_a^b \rho(z')H^\dagger(x, z, z')\,dz'. \quad \text{(A29)}$$

From (A12), (A5), and (21), we obtain the initial condition

$$I(0, z) = 0. \quad \text{(A30)}$$

We see that Eqs. (A20), (A23), (A26), and (A29) constitute a set of four coupled linear homogeneous first-order differential equations in the variables $E^\dagger(x, z')$, $H^\dagger(x, z, z')$, $u^\dagger(x)$, and $I^\dagger(x, z)$ subject to the homogeneous initial conditions (A21), (A24), (A27), and (A30), the *unique* solution of which is zero for all four variables. Hence, from (A9)–(A12),

$$E(x, z) = E^*(x, z), \quad \text{(A31)}$$

$$H(x, z, z') = H^*(x, z, z'), \quad \text{(A32)}$$

$$u(x) = u^*(x), \quad \text{(A33)}$$

$$I(x, z) = I^*(x, z). \quad \text{(A34)}$$

Next, we obtain differential equations for the variables $u^\dagger(t, x)$, $v^\dagger(t, x)$, $I^\dagger(t, x, z)$, and $J^\dagger(t, x, z)$.

Differentiating (A5) with respect to x and using (72), we obtain

$$u_x^*(t, x) = -i\int_0^t d\tau\int_0^x dy e^{ik(t-\tau)}R(|\tau - y|) \times [u_x(y, x) + v_x(y, x)] - i\int_0^t d\tau e^{ik(t-\tau)}R(x - \tau)g(x). \quad \text{(A35)}$$

Substituting (23) and (25) into the first integrand and using (A5), (A7), (A13), (A14), and (8), we obtain

$$u_x^\dagger(t, x) = iku^\dagger(t, x) - ig(x)\int_a^b \rho(z)I^\dagger(t, x, z)\,dz - \tfrac{1}{2}iu^\dagger(t, x)\int_a^b \rho(z)E(x, z)\,dz. \quad \text{(A36)}$$

From (24), (A5), (A3), (A33), and (A13) (with x replaced by t), we obtain the initial condition

$$u^\dagger(t, t) = 0. \quad \text{(A37)}$$

Differentiating (A6) with respect to x and using (72), we obtain

$$v_x^*(t, x) = -i\int_t d\tau\int_0^x dy e^{-ik(t-\tau)}R(|\tau - y|) \times [u_x(y, x) + v_x(y, x)] + 2ike^{ik(x-t)} - i\int_t^x d\tau e^{-ik(t-\tau)}R(x - \tau)g(x) - i\int_0^x dy e^{ik(x-t)}R(x - y)[u(y, x) + v(y, x)]. \quad \text{(A38)}$$

Substituting (23) and (25) into the first integrand and using (A6), (A8), (A14), (A16), and (8), we obtain

$$v_x^\dagger(t, x) = ikv^\dagger(t, x) - \tfrac{1}{2}iv^\dagger(t, x)\int_a^b \rho(z)E(x, z)\,dz - ig(x)\int_a^b \rho(z)J^\dagger(t, x, z)\,dz. \quad \text{(A39)}$$

From (A6), (28), and (A14), we obtain the initial condition

$$v^\dagger(t, t) = 0. \quad \text{(A40)}$$

Differentiating (A7) with respect to x and using (28) and (30), we obtain

$$I_x^*(t, x, z) = -i\int_0^t d\tau\int_0^x dy e^{ik(t-\tau)}R(|\tau - y|) \times [I_x(y, x, z) + J_x(y, x, z)] - i\int_0^t d\tau e^{ik(t-\tau)}R(x - \tau)I(x, z) - z^{-1}\int_0^t d\tau e^{ik(t-\tau)}e^{-(x-\tau)/z}. \quad \text{(A41)}$$

Substituting (27) and (29) into the first integrand and using (A5), (A7), (A13), (A15), and (8), we obtain

$$I_x^\dagger(t, x, z) = -z^{-1}I^\dagger(t, x, z) - iI(x, z)\int_a^b \rho(z')I^\dagger(t, x, z')\,dz' + \tfrac{1}{2}u^\dagger(t, x)\left(1 - i\int_a^b \rho(z')H(x, z, z')\,dz'\right). \quad \text{(A42)}$$

From (28), (A7), (A4), (A34), and (A15) (with x replaced by t), we obtain the initial condition

$$I^\dagger(t, t) = 0. \quad \text{(A43)}$$

Differentiating (A8) with respect to x and using (28) and (30), we obtain

$$J_x^*(t, x, z) = -i\int_t^x d\tau\int_0^x dy e^{-ik(t-\tau)}R(|\tau - y|) \times [I_x(y, x, z) + J_x(y, x, z)] - i\int_0^x dy e^{-ik(t-x)}R(x - y)[I(y, x, z) + J(y, x, z)] - i\int_t^x d\tau e^{-ik(t-\tau)}R(x - \tau)I(x, z) + e^{ik(x-t)} - z^{-1}\int_t^x d\tau e^{-ik(t-\tau)}e^{-(x-\tau)/z}. \quad \text{(A44)}$$

Substituting (27) and (29) into the first integrand and using (A6), (A8), (A14), (A16), and (8), we obtain

$$J_x^\dagger(t, x, z) = -z^{-1}J^\dagger(t, x, z) - iI(x, z)\int_a^b \rho(z')J^\dagger(t, x, z')\,dz' + \tfrac{1}{2}v^\dagger(t, x)\left(1 - i\int_a^b \rho(z')H(x, z, z')\,dz'\right). \tag{A45}$$

From (A16), (A8), and (30), we obtain the initial condition

$$J^\dagger(t, t, z) = 0. \tag{A46}$$

We see that Eqs. (A36), (A39), (A42), and (A45) constitute a set of four coupled linear homogeneous first-order differential equations in the variables $u^\dagger(t, x)$, $v^\dagger(t, x)$, $I^\dagger(t, x, z)$, and $J^\dagger(t, x, z)$ subject to the homogeneous initial conditions (A37), (A40), (A43), and (A46).

Since the unique solution vanishes, Eqs. (A17) and (A18) follow from (A13) and (A14), respectively. This completes the proof of the theorem.

APPENDIX B

Theorem: Assume that $p(x)$, $L(x, z')$, $K(x, z, z')$, and $I(x, z)$ are a solution to Eqs. (52)–(59), and $p(t, x)$, $q(t, x)$, $I(t, x, z)$, and $J(t, x, z)$ are a solution to Eqs. (61)–(68), $a \le z, z' \le b$, where $\rho(x)$ is given and $f(x)$ is defined by (60). Let $s(y, x)$ and $M(y, x, z)$ be defined by

$$s(y, x) \equiv e^{iky}p(y, x) + e^{-iky}q(y, x) \tag{B1}$$

and

$$M(y, x, z) \equiv e^{iky}I(y, x, z) + e^{-iky}J(y, x, z), \tag{B2}$$

and assume also that the following quantities exist:

$$L^*(x, z') = \int_0^x e^{-(x-y)/z'}s(y, x)\,dy, \tag{B3}$$

$$K^*(x, z, z') = \int_0^x e^{-(x-y)/z'}M(y, x, z)\,dy, \tag{B4}$$

$$p^*(x) = -i\int_0^x d\tau\int_0^x dy e^{-ik\tau}R(|y - \tau|)s(y, x), \tag{B5}$$

$$I^*(x, z) = -i\int_0^x d\tau\int_0^x dy e^{-ik\tau}R(|y - \tau|)M(y, x, z) + \int_0^x e^{-ik\tau}e^{-(x-\tau)/z}\,d\tau, \tag{B6}$$

$$p^*(t, x) = -i\int_0^t d\tau\int_0^x dy e^{-ik\tau}R(|y - \tau|)s(y, x), \tag{B7}$$

$$q^*(t, x) = 2 - i\int_t^x d\tau\int_0^x dy e^{ik\tau}R(|y - \tau|)s(y, x), \tag{B8}$$

$$I^*(t, x, z) = -i\int_0^t d\tau\int_0^x dy e^{-ik\tau}R(|y - \tau|)M(y, x, z) + \int_0^t e^{-ik\tau}e^{-(x-\tau)/z}\,d\tau, \tag{B9}$$

$$J^*(t, x, z) = -i\int_t^x d\tau\int_0^x dy e^{ik\tau}R(|y - \tau|)M(y, x, z) + \int_t^x e^{ik\tau}e^{-(x-\tau)/z}\,d\tau. \tag{B10}$$

In these equations $R(|\tau - y|)$ is defined in terms of $\rho(z)$ by Eq. (8). Then $p(t, x)$ and $q(t, x)$ satisfy the two-point boundary value problem defined by (49) and (50).

Proof: The proof is similar to that given in Appendix A for the nontransformed case. Define the following quantities:

$$L^\dagger(x, z') = L^*(x, z') - L(x, z), \tag{B11}$$

$$K^\dagger(x, z, z') = K^*(x, z, z') - K(x, z, z'), \tag{B12}$$

$$p^\dagger(x) = p^*(x) - p(x), \tag{B13}$$

$$I^\dagger(x, z) = I^*(x, z) - I(x, z), \tag{B14}$$

$$p^\dagger(t, x) = p^*(t, x) - p(t, x), \tag{B15}$$

$$q^\dagger(t, x) = q^*(t, x) - q(t, x), \tag{B16}$$

$$I^\dagger(t, x, z) = I^*(t, x, z) - I(t, x, z), \tag{B17}$$

$$J^\dagger(t, x, z) = J^*(t, x, z) - J(t, x, z). \tag{B18}$$

We first show that the quantities $L^\dagger(x, z')$, $K^\dagger(x, z, z')$, $p^\dagger(x)$, and $I^\dagger(x, z)$ are the unique vanishing solutions to a set of differential equations.

Differentiating (B3) with respect to x, we obtain

$$L_x^*(x, z') = 2f(x) - (z')^{-1}L^*(x, z') + \int_0^x e^{-(x-y)/z'}s_x(y, x)\,dy, \tag{B19}$$

since, by (B1) and (60),

$$s(x, x) = 2f(x). \tag{B20}$$

The quantity $s_x(y, x)$ is obtained from (B1), (B2), (61), and (63):

$$s_x(y, x) = -2if(x)\int_a^b \rho(z')M(y, x, z')\,dz' - \tfrac{1}{2}ie^{ikx}s(y, x)\int_a^b \rho(z')L(x, z')\,dz'. \tag{B21}$$

Substituting (B21) into the integrand of (B19) and using (B3), (B4), (B11), and (B12), one obtains

$$L_x^\dagger(x, z') = -(1/z')L^\dagger(x, z') - 2if(x)\int_a^b \rho(z)K^\dagger(x, z, z')\,dz - \tfrac{1}{2}ie^{ikx}L^\dagger(x, z')\int_a^b \rho(z)L(x, z)\,dz. \quad (B22)$$

From (55), (B3), and (B11), one obtains the initial condition

$$L^\dagger(0, z') = 0. \quad (B23)$$

Differentiating (B4) with respect to x, we obtain

$$K_x^*(x, z, z') = e^{ikx}I(x, z) - (z')^{-1}K^*(x, z, z') + \int_0^x e^{-(x-y)/z'}M_x(y, x, z)\,dy \quad (B24)$$

since, by (B2), (66), and (68),

$$M(x, x, z) = e^{ikx}I(x, z). \quad (B25)$$

The quantity $M_x(y, x, z)$ is obtained from (B1), (B2), (65), and (67):

$$M_x(y, x, z) = -z^{-1}M(y, x, z) - ie^{ikx}I(x, z)\int_a^b \rho(z')M(y, x, z')\,dz' + \tfrac{1}{2}s(y, x)e^{ikx}\left(1 - i\int_a^b \rho(z')K(x, z, z')\,dz'\right). \quad (B26)$$

Substituting (B26) into the integrand of (B24) and using (B3), (B4), (B11), and (B12), one obtains

$$K_x^\dagger(x, z, z') = \tfrac{1}{2}L^\dagger(x, z')e^{ikx}\left(1 - i\int_a^b \rho(z')K(x, z, z')\,dz'\right) - iI(x, z)e^{ikx}\int_a^b \rho(z)K^\dagger(x, z, z')\,dz - [z^{-1} + (z')^{-1}]K^\dagger(x, z, z'). \quad (B27)$$

From (57), (B4), and (B11), one obtains the initial condition

$$K^\dagger(0, z, z') = 0. \quad (B28)$$

Differentiating (B5) with respect to x and using (B20), we obtain

$$p_x^*(x) = -i\int_0^x dy e^{-ikx}R(x - y)s(y, x) - 2if(x)\int_0^x e^{-ik\tau}R(x - \tau)\,d\tau - i\int_0^x d\tau\int_0^x dy e^{-ik\tau}R(|y - \tau|)s_x(y, x). \quad (B29)$$

Substituting (B21) into the last integrand and using (B5), (B6), (B13), (B14), (60), and (8), we obtain

$$p_x^\dagger(x) = -\tfrac{1}{2}ip^\dagger(x)\int_a^b \rho(z')L(x, z')\,dz' - 2if(x)\int_a^b \rho(z')I^\dagger(x, z')\,dz'. \quad (B30)$$

From (53), (B5), and (B15), we obtain the initial condition

$$p^\dagger(0) = 0. \quad (B31)$$

Differentiating (B6) with respect to x and using (B25), we obtain

$$I_x^*(x, z) = -i\int_0^x d\tau\int_0^x dy e^{-ik\tau}R(|y - \tau|)M_x(y, x, z) - i\int_0^x dy e^{-ikx}R(x - y)M(y, x, z) - iI(x, z)\int_0^x e^{ik(x-\tau)}R(y - \tau)\,d\tau + z^{-1}\int_0^x e^{-ik\tau}e^{-(x-\tau)/z}\,d\tau + e^{-ikx}. \quad (B32)$$

Substituting (B26) into the first integrand and using (B5), (B6), (B13), (B14), (B12), (58), (60), and (8), we obtain

$$I_x^\dagger(x, z) = -z^{-1}I^\dagger(x, z) - ie^{ikx}I(x, z)\int_a^b \rho(z')I^\dagger(x, z')\,dz' + \tfrac{1}{2}e^{ikx}p^\dagger(x)\left(1 - i\int_a^b \rho(z')K(x, z, z')\,dz'\right) - ie^{-ikx}\int_a^b \rho(z')K^\dagger(x, z, z')\,dz'. \quad (B33)$$

From (59), (B6), and (B14), we obtain the initial condition

$$I^\dagger(0) = 0. \quad (B34)$$

We see that Eqs. (B22), (B27), (B30), and (B33) constitute a set of four linear homogeneous first-order differential equations in the variables $L^\dagger(x, z)$, $K^\dagger(x, z, z')$, $p^\dagger(x)$, and $I^\dagger(x, z)$ subject to the homogeneous initial conditions (B23), (B28), (B31), and (B34). Since the unique solution of these equations vanishes, it follows from (B11)–(B14) that

$$L(x, z') = L^*(x, z'), \quad (B35)$$

$$K(x, z, z') = K^*(x, z, z'), \quad (B36)$$

$$p(x) = p^*(x), \quad (B37)$$

$$I(x, z) = I^*(x, z). \quad (B38)$$

Next, we show that $p^\dagger(t, x)$, $q^\dagger(t, x)$, $I^\dagger(t, x, z)$, and $J^\dagger(t, x, z)$ are the unique vanishing solutions to a set of differential equations.

Differentiating (B7) with respect to x and using (B20), we obtain

$$p^*_x(t, x) = -i\int_0^t d\tau \int_0^x dy e^{-ik\tau} R(|y-\tau|) s_x(y, x) - 2if(x)\int_0^t d\tau e^{-ik\tau} R(x-\tau). \quad \text{(B39)}$$

Substituting (B21) into the first integrand and using (B21), (B7), (B9), (B15), (B17), (61), and (8), we obtain

$$p^\dagger_x(t, x) = (-i/2) e^{ikx} p^\dagger(t, x) \int_a^b \rho(z) L(x, z)\, dz - 2if(x)\int_a^b \rho(z) I^\dagger(t, x, z)\, dz. \quad \text{(B40)}$$

From (B15), (B7), (B5), (62), and (B37) with x replaced by t, we obtain the initial condition

$$p^\dagger(t, t) = 0. \quad \text{(B41)}$$

Differentiating (B8) with respect to x and using (B20), we obtain

$$q^*_x(t, x) = -i\int_0^x dy e^{ikx} R(x-y) s(y, x) - 2if(x)\int_t^x e^{ik\tau} R(x-\tau)\, d\tau - i\int_t^x d\tau \int_0^x dy e^{ik\tau} R(|y-\tau|) s_x(y, x). \quad \text{(B42)}$$

Substituting (B21) into the last integrand and using (B8), (B10), (B16), (B18), (B11), and (8), we obtain

$$q^\dagger_x(t, x) = -ie^{ikx}\int_a^b \rho(z') L^\dagger(x, z') - 2if(x)\int_a^b \rho(z') J^\dagger(t, x, z')\, dz' - \tfrac{1}{2} i e^{ikx} q^\dagger(t, x)\int_a^b \rho(z') L(x, z')\, dz'. \quad \text{(B43)}$$

From (64), (B8), and (B16), we obtain the initial condition

$$q^\dagger(t, t) = 0. \quad \text{(B44)}$$

Differentiating (B9) with respect to x and using (B25), we obtain

$$I^*_x(t, x, z) = -i\int_0^t d\tau \int_0^x dy e^{-ik\tau} R(|y-\tau|) M_x(y, x, z) + e^{ikx} I(x, z)\int_0^t e^{-ik\tau} R(x-\tau)\, d\tau - z^{-1}\int_0^t e^{-ik\tau} e^{-(x-\tau)/z}\, d\tau. \quad \text{(B45)}$$

Substituting (B26) into the first integrand and using (B7), (B9), (65), (B15), (B17), and (8), we obtain

$$I^\dagger_x(t, x, z) = -z^{-1} I^\dagger(t, x, z) - ie^{ikx} I(x, z)\int_a^b \rho(z') I^\dagger(t, x, z')\, dz' + \tfrac{1}{2} p^\dagger(t, x) e^{ikx}\left(1 - i\int_a^b \rho(z') K(x, z, z')\, dz'\right). \quad \text{(B46)}$$

From (B17), (B9), (B6), (66), and (B38) with x replaced by t, we obtain the initial condition

$$I^\dagger(t, t, z) = 0. \quad \text{(B47)}$$

Differentiating (B10) with respect to x and using (B25), we obtain

$$J^*_x(t, x, z) = -i\int_t^x d\tau \int_0^x dy e^{-ik\tau} R(|y-\tau|) M_x(y, x, z) - i\int_0^x dy e^{ikx} R(x-y) M(y, x, z) - iI(x, z)\int_t^x d\tau e^{ik(x+\tau)} R(x-\tau) - z^{-1}\int_t^x e^{ik\tau} e^{-(x-\tau)/z}\, d\tau + e^{ikx}. \quad \text{(B48)}$$

Substituting (B26) into the first integrand and using (B7), (B9), (67), (B16), (B18), and (8), we obtain

$$J^\dagger_x(t, x, z) = -z^{-1} J^\dagger(t, x, z) - ie^{ikx} I(x, z)\int_a^b \rho(z') J^\dagger(t, x, z')\, dz' + \tfrac{1}{2} q^\dagger(t, x) e^{ikx}\left(1 - i\int_a^b \rho(z') K(x, z, z')\, dz'\right) - ie^{ikx}\int_a^b \rho(z') K^\dagger(x, z, z')\, dz'. \quad \text{(B49)}$$

From (68), (B10), and (B18), we obtain the initial condition

$$J^\dagger(t, t, z) = 0. \quad \text{(B50)}$$

Now Eqs. (B40), (B43), (B46), and (B49) constitute a set of linear homogeneous first-order differential equations in the variables $p^\dagger(t, x)$, $q^\dagger(t, x)$, $I^\dagger(t, x, z)$, and $J^\dagger(t, x, z)$, subject to the homogeneous initial conditions (B41), (B44), (B47), and (B50). Since their vanishing solution is unique, it follows from (B15), (B16), (B7), and (B8) that

$$p(t, x) = p^*(t, x) = -i\int_0^t d\tau \int_0^x dy e^{-ik\tau} R(|y-\tau|) s(y, x) \quad \text{(B51)}$$

and

$$q(t, x) = q^*(t, x) = 2 - \int_t^x d\tau \int_0^x dy e^{ik\tau} R(|y-\tau|) s(y, x). \quad \text{(B52)}$$

One readily verifies that (B51) and (B52) satisfy the two-point boundary value problem defined by (49) and (50). QED

* Supported by the National Science Foundation under Grant No. GF-294 and the National Institutes of Health under Grants No. GM-16197-01 and No. GM-16437-01.

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[1] G. A. Baraff, J. Math. Phys. **9**, 372 (1968).
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[3] G. A. Baraff, Phys. Rev. **178**, 1155 (1969).
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[5] Aside from the fact that we have chosen the wave to be incident from the right rather than the left, these boundary conditions are the same as those of Baraff, Ref. 1, Eqs. (2.6b) and (2.6c). We have chosen the wave to be incident from the right since this facilitates the derivation by the invariant imbedding method. Of course, the case where the wave is incident from the left may be obtained from our results by a simple transformation.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Self-Adjoint Operators in Indefinite Metric Spaces*

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(Received 4 December 1970)

Some properties of self-adjoint operators in indefinite metric spaces are explored, with emphasis on the problem of the completeness of the set of eigenvectors. For operators in spaces of finite dimension, some simple criteria are deduced regarding the existence of such a complete set. Implications of completeness of eigenvectors for operators in infinite-dimensional spaces are discussed, and some partial extensions of the results for finite dimensions given.

I. INTRODUCTION

Lee and Wick have recently put forward a number of field-theoretic models set in indefinite metric spaces,[1,2] primarily with a view towards eliminating the divergences in physically interesting theories such as quantum electrodynamics.[3] Their work (and that of Sudarshan,[4] who has been critical of the Lee–Wick approach[5]) makes it seem worthwhile to examine some of the general properties of self-adjoint operators in such spaces. Lee has remarked that the problem of the completeness of the set of eigenvectors is an open question even for spaces of finite dimension. Yet it seems altogether reasonable to require this completeness for the Hamiltonian operator if the usual manipulations involving sums over intermediate eigenstates are to be meaningful.

In the next section of this paper, we give some definitions and elementary properties of indefinite metric spaces and of self-adjoint operators defined on them. For a more complete treatment, the reader should consult the review article of Pandit.[6] In his review, Pandit shows that the eigenvectors of a self-adjoint operator can fail to span the space when one of them has zero norm in the indefinite metric and corresponds to a real eigenvalue. In Sec. III, we sharpen this result somewhat and derive a set of necessary and sufficient conditions for completeness of the eigenvectors in finite-dimensional spaces. Section IV is concerned with some aspects of the infinite-dimensional case, including a partial extension of the results for finite dimensions.

II. DEFINITIONS AND PRELIMINARIES

The class of linear vector spaces which we shall be considering, and which we will call indefinite metric spaces, are a subset of the more general class of spaces with scalar product. Let S be a linear vector space; then a scalar product defined on S is a rule which associates with any two vectors ψ and ϕ in S, a complex number denoted by

$$\langle\psi, \phi\rangle.$$

Furthermore, the scalar product must have the properties

(i) $\langle\psi, \phi\rangle = \overline{\langle\phi, \psi\rangle}$,

where the bar denotes complex conjugation,

(ii) $\langle\psi, a_1\phi_1 + a_2\phi_2\rangle = a_1\langle\psi, \phi_1\rangle + a_2\langle\psi, \phi_2\rangle$,

and

(iii) $\langle\psi, \phi\rangle = 0$ for all ϕ in S implies $\psi = 0$.

Let L be a linear operator defined on S. Then its adjoint L^A is defined by

$$(L^A\psi, \phi) = (\psi, L\phi).$$

An operator is said to be self-adjoint if $L = L^A$.

One readily verifies that (B51) and (B52) satisfy the two-point boundary value problem defined by (49) and (50). QED

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In the next section of this paper, we give some definitions and elementary properties of indefinite metric spaces and of self-adjoint operators defined on them. For a more complete treatment, the reader should consult the review article of Pandit.[6] In his review, Pandit shows that the eigenvectors of a self-adjoint operator can fail to span the space when one of them has zero norm in the indefinite metric and corresponds to a real eigenvalue. In Sec. III, we sharpen this result somewhat and derive a set of necessary and sufficient conditions for completeness of the eigenvectors in finite-dimensional spaces. Section IV is concerned with some aspects of the infinite-dimensional case, including a partial extension of the results for finite dimensions.

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and

(iii) $\langle \psi, \phi \rangle = 0$ for all ϕ in S implies $\psi = 0$.

Let L be a linear operator defined on S. Then its adjoint L^A is defined by

$$(L^A\psi, \phi) = (\psi, L\phi).$$

An operator is said to be self-adjoint if $L = L^A$.

We will say that S is an indefinite metric space if it has the orthogonal decomposition

$$S = S_P \oplus S_N,$$

such that

$$\psi \in S_P \quad \text{implies} \quad \langle\psi, \psi\rangle > 0,$$
$$\psi \in S_N \quad \text{implies} \quad \langle\psi, \psi\rangle < 0.$$

Every finite-dimensional scalar product space has such a decomposition. Now let P be the projection onto S_P, and N, the projection onto S_N. P and N are clearly self-adjoint, and hence so is the metric

$$\eta = P - N.$$

Note that

$$\eta^2 = I \text{ (the identity).}$$

Using the metric η, we can define an auxiliary scalar product

$$(\psi, \phi) = \langle\psi, \eta\phi\rangle,$$

which in addition to satisfying (i), (ii), and (iii) above also has the property that

$$(\psi, \psi) > 0 \quad \text{if} \quad \psi \neq 0.$$

This auxiliary scalar product is thus of the familiar positive-definite sort. We may use it to define the Hermitian conjugate of L, called L^*, by

$$(L^*\psi, \phi) = (\psi, L\phi).$$

The adjoint and Hermitian conjugate are related by

$$L^A = \eta L^* \eta.$$

If $L = L^*$, we say L is Hermitian. The metric η is both self-adjoint and Hermitian.

We are now at the usual starting point for discussions of indefinite metric spaces. Consider the set of eigenvectors $\psi_1, \psi_2, \cdots$ of a self-adjoint operator L, with corresponding eigenvalues $\lambda_1, \lambda_2, \cdots$. Then the usual manipulations give

$$(\bar{\lambda}_m - \lambda_n)\langle\psi_m, \psi_n\rangle = 0. \tag{1}$$

If $m = n$, there are three possibilities. First, the eigenvalue can be real while $\langle\psi_n, \psi_n\rangle$ is nonzero. Second, the eigenvalue can be complex while $\langle\psi_n, \psi_n\rangle = 0$. We will call vectors satisfying $\langle\psi, \psi\rangle = 0$ null vectors. Third, we can have a real eigenvalue *and* a null eigenvector. In the next section we will see that the latter case is closely connected with the completeness of the eigenvectors.

There is another property of self-adjoint operators which will prove useful later. Suppose

$$L\psi = \lambda\psi.$$

Then consider

$$L^*(\eta\psi) = \eta L \eta(\eta\psi) = \eta L\psi = \lambda(\eta\psi).$$

Thus L and L^* have the same eigenvalues and, if ψ is the eigenvector of L, $\eta\psi$ is the corresponding eigenvector of L^*.

III. SPACES OF FINITE DIMENSION

We would like to know whether or not the eigenvectors of a self-adjoint operator span the space. In finite dimensions, it is a general result that the *generalized* eigenvectors of any linear operator do span the space. A generalized eigenvector of rank k is defined to be a vector ψ for which

$$(L - \lambda)^{k-1}\psi \neq 0,$$

but

$$(L - \lambda)^k\psi = 0.$$

Note that this implies that λ is an eigenvalue, since if we define

$$\phi = (L - \lambda)^{k-1}\psi,$$

then

$$L\phi = \lambda\phi.$$

The following theorem indicates an interesting relationship between the generalized eigenvectors of a linear operator L and those of its Hermitian conjugate L^*.

Theorem 1 [7]*:* Let λ be an eigenvalue of L; then $\bar{\lambda}$ is an eigenvalue of L^*. Furthermore, to any chain of maximum length k of generalized eigenvectors of L, namely, vectors $\psi_1, \psi_2, \cdots, \psi_k$ such that

$$\psi_j = (L - \lambda)^{j-1}\psi_1,$$

there corresponds a chain of length k of generalized eigenvectors of L^*, namely, vectors $\phi_1, \phi_2, \cdots, \phi_k$ such that

$$\phi_j = (L^* - \bar{\lambda})^{k-j}\phi_k$$

and such that

$$(\phi_i, \psi_j) = \delta_{ij}.$$

The proof of this hinges on the result[8] that

$$(L - \lambda)\psi' = \psi \tag{2}$$

has a nontrivial solution $\psi' \neq 0$ if and only if ψ is orthogonal (via the positive-definite scalar product) to every solution of

$$(L^* - \bar{\lambda})\phi = 0. \tag{3}$$

Consider the simplest case, $k = 1$. If Eq. (3) has only the trivial solution, $\phi = 0$, then Eq. (2) would have a nontrivial solution. The vectors ψ and ψ' would form a chain of length 2, in contradiction to the assumption that $k = 1$. Hence L^* must have an eigenvector corresponding to eigenvalue $\bar{\lambda}$, and this eigenvector cannot be orthogonal to ψ by the same reasoning.

The generalization of this argument to chains of arbitrary length is not difficult.

Note that whenever L has a generalized eigenvector of rank greater than 1, then it has an ordinary eigenvector ψ satisfying Eq. (2). This is the key point in the proof of the main results of this section.

Theorem 2: The eigenvectors of a self-adjoint operator L span the space S unless L has a null eigenvector which is orthogonal to every other eigenvector of L.

To prove this, suppose that the eigenvectors of L do not span S; then there must be at least one generalized eigenvector of rank greater than 1. Hence we have vectors ψ and ψ' satisfying Eq. (2), where ψ is an eigenvector of L corresponding to some eigenvalue λ. Suppose λ is real. Then,

$$\langle \psi, \psi \rangle = \langle (L - \lambda)\psi', \psi \rangle = \langle \psi', (L - \lambda)\psi \rangle = 0.$$

Thus, if λ is real, ψ is null; if λ is not real, ψ is null by virtue of Eq. (1). We have shown that the set of eigenvectors will be complete unless at least one of them is null. Now let us consider the scalar product of ψ with the other eigenvectors of L. By Eq. (1), this scalar product must vanish except for eigenvectors corresponding to eigenvalue $\bar{\lambda}$. In the case that λ is real, the existence of such eigenvectors will depend on the degeneracy of the eigenvalue. For complex λ, Theorem 1 and the remark at the end of Sec. II guarantee at least one such eigenvector. However, for either case, let ϕ be any eigenvector of L corresponding to eigenvalue $\bar{\lambda}$ (which is the same as λ, of course, if λ is real). Then,

$$\langle \psi, \phi \rangle = \langle (L - \lambda)\psi', \phi \rangle = \langle \psi', (L - \bar{\lambda})\varphi \rangle = 0.$$

Hence ψ is orthogonal to all the eigenvectors of L.

The converse of Theorem 2 is also true; we state it below as a separate theorem since it will be extended in Sec. IV to spaces of infinite dimension. For finite dimensions, the two theorems together provide a necessary and sufficient condition for the eigenvectors of a self-adjoint operator to span the space, namely, the absence of a null eigenvector orthogonal to all other eigenvectors. It is interesting to note that such eigenvectors are associated with the simultaneous vanishing of both the factors in Eq. (1).

Theorem 3: If a self-adjoint operator L has a null eigenvector which is orthogonal to every other eigenvector of L, then these eigenvectors do not span the space S.

This follows almost trivially from one of the properties of the scalar product as defined in Sec. I, for if ψ were such an eigenvector, it would be orthogonal to the subspace spanned by the eigenvectors of L. If this were the whole space S, ψ would have to be the zero vector.

IV. SOME REMARKS ON THE GENERAL CASE

Once we abandon the terrain of finite-dimensional spaces, many simple ideas have to be replaced by more abstract notions. The question of the completeness of the eigenvectors of an operator, for example, is generally not an important one since many quite reasonable operators have no eigenvectors at all. Instead the analogous problem is that of the spectrum of an operator, which for Hermitian and normal operators is solved by the spectral theorems. It is not our ambition here to attempt an extension of the formidable machinery of spectral theory to self-adjoint operators in indefinite metric spaces, however desirable such an extension might be in principle. Fortunately, most physicists are generally content to circumvent these difficulties by tricks such as "normalization in a box," which convert the continuous spectrum into a discrete spectrum, and to equip the operator with properly normalized eigenvectors. We will sidestep the problem of whether or not this procedure is valid and instead investigate a few of its consequences. Suppose that when a self-adjoint operator is supplied with eigenvectors, these eigenvectors do span the space in the sense of convergence in the topology defined by the norm

$$\|\psi\|^2 = (\psi, \psi) = \langle \psi, \eta\psi \rangle.$$

In this case, we can show that complex eigenvalues must occur in complex-conjugate pairs.

Lemma 1: If the eigenvectors of a self-adjoint operator L span the space S and if λ is a complex eigenvalue of L, so is $\bar{\lambda}$.

Assume the contrary. Let ψ_1 be an eigenvector corresponding to complex eigenvalue λ such that $\bar{\lambda}$ is not an eigenvalue. Then, according to (1),

$$\langle \psi_k, \psi_1 \rangle = 0,$$

where ψ_k is *any* eigenvector, including ψ_1. Since L has a complete set of eigenvectors, for any ϕ in S we have

$$\phi_N = \sum_{i=1}^{N} \alpha_i \psi_i$$

such that

$$\|\phi - \phi_N\|$$

is arbitrarily small for sufficiently large N. Consider

$$|\langle\phi, \psi_1\rangle|^2 = |\langle\phi - \phi_N, \psi_1\rangle|^2 = |(\phi - \phi_N, \eta\psi_1)|^2 \leq \|\phi - \phi_N\| \, \|\eta\psi_1\| = \|\phi - \phi_N\| \, \|\psi_1\|.$$

This can be made arbitrarily small by choosing N large enough, so in fact

$$\langle\phi, \psi_1\rangle = 0$$

for any ϕ in S. But this is only possible if $\psi_1 = 0$; so there must be some k for which

$$\langle\psi_k, \psi_1\rangle \neq 0.$$

Then, by (1), this ψ_k must correspond to eigenvalue $\bar{\lambda}$.

Reasoning analogous to that used in the proof of Lemma 1 implies that *Theorem 3 remains valid in the general case.*

We have assumed that by some means the continuous spectrum of L has been replaced by a discrete spectrum. It seems reasonable to conjecture that the resulting operator has only a discrete spectrum; i.e., every λ in the spectrum of L is actually an eigenvalue. But the spectrum of L also contains the residual spectrum; this is made up of those values of λ for which the closure of the range of $L-\lambda$ is a proper subset of S, but which are not eigenvalues. The next lemma shows that operators of the type we have been discussing have no residual spectrum, so that our speculation is correct.

Lemma 2: A self-adjoint operator with a complete set of eigenvectors has no residual spectrum.

Suppose λ is such that the closure of the range of $L-\lambda$ is a proper subset of S. We must show that λ is an eigenvalue. There is some ϕ in S such that

$$(\phi, (L - \lambda)\psi) = 0$$

for all ψ in S. But then

$$((L^* - \bar{\lambda})\phi, \psi) = 0$$

for all ψ in S, which implies that ϕ is an eigenvector of L^* with eigenvalue $\bar{\lambda}$. The vector $\eta\phi$ is therefore an eigenvector of L with eigenvalue $\bar{\lambda}$. But, according to Lemma 1, if $\bar{\lambda}$ is an eigenvalue, so is λ.

An interesting application of the results of this section is in allowing a slight weakening of the quarantine condition imposed by Lee and Wick on their models to guarantee a unitary S matrix.[9] They require that any eigenstate of the Hamiltonian satisfy

$$\langle\psi, \psi\rangle \geq 0 \tag{4}$$

and furthermore that no null eigenvector correspond to a real eigenvalue. However, if we agree that requiring the eigenstates of the Hamiltonian to span the space is reasonable on other grounds, then this assumption plus the inequality (4) is sufficient, for completeness would require that any null eigenvector corresponding to a real eigenvalue have a nonzero scalar product with some other degenerate eigenvector. Let ψ_1 be the null eigenvector and ψ_2 another eigenvector with the same eigenvalue, normalized so that

$$\langle\psi_1, \psi_2\rangle = 1$$

and

$$\langle\psi_2, \psi_2\rangle < 1.$$

Then H would have the eigenvector

$$\psi = \psi_1 - \psi_2$$

such that

$$\langle\psi, \psi\rangle = -2 + \langle\psi_2, \psi_2\rangle < -1 < 0,$$

which violates inequality (4). Hence, this inequality and the assumption of completeness of the eigenstates of H rules out any eigenstate with real eigenvalue being null.

* Work supported in part by the U.S. Atomic Energy Commission.

[1] T. D. Lee and G.-C. Wick, Nucl. Phys. **B9**, 209 (1969).
[2] T. D. Lee and G.-C. Wick, Nucl. Phys. **B10**, 1 (1969).
[3] T. D. Lee and G.-C. Wick, Phys. Rev. D **2**, 1033 (1970).
[4] E. C. G. Sudarshan, "Indefinite Metric and Nonlocal Field Theories," in *Fundamental Problems in Elementary Particle Physics*, Solvay Institute 14th Physics Conference (Interscience, New York, 1968), pp. 97–127.
[5] A. M. Gleeson and E. C. G. Sudarshan, Phys. Rev. D **1**, 474 (1970).
[6] L. K. Pandit, Nuovo Cimento Suppl. **10**, 157 (1959).
[7] This is a paraphrase of a result in B. Friedman, *Principles and Techniques of Applied Mathematics* (Wiley, New York, 1956), p. 131. This reference provides the details of the proof.
[8] For a proof, see B. Friedman, Ref. 7, p. 45.
[9] Sudarshan's criticism of the work of Lee and Wick centers on the claim that the restriction (5) must break down in higher sectors of a field-theoretic model.

Propagation of Random Electromagnetic Fields*

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The propagation of a random electromagnetic field in a uniform medium is investigated. It is assumed that the two-point mutual coherence γ is stationary over an initial plane. It is shown that the mean intensity will be conserved if and only if $\gamma(k_x, k_y)$, the spectrum of γ, is zero for $k_x^2 + k_y^2 > k^2$, where k is the wavenumber in the medium, meaning that evanescent waves are not considered; and it is proved that, under this condition, the transverse coherence is unchanged from plane to plane.

I. INTRODUCTION

Many modern problems involve electromagnetic fields which have been spatially randomized by such processes as passage through a turbulent dielectric. In this paper we consider such a field after randomization by such processes and its propagation from an initial plane on which the mutual coherence is stationary into a homogeneous isotropic medium. More specifically, we determine the mutual coherence function in the medium in terms of the mutual coherence on the initial plane. Because of the existence of turbulence in the ionosphere and in tropospheric layers, this geometry is applicable to many problems and is, of course, different from that which is considered in the well-known van Cittert–Zernike theorem in which a small planar source is considered. An infinite plane source has been considered by Beran,[1] who derived a result which may be considered as the high frequency case (for isotropic waves) of one of the general results we prove in this paper. The more general results obtained here follow from the inclusion of the assumption that the mean intensity will remain constant for a lossless medium. We find that the spectrum of the mutual coherence, $\gamma(k_x, k_y)$, is nonzero only for $k_x^2 + k_y^2 \leq k^2$, where k is the wavenumber in the medium, and that the transverse coherence propagates unchanged. Beran[1] showed previously that mutual coherence is conserved if $k_x^2 + k_y^2 \ll k^2$. The present restriction on the spectrum can be interpreted, in terms of the angular spectrum of plane waves,[2] to mean, consistently, that evanescent waves are not included. (If such waves are generated during the randomization, they will be rapidly attenuated in any case.)

Because we are treating the propagation of an electromagnetic field in a uniform isotropic medium, we can employ the scalar wave equation because the rectangular components of the electromagnetic field obey the scalar wave equation in such media.[3] The mutual coherence is usually taken between similar polarizations, but this interpretation is not required and our results also apply to the coherence between cross polarizations.

II. BASIC FORMULATION

We consider the propagation of a wave $\psi(r)$ obeying the scalar wave equation

$$(\nabla^2 + k^2)\psi(\mathbf{r}) = 0. \tag{1}$$

As usual, $\psi(\mathbf{r})$ represents a monochromatic wave with $k_0 = \omega/c$ and $k^2 = \epsilon_R k_0^2$. We shall assume that the boundary values are given over the $z = 0$ plane, use Green's theorem, and obtain the Helmholtz–Kirchhoff integral

$$\psi(\mathbf{r}) = \frac{1}{4\pi}\iint\left(\frac{\partial\psi(\mathbf{r}')}{\partial n}G(\mathbf{r},\mathbf{r}') - \psi(\mathbf{r}')\frac{\partial G(\mathbf{r},\mathbf{r}')}{\partial n}\right)dS', \tag{2}$$

where $G(\mathbf{r}, \mathbf{r}')$ is an appropriate Green's function and n is the outward normal. The integral is over the plane $z = 0$, the contribution over the infinite hemisphere having been eliminated by the application of the Sommerfeld radiation condition. We employ the Green's function

$$G(\mathbf{r},\mathbf{r}') = \frac{\exp\{jk[(x-x')^2+(y-y')^2+(z-z')^2]^{\frac12}\}}{[(x-x')^2+(y-y')^2+(z-z')^2]^{\frac12}} - \frac{\exp\{jk[(x-x')^2+(y-y')^2+(z+z')^2]^{\frac12}\}}{[(x-x')^2+(y-y')^2+(z+z')^2]^{\frac12}}. \tag{3}$$

Then $G(\mathbf{r}, \mathbf{r}') = 0$ on the boundary plane. On this plane, the outward normal is in the $-z$ direction. Consequently, Eq. (5) takes the form

$$\psi(\mathbf{r}) = \frac{1}{4\pi}\iint\psi(\mathbf{r}')\frac{\partial G(\mathbf{r},\mathbf{r}')}{\partial z'}dS'. \tag{4}$$

Equation (4) is a standard form.[3] We now cast this equation into a form more useful for our purposes by noting that by direct calculation

$$\frac{\partial G(\mathbf{r},\mathbf{r}')}{\partial z'}\bigg|_{z'=0} = -\frac{2z}{R^2}\left(jk - \frac{1}{R}\right)e^{jkR} = -2\frac{\partial}{\partial z}\left(\frac{e^{jkR}}{R}\right), \tag{5}$$

where $R = [(x-x')^2 + (y-y')^2 + z^2]^{\frac{1}{2}}$. Thus

$$\psi(\mathbf{r}) = -\frac{1}{2\pi}\frac{\partial}{\partial z}\iint \psi(\mathbf{r}')\frac{e^{jkR}}{R}\,dS'. \tag{6}$$

Using Eq. (6), we now obtain the following expression for the mutual coherence function[4] $\gamma(\mathbf{r}_1, \mathbf{r}_2) = \langle\psi(\mathbf{r}_1)\psi^*(\mathbf{r}_2)\rangle$, in the space $z > 0$ in terms of the mutual coherence on the boundary plane:

$$\gamma(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{4\pi^2}\frac{\partial}{\partial z_1}\frac{\partial}{\partial z_2}\iint dS \iint dS'' \frac{e^{jk|\mathbf{r}_1-\mathbf{r}'|}}{|\mathbf{r}_1-\mathbf{r}'|} \times \frac{\exp(jk|\mathbf{r}_2-\mathbf{r}''|)}{|\mathbf{r}_2-\mathbf{r}''|}\gamma_0(\mathbf{r}',\mathbf{r}''). \tag{7}$$

The zero subscript has been placed on the function γ inside the integral as a reminder that it is being evaluated over the $z = 0$ plane. We shall assume that the mutual coherence is spatially stationary on the boundary plane, that is,

$$\gamma_0(\mathbf{r}',\mathbf{r}'') = \gamma_0(x'-x'', y'-y'') = \gamma_0(\xi,\eta), \tag{8}$$

where $\xi = x' - x''$ and $\eta = y' - y''$. We can now introduce the Fourier transform relations

$$\gamma_0(\mathbf{r}',\mathbf{r}'') = \frac{1}{4\pi^2}\iint_{-\infty}^{\infty} dk_x\,dk_y \times \exp[j(k_x\xi + k_y\eta)]\hat{\gamma}_0(k_x,k_y),$$
$$\hat{\gamma}_0(k_x,k_y) = \iint_{-\infty}^{\infty} d\xi\,d\eta \exp[-j(k_x\xi+k_y\eta)]\gamma_0(\xi,\eta). \tag{9}$$

Substituting in Eq. (7) and reversing the order of differentiation and integration, we obtain

$$\gamma(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{(2\pi)^2}\iint_{-\infty}^{\infty} dk_x\,dk_y\hat{\gamma}_0(k_x,k_y)\frac{\partial}{\partial z_1}\frac{\partial}{\partial z_2}T(\mathbf{r}_1)T^*(\mathbf{r}_2), \tag{10}$$

where, for example,

$$T(\mathbf{r}_1) = \frac{1}{2\pi}\iint_{-\infty}^{\infty}\frac{\exp[jk|\mathbf{r}'-\mathbf{r}_1|]}{|\mathbf{r}'-\mathbf{r}_1|} \times \exp[j(k_xx'+k_yy')]\,dx'\,dy'. \tag{11}$$

III. EVALUATION OF $T(\mathbf{r})$

We evaluate the expression for $T(\mathbf{r}_1)$, using the representation of a spherical wave as a sum of elementary cylindrical waves[5]:

$$\frac{\exp(jk|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} = \int_0^\infty \frac{\lambda\,d\lambda}{(\lambda^2-k^2)^{\frac{1}{2}}}J_0(\lambda\rho) \times \exp[-(z-z')[\lambda^2-k^2]^{\frac{1}{2}}], \tag{12}$$

where $z - z' > 0$, $|\mathbf{r}-\mathbf{r}'| = [(x-x')^2 + (y-y')^2 + (z-z')]^{\frac{1}{2}}$, and $\rho = [(x-x')^2 + (y-y')^2]^{\frac{1}{2}}$. Thus, from Eqs. (11) and (12), setting $z' = 0$ and interchanging the order of integration, we obtain

$$T(\mathbf{r}_1) = \frac{1}{2\pi}\int_0^\infty d\lambda \iint_{-\infty}^{\infty} dx'\,dy'\frac{\lambda}{(\lambda^2-k^2)^{\frac{1}{2}}}J_0(\lambda\rho_1) \times \exp[-z_1(\lambda^2-k^2)^{\frac{1}{2}}]\exp[j(k_xx'+k_yy')], \tag{13}$$

with $\rho_1 = [(x_1-x')^2 + (y_1-y')]^{\frac{1}{2}}$.

We introduce polar coordinates, setting $x' - x_1 = \rho_1\cos\theta$ and $y' - y_1 = \rho_1\sin\theta$ and defining $k_x = K\cos\varphi$ and $k_y = K\sin\varphi$. We obtain

$$T(\mathbf{r}_1) = \frac{\exp[j(k_xx_1+k_yy_1)]}{2\pi}\int_0^\infty d\lambda \times \int_0^\infty \frac{\lambda\rho_1\,d\rho_1}{(\lambda^2-k^2)^{\frac{1}{2}}}J_0(\lambda\rho_1)\exp[-z_1(\lambda^2-k^2)^{\frac{1}{2}}] \times \int_0^{2\pi}\exp[jk\rho_1\cos(\theta-\varphi)]\,d\theta. \tag{14}$$

The inner integral is recognized as $2\pi J_0(k\rho_1)$. Thus, interchanging the order of integration of ρ_1 and λ, we obtain

$$T(\mathbf{r}_1) = \exp[j(k_xx_1+k_yy_1)] \times \int_0^\infty \rho_1\,d\rho_1\int_0^\infty \lambda\,d\lambda J_0(\lambda\rho_1)J_0(k\rho_1) \times \left(\frac{\exp[-z_1(\lambda^2-k^2)^{\frac{1}{2}}]}{[\lambda^2-k^2]^{\frac{1}{2}}}\right). \tag{15}$$

The double integral on the right is recognized as the Fourier–Bessel integral transform of the term in brackets,[6] provided that

$$\int_0^\infty \lambda\left|\frac{\exp[-z_1(\lambda^2-k^2)^{\frac{1}{2}}]}{(\lambda^2-k^2)^{\frac{1}{2}}}\right| < \infty. \tag{16}$$

This condition is clearly met because the integrand will decrease exponentially with λ for large λ. Thus we obtain

$$T(\mathbf{r}_1) = \exp [j(k_x x_1 + k_y y_1)] \times \exp [-z_1(K^2 - k^2)^{\frac{1}{2}}]/(K^2 - k^2)^{\frac{1}{2}}, \quad (17)$$

where $K^2 = k_x^2 + k_y^2$.

IV. MATHEMATICAL RESULTS

Our general result is obtained from Eq. (10), using Eq. (17). Substituting, we find, upon carrying through the differentiation,

$$\gamma(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{4\pi^2} \iint_{-\infty}^{\infty} dk_x \, dk_y \hat{\gamma}_0(k_x, k_y) \times \exp [-z_1(k_x^2 + k_y^2 - k^2)^{\frac{1}{2}}] \times \exp [-z_2(k_x^2 + k_y^2 - k^2)^{\frac{1}{2}}]^* \times \exp \{j[k_x(x_1 - x_2) + k_y(y_1 - y_2)]\}. \quad (18)$$

The validity of Eq. (18) may readily be checked by considering the example of an incident plane wave. In this case, $\hat{\gamma}_0(k_x, k_y)$ is a delta function, and we have $\gamma(\mathbf{r}_1, \mathbf{r}_2) = \exp [jk(z_1 - z_2)]$, as expected. A considerable simplification is available when the mutual coherence is assumed to be isotropic in x and y over the boundary plane. In this case $\hat{\gamma}_0(k_x, k_y) = \hat{\gamma}_0(K)$, where $K = (k_x^2 + k_y^2)^{\frac{1}{2}}$. We again set $k_x = K \cos \varphi$ and $k_y = K \sin \varphi$ and define $x_1 - x_2 = s \cos \delta$ and $y_1 - y_2 = s \sin \delta$. As a result,

$$\gamma(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{4\pi^2} \int_0^{\infty} K \, dK \hat{\gamma}_0(K) \exp [-z_1(K^2 - k^2)^{\frac{1}{2}}] \times \exp [-z_2(K^2 - k^2)^{\frac{1}{2}}]^* \times \int_0^{2\pi} \exp [jKs \cos (\varphi - \delta)] \, d\varphi$$

$$= \frac{1}{2\pi} \int_0^{\infty} K \, dK \hat{\gamma}_0(K) J_0(Ks) \times \exp [-z_1(K^2 - k^2)^{\frac{1}{2}}] \times \exp [-z_2(K^2 - k^2)^{\frac{1}{2}}]^*, \quad (19)$$

with $s = [(x_1 - x_2)^2 + (y_1 - y_2)^2]^{\frac{1}{2}}$.

V. THE MEAN INTENSITY

We readily calculate the mean intensity $\langle I \rangle = \gamma(\mathbf{r}, \mathbf{r}) = \langle \psi(\mathbf{r}) \psi^*(\mathbf{r}) \rangle$, using Eq. (18). Thus,

$$\langle I \rangle = \frac{1}{4\pi^2} \iint_{-\infty}^{\infty} dk_x \, dk_y \hat{\gamma}_0(k_x, k_y) \times |\exp [-z(k_x^2 + k_y^2 - k^2)^{\frac{1}{2}}]|^2, \quad (20)$$

and for the isotropic case

$$\langle I \rangle = \frac{1}{2\pi} \int_0^{\infty} K \, dK \hat{\gamma}_0(K) \, |\exp [-z(K^2 - k^2)^{\frac{1}{2}}]|^2. \quad (21)$$

It is clear from Eq. (21) that if $\hat{\gamma}_0(K)$ is zero for $K > k$, then $\langle I \rangle$ is not a function of z. We shall now show that if $\langle I \rangle$ is independent of z, then $\hat{\gamma}_0(K) = 0$ for $K > k$.

Write Eq. (21) in the form

$$\langle I \rangle = \frac{1}{2\pi} \int_0^{k} K \, dK \hat{\gamma}_0(K) + \frac{1}{2\pi} \int_k^{\infty} K \, dK \hat{\gamma}_0(K) \exp [-2z(K^2 - k^2)^{\frac{1}{2}}]. \quad (22)$$

If $\langle I \rangle$ is independent of z, the second integral on the right must also be independent of z. Setting $t = [K^2 - k^2]^{\frac{1}{2}}$, we write this integral in the form

$$S = \int_0^{\infty} t \, dt \hat{\gamma}_0([t^2 + k^2]^{\frac{1}{2}}) e^{-tz'}, \quad (23)$$

where we have set $z' = 2z \geq 0$. Because $\hat{\gamma}_0$ is piecewise continuous, we may continue the integral analytically into the complex z' plane. The integral now represents a Laplace transform. Taking the inverse transform of both sides of Eq. (23), we obtain

$$L^{-1}[S] = t\hat{\gamma}_0((t^2 + k^2)^{\frac{1}{2}}). \quad (24)$$

Since S is not a function of z', the left-hand side of Eq. (24) is a delta function of t or zero. Thus $\hat{\gamma}_0((t^2 + k^2)^{\frac{1}{2}})$ is zero for $t > 0$, which implies it is zero for $K > k$. QED

With this result, we may write Eq. (19) in a form that is valid for lossless media (k real),

$$\gamma(\mathbf{r}_1, \mathbf{r}_2) = \gamma(s, z_2 - z_1) = \frac{1}{2\pi} \int_0^{k} K \, dK \hat{\gamma}_0(K) J_0(Ks) \times \exp [j(z_2 - z_1)(k^2 - K^2)^{\frac{1}{2}}]. \quad (25)$$

Since $\hat{\gamma}_0(K) = 0$ for $K > k$, we may extend the integral to infinity:

$$\gamma(s, z_2 - z_1) = \frac{1}{2\pi} \int_0^{\infty} K \, dK \hat{\gamma}_0(K) J_0(Ks) \times \exp [j(z_2 - z_1)(k^2 - K^2)^{\frac{1}{2}}]. \quad (26)$$

We observe that, in the transverse plane $z_1 = z_2 = z$, Eq. (26) reduces to

$$\gamma(s, z) = \frac{1}{2\pi} \int_0^{\infty} K \, dK \hat{\gamma}_0(K) J_0(Ks) = \gamma_0(s). \quad (27)$$

In order to arrive at the final result in Eq. (27), we observed that the integral was the inverse Hankel transform. We have thus demonstrated that the coherence function propagates unchanged from plane to plane. A restricted form of this result was derived by Beran,[1] using an approximation for the Green's functions.

We may easily extend our result to anisotropic γ, beginning with Eq. (20). We find, corresponding to Eq. (23),

$$S' = \iint_{k_x^2+k_y^2>k^2} dk_x\, dk_y \hat{\gamma}_0(k_x, k_y) \times \exp[-2z(k_x^2 + k_y^2 - k^2)^{\frac{1}{2}}], \quad (28)$$

where S' is not a function of z. Using the same transformations and converting to polar coordinates in the k plane, we obtain

$$S' = \int_0^\infty e^{-z't} dt \int_0^{2\pi} d\varphi t \hat{\gamma}_0((k^2 + t^2)^{\frac{1}{2}} \cos\varphi, (k^2 + t^2)^{\frac{1}{2}} \sin\varphi). \quad (29)$$

We again take the inverse Laplace transform, and find that if $\hat{\gamma}_0(k_x, k_y) \geq 0$ for all (k_x, k_y), then $\hat{\gamma}_0(k_x, k_y) = 0$ for $k_x^2 + k_y^2 > k^2$. We then obtain, in an exactly similar manner to Eq. (27), that

$$\gamma(x_1 - x_2, y_1 - y_2, z) = \gamma_0(x_1 - x_2, y_1 - y_2) \quad (30)$$

is valid for anisotropic waves.

VI. LONGITUDINAL SEPARATIONS

When $\gamma(k_x, k_y) = 0$ for $k_x^2 + k_y^2 > K_c^2$ and

$$K_c^4 |z_2 - z_1| \ll 8k^3,$$

our general expression, Eq. (18), may be simplified using

$$[k_x^2 + k_y^2 - k^2]^{\frac{1}{2}} = -jk + j(k_x^2 + k_y^2)/2k \quad (31)$$

and observing that

$$\exp[j(z_1 - z_2)(k_x^2 + k_y^2)/2k] = \frac{-jk}{2\pi(z_1 - z_2)} \mathcal{F}\{\exp[jk(\xi^2 + \eta^2)/2(z_1 - z_2)]\}. \quad (32)$$

Substituting, we find

$$\begin{aligned} \gamma(\mathbf{r}_1, \mathbf{r}_2) &= -\{jk \exp[jk(z_1 - z_2)]/2\pi(z_1 - z_2)\} \\ &\quad \times \mathcal{F}^{-1}\{\hat{\gamma}_0(k_x, k_y) \\ &\quad \times \mathcal{F}\{\exp[jk(\xi^2 + \eta^2)/2(z_1 - z_2)]\}\} \\ &= \{-jk \exp[jk(z_1 - z_2)]/2\pi(z_1 - z_2)\} \\ &\quad \times \gamma_0(\xi, \eta) * \exp[jk(\xi^2 + \eta^2)/2(z_1 - z_2)], \end{aligned} \quad (33)$$

where the asterisk indicates the convolution.

* Research supported by a grant from the Atmospheric Sciences Section, National Science Foundation.

† Work submitted in partial fulfillment of the requirements for the Ph.D. degree in Electrical Engineering, University of Maryland.

[1] M. J. Beran, in *Statistical Methods in Radio Wave Propagation*, edited by W. C. Hoffman (Pergamon, New York, 1960), pp. 93–98.

[2] J. R. Shewell and E. Wolf, J. Opt. Soc. Am. **58**, 1596 (1968).

[3] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill, New York, 1941).

[4] M. Born and E. Wolf, *Principles of Optics* (Pergamon, New York, 1959), Chap. X.

[5] Reference 3, p. 576.

[6] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1953), Vol. I, p. 490.

Eigenfunctions of the Integral Equation for the Potential of the Charged Disk

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(Received 17 December 1970)

The integral equation

$$f(r,\theta)=\int_0^{2\pi}\int_0^1 \frac{u(r',\theta')}{[r^2+r'^2-2rr'\cos(\theta-\theta')]^{\frac{1}{2}}}\cdot\frac{r'}{(1-r'^2)^{\frac{1}{2}}}\,dr'\,d\theta'$$

arises in connection with the problem of the electrostatic potential due to a charged disk. We solve the equation by computing a complete set of eigenfunctions and eigenvalues for the integral operator. The eigenfunctions have the form $F^{\pm}_{m,n}(r,\theta)=P_n^m[(1-r^2)^{\frac{1}{2}}]e^{\pm im\theta}$, $0\le m\le n$, $m+n$ even. Here $P_n^m(x)$ is the associated Legendre function of the first kind.

The main result we wish to prove is as follows: Let

$$F^{\pm}_{m,n}(r,\theta)=P_n^m[(1-r^2)^{\frac{1}{2}}]e^{\pm im\theta},$$
$$0\le r\le 1,\quad 0\le m\le n,\quad m+n \text{ even.} \tag{1}$$

Then

$$\frac{1}{\pi^2}\int_0^{2\pi}\int_0^1 \frac{F^{\pm}_{m,n}(r',\theta')}{[r^2+r'^2-2rr'\cos(\theta-\theta')]^{\frac{1}{2}}}\times\frac{r'}{(1-r'^2)^{\frac{1}{2}}}\,dr'\,d\theta' = \lambda_{m,n}F^{\pm}_{m,n}(r,\theta),\quad 0\le r\le 1, \tag{2}$$

where

$$\lambda_{m,n}=\frac{1}{\pi}\frac{\Gamma((n+m+1)/2)\Gamma((n-m+1)/2)}{\Gamma((n-m+2)/2)\Gamma((n+m+2)/2)}. \tag{3}$$

The problem arises in the following way. Suppose we wish to find the electrostatic potential due to the presence of a charged circular disk when the potential on the disk is given. The mathematical problem then is to find a function $u(x,y,z)$ continuous for all (x,y,z), tending to zero at infinity, and harmonic for all (x,y,z) except for (x,y,z) on the disk, $x^2+y^2\le 1$, $z=0$. On the disk, u is to be equal to a given function $\tilde f(x,y)$. We look for a solution of the form

$$u(x,y,z)=\iint_{x'^2+y'^2\le 1}\frac{\tilde\phi(x',y')}{[(x-x')^2+(y-y')^2+z^2]^{\frac{1}{2}}}\,dx'\,dy'.$$

Here $\tilde\phi$ is the jump in the normal derivative of u across the disk. In order to satisfy the boundary condition, we must have

$$\tilde f(x,y)=\iint_{x'^2+y'^2\le 1}\frac{\tilde\phi(x',y')}{[(x-x')^2+(y-y')^2]^{\frac{1}{2}}}\,dx'\,dy',\quad x^2+y^2\le 1,$$

or, switching to polar coordinates and setting $f(r,\theta)=\tilde f(r\cos\theta, r\sin\theta)$, $\phi(r',\theta')=\tilde\phi(r'\cos\theta', r'\sin\theta')$, we have

$$f(r,\theta)=\int_0^{2\pi}\int_0^1\frac{\phi(r',\theta')}{[r^2+r'^2-2rr'\cos(\theta-\theta')]^{\frac{1}{2}}}\,r'\,dr'\,d\theta'. \tag{4}$$

To see why a result such as (2) must hold, we observe the following. The problem as described above can be solved by separation of variables in oblate spherical coordinates,[1]

$$x=\cosh\eta\sin\nu\cos\phi,$$
$$y=\cosh\eta\sin\nu\sin\phi,$$
$$z=\sinh\eta\cos\nu.$$

The range of the variables is $0\le\eta<\infty$, $0\le\nu\le\pi$, $0\le\phi\le 2\pi$. The surface $\eta=0$, $0\le\nu\le\pi/2$ corresponds to the top of the disk $x^2+y^2\le 1$, $z=0$, while the surface $\eta=0$, $\pi/2\le\nu\le\pi$ corresponds to the bottom of the disk. The solutions found by separation of variables are $P_n^m(\cos\nu)Q_n^m(i\sinh\eta)e^{\pm im\phi}$, $m+n$ even, where $Q_n^m(x)$ is the associated Legendre function of the second kind. The condition $m+n$ even assures that the function is single valued on the disk. If we take $0\le\nu\le\pi/2$ on the disk, the jump in the normal derivative of this function across the disk is

$$2P_n^m(\cos\nu)\lim_{\eta\to 0+}\frac{dQ_n^m(i\sinh\eta)}{d\eta}\,\frac{1}{\cos\nu}\,e^{\pm im\phi}.$$

In terms of the usual polar coordinates on the disk, we have $r=\sin\nu$. Thus from (4) we see that (2) holds with

$$\lambda_{m,n}=\frac{1}{2i}\lim_{t\to 0+}\frac{Q_n^m(it)}{(d/dt)Q_n^m(it)}.$$

Unfortunately, the value of $\lambda_{m,n}$ does not seem to be readily available, and so we will use a different method to compute it. We will derive the result for $F^{+}_{m,n}(r,\theta)$. The result for $F^{-}_{m,n}(r,\theta)$ will follow by taking complex conjugates.

We will use the method of Fourier transforms. We note that the left hand side of (2) is a convolution of $1/r$ and $G_{m,n}(r,\theta)$, where

$$G_{m,n}(r,\theta)=\begin{cases}F^{+}_{m,n}(r,\theta)\cdot(1-r^2)^{-\frac{1}{2}}, & r<1,\\ 0, & r>1.\end{cases}$$

We will proceed formally to take the Fourier transform of the left-hand side of (2) and invert it. This can be made rigorous by considering our operations to be taking place in the space of temperate distributions.[2]

Thus, if $H_{m,n}(\rho,\phi)$ is the Fourier transform of $G_{m,n}(r,\theta)$,

$$\begin{aligned}H_{m,n}(\rho,\phi)&=\frac{1}{4\pi^2}\int_0^1\frac{P_n^m[(1-r^2)^{\frac{1}{2}}]}{(1-r^2)^{\frac{1}{2}}}\,r\,dr\int_0^{2\pi}e^{im\theta}e^{-ir\rho\cos(\theta-\phi)}\,d\theta\\&=\frac{1}{2\pi}e^{im\pi/2}e^{im\phi}\int_0^1\frac{P_n^m[(1-r^2)^{\frac{1}{2}}]}{(1-r^2)^{\frac{1}{2}}}\,rJ_m(\rho r)\,dr.\end{aligned}\qquad(5)$$

Using the relations[3]

$$P_n^m(x)=(-1)^m[\Gamma(n+m+1)/\Gamma(n-m+1)]P_n^{-m}(x)\qquad(6a)$$

and

$$C_{n-m}^{m+\frac{1}{2}}(x)=2^m\frac{\Gamma(n+m+1)}{\Gamma(2m+1)}(-1)^n\frac{\Gamma(m+1)}{\Gamma(n-m+1)}\times P_n^{-m}(x)(1-x^2)^{-m/2},\qquad(6b)$$

where $C_l^\lambda(x)$ is a Gegenbauer polynomial, we find

$$\int_0^1\frac{P_n^m[(1-r^2)^{\frac{1}{2}}]}{(1-r^2)^{\frac{1}{2}}}\,rJ_m(\rho r)\,dr=\frac{\Gamma(2m+1)}{2^m\Gamma(m+1)}\int_0^1 r^{m+1}C_{n-m}^{m+\frac{1}{2}}[(1-r^2)^{\frac{1}{2}}]J_m(\rho r)\,dr.$$

The integral on the right has been tabulated.[4] Using this result, we find

$$\int_0^1\frac{P_n^m[(1-r^2)^{\frac{1}{2}}]}{(1-r^2)^{\frac{1}{2}}}\,rJ_m(\rho r)\,dr=[\Gamma(2m+1)/2^m\Gamma(m+1)](-1)^{(n-m)/2}\times(\pi/2)^{\frac{1}{2}}\rho^{-\frac{1}{2}}C_{n-m}^{m+\frac{1}{2}}(0)J_{n+\frac{1}{2}}(\rho).$$

On substituting in the value[5] of $C_{n-m}^{m+\frac{1}{2}}(0)$ and substituting in (5), we find

$$\begin{aligned}G_{m,n}(\rho,\phi)&=\tfrac{1}{4}(2/\pi)^{\frac{1}{2}}\rho^{-\frac{1}{2}}J_{n+\frac{1}{2}}(\rho)\times\frac{\Gamma((n+m+1)/2)\Gamma(2m+1)}{2^m\Gamma(m+1)\Gamma((2m+1)/2)\Gamma((n-m+2)/2)}e^{im(\phi+\pi/2)}\\&=\frac{2^{m-\frac{3}{2}}}{\pi}\rho^{-\frac{1}{2}}J_{n+\frac{1}{2}}(\rho)\frac{\Gamma((n+m+1)/2)}{\Gamma((n-m+2)/2)}e^{im(\phi+\pi/2)},\end{aligned}$$

where in the last step we have used the multiplication theorem for the Gamma function.

Now the (distributional) Fourier transform of $1/r$ is $1/2\pi\rho$.[6] Thus, if $I_{m,n}(\rho,\phi)$ denotes the Fourier transform of $G_{m,n}(r,\theta)*(1/r)$, we have

$$I_{m,n}(\rho,\theta)=[(2^{m-5/2})/\pi^2]\rho^{-\frac{3}{2}}J_{n+\frac{1}{2}}(\rho)\times\frac{\Gamma((n+m+1)/2)}{\Gamma((n-m+2)/2)}e^{im(\phi+\pi/2)}.$$

Denote the left-hand side of (2) by $J_{m,n}(r,\theta)$. We have

$$\begin{aligned}J_{m,n}(r,\theta)&=\frac{2^{m-\frac{1}{2}}}{\pi^2}\frac{\Gamma((n+m+1)/2)}{\Gamma((n-m+2)/2)}e^{\frac{1}{2}im\pi}\int_0^\infty\rho^{-\frac{1}{2}}J_{n+\frac{1}{2}}(\rho)\,d\rho\times\int_0^{2\pi}e^{i\rho r\cos(\theta-\phi)+im\phi}\,d\phi\\&=(-1)^m e^{im\theta}\frac{2^{m+\frac{1}{2}}}{\pi}\frac{\Gamma((n+m+1)/2)}{\Gamma((n-m+2)/2)}\times\int_0^\infty\rho^{-\frac{1}{2}}J_{n+\frac{1}{2}}(\rho)J_m(\rho r)\,d\rho\\&=(-1)^m e^{im\theta}\frac{2^m}{\pi}\frac{\Gamma^2((n+m+1)/2)}{\Gamma^2((n-m+2)/2)}\frac{1}{\Gamma(m+1)}\times{}_2F_1\left(\frac{n+m+1}{2},\frac{m-n}{2};m+1,r^2\right).\end{aligned}$$

In the last step we have used Eq. (9) on p. 48 of Ref. 4. Now if we use the identity[7]

$$\Gamma(1+m)P_n^{-m}[(1-r^2)^{\frac{1}{2}}]=r^m2^{-m}{}_2F_1((m+n+1)/2,(m-n)/2,m+1;r^2)$$

and (6), we find

$$J_{m,n}(r,\theta)=\frac{2^{2m}}{\pi}\frac{\Gamma^2((n+m+1)/2)}{\Gamma^2((n-m+2)/2)}\frac{\Gamma(n-m+1)}{\Gamma(n+m+1)}F^{+}_{m,n}(r,\theta).$$

We again apply the multiplication theorem for the Gamma function to obtain (2) and (3). This result is a partial generalization of a result of Bouwkamp.[8] Our results agree with his on their intersection. His methods are different from ours. Ashour[9] considers an integral closely related to ours. However, we believe that his result for the eigenvalues is incorrect.

The set $F^{\pm}_{m,n}(r, \theta)$, $0 \leq m \leq n$, $m + n$ even, forms a complete orthogonal set in the space of functions square integrable over the unit disk with weight function $(1 - r^2)^{-\frac{1}{2}}$. To see this, we note that the set of spherical harmonics

$$Y_{n,m}(\nu, \theta) = \left(\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}\right)^{\frac{1}{2}} P_n^m(\cos\nu)e^{im\theta}, \qquad |m| \leq n,$$

are a complete orthonormal set on the unit sphere, i.e.,

$$\int_0^{2\pi} d\theta \int_0^{\pi} \sin\nu \bar{Y}_{n',m'}(\nu, \theta) Y_{n,m}(\nu, \theta)\, d\nu = \delta_{n,n'}\delta_{m,m'}, \tag{7}$$

and, if $\tilde{f}$ is square integrable over the sphere, i.e.,

$$\int_0^{2\pi} d\theta \int_0^{\pi} \sin\nu\, |\tilde{f}(\nu, \theta)|^2\, d\nu < \infty, \tag{8}$$

then f may be expanded in a Fourier series with respect to the $Y_{n,m}$.

Now, for $n + m$ even, $Y_{n,m}(\pi - \nu, \theta) = Y_{n,m}(\nu, \theta)$, while, for $n + m$ odd, $Y_{n,m}(\pi - \nu, \theta) = -Y_{n,m}(\nu, \theta)$. Thus, if $\tilde{f}(\pi - \nu, \theta) = \tilde{f}(\nu, \theta)$, the Fourier expansion of $\tilde{f}$ will contain only terms with $n + m$ even. Thus, if $\tilde{f}(\nu, \theta)$ is defined and square integrable over the upper hemisphere, we can extend it to the lower hemisphere by $\tilde{f}(\nu, \theta) = \tilde{f}(\pi - \nu, \theta)$, $\pi/2 < \nu < \pi$. Then the extended $\tilde{f}$ will be square integrable over the sphere and have a Fourier expansion in terms of the $Y_{n,m}(\nu, \theta)$ with $n + m$ even. Thus the set $2^{\frac{1}{2}} Y_{n,m}(\nu, \theta)$, $n + m$ even, is a complete orthonormal sequence on the upper hemisphere, $0 < \nu < \pi/2$, $0 \leq \theta \leq 2\pi$. Now make the change of variable $\sin\nu = r$. This maps the hemisphere into the disk. The condition of square integrability [(8) with π replaced by $\pi/2$] now becomes [with $f(r, \theta) = \tilde{f}(\sin^{-1} r, \theta)$]

$$\int_0^{2\pi} d\theta \int_0^1 \frac{r}{(1 - r^2)^{\frac{1}{2}}} |f(r, \theta)|^2\, dr < \infty. \tag{9}$$

The complete orthonormal set now becomes

$$\left(\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}\right)^{\frac{1}{2}} P_n^m[(1 - r^2)^{\frac{1}{2}}]e^{im\theta}, \quad |m| \leq n, \quad m + n \text{ even}.$$

If $m \geq 0$, this is

$$\left(\frac{2n+1}{2}\frac{(n-m)!}{(n+m)!}\right)^{\frac{1}{2}} F^{+}_{m,n}(r, \theta)$$

and, if $m < 0$, this is

$$(-1)^m \left(\frac{2n+1}{2\pi}\frac{(n+m)!}{(n-m)!}\right)^{\frac{1}{2}} F^{-}_{-m,n}(r, \theta).$$

Thus, if $f(r, \theta)$ satisfies (9), we may write

$$f = \sum_{n=0}^{\infty} \sum_{m=0}^{n} (c^{+}_{m,n}F^{+}_{m,n} + c^{-}_{m,n}F^{-}_{m,n}), \tag{10}$$

$$c^{+}_{m,n} = \frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}\int_0^{2\pi} d\theta \times \int_0^1 \frac{r}{(1 - r^2)^{\frac{1}{2}}} F^{-}_{m,n}(r, \theta) f(r, \theta)\, dr,$$

$$c^{-}_{m,n} = (-1)^m \frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}\int_0^{2\pi} d\theta \times \int_0^1 \frac{r}{(1 - r^2)^{\frac{1}{2}}} F^{+}_{m,n}(r, \theta) f(r, \theta)\, dr.$$

We now consider the integral equation (4), with f satisfying (9). This equation will have a solution in the class of functions satisfying

$$\int_0^1 \int_0^{2\pi} r(1 - r^2)^{\frac{1}{2}}\, |\phi(r, \theta)|^2\, dr\, d\theta < \infty \tag{11}$$

if and only if

$$\sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{1}{\lambda^2_{m,n}} \left(\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}\right)^{-1} \times (|c^{+}_{m,n}|^2 + |c^{-}_{m,n}|^2) < \infty. \tag{12}$$

If (12) is satisfied, the solution to (4) is

$$\phi(r, \theta) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{1}{\lambda_{m,n}} (c^{+}_{m,n}F^{+}_{m,n} + c^{-}_{m,n}F^{-}_{m,n})(1 - r^2)^{-\frac{1}{2}}, \tag{13}$$

with the c's given by (10).

It would be desirable to give an alternate description of the range of the integral operator. We can state a necessary condition for a function to be in the range of the operator. Let $g(r, \theta)$ satisfy (11). An application of Hölder's inequality shows that if $1 < p < \frac{4}{3}$,

$$\int_0^{2\pi} \int_0^1 r\, |g(r, \theta)|^p\, dr\, d\theta < \infty, \tag{14}$$

i.e., $g \in L_p(\Omega)$, where Ω is the unit disk. Now let

$$f(r, \theta) = \int_0^{2\pi} \int_0^1 \frac{r' g(r', \theta')}{[r^2 + r'^2 - 2rr'\cos(\theta - \theta')]^{\frac{1}{2}}}\, dr'\, d\theta'.$$

If we apply a theorem of Mikhlin,[10] we see that f has generalized first derivatives in $L_p(\Omega)$.

* This research was supported in part by the National Science Foundation under Grant GP-12838 with the University of Maryland.

[1] E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics* (Cambridge U.P., New York, 1951), p. 421.

[2] L. Schwartz, *Théorie des distributions* (Hermann, Paris, 1951), Tome II, p. 93.

[3] W. Magnus, F. Oberhettinger, and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer-Verlag, Berlin, 1966), pp. 170–219.

[4] A. Erdélyi *et al.*, *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. II, p. 43, Formula (13). There is a slight error in this result. The exponent of y should be $\nu + \frac{3}{2}$ instead of $\nu + \frac{1}{2}$.

[5] Reference 3, p. 218.

[6] Reference 2, p. 113. (The constants may differ due to different definitions of the Fourier transform.)

[7] A. Erdélyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. I, p. 147, Formula (7).

[8] C. J. Bouwkamp, Indagationes Math. **12**, 208 (1950).

[9] A. A. Ashour, J. Math. Phys. **5**, 1421 (1964).

[10] S. G. Mikhlin, *Multidimensional Singular Integrals and Integral Equations* (Pergamon, Oxford, 1965), p. 134.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Geometrization of a Massless Complex Scalar Field*

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(Received 21 December 1970)

This paper presents the necessary and sufficient conditions that a Riemannian geometry have as its source a massless complex scalar field.

1. INTRODUCTION

The purpose of this paper is to show that a complex scalar field satisfying the massless Klein–Gordon equation can be geometrized in the spirit of the already unified field theory. Partial results to this problem have been obtained previously by Penney.[1,2] In previous work[3,4] we have shown how to geometrize a real scalar field and null and nonnull electromagnetic fields using a certain classification of the Ricci tensor.

In Sec. 2 we obtain the algebraic conditions in terms of this classification. The differential conditions, which together with the algebraic ones are necessary and sufficient for a Riemannian geometry to have as its source a complex scalar field, are derived in Sec. 3. In the final section we present a brief discussion.

2. ALGEBRAIC CONDITIONS

Of the various classes for the Ricci tensor $R_{\alpha\beta}$ we shall need mainly C and B_1. If $R_{\alpha\beta}$ belongs to class $C_\pm$, we have

$$R_{\alpha\beta} = \pm R_{(\alpha}\bar{R}_{\beta)} + \kappa g_{\alpha\beta}, \tag{2.1}$$

where R_α is a complex vector which cannot be chosen real, $R \cdot R \neq 0$, $g_{\alpha\beta}$ is the metric tensor, and κ is a constant. The invariant I, defined by

$$I = \tfrac{1}{4}\,|R \cdot R|^2 - \tfrac{1}{4}(R \cdot \bar{R})^2,$$

distinguishes between subclasses $C_{1\pm}$ ($I > 0$), $C_{2\pm}$ ($I = 0$), and $C_{3\pm}$ ($I < 0$). It is quite easy to show that a Ricci tensor of class B_1 may be expressed as in Eq. (2.1) but with $R \cdot R = 0$, the plus sign corresponding to class B_{1a}, and the minus sign to class B_{1b}.

We want to find necessary and sufficient conditions on a Riemannian geometry in order that it have as its source a complex (massless) scalar field ϕ. We assume that $\phi_{,\alpha}$ cannot be made real by multiplying by a phase factor.

From the Lagrangian

$$L = \phi^{,\alpha}\bar{\phi}_{,\alpha},$$

we obtain the equations of motion

$$\phi_{,\alpha}{}^{;\alpha} = 0 \tag{2.2}$$

as well as the stress–energy tensor

$$T_{\alpha\beta} = \phi_{,(\alpha}\bar{\phi}_{,\beta)} - \tfrac{1}{2}g_{\alpha\beta}\phi_{,\gamma}\bar{\phi}^{,\gamma}.$$

Because of the Einstein field equations, the Ricci tensor is then given by

$$R_{\alpha\beta} = -\phi_{(\alpha}\bar{\phi}_{\beta)} \tag{2.3}$$

and the Ricci scalar by

$$R = -\phi_\alpha\bar{\phi}^\alpha, \tag{2.4}$$

where ϕ_α is the gradient of ϕ. Therefore, we have two necessary conditions. $R_{\alpha\beta}$ must be in class C_- or B_{1b}, and R must be given in terms of the corresponding complex vector ϕ_α by Eq. (2.4).

Conversely, suppose these two conditions are fulfilled. The complex vector ϕ_α is determined only up

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[6] Reference 2, p. 113. (The constants may differ due to different definitions of the Fourier transform.)

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[8] C. J. Bouwkamp, Indagationes Math. **12**, 208 (1950).

[9] A. A. Ashour, J. Math. Phys. **5**, 1421 (1964).

[10] S. G. Mikhlin, *Multidimensional Singular Integrals and Integral Equations* (Pergamon, Oxford, 1965), p. 134.

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Geometrization of a Massless Complex Scalar Field*

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1. INTRODUCTION

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In Sec. 2 we obtain the algebraic conditions in terms of this classification. The differential conditions, which together with the algebraic ones are necessary and sufficient for a Riemannian geometry to have as its source a complex scalar field, are derived in Sec. 3. In the final section we present a brief discussion.

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We want to find necessary and sufficient conditions on a Riemannian geometry in order that it have as its source a complex (massless) scalar field ϕ. We assume that $\phi_{,\alpha}$ cannot be made real by multiplying by a phase factor.

From the Lagrangian

$$L = \phi^{,\alpha}\bar{\phi}_{,\alpha},$$

we obtain the equations of motion

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where ϕ_α is the gradient of ϕ. Therefore, we have two necessary conditions. $R_{\alpha\beta}$ must be in class C_- or B_{1b}, and R must be given in terms of the corresponding complex vector ϕ_α by Eq. (2.4).

Conversely, suppose these two conditions are fulfilled. The complex vector ϕ_α is determined only up to the transformations

$$\phi_\alpha \to \phi_\alpha e^{-i\gamma}, \quad \gamma \text{ real}, \tag{2.5}$$

and

$$\phi_\alpha \to \bar{\phi}_\alpha. \tag{2.6}$$

Choosing any one of these as "extremal field" ϕ'_α, we now ask whether there is a real function θ (the "complexion") such that ϕ_α, given by

$$\phi_\alpha = \phi'_\alpha e^{-i\theta}, \tag{2.7}$$

satisfies

$$\phi_{[\alpha;\beta]} = 0 \tag{2.8}$$

and Eq. (2.2). If so, there exists a complex scalar field ϕ with gradient ϕ_α satisfying Eqs. (2.2)–(2.4).

3. DIFFERENTIAL CONDITIONS

Let us now find necessary and sufficient conditions for the existence of such a function θ. If θ exists, substitution of Eq. (2.7) into Eqs. (2.8) and (2.2) gives

$$\phi'_{[\alpha;\beta]} - i\phi'_{[\alpha}\theta_{,\beta]} = 0, \tag{3.1}$$

$$\phi'^{;\alpha}_{\alpha} - i\theta_{,\alpha}\phi'^{\alpha} = 0. \tag{3.2}$$

If $\phi'_\alpha\phi'^\alpha \neq 0$, multiplying Eq. (3.1) by ϕ'^α and using Eq. (3.2), we obtain

$$\theta_{,\beta} = H_\beta, \tag{3.3}$$

where

$$H_\beta = -i[2\phi'^\alpha\phi'_{[\alpha;\beta]} + \phi'^{;\alpha}_{\alpha}\phi'_\beta]/\phi'^\mu\phi'_\mu.$$

From Eqs. (3.1) and (3.3) we then find

$$\phi'_{[\alpha;\beta]} - i\phi'_{[\alpha}H_{\beta]} = 0. \tag{3.4}$$

It is not hard to show that Eqs. (3.3) and (3.4) are equivalent to Eqs. (3.1) and (3.2). We also have

$$H_\beta - \bar{H}_\beta = 0, \tag{3.5}$$

since θ is real, and

$$H_{[\alpha;\beta]} = 0 \tag{3.6}$$

due to Eq. (3.3).

In a similar fashion we can show that, provided that $\phi'_\alpha\bar{\phi}'^\alpha \neq 0$, the equations

$$\theta_{,\beta} = K_\beta, \tag{3.7}$$

$$\phi'_{[\alpha;\beta]} - i\phi'_{[\alpha}K_{\beta]} = 0, \tag{3.8}$$

are equivalent to Eqs. (3.1) and (3.2), where K_β, defined by

$$K_\beta = -i[2\bar{\phi}'^\alpha\phi'_{[\alpha;\beta]} - \phi'_\beta\bar{\phi}'^{;\alpha}_{\alpha}]/\phi'_\mu\bar{\phi}'^\mu,$$

satisfies

$$K_\beta - \bar{K}_\beta = 0 \tag{3.9}$$

and

$$K_{[\alpha;\beta]} = 0. \tag{3.10}$$

Equations (3.4)–(3.6) and (3.8)–(3.10) are conditions on the geometry since they are independent of the particular choice of extremal field. To see this, note that under the transformation (2.5)

$$H_\alpha \to H_\alpha - \gamma_{,\alpha}, K_\alpha \to K_\alpha - \gamma_{,\alpha},$$

and under the transformation Eq. (2.6) H_α and K_α become the negatives of their complex conjugates.

Thus, if $\phi'_\alpha\phi'^\alpha \neq 0$, Eqs. (3.4)–(3.6) are necessary conditions on the geometry in order that a function θ with the desired properties exist. They are also sufficient. Equations (3.5) and (3.6) ensure the existence of a real function θ satisfying Eq. (3.3). Since Eqs. (3.3) and (3.4) are equivalent to Eqs. (3.1) and (3.2), ϕ_α, given by Eq. (2.7), satisfies Eqs. (2.2) and (2.8).

Similarly, when $\phi'_\alpha\phi'^\alpha \neq 0$, we find the necessary and sufficient conditions to be Eqs. (3.8)–(3.10).

4. DISCUSSION

We have found necessary and sufficient conditions on a Riemannian geometry so that its source is a complex scalar field satisfying the massless Klein–Gordon equation. The algebraic conditions are that the Ricci tensor belongs to class C_- or B_{1b} and that the Ricci scalar be given in terms of the associated complex vector ϕ_α by Eq. (2.4). If $\phi_\alpha\phi^\alpha \neq 0$, the differential conditions are given by Eqs. (3.4)–(3.6), if $\phi_\alpha\bar{\phi}^\alpha \neq 0$ by Eqs. (3.8)–(3.10). If neither $\phi_\alpha\phi^\alpha$ nor $\phi_\alpha\bar{\phi}^\alpha$ vanish, either set of conditions will do.

The scalar field ϕ is not uniquely determined by these conditions. θ is determined up to an additive arbitrary constant θ_0 for any choice of ϕ'_α. A different choice of extremal field may yield a different θ, but ϕ_α is determined uniquely up to Eqs. (2.5) and (2.6) with $\gamma = \theta_0$. It follows that ϕ is unique up to the transformations

$$\phi \to \phi + \phi_0, \tag{4.1}$$

$$\phi \to \phi e^{i\theta_0}, \tag{4.2}$$

$$\phi \to \bar{\phi}, \tag{4.3}$$

where ϕ_0 is another arbitrary constant. This is not surprising. Given a complex scalar field which satisfies Eqs. (2.2)–(2.4), then the fields obtained from ϕ by transformations (4.1)–(4.3) also satisfy (2.2)–(2.4).

It should be noted that our geometrization procedure also holds for the degenerate case for which ϕ may become real provided that $\phi_{,\alpha}$ is not null. (Of course, the algebraic conditions are then different.) At points where $\phi_{,\alpha}$ is real (or real but for a phase factor) and null, our procedure breaks down.

In the nondegenerate case the equations of motion (2.2) follow from Eq. (2.8) and the contracted Bianchi identity, just as in the case of a real scalar field.[3,5]

* Supported in part by the National Research Council of Canada.

[1] R. Penney, J. Math. Phys. 7, 479 (1966).
[2] R. Penney, J. Math. Phys. 8, 2297 (1967).
[3] G. Ludwig and G. Scanlan, Commun. Math. Phys. 20, 291 (1971).
[4] G. Ludwig, Commun. Math. Phys. 17, 98 (1970).
[5] D. Brill, Nuovo Cimento Suppl. 2, 1 (1964).

Geometrization of a Massive Scalar Field*

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(Received 23 March 1971)

This paper presents the necessary and sufficient conditions that a Riemannian geometry have as its source a real or complex massive scalar field.

1. INTRODUCTION

In a recent paper[1] a classification of the Ricci tensor was obtained which enabled us to geometrize[2] the null and nonnull electromagnetic fields[3] as well as the real[1] and complex[4] massless scalar fields. The present article deals with the geometrization of a massive scalar field. This problem has been tackled previously by Penney[5] and Nagaraj[6] for the real field and by Peres[7] and Kuchař[8] for both the real and the complex case. These authors expressed the conditions for geometrization explicitly in terms of the Ricci tensor, whereas in our approach the Ricci tensor is involved only implicitly. This results in considerable simplification.

The notation employed here is as follows. Tensor indices are given by small Greek letters; the summation convention is used throughout. Ordinary differentiation is indicated by a comma, covariant differentiation by a semicolon. Round brackets around suffixes denote symmetrization; square brackets denote antisymmetrization. A bar over a quantity stands for complex conjugation of that quantity. "Re" stands for the real part, "Im" for the imaginary part of a number. The signature and the Ricci tensor are defined as in Ref. 3.

2. THE MASSIVE REAL SCALAR FIELD

The Ricci tensor for a real massive scalar field ϕ satisfying the Klein–Gordon equation

$$\phi^{,\alpha}{}_{;\alpha} + \mu^2\phi = 0 \tag{2.1}$$

has the trace-free part

$$S_{\alpha\beta} = -\phi_{,\alpha}\phi_{,\beta} + \tfrac{1}{4}g_{\alpha\beta}\phi^{,\gamma}\phi_{,\gamma} \tag{2.2}$$

and the trace

$$R = -\phi_{,\gamma}\phi^{,\gamma} + 2\mu^2\phi^2. \tag{2.3}$$

We shall assume that

$$\phi_{,\alpha} \neq 0 \tag{2.4}$$

anywhere in the region D of space–time under consideration. The degenerate case with vanishing $\phi_{,\alpha}$ may be treated separately. We wish to find necessary and sufficient conditions on a Riemannian geometry for the existence of a real scalar field ϕ satisfying (2.1)–(2.4) at each point in D. Let us exhibit sufficient conditions.

Suppose[1]

$$S_{\alpha\beta} \text{ belongs to class } A_- \tag{2.5}$$

at every point of D. This defines a nowhere vanishing vector field A_α uniquely up to sign satisfying (2.2) with $\phi_{,\alpha}$ replaced by A_α. Assume further that the condition

$$R + A^\gamma A_\gamma > 0 \tag{2.6}$$

is obeyed by the geometry, and define the geometrical entity

$$H = [\tfrac{1}{2}(R + A^\gamma A_\gamma)]^{\frac{1}{2}}.$$

If

$$H_{,\alpha} \neq 0 \tag{2.7}$$

anywhere in D and if the vectors

$$H_{,\alpha} \text{ and } A_\alpha \text{ are linearly dependent} \tag{2.8}$$

at every point in D, then

$$H_{,\alpha} = \mu A_\alpha$$

for some nonzero μ (defined by the geometry up to sign only). Assuming that μ is a constant, i.e., that

$$\mu_{,\alpha} = 0, \tag{2.9}$$

we define a real scalar function ϕ by

$$\phi = H/\mu.$$

Since $\phi_{,\alpha} = A_\alpha$, ϕ satisfies (2.2)–(2.4). That ϕ also obeys (2.1) follows from the contracted Bianchi identity and (2.4). It is easily verified that (2.5)–(2.9) are not only sufficient but also necessary conditions for the existence of a real scalar function ϕ with the desired properties. These conditions determine ϕ up to sign only. Conversely, (2.1)–(2.4) are invariant under such a change of sign.

It should be noted that the massless case ($\mu = 0$) has to be treated separately.[1]

3. THE MASSIVE COMPLEX SCALAR FIELD

The complex massive scalar field ϕ satisfying (2.1) and its complex conjugate is geometrized in a similar fashion. The Ricci tensor whose source is ϕ has trace-free part

$$S_{\alpha\beta} = -\phi_{,(\alpha}\bar{\phi}_{,\beta)} + \tfrac{1}{4}g_{\alpha\beta}\phi_{,\gamma}\bar{\phi}^{,\gamma} \quad (3.1)$$

and trace

$$R = -\phi_{,\gamma}\bar{\phi}^{,\gamma} + 2\mu^2\phi\bar{\phi}. \quad (3.2)$$

We shall assume that $\phi_{,\alpha}$ is nowhere proportional to a real vector in the region D of interest. The degenerate case where $\phi_{,\alpha}$ is essentially real in a subregion of D may be treated separately in an analogous manner.

We shall exhibit sufficient (and necessary) conditions on the geometry in order that there exist a complex scalar field ϕ satisfying (2.1), (3.1), and (3.2). We shall also show how to find ϕ provided that these conditions are satisfied.

Suppose[1]

$$S_{\alpha\beta} \text{ is in class } B_{1b} \text{ or } C_{-}. \quad (3.3)$$

This specifies a vector A_α (which is nowhere proportional to a real vector) up to the transformations

$$A_\alpha \to A_\alpha e^{-i\psi} \quad (3.4)$$

and

$$A_\alpha \to \bar{A}_\alpha. \quad (3.5)$$

Conditions involving A_α (explicitly or implicitly) can be geometrical conditions only if they are invariant under (3.4) and (3.5).

Suppose further that

$$R + A_\gamma\bar{A}^\gamma > 0. \quad (3.6)$$

Then, as in the previous section, we may define the geometrical entity

$$H = [\tfrac{1}{2}(R + A_\gamma\bar{A}^\gamma)]^{\frac{1}{2}}.$$

We also define $B_\alpha = \text{Re}\, A_\alpha$ and $C_\alpha = \text{Im}\, A_\alpha$ and note that these vectors are linearly independent due to the fact that A_α is not proportional to a real vector. Assuming

$$H_{,\alpha} \neq 0 \quad (3.7)$$

and

$$H_{,\alpha},\ B_\alpha, \text{ and } C_\alpha \text{ are linearly dependent}, \quad (3.8)$$

we have

$$H_{,\alpha} = aB_\alpha + bC_\alpha \quad \text{for some } a, b.$$

We note that (3.8) is a geometrical condition since the B–C plane is invariant under (3.4) and (3.5). Under these transformations

$$a \to a\cos\psi + b\sin\psi, \quad b \to -a\sin\psi + b\cos\psi$$

and

$$a \to a, \quad b \to -b,$$

respectively. Denoting the nonzero invariant $a^2 + b^2$ by μ^2, we require that μ (defined by the geometry up to sign) be a constant, i.e., that

$$\mu_{,\alpha} = 0. \quad (3.9)$$

The function σ given by

$$a = \mu\cos\sigma, \quad b = -\mu\sin\sigma$$

is determined up to additive multiples of 2π for any given choice of A_α but transforms as $\sigma \to \sigma + \psi$, $\sigma \to -\sigma$ under (3.4) and (3.5), respectively; that is, (3.4) leaves $A_\alpha e^{i\sigma}$ invariant and (3.5) maps it into its complex conjugate.

The geometrical condition

$$[(\mu/H)\,\text{Im}\, A_{[\alpha}e^{i\sigma}]_{;\beta]} = 0 \quad (3.10)$$

is then necessary and sufficient for the existence of a function θ satisfying

$$\theta_{,\alpha} = (\mu/H)\,\text{Im}\,(A_\alpha e^{i\sigma}).$$

θ is determined up to an additive constant θ_0 for any given A_α, remains invariant under (3.4), and changes sign under (3.5). Since

$$H_{,\alpha} = \mu\,\text{Re}\,(A_\alpha e^{i\sigma}),$$

we have

$$[(H/\mu)e^{i\theta}]_{,\alpha} = A_\alpha e^{i(\sigma+\theta)}.$$

The complex scalar function ϕ given by

$$\phi = (H/\mu)e^{i\theta}$$

is, therefore, defined by the geometry up to

$$\phi \to \phi e^{i\theta_0} \quad (3.11)$$

and

$$\phi \to \bar{\phi} \quad (3.12)$$

and has the gradient

$$\phi_{,\alpha} = A_\alpha e^{i(\sigma+\theta)}.$$

Therefore, ϕ satisfies (3.1) and (3.2). That it also satisfies (2.1) follows from the contracted Bianchi identity and the fact that A_α is nowhere proportional to a real vector. The conditions (3.3) and (3.6)–(3.10) are easily seen to be necessary as well as sufficient conditions on a Riemannian geometry in order that it have as its source a complex scalar function ϕ satisfying the Klein–Gordon equation. Provided that these conditions are satisfied, we have shown how to extract ϕ from the geometry uniquely up to the transformations (3.11) and (3.12). Conversely, from any solution ϕ of (2.1), (3.1), and (3.2), others may be obtained by applying transformations (3.11) and (3.12).

Again, we see that the massless case must be considered separately.

* Supported in part by the National Research Council of Canada.

1 G. Ludwig and G. Scanlan, Commun. Math. Phys. **20**, 291 (1971).
2 J. A. Wheeler, *Geometrodynamics* (Academic, New York, 1962).
3 G. Ludwig, Commun. Math. Phys. **17**, 98 (1970).
4 G. Ludwig, J. Math. Phys. **12**, 1218 (1971).
5 R. Penney, J. Math. Phys. **6**, 1029 (1965).
6 M. Nagaraj, Tensor **22**, 53 (1971).
7 A. Peres, Bull. Res. Council Israel **9F**, 129 (1960).
8 K. Kuchař, Czech. J. Phys. B **13**, 551 (1963).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Radiation and Energy in an Asymptotically Friedmann Space-Time

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(Received 18 November 1970)

A bounded gravitating system in an asymptotically hyperbolic Friedmann space is examined. The Bondi-Metzner-Sachs (BMS) group is shown to be the asymptotic symmetry group. The BMS generators and the Weyl tensor are used to construct an asymptotic invariant which allows the energy of the gravitating system to be calculated without infinite contributions from the cosmological dust. It is shown that a bounded gravitating system in a cosmological space can be understood in much the same manner as a similar physical system in an asymptotically flat space-time.

1. INTRODUCTION

Gravitational radiation in asymptotically flat space-times has been intensively studied over the past decade.[1] Asymptotic flatness is an excellent approximation for a system whose boundaries are large compared to the "disturbance" and small compared to the radius of curvature of the universe. In this context, general relativity has been brought within the mainstream of physics. Questions of advanced and retarded gravitational waves have been clarified and the concepts of the momentum and angular momentum of both the waves and gravitating object have been defined. Bondi *et al.*[2] and Sachs[3] have identified the mass and mass loss of a bounded radiating system, and Penrose[4,5] and Tamburino and Winicour[6] have introduced invariant techniques to relate the momenta to the Bondi-Metzner-Sachs (BMS) group, the symmetry group of asymptotically flat space-time.[5-7] This paper considers how these concepts can be extended to a cosmological space-time.

For cosmological studies, one examines gravitational radiation propagating over large distances where the effects of matter and the expansion and curvature of the universe must be included. Hawking[8] has used the Newman-Penrose method of asymptotic expansions along null rays to study outgoing radiation in an expanding dust-filled universe. With the boundary condition that space-time asymptotically approaches an hyperbolic Friedmann universe, Hawking found the asymptotic symmetry group to have no super-translations and to be the same as the isometry group of the unperturbed Friedmann model, i.e., a group isomorphic to the six-parameter homogeneous Lorentz group. With no translations as symmetries, he defines the mass as an integral over a spacelike 2-surface sliced from an outgoing null surface. In the limit of future null infinity, this mass expression becomes infinite because of the infinite amount of matter which contributes to the mass via the Ricci tensor. Hawking points out that his mass expression can be separated into a part which remains finite and a part which becomes infinite. The finite part is then interpreted (following Bondi and Sachs[2,3]) as the mass of the bounded perturbing source plus the energy of the outgoing radiation.

In this work we consider the same physical system as Hawking, but take a different approach. The "mass renormalization" is achieved by constructing an asymptotic invariant from the intrinsic geometric quantities of the system, and, since a meaningful energy expression should be defined in an invariant manner which directly relates the energy to a symmetry, we are led to a view of the asymptotic symmetries which is alternative to Hawking's. Following Penrose,[5] the asymptotic symmetry group of the physical manifold is defined as the group of conformal motions of the boundary of the compactified manifold.

The conformal technique of Penrose[5] is used to construct future null infinity ($\mathscr{I}^+$). The Einstein field equations, in the conformal space, then tell us that $\mathscr{I}^+$ is a shear-free null hypersurface. Solving the Killing equations on $\mathscr{I}^+$ provides the *BMS group* as the asymptotic symmetry group.

To measure the energy of the bounded source plus gravitational radiation, an asymptotic invariant is constructed which is a function of the Weyl tensor, the normal vector field of the outgoing null hypersurfaces, and the asymptotic Killing vectors. For an asymptotically flat space-time, with Newman-Unti[9] or Bondi-Sachs[2,3] coordinate conditions, the invariant reduces to the usual Bondi mass result. The asymptotic solutions of the Einstein field equations (in their Newman-Penrose[10] form) allow us to evaluate the mass and mass loss of the radiation and bounded source in an asymptotically Friedmann universe. There are no infinities in the result since the Ricci tensor, in which the cosmological matter appears, plays no role in the energy expression.

The question of boundary conditions is interesting. Penrose has shown,[11] for asymptotically flat spaces, that a shear-free null $\mathcal{J}^+$, together with asymptotic simplicity and the asymptotically vacuum Bianchi identities (which are conformally covariant), provides the peeling of the Weyl tensor. This is fully equivalent to the Newman–Penrose condition $\Psi_0 = O(r^{-5})$. However, in the asymptotically Friedmann space the vacuum Bianchi identities no longer obtain (even asymptotically). The existence of a null shear-free $\mathcal{J}^+$ provides the weak condition $\Psi_4 = o(r_l^{-1})$ or, if sufficient differentiability is also assumed, $\Psi_4 = O(r_l^{-1})$, where r_l is a luminosity distance. Conformal considerations alone produce no further information about the falloff of the Weyl tensor.

Hawking's boundary conditions were found by a physically reasonable approach essentially equivalent to examining perturbations of the linearized field equations in a background hyperbolic Friedmann space. The conditions $\psi_0 = O(r^{-\frac{7}{2}})$ and $\Phi_{01} = O(r^{-\frac{7}{2}})$, have the lowest order (in r^{-n}) for which $\dot{\psi}_0$ and $\dot{\Phi}_{01}$ are driven by the gravitational news function and the highest order which can be maintained when $\psi_4 = O(r^{-1})$. These boundary conditions do allow the momenta of a bounded gravitating system to be evaluated in an invariant manner.

Section 2 presents the exact hyperbolic Friedmann metric in outgoing null coordinates. In Sec. 3, Penrose's conformal technique is introduced and used to compactify the asymptotically Friedmann space. The geometry of $\mathcal{J}^+$ is examined, and it is shown to be a shear-free null hypersurface. Killing's equations are solved on $\mathcal{J}^+$ in Sec. 4, and the BMS group is found to be the asymptotic symmetry group. Section 5 discusses the Tamburino–Winicour linkage expressions for asymptotically flat spaces. A new asymptotic invariant is introduced which is independent of the Ricci tensor. It is shown to be equivalent to the Tamburino–Winicour expression in asymptotically flat space–time (vacuum or Einstein–Maxwell) when the BMS descriptors are restricted to the translations and conformal rotations ($l \leq 1$). In Sec. 6 the new asymptotic invariant is used to define the momentum and angular momentum of a bounded radiating source in an asymptotically Friedmann space–time.

Appendix A presents Hawking's asymptotic solution of the Newman–Penrose field equations, and Appendix B proves the equivalence of the Tamburino–Winicour linkage expression with our asymptotic invariant for asymptotically flat space–time.

2. ASYMPTOTIC FORM OF THE METRIC

Following Hawking,[8] we restrict our attention to the hyperbolic Friedmann model (dust with zero pressure) as an asymptotic metric:

$$ds^2 = R^2(\tau)[d\tau^2 - d\chi^2 - \sinh^2\chi(d\theta^2 + \sin^2\theta\, d\varphi^2)],$$
$$R(\tau) = A(\cosh\tau - 1), \quad A > 0. \tag{2.1}$$

The parameter A^{-1} represents the kinetic plus potential energy of the matter, and the energy–momentum tensor for this model is given by[12]

$$T_{\mu\nu} = 6AR^{-1}\tau_{,\mu}\tau_{,\nu}. \tag{2.2}$$

All the Friedmann metrics are conformally flat, and the work of Infeld and Schild[13] provides us with the conformal relation between (2.1) and the Minkowski metric. In the usual null Minkowski coordinates, the Friedmann metric (2.1) can be written as

$$ds^2 = F^2(u, r)[du^2 + 2\, du\, dr - r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)],$$

where (2.3)

$$F(u, r) = \tfrac{1}{2}A\{1 - [u(u + 2r)]^{-\frac{1}{2}}\}^2,$$

along with the coordinate transformation

$$u = e^{\tau-\chi}, \quad r = e^{\tau}\sinh\chi.$$

We see that the infinite past in Minkowski coordinates corresponds to the $u = 0$ surface and in the following work the range of u is restricted to $u > 0$. The six-parameter isometries of the spacelike Friedmann hypersurfaces $\tau = \text{const}$ are now seen as isometries of the hyperbolas $t^2 - r^2 = \text{const} > 1$ in Minkowski coordinates.

3. GEOMETRY OF FUTURE NULL INFINITY

In order to study null infinity in a covariant manner, Penrose's conformal technique[4,5,11] is used. Null infinity is to be thought of as a boundary to space–time consisting of the limit points of null rays. By means of a coordinate transformation, finite values can be assigned to these limit points. Clearly, in such a coordinate system the metric must be singular at the points representing null infinity in order that neighboring points be infinitely distant. By performing a conformal transformation on this metric, it is possible to arrive at a conformal metric which is regular at null infinity.

Denoting the physical space metric by $\tilde{g}_{\mu\nu}$, the relation to the conformal metric is[14]

$$\tilde{g}_{\mu\nu} = \Omega^{-2}g_{\mu\nu}. \tag{3.1}$$

Before proceeding to the compactification of the asymptotic Friedmann manifold, it is instructive to examine the compactified exact Friedmann manifold.

Introducing a new coordinate $z = r^{-1}$ and conformal factor $\Omega = zF^{-1}$, we give the metric conformal to (2.3) via (3.1) by

$$ds^2 = z^2\,du^2 - 2\,du\,dz - (d\theta^2 + \sin^2\theta\,d\varphi^2), \quad (3.2)$$

with

$$\Omega = (2/A)zu(uz+2)\{[u(uz+2)]^{\frac{1}{2}} - z^{\frac{1}{2}}\}^{-2}.$$

This conformal metric is manifestly regular (C^∞) in the neighborhood of, and at, the hypersurface $\mathcal{J}^+$ given by $z = 0$, u finite. It should be noted that the conformal factor[15] Ω (and hence the conformal manifold) is C^1, but the in-surface derivatives on $\mathcal{J}^+$ are C^∞ so that Ω properly determines the geometry of $\mathcal{J}^+$. By direct differentiation, $\mathcal{J}^+$ is found to be a shear-free null hypersurface with nonzero normal $\Omega_{,\mu}$.

At this point, one may note that the conformal metric (3.2) is the same as the compactified Minkowski metric and inquire where the difference lies. It lies in the fact that the conformal factor for the Minkowski compactification is C^∞, and the one we have chosen for Friedmann is C^1. The Ricci tensor in the unphysical conformal space with a C^1 conformal factor will be infinite on $\mathcal{J}^+$, and this is interpreted physically as the result of confining an infinite amount of dust in a finite region.

Since the conformal Ricci tensor is related to the physical one by

$$\tilde{R}_{\mu\nu} = R_{\mu\nu} - 2\Omega^{-1}\Omega_{;\mu\nu} + g_{\mu\nu}(3\Omega^{-2}\Omega_{,\alpha}\Omega^{,\alpha} - \Omega^{-1}\Omega_{;\alpha}{}^{\alpha})$$

and is thus clearly not a conformal covariant, a possible objection to the interpretation above is that a poor choice was made for Ω. However, after a detailed examination of the Friedmann metric (2.3), we conjecture that this is not the case and that there is no conformal map better than C^1 which provides a sufficiently regular conformal metric (say C^3) for the compactified manifold while maintaining $\Omega_{,\mu} \overset{\mathcal{J}}{\neq} 0$. Thus, while the geometry (and, as we will see below, the symmetry group) of $\mathcal{J}^+$ is identical for compactified Minkowski space and compactified hyperbolic Friedmann space, its embedding as a hypersurface in a 4-manifold is different for each case.

In null coordinates, the Friedmann metric (2.3) is a special case of

$$d\tilde{s}^2 = \tilde{g}_{00}\,du^2 + 2(\tilde{g}_{01}\,dr_l + \tilde{g}_{0i}\,dx^i)\,du - r_l^2\tilde{h}_{ij}\,dx^i\,dx^j \quad (3.3)$$

where solutions of $\tilde{g}^{\mu\nu}u_{,\mu}u_{,\nu} = 0$ define a family of $x^0 = u = \text{const}$ null hypersurfaces. The null hypersurfaces with normal $\tilde{l}_\mu = u_{,\mu}$ are generated by a two-parameter system of null geodesics tangent to $\tilde{l}_\mu$, called rays. Two additional coordinates x^i are chosen as parameters constant along each ray:

$$x^i{}_{,\nu}\tilde{l}^\nu = 0, \quad i = 2, 3.$$

The coordinate $x^1 = r_l$ is defined as a luminosity distance along the null rays by the algebraic condition

$$|\tilde{h}_{ij}| = f^2(x^i),$$

where $f(x^i)$ is some known function characterizing the type of angular variable used to label the null rays. For the usual spherical coordinates $x^2 = \theta$, $x^3 = \varphi$, we have $f(x^i) = \sin\theta$. The determinant of (3.3) satisfies

$$\sqrt{-\tilde{g}} = \tilde{g}_{01}r_l^2 f. \quad (3.4)$$

The exact Friedmann metric (2.3) in null Bondi–Sachs coordinates is given by (with $A = 2$ for convenience)

$$\begin{aligned}
\tilde{g}_{00} &= -(\sqrt{2})u^{-\frac{3}{2}}r_l^{\frac{1}{2}} + 1 + 3u^{-2} + O(r_l^{-\frac{1}{2}}),\\
\tilde{g}_{01} &= 1 - 3(\sqrt{2})u^{-\frac{1}{2}}r_l^{-\frac{1}{2}} + (3u^{-1})r_l^{-1} + O(r_l^{-\frac{3}{2}}),\\
\tilde{g}_{0i} &= 0,\\
\tilde{h}_{ij} &= \delta_{22} + \sin^2\theta\,\delta_{33}.
\end{aligned} \quad (3.5)$$

(See Appendix A for Hawking's asymptotic solution.) To compactify (3.3), we introduce the coordinate $z = Fr_l^{-1}$ with $F(u, z) = \frac{1}{2}A\{1 - [z/u(uz+2)]^{\frac{1}{2}}\}^2$ and conformal factor

$$\Omega = r_l^{-1} = zF^{-1}. \quad (3.6)$$

The hypersurface $\mathcal{J}^+$ will be given by $z = 0$, u finite ($u > 0$). Since (3.3) is a solution of the Einstein equations

$$\tilde{G}_{\mu\nu} = -\tilde{T}_{\mu\nu}, \quad (3.7)$$

the geometry of $\mathcal{J}^+$ will be determined by the conformal Einstein equations. With the relation between the physical and conformal spaces given by (3.1), the Einstein equations take the form

$$-\tilde{T}_{\mu\nu} = G_{\mu\nu} - 2\Omega^{-1}\Omega_{;\mu\nu} + g_{\mu\nu}(2\Omega^{-1}\Omega_{;\alpha}{}^{\alpha} - 3\Omega^{-2}\Omega_{,\alpha}\Omega^{,\alpha}), \quad (3.8)$$

where

$$\tilde{T}_{\mu\nu} = (3A/2)\Omega z^{-1}y^{-\frac{3}{2}}y_{,\mu}y_{,\nu} + \tilde{I}_{\mu\nu} \quad (3.9)$$

with

$$y = u(u + 2z^{-1}).$$

$\tilde{I}_{\mu\nu}$ represents the energy–momentum contribution of the bounded perturbing source. In the physical space the asymptotic behavior of this term is of higher order in r_l^{-1} than the energy–momentum of the cosmological dust given by (2.2). This is in keeping with our model of a space–time which is asymptotically Friedmann and in which the interaction between the dust and the perturbing source dies out as infinity is approached along the null rays. In the conformal space, $I_{\mu\nu}$ and its divergence vanish more strongly on $\mathfrak{J}^+$ than the first term of (3.9), and thus $I_{\mu\nu}$ plays no role in the geometry of $\mathfrak{J}^+$.

Multiplying (3.8) by Ω^2 and evaluating at $z = \Omega = 0$ immediately tells us that $\mathfrak{J}^+$ is a null hypersurface:

$$\Omega_{,\alpha}\Omega^{,\alpha} \stackrel{\mathfrak{J}}{=} 0. \qquad (3.10)$$

In addition, with (3.8) multiplied by Ω, we have the result

$$\Omega_{;\mu\nu}m^i\delta_i{}^\mu m^j\delta_j{}^\nu \stackrel{\mathfrak{J}}{=} 0, \qquad (3.11)$$

where a polarization dyad has been introduced:

$$\begin{aligned} -g^{ij} &= m^i\bar{m}^j + \bar{m}^i m^j, \quad i, j = 2, 3, \\ m^i &= g^{ij}m_j, \quad m^i m_i = 0, \quad m^i\bar{m}_i = -1. \end{aligned} \qquad (3.12)$$

Equation (3.11) provides the conformally covariant result that $\mathfrak{J}^+$ is shear-free.

The divergence of $\mathfrak{J}^+$, $\Omega_{;\mu\nu}m^i\delta_i{}^\mu\bar{m}^j\delta_j{}^\nu$, is not a conformally covariant property. We happen to have chosen a gauge in which the divergence can be zero (Ω is the inverse luminosity distance), but no direct use will be made of this condition.

We shall see below that the supertranslations are an asymptotic symmetry and this is possible only because $\mathfrak{J}^+$ is shear-free. The topology of $\mathfrak{J}^+$ is $S^2 \times E^1$ (see Penrose[11] and Geroch[16] for proofs of the topological structure), and it is this structure which ultimately allows only the boosts and rotations (conformal transformations of the 2-sphere) as symmetries and rules out the superboosts.

4. ASYMPTOTIC SYMMETRIES

The conditions for an infinitesimal transformation $\bar{x}^\mu = x^\mu + k^\mu$ to be an asymptotic symmetry are that Killing's equations in the conformal space vanish on $\mathfrak{J}^+$:

$$k^{(\mu;\nu)} - \Omega^{-1}\Omega_{,\alpha}k^\alpha g^{\mu\nu} \stackrel{\mathfrak{J}}{=} 0. \qquad (4.1)$$

We immediately have the regularity condition

$$\Omega_{,\alpha}k^\alpha \stackrel{\mathfrak{J}}{=} 0. \qquad (4.2)$$

In the conformal Bondi frame above, the metric on $\mathfrak{J}^+$ takes the form

$$[g^{\mu\nu}] \stackrel{\mathfrak{J}}{=} \begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & \multicolumn{2}{c}{\multirow{2}{*}{$-h^{ij}(x^k)$}} \\ 0 & 0 & & \end{bmatrix},$$

where $h_{ij,0} \stackrel{\mathfrak{J}}{=} 0$. Since $\mathfrak{J}^+$ has topology $S^2 \times E^1$, h_{ij} can be restricted to one of the usual spherical metrics (with components depending on the particular choice of ray labels). Equation (4.2) provides[17]

$$k^1 \stackrel{\mathfrak{J}}{=} 0, \qquad (4.3)$$

and, using l'Hospital's rule, we can write (4.1) as

$$g^{\mu\rho}k^\nu{}_{,\rho} + g^{\nu\rho}k^\mu{}_{,\rho} - g^{\mu\nu}{}_{,\rho}k^\rho - 2k^1{}_{,1}g^{\mu\nu} \stackrel{\mathfrak{J}}{=} 0. \quad (4.4)$$

From (4.4) the following conditions obtain (with the two-dimensional covariant derivative abbreviated by a colon):

$$\begin{aligned} k^1{}_{,0} = k^i{}_{,0} = k^0{}_{,1} &\stackrel{\mathfrak{J}}{=} 0, \\ k^1{}_{,1} \stackrel{\mathfrak{J}}{=} \tfrac{1}{2}k^i{}_{:i}, \quad k^i{}_{,1} &\stackrel{\mathfrak{J}}{=} k^{0,i}; \\ f^{(i:j)} &\stackrel{\mathfrak{J}}{=} \tfrac{1}{2}h^{ij}f^k{}_{:k}. \end{aligned} \qquad (4.5)$$

The solutions of (4.4) are

$$k^i \stackrel{\mathfrak{J}}{=} f^i(x^j), \quad k^0 \stackrel{\mathfrak{J}}{=} \tfrac{1}{2}uf^i{}_{:i} + \alpha(x^j), \qquad (4.6)$$

where α is an arbitrary function of angle. Equations (4.6) are the defining equations of the BMS group as given by Sachs.[7] The functions f^i and α determine the transformation freedom at $\mathfrak{J}^+$. The transformations with $\alpha = 0$ describe the six-parameter subgroup of conformal transformations of the 2-sphere which are isomorphic to $L_+^\uparrow$ (the orthochronous homogeneous Lorentz group). The transformations with $f^i = 0$ form the invariant subgroup of supertranslations.

Note added in proof: It is possibly surprising that the constant density surfaces of the Friedmann space (which in the conformal Minkowski picture appear as hyperbolas all asymptotically tangent to the $u = 0$ null cone) do not rule out the translations. However, the dust and radiation end up asymptotically in different places, and a point on $\mathfrak{J}^+$ which the radiation reaches is inaccessible to $u = 0$.

5. ASYMPTOTIC INVARIANTS

For asymptotically flat space–time, the Bondi mass has been linked geometrically to the asymptotic symmetry group, the BMS group, through the work of Tamburino and Winicour.[6,18] They have introduced functionals defined on closed two-dimensional cross sections of nonsingular outgoing null hypersurfaces. If Σ is a closed spacelike cross section of the outgoing null hypersurface $\mathcal{N}$, given by $u = \text{const}$, with normal $l_\mu = u_{,\mu}$, their linkage expression is given by[19]

$$L(\Sigma) = \oint_\Sigma (k^{[\mu;\nu]} + k^\alpha{}_{;\alpha}l^{[\mu}n^{\nu]})\, dS_{\mu\nu}, \qquad (5.1)$$

where n^μ is a vector field on Σ normalized by $n^\mu l_\mu = 1$.

The BMS descriptors k^μ_p, which are associated with two infinitesimally differing null polar-coordinate systems on $\mathfrak{J}^+$,

$$\bar{x}^\mu \stackrel{\mathfrak{J}}{=} x^\mu + k^\mu_p\epsilon^p + O(\epsilon^2),$$

are determined by solving Killing's equations on $\mathfrak{J}^+$ and then are uniquely evaluated everywhere on $\mathcal{N}$

according to the propagation equation[6]

$$k^{(\mu;\nu)}l_\nu = \tfrac{1}{2}k^\alpha{}_{;\alpha}l^\mu. \quad (5.2)$$

The linkage expression transforms as an adjoint representation of the BMS group:

$$L'_Q(\Sigma) \overset{\mathfrak{J}}{=} L_Q(\Sigma) + C_{PQ}{}^R L_R(\Sigma)\epsilon^P,$$

where the $C_{PQ}{}^R$ are the BMS structure constants.[20]

The asymptotic invariance of (5.1) is best discussed by casting the linkages into the usual form of a conservation law,[21]

$$L(\Sigma_2) - L(\Sigma_1) = \text{flux} - \int_{\mathcal{N}} T^\mu{}_\nu k^\nu \, dS_\mu, \quad (5.3)$$

through the use of the Ricci identity and the Einstein field equations (3.7), where

$$\text{flux} := \int_{\mathcal{N}} (k^{(\mu;\nu)}{}_{;\nu} - k^\nu{}_{;\nu}{}^\mu + \tfrac{1}{2}Rk^\mu)\, dS_\mu - \int_{\mathcal{N}} \tfrac{1}{2}(k^\alpha_{;\alpha}l^\nu)_{;\nu}\, dV.$$

Winicour and Tamburino have shown that for an empty, asymptotically flat, space-time the local flux across an outgoing null hypersurface, i.e., the right-hand side of (5.3), vanishes at $\mathfrak{J}^+$. (This is also true for an asymptotically flat Einstein-Maxwell space.) Furthermore, in a Bondi-Sachs or Newman-Unti coordinate system, with the usual tetrad

$$l^\mu n_\mu = 1, \quad m^\mu \bar{m}_\mu = -1,$$

all other contractions zero, and completeness relation

$$g_{\mu\nu} = 2l_{(\mu}n_{\nu)} - 2m_{(\mu}\bar{m}_{\nu)},$$

the linkage expression (5.1), in the limit of future null infinity, reduces to[22,23]

$$L(\Sigma^+) \overset{\mathfrak{J}}{=} \mathrm{Re} \oint_{\Sigma^+} \{-k^0(\psi_2^0 + \sigma^0\dot{\bar{\sigma}}^0 - \eth^2\bar{\sigma}^0) + k_+[2\bar{\psi}_1^0 - \bar{\eth}(\sigma^0\bar{\sigma}^0) - 2\bar{\sigma}^0\bar{\eth}\sigma^0]\}\, d\omega, \quad (5.4)$$

where $d\omega$ is the area element of the unit sphere and

$$k_+ := \lim_{r\to\infty} r^{-1}k^\alpha m_\alpha = a^m{}_1 Y_{1,m}$$

for three complex constants a^m. When the angular dependence of $k^0 := k^\alpha l_\alpha$ is restricted to spherical harmonics with $l \le 1$, this angular restriction of the translation descriptor singles out the four-parameter translation subgroup of the BMS group. When the conformal transformations (isomorphic to the homogeneous Lorentz group) are turned off, the linkages (5.4) are called P_a, the energy-momentum linkages associated with the translational descriptors Y_a, where

$$k^0 = \alpha = Y_a\epsilon^a, \quad a = 0, 1, 2, 3,$$

with

$$Y_0 := (4\pi)^{\frac{1}{2}} Y_{00}, \quad Y_1 + iY_2 := -(8\pi/3)^{\frac{1}{2}} Y_{11}, \quad Y_3 := (4\pi/3)^{\frac{1}{2}} Y_{10},$$

the Y_{lm} being the usual spherical harmonics. The parameter choices ϵ^a represent unit translations along four orthogonal axes, with $a = 0$ corresponding to a timelike translation. Thus, from (5.4),

$$P_a(u) \overset{\mathfrak{J}}{=} -\oint Y_a(\psi_2^0 + \sigma^0\dot{\bar{\sigma}}^0)\, d\omega \quad (5.5)$$

and, as Sachs has shown,[7] the rate of radiation of energy and momentum is given by the spacelike (null if the news is zero) 4-vector $\dot{P}_a$:

$$\dot{P}_a \overset{\mathfrak{J}}{=} -\oint |\dot{\sigma}^0|^2\, Y_a\, d\omega. \quad (5.6)$$

In order to treat the mass and mass loss of a radiating system in an asymptotically Friedmann space-time, we cannot appeal directly to the linkage expression (5.1). Any expression which integrates the Ricci tensor and hence the energy-momentum tensor, as is evident from (5.3), over spheres of increasing radius must have an infinite limit whenever $T_{\mu\nu}$ includes cosmological dust. [In fact, $T^\mu{}_\nu l_\mu k^0 n^\nu = O(r_l^{-\frac{1}{2}})$ for asymptotic hyperbolic Friedmann.] Thus a new expression is called for, one which does not depend on the Ricci tensor. The generic form of this expression will be[19]

$$E(\Sigma) = \oint_\Sigma U^{\mu\nu}\, dS_{\mu\nu}, \quad (5.7a)$$

with $U^{\mu\nu}$ a bivector to be specified. The integral (5.7a) must (a) have a finite value in the limit of future null infinity and reduce to (5.4) when evaluated in an asymptotically flat space-time, (b) transform properly under the BMS group, and (c) be independent of the 2-surface Σ embedded in $\mathcal{N}$. Guided by early work of Goldberg[24] and the need for agreement with (5.4) and (5.5), we propose

$$U^{\mu\nu} = \rho^{-1}[C^{\mu\nu\rho\sigma}k_\rho l_\sigma + 2l^{[\mu}n^{\nu]}(A + k^{(\alpha;\beta)}l_{\alpha;\beta})], \quad (5.7b)$$

where[22]

$$A = \rho^{-1}\,\mathrm{Re}\,\{k^\alpha m_\alpha[(D - 3\rho)\bar{\psi}_1 - \bar{\delta}(\sigma\bar{\sigma}) - 2\bar{\sigma}(\bar{\delta} - 2\alpha + 2\bar{\beta})\sigma]\}.$$

For asymptotically flat spaces, (5.7) can be evaluated directly, or (B4) can be mapped back to the physical space; and, in Newman-Unti or Bondi-Sachs coordinates, (5.7) reduces to (5.4). Equation (B4) verifies the agreement of our expression with the Tamburino-Winicour linkage in the conformal space (for asymptotically flat space-time). The term A, in (5.7b) above, appears in order that the angular momentum part of (5.7) agree with the Tamburino–Winicour (TW) angular momentum. The transformation properties are identical with the TW linkages, i.e., (5.7) transforms on $\mathfrak{J}^+$ as a representation (adjoint) of the BMS group. The in-surface flux must satisfy

$$U^{\mu\nu}{}_{;\nu} l_\mu = O(r^{-3-\epsilon}) \qquad (5.8)$$

for $\epsilon > 0$ in order that condition (c) be satisfied. Tamburino and Winicour have already demonstrated this to hold for asymptotically flat space–time.

6. MOMENTA IN AN ASYMPTOTICALLY FRIEDMANN SPACE-TIME

The asymptotic invariant, (5.7) presented above, must be re-examined in the asymptotically Friedmann space–time to ensure that it has a finite value on $\mathfrak{J}^+$ and that the in-surface flux (5.8) falls off fast enough. Via the propagation law (5.2) and $l_\mu = u_{,\mu}$, (5.7) reduces to[22]

$$\begin{aligned} E(\Sigma) = -\mathrm{Re} \oint_\Sigma \rho^{-1}\{&-k^\alpha l_\alpha(\psi_2 + \sigma\lambda) + k^\alpha m_\alpha \bar{\psi}_1 \\ &+ 2k^\alpha n_\alpha \sigma\bar{\sigma} + \bar{\sigma}(\delta + \bar{\alpha} - \beta)k^\alpha m_\alpha \\ &+ \rho^{-1}k^\alpha m_\alpha[(D - 3\rho)\bar{\psi}_1 - \bar{\delta}(\sigma\bar{\sigma}) \\ &- 2\bar{\sigma}(\bar{\delta} - 2\alpha + 2\bar{\beta})\sigma]\}\, dS \end{aligned} \qquad (6.1)$$

with $dS = \sqrt{-g}\, dx^2\, dx^3$.

With the rotations turned off and the asymptotic solutions of Appendix A substituted, (6.1) has a finite limit on[25] $\mathfrak{J}^+$:

$$P(u) \overset{\mathfrak{J}}{=} -\mathrm{Re} \oint k^0(\psi_2^0 + \sigma^0\lambda^0)\, d\omega, \qquad (6.2)$$

where $k^0 = \alpha$ is restricted to the translations ($l \leq 1$). The in-surface flux falls off properly for (6.2) to be an asymptotic invariant, i.e.,

$$U^{\mu\nu}{}_{;\nu} l_\mu = O(r^{-\frac{7}{2}}).$$

Thus, the Bondi mass of a bounded radiating system in an asymptotically hyperbolic Friedmann space–time can be defined in precisely the same manner as for asymptotically flat spaces. In addition, there is a mass loss expression similar to the one for asymptotically flat spaces[25]:

$$\dot{P}(u) \overset{\mathfrak{J}}{=} -\oint k^0\, |\lambda^0|^2\, d\omega.$$

When we turn to the angular momentum, however, it is not as easily seen that (6.1) is finite as $r \to \infty$ along the outgoing null surface. This is so because (see Appendix A)

$$\psi_1 = [2P^3\bar{\nabla}(\psi_0^0 P^{-2}) - 3\Phi_{01}^0 + 3A\tau^0/2\sqrt{2}]r^{-\frac{7}{2}} + O(r^{-4})$$

is a solution of the hypersurface equation[26]

$$\begin{aligned}(D - 4\rho)\psi_1 = (\bar{\delta} - 4\alpha + \bar{\tau})\psi_0 + (D - 2\rho)\Phi_{01} \\ - (\delta - \tau)\Phi_{00} - 2\sigma\Phi_{10}.\end{aligned} \qquad (6.3)$$

With Hawking's boundary conditions (A2), (A3), and (A4), each of the first three terms on the right-hand side of (6.3) contributes to the leading order of ψ_1.

In order to see that the angular momentum has a finite limit, we must understand the angular behavior of the leading part of ψ_1 in terms of an expansion $a^{lm}{}_1 Y_{l,m}$. Since ψ_0^0 is a spin-weight-2 quantity, its lowest l value is 2. Similarly, since $\tau^0 = -\bar{\eth}\sigma^0$ up to a numerical factor,[23] its lowest l is also 2. Φ_{01}^0 has spin weight 1, but when the $\Delta\Phi_{01}$ field equation is examined, one finds that Φ_{01} is driven only by $\bar{\eth}\sigma^0$ and $\bar{\eth}\dot{\sigma}^0$ and thus Φ_{01}^0 has a lowest l of 2. It is now clear that the leading term of ψ_1, when integrated over the sphere in (6.1), will vanish. Thus, the angular momentum is given by[25]

$$L(u) \overset{\mathfrak{J}}{=} \mathrm{Re} \oint k_+[2\bar{\psi}_1^0 - \bar{\eth}(\sigma^0\bar{\sigma}^0) - 2\bar{\sigma}^0\bar{\eth}\sigma^0]\, d\omega$$

with $k_+ = a^m{}_1 Y_{1,m}$ for three complex constants a^m. $L(u)$ can be given bivector labels corresponding to the six real independent parts of k_+, which in turn correspond to the six generators of the Lorentz boosts and rotations.[27]

7. SUMMARY

The goal of this work was to show that the physically interesting characteristics of a bounded radiating source, in a cosmological space, can be understood in much the same manner that we have come to understand a similar physical system in asymptotically flat space–time.

Future null infinity, for an asymptotically hyperbolic Friedmann space, has been shown to be a null, shear-free, hypersurface. The asymptotic symmetry group is the BMS group, and, from the BMS descriptors, the Weyl tensor, and the normal of the outgoing null hypersurfaces, an asymptotic invariant has been constructed which defines the energy and angular momentum of the gravitating system. For asymptotically flat spaces, this invariant is identical to the Tamburino–Winicour linkages.

$\mathfrak{J}^-$ is not discussed other than to note it must be spacelike, which follows from the existence of a particle horizon.[5] Future work will consider Einstein–Maxwell-dust solutions and Newman–Penrose constants.

ACKNOWLEDGMENTS

In the course of this research, the author has profited from many discussions with Dr. J. Winicour and Dr. D. Robinson and correspondence with Dr. S. W. Hawking.

APPENDIX A

For the purpose of easy reference, we list here Hawking's asymptotic solution[8] of the Newman–Penrose field equations. The notation, definitions, and sign conventions are those of Newman and Penrose[10] with the exception that Greek indices here range from 0 to 3.

The twelve complex spin coefficients are defined below:

$$\kappa := m^\mu D l_\mu, \quad \epsilon := \tfrac{1}{2}(n^\mu D l_\mu - \bar{m}^\mu D m_\mu),$$
$$\pi := -\bar{m}^\mu D n_\mu,$$
$$\rho := m^\mu \bar{\delta} l_\mu, \quad \alpha := \tfrac{1}{2}(n^\mu \bar{\delta} l_\mu - \bar{m}^\mu \bar{\delta} m_\mu),$$
$$\lambda := -\bar{m}^\mu \bar{\delta} n_\mu,$$
$$\sigma := m^\mu \delta l_\mu, \quad \beta := \tfrac{1}{2}(n^\mu \delta l_\mu - \bar{m}^\mu \delta m_\mu),$$
$$\mu := -\bar{m}^\mu \delta n_\mu,$$
$$\tau := m^\mu \Delta l_\mu, \quad \gamma := \tfrac{1}{2}(n^\mu \Delta l_\mu - \bar{m}^\mu \Delta m_\mu),$$
$$\nu := -\bar{m}^\mu \Delta n_\mu,$$

with tetrad derivatives defined as

$$D := l^\nu \nabla_\nu, \quad \Delta := n^\nu \nabla_\nu, \quad \delta := m^\nu \nabla_\nu.$$

The Weyl tensor components are five complex scalars:

$$\psi_0 := -C_{\mu\nu\rho\sigma} l^\mu m^\nu l^\rho m^\sigma, \quad \psi_1 := -C_{\mu\nu\rho\sigma} l^\mu n^\nu l^\rho m^\sigma,$$
$$\psi_2 := -C_{\mu\nu\rho\sigma} \bar{m}^\mu n^\nu l^\rho m^\sigma, \quad \psi_3 := -C_{\mu\nu\rho\sigma} \bar{m}^\mu n^\nu l^\rho n^\sigma,$$
$$\psi_4 := -C_{\mu\nu\rho\sigma} \bar{m}^\mu n^\nu \bar{m}^\rho n^\sigma.$$

The Ricci tensor components are four real and three complex scalars:

$$\Phi_{00} = \bar{\Phi}_{00} := -\tfrac{1}{2} R_{\mu\nu} l^\mu l^\nu,$$
$$\Phi_{11} = \bar{\Phi}_{11} := -\tfrac{1}{4} R_{\mu\nu}(l^\mu n^\nu + m^\mu \bar{m}^\nu),$$
$$\Phi_{22} = \bar{\Phi}_{22} := -\tfrac{1}{2} R_{\mu\nu} n^\mu n^\nu,$$
$$\Lambda = \bar{\Lambda} := \tfrac{1}{24} R,$$
$$\Phi_{01} = \bar{\Phi}_{10} := -\tfrac{1}{2} R_{\mu\nu} l^\mu m^\nu,$$
$$\Phi_{02} = \bar{\Phi}_{20} := -\tfrac{1}{2} R_{\mu\nu} m^\mu m^\nu,$$
$$\Phi_{12} = \bar{\Phi}_{21} := -\tfrac{1}{2} R_{\mu\nu} n^\mu m^\nu.$$

The coordinate $x^0 = u$ labels the outgoing null hypersurfaces, with $l_\mu := u_{,\mu}$. $x^1 = r$ is chosen to be an affine parameter:

$$r_{,\mu} l^\mu = 1.$$

x^2 and x^3 are the ray labels in the const u surfaces. m^μ and $\bar{m}^\mu$ are chosen to be surface forming and lie in the 2-surfaces of const u and r. These coordinate and tetrad conditions imply (with the propagation of m^μ chosen such that $\epsilon = 0$)

$$\kappa = \epsilon = 0, \quad \rho = \bar{\rho},$$
$$\mu = \bar{\mu}, \quad \tau = \bar{\alpha} + \beta = \bar{\pi}.$$

In these coordinates, the tetrad vectors are expressed as

$$l_\mu = \delta^0_\mu, \quad l^\mu = \delta^\mu_1,$$
$$n^\mu = \delta^\mu_0 + U\delta^\mu_1 + X^i \delta^\mu_i,$$
$$m^\mu = \xi^i \delta^\mu_i.$$

The boundary conditions are chosen to be[28]

$$\Lambda = \tfrac{1}{4} A(R)^{-3} + O(r^{-\frac{7}{2}}), \tag{A1}$$
$$\Phi_{00} = 3A(R)^{-5} + O(r^{-\frac{9}{2}}), \tag{A2}$$
$$\Phi_{01} = O(r^{-\frac{7}{2}}), \tag{A3}$$
$$\psi_0 = O(r^{-\frac{7}{2}}). \tag{A4}$$

The leading terms of Λ and Φ_{00} come from the exact, unperturbed, metric (2.1). The critical choice for ψ_0 and Φ_{01} was the highest order which preserves $\psi_4 = O(r^{-1})$ and where the u derivatives of ψ_0 and Φ_{01} depend on σ^0 (interpreted by Hawking as having the perturbations to exact hyperbolic Friedmann arise only from the gravitational radiation of the perturbing source). Below, the leading terms of Hawking's asymptotic solution of the Newman–Penrose field equations are listed:

$$\rho = -r^{-1} + 3A(2r)^{-\frac{3}{2}} + O(r^{-2}\log r), \tag{A5}$$
$$\sigma = \sigma^0 r^{-2} + O(r^{-\frac{5}{2}}), \tag{A6}$$
$$\tau = \bar{\pi} = \tau^0 r^{-2} + O(r^{-\frac{5}{2}}), \tag{A7}$$
$$\alpha = \alpha^0 r^{-1} + O(r^{-\frac{3}{2}}), \tag{A8}$$
$$\beta = -\bar{\alpha}^0 r^{-1} + O(r^{-\frac{3}{2}}), \tag{A9}$$
$$\lambda = 2(\dot{\bar{\sigma}}^0 - \bar{\sigma}^0) r^{-1} + O(r^{-\frac{3}{2}}), \tag{A10}$$
$$\mu = (A/2\sqrt{2}) r^{-\frac{1}{2}} + O(r^{-1}), \tag{A11}$$
$$\gamma = -\tfrac{1}{2} - (A/2\sqrt{2}) r^{-\frac{1}{2}} + O(r^{-1}), \tag{A12}$$
$$\nu = \psi^0_3 r^{-1} + O(r^{-\frac{3}{2}}), \tag{A13}$$
$$U = r + (2\sqrt{2A}) r^{\frac{1}{2}} + O(\log r), \tag{A14}$$
$$X^i = -(\tau^0 \bar{\xi}^{i0} + \bar{\tau}^0 \xi^{i0}) r^{-2} + O(r^{-\frac{5}{2}}), \tag{A15}$$
$$\xi^i = \xi^{i0} r^{-1} + O(r^{-\frac{3}{2}}), \tag{A16}$$
$$\psi_0 = \psi^0_0 r^{-\frac{7}{2}} + O(r^{-4}), \tag{A17}$$
$$\psi_1 = H r^{-\frac{7}{2}} + \psi^0_1 r^{-4} + O(r^{-\frac{9}{2}}\log r), \tag{A18}$$
$$\psi_2 = \psi^0_2 r^{-3} + O(r^{-\frac{7}{2}}), \tag{A19}$$
$$\psi_3 = \psi^0_3 r^{-2} + O(r^{-\frac{5}{2}}), \tag{A20}$$
$$\psi_4 = \psi^0_4 r^{-1} + O(r^{-\frac{3}{2}}), \tag{A21}$$

where $\xi^{02} = P(u, x^i)$, $\xi^{03} = iP$, and $P := (Ae^u/\sqrt{2}) \times (1 + \frac{1}{4}\zeta\bar{\zeta})$ with $\zeta := x^2 + ix^3$. Additionally,

$$\alpha^0 = (2)^{-\frac{3}{2}}A\zeta, \quad \tau^0 = 2P^3\bar{\nabla}(\sigma^0 P^{-2}),$$
$$\psi_4^0 = -2(\dddot{\bar{\sigma}}^0 - 3\dot{\bar{\sigma}}^0 + 2\bar{\sigma}^0), \quad \psi_3^0 = -\tfrac{1}{2}P^3\nabla(\lambda^0 P^{-2}),$$
$$\psi_2^0 - \bar{\psi}_2^0 = P^2\bar{\nabla}(\tau^0 P^{-1}) - P^2\nabla(\bar{\tau}^0 P^{-1}) + 4\bar{\sigma}^0\bar{\lambda}^0 - 4\sigma^0\lambda^0,$$
$$H = 2P^3\bar{\nabla}(\psi_0^0 P^{-2}) - 3\Phi_{01}^0 + 3A\tau^0/2\sqrt{2},$$

where

$$\nabla := \frac{\partial}{\partial x^2} + i\frac{\partial}{\partial x^3};$$

$\psi_2^0 + \bar{\psi}_2^0$ is undetermined;

$$\dot{\Phi}_{00} = O(r^{-\frac{9}{2}}), \quad \dot{\Lambda} = O(r^{-\frac{7}{2}}),$$
$$\dot{\Phi}_{01} = O(r^{-\frac{7}{2}}), \quad \dot{\psi}_0 = O(r^{-\frac{7}{2}}),$$

with the four u-derivatives above depending on σ^0. The remaining Ricci tensor components are related to the ones above by

$$\Phi_{11} = 3\Lambda + \Phi_{00}^{-1}\Phi_{01}\Phi_{10},$$
$$\Phi_{12} = 6\Lambda\Phi_{01}\Phi_{00}^{-1}(1 + \tfrac{1}{6}\Lambda^{-1}\Phi_{00}^{-1}\Phi_{01}\Phi_{10})^2,$$
$$\Phi_{22} = 6\Lambda\Phi_{01}^{-1}\Phi_{12}, \quad \Phi_{02} = \Phi_{00}^{-1}\Phi_{01}^2.$$

APPENDIX B

In order to compare our asymptotic invariant with the Winicour–Tamburino linkage expression[18] in asymptotically flat space–time, we will work in the conformal space. The definitions and conventions of Ref. 18 will be followed in this appendix with the exception of the relabeling

$$\xi^\mu \to k^\mu, \quad k^\mu \to l^\mu, \quad t^\mu \to m^\mu, \quad m^\mu \to n^\mu,$$
$$g_{\mu\nu} \to -g_{\mu\nu}, \quad \eth \to -\eth$$

where the arrow points from Winicour's notation to ours and the normalization

$$l^\mu n_\mu = -m^\mu \bar{m}_\mu = 1.$$

The final linkage expression, on $\mathscr{I}^+$ in the conformal space, is given by Eq. W(5.5),[29]

$$L(\Sigma) \overset{\mathscr{I}}{=} -\text{Re}\oint_\Sigma \{\Xi + k^\mu l_\mu \Phi + k^\mu m_\mu[2\Psi + \bar{\eth}(\sigma\bar{\sigma}) + 2\bar{\sigma}\bar{\eth}\sigma]\}\, dS \quad \text{(B1)}$$

with the definitions

$$\Xi := \sigma(k^{\alpha;\beta}\bar{m}_\alpha\bar{m}_\beta)_{;\nu}l^\nu,$$
$$\Phi := C^{\mu\alpha\beta\nu;\gamma}n_\mu m_\alpha\bar{m}_\beta l_\nu l_\gamma,$$
$$\Psi := C^{\mu\alpha\beta\nu;\gamma}m_\mu\bar{m}_\alpha\bar{m}_\beta l_\nu l_\gamma.$$

To show the equivalence of the asymptotic invariant (5.7) with (B1), we will map (5.7) into the conformal space. Following W(2.8), the conformal map is given by

$$\tilde{g}_{\mu\nu} = \Omega^{-2}g_{\mu\nu},$$
$$\tilde{l}_\mu = l_\mu, \quad \tilde{n}_\mu = \Omega^{-2}n_\mu, \quad \tilde{m}_\mu = \Omega^{-1}m_\mu.$$

The Weyl tensor maps as $\tilde{C}^\mu{}_{\nu\rho\sigma} = C^\mu{}_{\nu\rho\sigma}$, and the tensor surface element as $d\tilde{S}_{\mu\nu} = \Omega^{-4}\, dS_{\mu\nu}$. Rewriting (5.7), we have

$$E(\Sigma) = \oint_\Sigma \tilde{\rho}^{-1}[\tilde{C}^{\mu\nu\rho\sigma}\tilde{k}_\rho\tilde{l}_\sigma + 2\tilde{A}\tilde{l}^{[\mu}\tilde{n}^{\nu]} + 2\tilde{k}^{\alpha;\beta}(\tilde{\bar{\sigma}}\tilde{m}_\alpha\tilde{m}_\beta + \tilde{\sigma}\tilde{\bar{m}}_\alpha\tilde{\bar{m}}_\beta)\tilde{l}^{[\mu}\tilde{n}^{\nu]}\, d\tilde{S}_{\mu\nu}, \quad \text{(B2)}$$

where the propagation law (5.2) has been used to reduce $\tilde{k}^{(\alpha;\beta)}\tilde{l}_{\alpha;\beta}$. Since the divergence of l_μ maps as

$$\tilde{\rho} = \Omega^2\rho + \Omega l^\nu\Omega_{,\nu},$$

we follow Winicour in setting $\rho = 0$ by choosing $\tilde{\rho} = \Omega D\Omega$. Equation (B2) maps over to the conformal space as

$$E(\Sigma) = -\oint_\Sigma (\Omega D\Omega)^{-1}[C^{\mu\nu\rho\sigma}l_\mu n_\nu l_\rho k_\sigma + k^{\alpha;\beta}(\sigma\bar{m}_\alpha\bar{m}_\beta + \bar{\sigma}m_\alpha m_\beta)]\, dS - \text{Re}\oint_\Sigma \xi^\alpha m_\alpha(D\Omega)^{-2}[D\bar{\psi}_1 - \bar{\delta}(\sigma\bar{\sigma}) - 2\bar{\sigma}(\bar{\delta} - 2\alpha + 2\bar{\beta})\sigma]\, dS, \quad \text{(B3)}$$

where we have used

$$(\tilde{D} - 3\tilde{\rho})\tilde{\bar{\psi}}_1 = \Omega^5(D - 3\rho)\psi_1,$$

and, with W(2.15),

$$\tilde{\bar{\delta}}(\tilde{\sigma}\tilde{\bar{\sigma}}) = \Omega^5\bar{\delta}(\sigma\bar{\sigma}).$$

L'Hospital's rule is used to evaluate the limit $\Omega \to 0$, which restricts the integral to $\mathscr{I}^+$. With $D\Omega \overset{\mathscr{I}}{=} -1$, W(1.8) and W(2.6), the limit of (B3) is evaluated as

$$E(\Sigma) \overset{\mathscr{I}}{=} -\text{Re}\oint_\Sigma \{\Xi + k^\alpha l_\alpha \Phi + k^\alpha m_\alpha[2\Psi + \bar{\eth}(\sigma\bar{\sigma}) + 2\bar{\sigma}\bar{\eth}\sigma]\}\, dS. \quad \blacksquare \quad \text{(B4)}$$

We note that the middle term of (B2), $(\tilde{A}/\tilde{\rho})\, d\tilde{S}$, maps conformally covariantly to the expression

$$\text{Re}\,\{k^\alpha m_\alpha[\Psi + \bar{\eth}(\sigma\bar{\sigma}) + 2\bar{\sigma}\bar{\eth}\sigma]\}\, dS,$$

which is essentially just the third term of W(3.19). The other two terms of (B2) map to the first two terms of W(3.19). Finally, we mention again that the above proof of agreement of our expression with Winicour's is for asymptotically flat vacuum, or Einstein–Maxwell, space–time.

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1 For an excellent summary, see F. Pirani, "Introduction to Gravitational Radiation Theory," in *Lectures on General Relativity*, 1964 Brandeis Summer Institute (Prentice-Hall, Englewood Cliffs, N.J., 1965), Vol. 1.

[2] H. Bondi, M. van der Burg, and A. Metzner, Proc. Roy. Soc. (London) **A269**, 21 (1962).

[3] R. K. Sachs, Proc. Roy. Soc. (London) **A270**, 103 (1962).

[4] R. Penrose, Phys. Rev. Letters **10**, 66 (1963).

[5] R. Penrose, in *Relativity, Groups, and Topology*, 1963 Les Houches Summer School (Gordon and Breach, New York, 1964), p. 565

[6] L. Tamburino and J. Winicour, Phys. Rev. **150**, 1039 (1966).

[7] R. K. Sachs, Phys. Rev. **128**, 2851 (1962).

[8] S. W. Hawking, J. Math. Phys. **9**, 598 (1968).

[9] E. T. Newman and T. Unti, J. Math. Phys. **3**, 891 (1962).

[10] E. T. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962); **4**, 998 (1963).

[11] R. Penrose, Proc. Roy. Soc. (London) **A284**, 159 (1965).

[12] We follow the usual convention that partial derivatives are denoted by a comma or ∂_ν, and covariant derivatives by a semicolon or ∇_ν.

[13] L. Infeld and A. Schild, Phys. Rev. **68**, 250 (1945).

[14] In this section and Appendix B, we follow Penrose's convention of placing tildes over the quantities in the physical space. In all other sections we omit the tildes.

[15] The second derivative of Ω, $\partial^2\Omega/\partial z^2$, blows up on the $z = 0$ surface.

[16] R. Geroch, "Space–Time Structure from a Global Viewpoint," lectures given at the 1969 "Enrico Fermi" Summer School (Varenna).

[17] Coordinate components of k^μ are used in this section.

[18] J. Winicour, J. Math. Phys. **9**, 861 (1968).

[19] Square brackets around indices denote antisymmetrization and $dS_{\mu\nu} := u_{,[\mu}r_{,\nu]}\, dS$. Symmetrization is correspondingly denoted by parentheses around indices.

[20] The BMS descriptors are given four labels $Q = a, a = 0, 1, 2, 3$, and six bivector labels $Q = [ab]$ analogous to the descriptors of the Poincaré group. The remaining BMS descriptors, corresponding to the supertranslations, are given the spherical-harmonic labels $Q = (lm)$ with $l \geq 2$.

[21] $dS_\mu = l_\mu\, dV$, $2A_{\nu;[\rho\sigma]} \equiv A^\alpha R_{\alpha\nu\rho\sigma}$, $R_{\nu\rho} := g^{\mu\sigma}R_{\mu\nu\rho\sigma}$.

[22] See Appendix A for definitions of the Newman–Penrose spin coefficients and Weyl tensor components.

[23] If η is a function of spin weight s, then $\eth\eta := -(\delta^0 + 2s\alpha^0)\eta$ and $\eth\eta$ has spin weight $s + 1$. Two additional properties of $\eth$ are used: (a) If η has spin weight -1, then $\eth\eta$ is a divergence on the sphere, and (b) $\eth_s Y_{s,m} = 0$.

[24] J. N. Goldberg, Phys. Rev. **131**, 1367 (1963).

[25] With the solutions of Appendix A in terms of a luminosity distance, coefficients e^{-u}, which appear in Hawking's expressions, are eliminated.

[26] The Newman–Penrose field equation (6.3) is given for Hawking's tetrad conditions, which are presented in Appendix A.

[27] A. Held, E. T. Newman, and R. Posadas, J. Math. Phys. **11**, 3145 (1970).

[28] $R(\tau)$ given in (2.1) is a function of the affine parameter $r = A^2(\frac{1}{4}\sinh 2\tau - 2\sinh\tau + \frac{3}{2}\tau)$, and has the expansion $R = (2r)^{\frac{1}{2}} + A + O(r^{-\frac{1}{2}}\log r)$.

[29] W will precede all equation numbers of Ref. 18.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Myriotic Fields in Quantum Statistical Mechanics

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(Received 26 October 1970)

A Hilbert space formulation of quantum statistical mechanics is developed by using the notion of myriotic fields. The nonseparable nature of the Hilbert space is investigated, and it is shown that in the classical limit, $\hbar \to 0$, the Hilbert space approaches, in the absence of point eigenvalues, that Hilbert space appropriate to classical statistical mechanics.

I. INTRODUCTION

In recent years a considerable amount of theoretical investigation has been devoted to quantum statistical mechanics. This has placed the field of statistical mechanics among the major branches of mathematical physics. One particular area of extensive research is in the extension to quantum statistical mechanics of the algebraic approach proposed by Segal and Haag in quantum field theory.[1,2] In essence, this approach emphasizes the purely algebraic structure of local observables. Presently, the development in the algebraic approach is in understanding the description of equilibrium states. Thus, one hopes from this to learn more about interacting equilibrium and nonequilibrium states. In particular, some general features of states in thermal equilibrium have been obtained,[3] and it has been shown that invariant states of infinite systems may be decomposed into elementary (extremal) invariant states.[4]

In recent works[5] a new formulation of quantum statistical mechanics has been developed. It suggests that the notions of "the approach to equilibrium" in statistical mechanics and that of the asymptotic condition in axiomatic quantum field theory are *one and the same*. This link implies a deep unity in physics and allows for a complete utilization, in quantum statistical mechanics, of procedures already developed in axiomatic quantum field theory.

One noteworthy feature of the algebraic approach (as applied to quantum statistical mechanics) is that one begins by considering a macroscopic or infinite system. This differs considerably from the usual consideration of a large, but finite, system and then taking the thermodynamic limit. Besides being more

[2] H. Bondi, M. van der Burg, and A. Metzner, Proc. Roy. Soc. (London) **A269**, 21 (1962).
[3] R. K. Sachs, Proc. Roy. Soc. (London) **A270**, 103 (1962).
[4] R. Penrose, Phys. Rev. Letters **10**, 66 (1963).
[5] R. Penrose, in *Relativity, Groups, and Topology*, 1963 Les Houches Summer School (Gordon and Breach, New York, 1964), p. 565
[6] L. Tamburino and J. Winicour, Phys. Rev. **150**, 1039 (1966).
[7] R. K. Sachs, Phys. Rev. **128**, 2851 (1962).
[8] S. W. Hawking, J. Math. Phys. **9**, 598 (1968).
[9] E. T. Newman and T. Unti, J. Math. Phys. **3**, 891 (1962).
[10] E. T. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962); **4**, 998 (1963).
[11] R. Penrose, Proc. Roy. Soc. (London) **A284**, 159 (1965).
[12] We follow the usual convention that partial derivatives are denoted by a comma or ∂_ν, and covariant derivatives by a semicolon or ∇_ν.
[13] L. Infeld and A. Schild, Phys. Rev. **68**, 250 (1945).
[14] In this section and Appendix B, we follow Penrose's convention of placing tildes over the quantities in the physical space. In all other sections we omit the tildes.
[15] The second derivative of Ω, $\partial^2\Omega/\partial z^2$, blows up on the $z = 0$ surface.
[16] R. Geroch, "Space–Time Structure from a Global Viewpoint," lectures given at the 1969 "Enrico Fermi" Summer School (Varenna).
[17] Coordinate components of k^μ are used in this section.
[18] J. Winicour, J. Math. Phys. **9**, 861 (1968).
[19] Square brackets around indices denote antisymmetrization and $dS_{\mu\nu} := u,_{[\mu}r,_{\nu]}\, dS$. Symmetrization is correspondingly denoted by parentheses around indices.
[20] The BMS descriptors are given four labels $Q = a, a = 0, 1, 2, 3$, and six bivector labels $Q = [ab]$ analogous to the descriptors of the Poincaré group. The remaining BMS descriptors, corresponding to the supertranslations, are given the spherical-harmonic labels $Q = (lm)$ with $l \geq 2$.
[21] $dS_\mu = l_\mu\, dV$, $2A_{\nu;[\rho\sigma]} \equiv A^\alpha R_{\alpha\nu\rho\sigma}$, $R_{\nu\rho} := g^{\mu\sigma}R_{\mu\nu\rho\sigma}$.
[22] See Appendix A for definitions of the Newman–Penrose spin coefficients and Weyl tensor components.
[23] If η is a function of spin weight s, then $\eth\eta := -(\delta^0 + 2s\alpha^0)\eta$ and $\eth\eta$ has spin weight $s + 1$. Two additional properties of $\eth$ are used: (a) If η has spin weight -1, then $\eth\eta$ is a divergence on the sphere, and (b) $\eth_s Y_{s,m} = 0$.
[24] J. N. Goldberg, Phys. Rev. **131**, 1367 (1963).
[25] With the solutions of Appendix A in terms of a luminosity distance, coefficients e^{-u}, which appear in Hawking's expressions, are eliminated.
[26] The Newman–Penrose field equation (6.3) is given for Hawking's tetrad conditions, which are presented in Appendix A.
[27] A. Held, E. T. Newman, and R. Posadas, J. Math. Phys. **11**, 3145 (1970).
[28] $R(\tau)$ given in (2.1) is a function of the affine parameter $r = A^2(\frac{1}{4}\sinh 2\tau - 2\sinh\tau + \frac{3}{2}\tau)$, and has the expansion $R = (2r)^{\frac{1}{2}} + A + O(r^{-\frac{1}{2}}\log r)$.
[29] W will precede all equation numbers of Ref. 18.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Myriotic Fields in Quantum Statistical Mechanics

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(Received 26 October 1970)

A Hilbert space formulation of quantum statistical mechanics is developed by using the notion of myriotic fields. The nonseparable nature of the Hilbert space is investigated, and it is shown that in the classical limit, $\hbar \to 0$, the Hilbert space approaches, in the absence of point eigenvalues, that Hilbert space appropriate to classical statistical mechanics.

I. INTRODUCTION

In recent years a considerable amount of theoretical investigation has been devoted to quantum statistical mechanics. This has placed the field of statistical mechanics among the major branches of mathematical physics. One particular area of extensive research is in the extension to quantum statistical mechanics of the algebraic approach proposed by Segal and Haag in quantum field theory.[1,2] In essence, this approach emphasizes the purely algebraic structure of local observables. Presently, the development in the algebraic approach is in understanding the description of equilibrium states. Thus, one hopes from this to learn more about interacting equilibrium and nonequilibrium states. In particular, some general features of states in thermal equilibrium have been obtained,[3] and it has been shown that invariant states of infinite systems may be decomposed into elementary (extremal) invariant states.[4]

In recent works[5] a new formulation of quantum statistical mechanics has been developed. It suggests that the notions of "the approach to equilibrium" in statistical mechanics and that of the asymptotic condition in axiomatic quantum field theory are *one and the same*. This link implies a deep unity in physics and allows for a complete utilization, in quantum statistical mechanics, of procedures already developed in axiomatic quantum field theory.

One noteworthy feature of the algebraic approach (as applied to quantum statistical mechanics) is that one begins by considering a macroscopic or infinite system. This differs considerably from the usual consideration of a large, but finite, system and then taking the thermodynamic limit. Besides being more logical, the direct treatment of infinite systems should give an insight into the true nature of states in statistical mechanics and bring forth the peculiar behaviors, e.g., phase transitions, condensation, etc., which appear only in infinite systems.

In the formulation of Ref. 5 one also considers infinite systems. If one attempts to extend the notion of asymptotic condition of field theory to these states, one is led naturally to the concept of an asymptotic approach to equilibrium. Thus, the infinite nature of the systems considered is of crucial importance in this formulation and noticeably distinguishes these states from those studied in scattering theories (which describe finite systems). This generalized notion of asymptotic condition, as applied to *any* vector in the general Hilbert space, serves as a foundation to both scattering theory and statistical mechanics.

Hence, a quantum field theory in its general form is applicable to both of the above situations with the distinguishing factor being the Hilbert space under consideration. The separable Hilbert space, the part in which the physical vacuum state appears as a vector and, thus, with zero particle density, is appropriate to scattering theory, whereas, the nonseparable Hilbert spaces, with nonvanishing particle density, are appropriate to statistical mechanics. This distinction of the Hilbert spaces is directly related to the existence of (infinitely) many unitarily inequivalent irreducible representations.[2]

II. OCCUPATION NUMBER REPRESENTATION

Classical statistical mechanics defines a state of statistical equilibrium with the aid of the ensemble of Gibbs.[6] Consequently, the probabilistic nature of the state of equilibrium (or for that matter *any* state of the system) is due to the association of the state of the system with an appropriate ensemble of states. On the other hand, quantum mechanics already contains an inherent probabilistic interpretation. Therefore, it is not absurd to suppose that the physical interpretation of quantum mechanics, in terms of probabilities, should suffice to give quantum statistical mechanics a probabilistic interpretation without the additional use of the concept of an ensemble of states.

In the formulation of quantum statistical mechanics of Ref. 5, *single* states of the system were introduced which represent states of statistical equilibrium. This differs from the usual concept of equilibrium as an ensemble of states. Friedrichs[7] has also considered these types of states and used them to describe noninteracting equilibrium states. The simple construction of Friedrichs will be used in this section to derive some well-known results in quantum statistical mechanics for noninteracting systems. This will also serve as an introduction to the mathematical aspect of the theory.

Throughout this work an occupation number representation will be employed since, as shown by Friedrichs,[7] particle representations do not exist for the case of interest in statistical mechanics, that is, when the total number of particles is expected to be infinite in every state of the system.

Let s denote any continuous quantum variable such as the momentum or the position of a single particle. The occupation number will be denoted by $\nu(s)$ and is a function of the continuous variable s but may assume only integer values $\nu = 0, 1, 2, \cdots$. The s-space is partitioned into bounded and semi-infinite cells, and a state is given by specifying the amplitude of the probability of finding each cell occupied by a certain number of particles. This probability is independent of the distribution of the particles within the cells. One considers refinements for such partitions and performs a limiting process.

The (reduced) representer of the state Φ is a functional $\phi(\nu)$ of the occupation function $\nu(s)$. The inner product of two states Φ_1 and Φ_2 will be expressed in the symbolic form

$$(\Phi_1, \Phi_2) = \sum_{\nu} \phi_1^*(\nu)\phi_2(\nu) \prod_{s} [\nu(s)!]^{-1}[d\omega(s)]^{\nu(s)}e^{-d\omega(s)}, \tag{1}$$

where $\omega(s)$ is called the weight and is a measure function. The above expression represents the following formal operation which can be justified rigorously by considering a limiting process: For a given occupation $\nu(s)$, one forms the infinite product

$$\prod_{s} [\nu(s)!]^{-1}[d\omega(s)]^{\nu(s)}e^{-d\omega(s)},$$

with the variable s extending over the whole of s-space. One multiplies this product by $\phi_1^*(\nu)\phi_2(\nu)$ and sums the result over all possible choices of the occupation $\nu(s)$. Since one requires states of finite norm, $(\Phi, \Phi) < \infty$, the series (1) is convergent by Schwarz's inequality.

The manifold of functionals which are compatible[8] (in the second manner) with some partition forms a linear space. This linear space is extended to a complete linear space by the addition of its ideal elements. The Hilbert space of all compatible and ideal occupation functionals $\phi(\nu)$ are the representers of the states. One can express the probability of an observable having a value in a given range for any state in terms of the representer $\phi(\nu)$ of the state.

The states of interest in statistical mechanics contain an infinite number of particles (but finite density). In the present formulation of quantum statistical mechanics these states are those of a field with infinite total weight W, $W = \int d\omega(s)$. Friedrichs denotes these fields by the term myriotic. In case $W = \infty$, it is not possible to introduce the total number of particles operator; however, operators denoting the number of particles in cells of finite weight do exist. Since the vacuum state is defined in terms of the preceding operators, a vacuum state does not exist for a myriotic field. Consequently, a particle representation for myriotic fields is also nonexistent. On the other hand, myriotic fields possess equidistribution states [with representer $\phi(\nu) \equiv 1$] which are closely related to (noninteracting) equilibrium states.

III. OCCUPATION NUMBER REPRESENTATION FOR BOSON FIELDS

The inner product defined by (1) is appropriate to Maxwell–Boltzmann statistics. This is the case treated by Friedrichs, and for equidistribution states it leads to the usual formula for the expected number of particles at s with the energy restricted by $\sum_s \lambda(s)\nu(s) = \kappa$. [See (20.58) in Ref. 7.]

As an extension to the above work and also an introduction to the formal operations, let us consider the statistics of Bose and Einstein and summarily that of Fermi and Dirac. The presentation of Friedrichs will be followed closely so that one may feel free to omit nonessentials and, hence, benefit both in clarity and conciseness. As stated previously, one is particularly interested in myriotic fields for the description of states in statistical mechanics. Accordingly, one considers directly the generalization of the usual occupation number representation (discussed in Ref. 7, Sec. 18), which will apply equally to myriotic, as well as to ordinary or amyriotic fields.

The s-space is as described above. A partition $\mathcal{T}$ of the s-space is given by a subdivision of the space into distinct, bounded, or semi-infinite, cells. The region formed by all bounded cells will be denoted by $\mathcal{R}$, and is composed by cells $\mathcal{C}_k$, $k = 1, 2, 3, \cdots$. The region formed by the remaining cells will be denoted by $\mathcal{C}_*$. For every occupation $\nu(s)$ one has

$$\nu_k = \sum_{s\in\mathcal{C}_k} \nu(s), \quad k = 1, 2, \cdots,$$

and

$$\nu_* = \sum_{s\in\mathcal{C}_*} \nu(s). \tag{2}$$

By assumption, the numbers ν_k are required to be finite, but not ν_*.

A functional $f(\nu)$ is compatible (in the second manner) with the partition $\mathcal{T}$ if it depends only on the values of ν_k, $k = 1, 2, \cdots$, but not on ν_*. Let g_k, $k = 1, 2, \cdots$, denote the number of elementary eigenvalues in the cell denoted by $\mathcal{C}_k$. Define the inner product of two functionals ϕ_1 and ϕ_2, which are compatible with the partition $\mathcal{T}$, by

$$(\Phi_1, \Phi_2)_\epsilon^{\mathcal{T}} = \sum_\nu \phi_1^{*\mathcal{T}}(\nu_1, \nu_2, \cdots)\phi_2^{\mathcal{T}}(\nu_1, \nu_2, \cdots) \times \prod_k (\nu_k + g_k - 1)!\,(\nu_k!)^{-1}[(g_k - 1)!]^{-1} \times \exp[g_k \ln(1-\epsilon)]\epsilon^{\nu_k}. \tag{3}$$

The constant ϵ, with $0 < \epsilon < 1$, is, so far, an arbitrarily chosen converging factor. However, its need is essential in the above definition of the inner product for functionals compatible in the second manner. [See the remark after Eq. (7).] The exponential factor in (3) is merely a normalization factor. The summation symbol in (3) indicates sums over $\nu_1 = 0, 1, 2, \cdots$, $\nu_2 = 0, 1, 2, \cdots$, etc.; the subscript k in the product symbol extends over all values of k for which cells $\mathcal{C}_k$ are assigned but not over $\mathcal{C}_*$.

A partition $\mathcal{T}'$ is called a refinement of the partition $\mathcal{T}$ if each cell of $\mathcal{T}'$ is contained in a cell of $\mathcal{T}$ and $\mathcal{C}_*'$ is contained in $\mathcal{C}_*$. Clearly a functional $\phi(\nu)$ which is compatible with the partition $\mathcal{T}$ is also compatible with its refinement $\mathcal{T}'$. Now any two partitions have a common refinement; therefore, the manifold of functionals compatible with a given partition forms a linear space with the inner product defined by (3). One of the properties required of the inner product is that the vanishing of the unit form, $(\Phi, \Phi) = 0$, implies the vanishing of the element, $\Phi \equiv 0$. This is accomplished by including the elements for which $(\Phi_1 - \Phi_2, \Phi_1 - \Phi_2) = 0$ into an equivalence class of compatible functionals and assigning a single element to each class of equivalent functionals.[9]

This linear space of compatible functionals is extended to a complete linear space, the Hilbert space of functionals, by assigning an ideal element to every Cauchy sequence of compatible functionals. The manifold of all these functionals forms the Hilbert space of interest and its elements represent possible representer of physical states.

The value of the inner product (Φ_1, Φ_2) of two functionals compatible with the partition $\mathcal{T}$ is unaltered by a refinement $\mathcal{T}'$ of $\mathcal{T}$. Let $\mathcal{C}_{rk}'$ and $\mathcal{C}_{r*}'$ denote all the cells of $\mathcal{T}'$ which compose $\mathcal{C}_k$ and $\mathcal{C}_*$ respectively, so that

$$\sum_r \nu_{rk}' = \nu_k \quad \text{and} \quad \sum_r g_{rk}' = g_k. \tag{4}$$

Now,

$$(\Phi_1, \Phi_2)_\epsilon^{\mathfrak{T}'} = \sum_{\nu_1,\nu_2,\cdots} \phi_1^{*\mathfrak{T}}(\nu_1, \nu_2, \cdots)\phi_2^{\mathfrak{T}}(\nu_1, \nu_2, \cdots) \times \prod_k \sum_{\nu_{1k}',\nu_{2k}',\cdots} \sum_{\nu_{1*}',\nu_{2*}',\cdots} \prod_r \frac{(\nu_{rk}' + g_{rk}' - 1)!}{(g_{rk}' - 1)!\, \nu_{rk}'!} \epsilon^{\nu_{rk}'} \times \exp[g_{rk}' \ln(1-\epsilon)] \frac{(\nu_{r*}' + g_{r*}' - 1)!}{(g_{r*}' - 1)!\, \nu_{r*}'!} \epsilon^{\nu_{r*}'} \times \exp[g_{r*}' \ln(1-\epsilon)]. \quad (5)$$

Since, by the binomial theorem,

$$\frac{(\nu_k + g_k - 1)!}{\nu_k!\,(g_k - 1)!} = \sum_{\nu_{1k}',\nu_{2k}',\cdots} \prod_r \frac{(\nu_{rk}' + g_{rk}' - 1)!}{(g_{rk}' - 1)!\, \nu_{rk}'!}, \quad (6)$$

where $\sum_r g_{rk}' = g_k$ and $\sum_r \nu_{rk}' = \nu_k$. Now,

$$\sum_{\nu_{1*}',\nu_{2*}',\cdots} \prod_r \epsilon^{\nu_{r*}'} \times \exp[g_{r*}' \ln(1-\epsilon)] \frac{(\nu_{r*}' + g_{r*}' - 1)!}{(g_{r*}' - 1)!\, \nu_{r*}'!} = 1, \quad (7)$$

where it is essential to have the converging factor ϵ to obtain a finite value for (7). Then, (5) becomes

$$(\Phi_1, \Phi_2)_\epsilon^{\mathfrak{T}'} = \sum_{\nu_1,\nu_2,\cdots} \phi_1^{*\mathfrak{T}}(\nu)\phi_2^{\mathfrak{T}}(\nu) \prod_k \epsilon^{\nu_k} \exp[g_k \ln(1-\epsilon)] \times (\nu_k + g_k - 1)!/\nu_k!\,(g_k - 1)! = (\Phi_1, \Phi_2)_\epsilon^{\mathfrak{T}}. \quad (8)$$

For the inner product of two occupation functionals $\phi_1(\nu)$ and $\phi_2(\nu)$ the following symbolic notation is adopted:

$$(\Phi_1, \Phi_2)_\epsilon^{B} = \sum_\nu \phi_1^*(\nu)\phi_2(\nu) \prod_s \epsilon^{\nu(s)} e^{g(s)\ln(1-\epsilon)} \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!}, \quad (9)$$

which indicates that the inner product originated from the expression (3) valid for functionals compatible with the partition $\mathfrak{T}$.

A. Equidistribution State

Myriotic fields have two rather important features. Friedrichs has proved that myriotic fields possess no vacuum state and, also, that the total number operator cannot be defined for myriotic fields. It can similarly be proved that the above features also exist for the modified inner product (9) provided that the fields are myriotic, that is, $\sum_k g_k = \infty$. However, just as in Friedrich's case, the myriotic fields considered here possess equidistribution states which play a fundamental role in the theory. The equidistribution state has reduced representer $\Phi_v(\nu) \equiv 1$. From the inner product (9) one has that the equidistribution state is normalized to unity.

Consider the expected value of the biquantized observable $\sum_s \zeta(s)\mathcal{N}(s)$ in the equidistribution state. [The number operator $\mathcal{N}(s)$ itself is not a proper operator. However, the expected value will be proper if certain integral (see below) is finite.] This can be obtained by formal manipulations which can be justified rigorously:

$$\left\langle \sum_{s'} \zeta(s')\mathcal{N}(s') \right\rangle = \sum_\nu \left(\sum_{s'} \zeta(s')\nu(s') \right) \times \prod_s \epsilon^{\nu(s)} e^{g(s)\ln(1-\epsilon)} \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!}$$

$$= \sum_{s'} \zeta(s') \sum_\nu \nu(s') \prod_s \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!} \epsilon^{\nu(s)} e^{g(s)\ln(1-\epsilon)}$$

$$= \sum_{s'} \zeta(s')\epsilon \sum_{\nu(s')=0}^{\infty} \frac{[\nu(s') + g(s')]!}{\nu(s')!\,[g(s') - 1]!} \epsilon^{\nu(s')} e^{g(s')\ln(1-\epsilon)}.$$

Therefore,

$$\left\langle \sum_{s'} \zeta(s')\mathcal{N}(s') \right\rangle = [\epsilon/(1-\epsilon)] \sum_{s'} \zeta(s')g(s') = (1-\epsilon)^{-1} \int \zeta(s)\, d\omega(s), \quad (10)$$

and the operator $\sum_s \zeta(s)\mathcal{N}(s)$ is proper if

$$\int |\zeta(s)|\, d\omega(s) < \infty.$$

A word on the limiting process on refinements seems to be appropriate. In this limit the number of elementary eigenvalues in a cell $g(s)$ approaches unity, that is, each point in the continuum of s-space is associated with a cell. Also, the passage to the limit in (10) presupposes that $\zeta(s)$ is a sufficiently regular function of s. (An example where such regular behavior is not satisfied arises later on and is due to Bose condensation.)

For the total number of particles operator

$$\left\langle \sum_{s'} \mathcal{N}(s') \right\rangle = (1-\epsilon)^{-1} \int d\omega(s) = W/(1-\epsilon), \quad (11)$$

which becomes infinite for a myriotic field, $W = \infty$, thus showing that the total number operator is an improper operator.

The introduction of the ϵ factor in the inner product (9) was a necessity dictated by convergence requirements. Nevertheless, after expectation values and probabilities are evaluated, one may inquire into their behavior as ϵ approaches unity. From (10) it seems that every biquantized observable $\sum_s \zeta(s)\mathcal{N}(s)$, with $\int |\zeta(s)|\, d\omega(s) < \infty$, becomes an improper operator in this limit. We shall introduce later on conditioned equidistribution states for which finite values are obtained for such observables as ϵ approaches unity. One must conclude from this that equidistribution states are nonexistent as $\epsilon \to 1$.

The equidistribution state may be studied further by considering the probability that $\mathcal{N}$ particles will be found in the region $\mathcal{R}$ when the field is in an equidistribution state Φ_v. One has for such probability

$$\mathrm{P}\,(\mathcal{N}(\mathcal{R}) = \mathcal{N}) = \{[\mathcal{N} + W(\mathcal{R}) - 1]!/\mathcal{N}!\,[W(\mathcal{R}) - 1]!\} \times \epsilon^{\mathcal{N}} e^{W(\mathcal{R}) \ln (1-\epsilon)}. \tag{12}$$

Letting $\mathcal{R}$ cover the whole space and for $\mathcal{N} < \infty$,

$$\mathrm{P}\,(\mathcal{N}(\infty) = \mathcal{N}) = 0. \tag{13}$$

Therefore, in the equidistribution state of a myriotic field the probability of finding a finite number of particles is equal to zero. This result can be extended to states with representers $\phi(\nu)$, which are bounded, but since these type of states are dense in the Hilbert space of all compatible and ideal functionals $\phi(\nu)$, the result (13) follows for any state of a myriotic fields.

B. Probabilities and Expectation Values for the Equidistribution State

Consider the evaluation of certain values of the inner product (9) for states which can be constructed from the equidistribution state, $\phi_v \equiv 1$. Let

$$I_\epsilon[\tau] \equiv \sum_\nu \tau(\nu) \prod_s \epsilon^{\nu(s)} e^{g(s) \ln (1-\epsilon)} \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!}. \tag{14}$$

A class of functionals $\tau(\nu)$ for which the value of (14) is of considerable importance is given by the form

$$\tau(\nu) = H\Big(\sum_s \lambda(s)\nu(s)\Big). \tag{15}$$

The function $\lambda(s)$ has properties to be specified later on and $H(\alpha)$ admits the representation

$$H(\alpha) = \int_{\mathfrak{L}} e^{z\alpha} h(z)\, dz, \tag{16}$$

with $h(z)$ analytic in the neighborhood of the path $\mathfrak{L}$, and behaves appropriately when z approaches infinity along the path. Specifically, one may view (16) as the formula for the inverse Laplace transform of the function $h(z)$ analytic in the right half-plane.

For such form of the functional τ, (14) becomes

$$I_\epsilon\Big[H\Big(\sum_s \lambda(s)\nu(s)\Big)\Big] = \int_{\mathfrak{L}} I_\epsilon\Big[\exp\Big(z \sum_s \lambda(s)\nu(s)\Big)\Big] h(z)\, dz. \tag{17}$$

Now,

$$\begin{aligned} I_\epsilon\Big[\exp\Big(z \sum_s \lambda(s)\nu(s)\Big)\Big] &= \sum_\nu \exp\Big(z \sum_s \lambda(s)\nu(s)\Big) \times \prod_s \epsilon^{\nu(s)} e^{g(s) \ln (1-\epsilon)} \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!} \\ &= \sum_\nu \prod_s [\epsilon e^{z\lambda(s)}]^{\nu(s)} e^{g(s) \ln (1-\epsilon)} \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!} \\ &= \prod_s \frac{e^{g(s) \ln (1-\epsilon)}}{[1 - \epsilon e^{z\lambda(s)}]^{g(s)}}, \end{aligned} \tag{18}$$

where (18) follows by interchanging the summation and product symbols and performing the summation. Hence,

$$I_\epsilon\Big[\exp\Big(z \sum_s \lambda(s)\nu(s)\Big)\Big] = e^{Y(z;\lambda)}, \tag{19}$$

where

$$Y(z; \lambda) = -\int \frac{d\omega(s)}{\epsilon} [\ln (1 - \epsilon e^{z\lambda(s)}) - \ln (1 - \epsilon)]. \tag{20}$$

The function $Y(z; \lambda)$ corresponds to the adjusted grand partition function in statistical mechanics. Substituting (19) into (17) gives the important result

$$I_\epsilon\Big[H\Big(\sum_s \lambda(s)\nu(s)\Big)\Big] = \int_{\mathfrak{L}} e^{Y(z;\lambda)} h(z)\, dz. \tag{21}$$

Let us establish the conditions on $\lambda(s)$, $\omega(\mathcal{C})$, and $h(z)$ which enable us to obtain formula (21) rigorously. The function $\lambda(s)$ is nonnegative,

$$\lambda(s) \geq 0, \tag{22}$$

and is integrable with respect to the weight $\omega(\mathcal{C})$, so that

$$\kappa_0 = \int \lambda(s)\, d\omega(s) < \infty. \tag{23}$$

The quantity in (23) multiplied by $(1 - \epsilon)^{-1}$ gives the expectation value of the observable $\sum_s \lambda(s)\mathcal{N}(s)$ [see (10)] in the equidistribution state ϕ_v. Now

$$\infty > \int \lambda(s)\, d\omega(s) \geq \int_{\lambda(s) \geq l} \lambda(s)\, d\omega(s) \geq l \int_{\lambda(s) \geq l} d\omega(s).$$

Consequently,

$$\int_{\lambda(s) \geq l} d\omega(s) < \infty, \quad l > 0. \tag{24}$$

Therefore, if the total weight $W = \int d\omega(s)$ is infinite, it must arise from the region of s for which $\lambda(s) = 0$. If $\lambda(s)$ denotes the energy of a particle and the weight function $\omega(s)$ is properly chosen, then the preceding situation applies to the problem of the infrared catastrophe. (See Ref. 7.)

The adjusted grand partition function $Y(z; \lambda)$ and its derivative $Y_z(z; \lambda)$ are defined in the left half-plane $\operatorname{Re} z = x \leq 0$. Now for the principal determination of the logarithm and for $0 < \epsilon < 1$ with $\operatorname{Re} z \leq 0$

$$\ln |1 - \epsilon e^z| \geq \ln (1 - \epsilon e^x) \geq \ln (1 - \epsilon)$$

and

$$|\ln [(1 - \epsilon e^z)/(1 - \epsilon)]| \leq [\epsilon/(1 - \epsilon)]\, |z|.$$

Therefore,

$$\operatorname{Re} Y(z; \lambda) = -\int d\omega(s) \times [\ln |1 - \epsilon e^{z\lambda(s)}| - \ln (1 - \epsilon)] \leq 0, \tag{25}$$

$$|Y(z; \lambda)| \leq \int \frac{d\omega(s)}{\epsilon} \left| \ln \frac{1 - \epsilon e^{z\lambda(s)}}{1 - \epsilon} \right| \leq \frac{1}{1 - \epsilon} \kappa_0 |z|, \tag{26}$$

and

$$|Y_z(z; \lambda)| \leq \int \frac{d\omega(s)}{\epsilon} \frac{\epsilon \lambda(s) e^{x\lambda(s)}}{1 - \epsilon e^{x\lambda(s)}} \leq \frac{1}{1 - \epsilon} \kappa_0. \tag{27}$$

Stronger conditions may be obtained for $Y(z; \lambda)$ as $|z| \to \infty$ when $\operatorname{Re} z \leq 0$ if further restrictions are imposed on $\lambda(s)$ and $\omega(\mathcal{C})$. Let

$$p(l) = -\int_{\lambda(s) \geq l} d\omega(s), \tag{28}$$

which by (24) is finite, and suppose there exists a nonnegative number β such that

$$\int_0^{l_0} \left| dp(l) - \beta \frac{dl}{l} \right| \leq m_0 \tag{29}$$

holds for appropriate positive numbers l_0 and m_0. If

$$\phi(z) \equiv \int_0^{l_0} \frac{dl}{l} [\ln (1 - \epsilon e^{zl}) - \ln (1 - \epsilon)], \tag{30}$$

then

$$|Y(z; \lambda) + \beta\phi(z)| \leq 2[m_0 + p(l_0)] \ln [(1 - \epsilon)^{-1}]. \tag{31}$$

But,

$$|\phi(z) + \ln (1 - \epsilon) \ln (-z)| \leq |\phi(-1)| + \left| \int_1^{-z} \frac{\ln (1 - \epsilon e^{-tl_0})}{t} dt \right| \tag{32}$$

so that for $|z| \geq \rho > 0$ and $\operatorname{Re} z \leq 0$

$$|\phi(z) + \ln (1 - \epsilon) \ln (-z)| \leq m_1, \tag{33}$$

where m_1 is obtained from (32). Therefore,

$$|Y(z; \lambda) - \beta \ln (1 - \epsilon) \ln (-z)| \leq 2(m_0 + p(l_0)) \times \ln [(1 - \epsilon)^{-1}] + \beta m_1, \tag{34}$$

or, what is the same,

$$|e^{Y(z;\lambda)}| \leq \gamma / |z|^{-\beta \ln (1-\epsilon)} \tag{35}$$

for $|z| \geq \rho$, $\operatorname{Re} z \leq 0$, with $\beta, \gamma, \rho > 0$.

The conditions under which the integral (21) is well defined are, therefore, established. If the function $e^{Y(z;\lambda)}$ vanishes sufficiently rapidly as $|z| \to \infty$ in the left half-plane, for instance as in (35), then it is sufficient that the function $h(z)$ vanish of first order at infinity. In what follows the case where $h(z) = z^{-1} e^{-z\kappa}$ with $\kappa \geq 0$ will be considered.

C. Evaluation of Probabilities

As an explicit application of (21) consider the evaluation of the probability $\mathsf{P}(\kappa)$ that the observable

$$\mathcal{K} = \sum_s \lambda(s) \mathcal{N}(s) \tag{36}$$

has a value less than κ if the field is in the equidistribution state Φ_v. Denote the shifted unit step function by

$$\eta_\kappa(\alpha) = 1, \quad \text{for} \quad \alpha < \kappa,$$
$$= 0, \quad \text{for} \quad \alpha \geq \kappa, \tag{37}$$

which, from the theory of Laplace transform, has the integral representation

$$\eta_\kappa(\alpha) = \frac{1}{2\pi i} \int_{\mathfrak{L}} e^{(\alpha - \kappa)z} \frac{dz}{z}, \tag{38}$$

where the path $\mathfrak{L}$ is any straight line $z = x + iy$, with fixed $x < 0$, and the integral goes from lower limit $y = +\infty$ to upper limit $y = -\infty$.

The probability $\mathsf{P}(\kappa)$ is given by

$$\mathsf{P}(\kappa) = (\Phi_v, \eta_\kappa(\kappa)\Phi_v), \tag{39}$$

where $\eta_\kappa(\kappa)$ is the operator obtained from (38). The result follows from (16), with $h(z) = (2\pi i)^{-1} e^{-\kappa z}$, and (21):

$$\mathsf{P}(\kappa) = \frac{1}{2\pi i} \int_{\mathfrak{L}} e^{[Y(z;\lambda) - \kappa z]} \frac{dz}{z}. \tag{40}$$

For $\kappa = 0$ the integral (40) may be evaluated by considering a semicircle with side $\mathfrak{L}$ in the left half-plane. Because of (35) the value of the integral is not altered and, since no poles are enclosed, one obtains

$$\mathsf{P}(0) = 0. \tag{41}$$

Also, if one considers

$$1 - \mathsf{P}(\kappa) = \frac{1}{2\pi i} \int_{\mathfrak{L}} (1 - e^{Y(z;\lambda)}) e^{-kz} \frac{dz}{z}, \tag{42}$$

the path of integration can be moved to coincide with the imaginary axis. Since

$$\int_{-\infty}^{\infty} |e^{Y(iy;\lambda)} - 1| \frac{dy}{y} < \infty,$$

then by the Riemann–Lebesgue theorem one has that

$$\lim_{\kappa\to\infty} [1 - \mathsf{P}(\kappa)] = 0. \tag{43}$$

Finally, it is clear, by the same arguments used to obtain (41), that

$$\mathsf{P}(\kappa) = 0 \quad \text{for} \quad \kappa < 0. \tag{44}$$

D. Conditioned Equidistribution State

The equidistribution state introduced in Sec. I gives an expected number of particles occupying the place s which is equally distributed over the s-space relative to the weight $d\omega(s)$. Let the energy of the system be restricted to lie between the value κ and κ_1 (with $\kappa_1 > \kappa$). The field is then in a state denoted by ϕ_{v,κ,κ_1} and is referred to as a conditioned equidistribution state. The representer of this normalized state is given by the functional

$$\phi(\nu) = \eta_{\kappa,\kappa_1}\Big(\sum_s \lambda(s)\nu(s)\Big)[\mathsf{P}(\kappa_1) - \mathsf{P}(\kappa)]^{-\frac{1}{2}}, \tag{45}$$

where

$$\eta_{\kappa,\kappa_1}(\alpha) \equiv \eta_{\kappa_1}(\alpha) - \eta_\kappa(\alpha). \tag{46}$$

Consider the evaluation of the expected value $\langle\Gamma\rangle_{\phi_{v,\kappa,\kappa_1}}$ for the observable $\Gamma = \sum_s \zeta(s)\mathcal{N}(s)$ in the state ϕ_{v,κ,κ_1}. Now

$$\langle\Gamma\rangle_{\phi_{v,\kappa,\kappa_1}} = \frac{\mathcal{Q}(\kappa_1;\zeta) - \mathcal{Q}(\kappa;\zeta)}{\mathsf{P}(\kappa_1) - \mathsf{P}(\kappa)}, \tag{47}$$

with

$$\mathcal{Q}(\kappa;\zeta) = I_\omega\Big[\sum_s \zeta(s)\nu(s)\eta_\kappa\Big(\sum_s \lambda(s)\nu(s)\Big)\Big]. \tag{48}$$

In what follows it will be shown that one obtains for $\mathcal{Q}(\kappa;\zeta)$ the simple expression

$$\mathcal{Q}(\kappa;\zeta) = \int \zeta(s)\, d\omega(s) \sum_{n=1}^{\infty} \epsilon^{n-1}\mathsf{P}(\kappa - n\lambda(s)). \tag{49}$$

Note that in the limit $\epsilon \to 0$ one recovers the result of Friedrichs. Result (49) may be obtained in a formal manner but, nevertheless, can be justified rigorously since

$$\begin{aligned}\mathcal{Q}(\kappa;\zeta) = \sum_\nu \Big(\sum_{s'} \zeta(s')\nu(s')\Big) \frac{1}{2\pi i} \\ \times \int_{\mathfrak{L}} \exp\Big(z\sum_s \lambda(s)\nu(s)\Big) e^{-\kappa z}\frac{dz}{z} \\ \times \prod_s \epsilon^{\nu(s)} e^{g(s)\ln(1-\epsilon)} \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!}.\end{aligned}$$

After performing the sums over all the $\nu(s)$, except $s = s'$, one obtains

$$\begin{aligned}\mathcal{Q}(\kappa;\zeta) = \sum_{s'} \zeta(s')\frac{1}{2\pi i}\int_{\mathfrak{L}} e^{-\kappa z}\frac{dz}{z}\sum_{\nu(s')=0}^{\infty} \nu(s')(\epsilon e^{z\lambda(s')})^{\nu(s')} \\ \times \frac{[\nu(s') + g(s') - 1]!}{\nu(s')!\,[g(s') - 1]!} e^{g(s')\ln(1-\epsilon)} \\ \times \prod_s{}' \frac{e^{g(s')\ln(1-\epsilon)}}{(1 - \epsilon e^{z\lambda(s)})^{g(s)}},\end{aligned}$$

where the prime in the product symbol indicates the $s = s'$ term is to be omitted. The sum over $\nu(s')$ may be done, and one has

$$\begin{aligned}\mathcal{Q}(\kappa;\zeta) &= \sum_{s'} \zeta(s')q(s')\frac{1}{2\pi i}\int_{\mathfrak{L}} e^{-\kappa z}\frac{dz}{z}\frac{\epsilon e^{z\lambda(s')}}{1 - \epsilon e^{z\lambda(s')}} \\ &\quad\times \prod_s \frac{e^{g(s)\ln(1-\epsilon)}}{(1 - \epsilon e^{z\lambda(s)})^{g(s)}} \\ &= \sum_{s'} \zeta(s')q(s')\frac{1}{2\pi i}\int_{\mathfrak{L}} e^{-\kappa z}\frac{dz}{z}\frac{\epsilon e^{z\lambda(s')}}{1 - \epsilon e^{z\lambda(s')}} e^{Y(z;\lambda)}.\end{aligned} \tag{50}$$

Finally, (49) follows from the form (40) for $\mathsf{P}(\kappa)$.

In the limit when the conditioned equidistribution state has a fixed well-defined energy κ, i.e., $\kappa_1 \to \kappa$, (47) becomes

$$\langle\Gamma\rangle_{\phi_{v,\kappa}} = \frac{\int \zeta(s)\, d\omega(s)\sum_{n=1}^{\infty}\epsilon^{n-1}\mathsf{P}'(\kappa - n\lambda(s))}{\mathsf{P}'(\kappa)}, \tag{51}$$

where the prime denotes differentiation with respect to κ. For the expected value $\langle\zeta(s)\mathcal{N}(s)\rangle_{\phi_{v,\kappa}}$, (51) gives

$$\langle\zeta(s)\mathcal{N}(s)\rangle_{\phi_{v,\kappa}} = \frac{\zeta(s)\, d\omega(s)\sum_{n=1}^{\infty}\epsilon^{n-1}\mathsf{P}'(\kappa - n\lambda(s))}{\mathsf{P}'(\kappa)}. \tag{52}$$

A case of considerable importance, for which expression (51) may be simplified greatly, occurs when the weight function $d\omega(s)$ is replaced by $M\, dm(s)$ with M large and positive. For large values of M the quantity $\mathsf{P}(\kappa)$ may be evaluated by the saddle point method. Suppose

$$\int \frac{dm(s)}{\epsilon^{-1}\exp[-x_0\lambda(s)] - 1} < \infty, \tag{53}$$

for given $x_0 < 0$, where $\lambda(s) \geq 0$. From (53) one has that $\int \exp[x_0\lambda(s)]\, dm(s) < \infty$. Therefore, for every $l > 0$

$$\int_{\lambda(s)\leq l} dm(s) < \infty. \tag{54}$$

Consequently, if $W = M\int dm(s)$ is infinite, this infinity must arise from the region s for which $\lambda(s) = \infty$. This situation is quite different from that of Sec.

II which is obviously applicable to the case of the infrared catastrophe.

Condition (53) implies that the integral

$$Z(z;\lambda) \equiv -\int \frac{d\omega(s)}{\epsilon} \ln(1 - \epsilon e^{z\lambda(s)}) \qquad (55)$$

converges uniformly and absolutely for $\operatorname{Re} z < x_0$. Hence, by the Riemann–Lebesgue theorem

$$\lim_{|\operatorname{Im} z| \to \infty} \int d\omega(s) \ln(1 - \epsilon e^{z\lambda(s)}) = 0. \qquad (56)$$

From the convergence of the integral (55) one has that the adjusted partition function $Y(z;\lambda)$ is not defined for myriotic fields. However, the unadjusted partition function $Z(z;\lambda)$ is well defined and is given by (55) with

$$e^{Y(z;\lambda)} = e^{Z(z;\lambda)} e^{(W/\epsilon)\ln(1-\epsilon)}. \qquad (57)$$

It follows from (40) and (57) that $\mathsf{P}(\kappa) = 0$ for κ finite and $W = \infty$.

For the present case, one has to revert to the concept of compatibility of a functional in the first manner[10] and proceed as in Sec. III for functionals compatible in the second manner. In (14) the exponential factor does not appear if the functional $\tau(\nu)$ is defined in the first manner and in result (21) the function $Z(z;\lambda)$ would occur instead of $Y(z;\lambda)$.

The quantity

$$\mathsf{F}(\kappa) = \frac{1}{2\pi i} \int_{\mathfrak{L}} e^{(Z(z;\lambda) - \kappa z)} \frac{dz}{z} \qquad (58)$$

takes the place of $\mathsf{P}(\kappa)$ in the preceding formulas. Note especially formulas (47) and (49). For large values of M the quantity $\mathsf{F}(\kappa)$ may be evaluated by the saddle point method. The saddle points are determined by the equation

$$\int \frac{\lambda(s)\, d\omega(s)}{e^{-z\lambda(s)} - \epsilon} = \kappa. \qquad (59)$$

As M approaches infinity, the ratio κ/M, by (53), approaches a finite limit. Therefore, in this limit, the unique saddle point, for $\operatorname{Re} z = x \leq 0$, is given by the real point $z_0 = -\theta_\kappa$ with

$$\kappa = \int \frac{\lambda(s)\, d\omega(s)}{\exp[\theta_\kappa \lambda(s)] - \epsilon}. \qquad (60)$$

From the behavior (56) one has that $\operatorname{Re}[Z(z;\lambda) - \kappa z - \ln z]$ approaches $-\infty$ at either end point of the path $\mathfrak{L}$. Therefore, the distant portions of the path of integration contributes an infinitesimally small amount to the value of the integral as M becomes infinite. Also, the total contribution to the integral comes from an infinitesimal neighborhood of the saddle point and gives for $\mathsf{F}(\kappa)$

$$\mathsf{F}(\kappa) = \frac{\exp[Z(-\theta_\kappa;\lambda) + \kappa\theta_\kappa]}{[2\pi^2\theta_\kappa^2 Z_{zz}(-\theta_\kappa;\lambda)]^{\frac{1}{2}}}. \qquad (61)$$

For α finite,

$$\mathsf{F}(\kappa - \alpha) = \exp(-\theta_\kappa \alpha)\mathsf{F}(\kappa), \qquad (62)$$

which, interestingly enough, is a derivation of the Boltzmann factor. Result (62), in conjunction with (49), yields

$$\mathfrak{Q}(\kappa;\zeta) = \int \frac{d\omega(s)}{\epsilon} \frac{\zeta(s)\mathsf{F}(\kappa)}{\epsilon^{-1}\exp[\theta_\kappa\lambda(s)] - 1}. \qquad (63)$$

Combining the results (47) and (63) gives a fundamental result in quantum statistical mechanics[11]:

$$\langle\Gamma\rangle_{\phi_{\zeta,\kappa}} = \int \frac{\zeta(s)}{\epsilon^{-1}\exp[\theta_\kappa\lambda(s)] - 1} \frac{d\omega(s)}{\epsilon}. \qquad (64)$$

Consequently, the conditioned equidistribution states are nothing else than the equilibrium states of a system of noninteracting bosons with ϵ taking the place of the fugacity. Thus, the arbitrarily chosen converging factor ϵ has a deep physical meaning and is related to the chemical potential of the system.

IV. OCCUPATION NUMBER REPRESENTATION FOR FERMIONS

The occupation number representation for boson fields, discussed in the preceding sections, may be extended to fermion fields. The presentation which follows differs considerably from that given by Friedrichs for fermion fields.

The main consideration of Friedrichs is to the space $\mathfrak{F}_\omega$ of reduced functionals $\phi(\nu)$ appropriate to the statistics of Boltzmann. The space $\mathfrak{F}_\omega^{\mathrm{F}}$ of fermion representer $\phi(\nu)$ is defined as the subspace of all functionals $\phi(\nu)$ in $\mathfrak{F}_\omega$ which are of the form

$$\phi(\nu) = F(\nu)\phi(\nu), \qquad (65)$$

where $F(\nu) = 1$ if $\nu(s) = 0$ or $\nu(s) = 1$, for all values of s, and $F(\nu) = 0$ otherwise. This approach leads to peculiar expressions which require care for their evaluation and to results which are already indicative of its limitations. Friedrichs shows that the functional $F(\nu)$ is identically equal to one if s has no point eigenvalue. Therefore, for the occupation representation of Boltzmann fields, when summing over all possible choices of the occupation $\nu(s)$, we might have had to restrict the values of $\nu(s)$ to $\nu(s) = 0$ and $\nu(s) = 1$ without altering the final results. Thus, the same results are obtained for Boltzmann or fermion fields. This, clearly, is unacceptable.

As for the boson case, a partition $\mathcal{T}$ of the s-space is introduced. The inner product of two functionals ϕ_1 and ϕ_2, which are compatible in the second manner with the partition $\mathfrak{T}$, is defined. The value of the inner product is unaltered by a refinement $\mathfrak{T}'$ of $\mathfrak{T}$. The inner product is given by the symbolic expression

$$(\Phi_1, \Phi_2)_\epsilon^{\mathrm{F}} = \sum_\nu \phi_1^*(\nu)\phi_2(\nu) \times \prod_s \{g(s)!/\nu(s)!\,[g(s) - \nu(s)]!\}\epsilon^{\nu(s)}e^{-g(s)\ln(1+\epsilon)}. \tag{66}$$

The summation symbol in (66) indicates a sum over $\nu_1 = 0, 1, 2, \cdots, g_1$; $\nu_2 = 0, 1, 2, \cdots, g_2$, etc. In contrast to the definition of the inner product for boson fields, the parameter ϵ in (66), with $\epsilon > 0$, is not needed for convergence purpose but is introduced as a convenient characterization of the Hilbert space. It will be shown later that in the limit ϵ approaching zero the corresponding states with the Boltzmann statistics are recovered.

The manifold of functionals compatible with a given partition forms a linear space with the above defined inner product. This linear manifold is closed by adding all its ideal elements. An equivalence class is introduced for functionals which differ only on a set of Lebesgue measure zero. This closed linear space is a Hilbert space and is denoted by $\mathfrak{F}_\epsilon^{\mathrm{F}}$.

The equidistribution state Φ_v is the state with reduced representer $\phi(\nu) \equiv 1$ which, according to (66), is normalized to unity.[12]

The expected value of the biquantized observable $\sum_s \zeta(s)\mathcal{N}(s)$ in the equidistribution state can be calculated by similar formal operations as for boson fields which may equally be justified rigorously,

$$\left(\Phi_v, \sum_s \zeta(s)\mathcal{N}(s)\Phi_v\right)_\epsilon^{\mathrm{F}} = \frac{1}{1+\epsilon}\int \zeta(s)\,d\omega(s), \tag{67}$$

where in the limit to the continuum the factor $\epsilon q(s)$ is replaced by the weight function $d\omega(s)$.

The probability that the biquantized observable $\sum_s \lambda(s)\mathcal{N}(s)$ has a value which lies below the value κ when the field is in the equidistribution state Φ_v is given by

$$\mathsf{P}(\kappa) = \frac{1}{2\pi i}\int_{\mathfrak{L}} \frac{dz}{z}\, e^{-\kappa z} e^{Y(z;\lambda)}, \tag{68}$$

with

$$Y(z;\lambda) = \int \frac{d\omega(s)}{\epsilon}\,[\ln(1 + \epsilon e^{z\lambda(s)}) - \ln(1+\epsilon)]. \tag{69}$$

As ϵ approaches zero, the equidistribution state for fermions approaches the corresponding state but with Boltzmann statistics.

The equidistribution state Φ_v is composed of states which give rise to all possible values of the observable $\kappa = \sum_s \lambda(s)\mathcal{N}(s)$. Let the operator κ represent the energy of the field and suppose the states composing Φ_v are restricted to have energies which lie between the values κ and κ_1. The state Φ_{v,κ,κ_1} so obtained is the conditioned equidistribution state and has the reduced representer

$$\phi(\nu) = \frac{\eta_{\kappa_1}\left(\sum_s \lambda(s)\nu(s)\right) - \eta_\kappa\left(\sum_s \lambda(s)\nu(s)\right)}{\mathsf{P}(\kappa_1) - \mathsf{P}(\kappa)}, \tag{70}$$

where $\eta_\kappa(\alpha)$ is defined by (38). For the state Φ_{v,κ,κ_1} the expected value of the observable $\sum_s \zeta(s)\mathcal{N}(s)$ is

$$\left(\Phi_{v,\kappa,\kappa_1}, \sum_s \zeta(s)\mathcal{N}(s)\Phi_{v,\kappa,\kappa_1}\right)_\epsilon^{\mathrm{F}} = \frac{\mathfrak{Q}(\kappa_1;\zeta) - \mathfrak{Q}(\kappa;\zeta)}{\mathsf{P}(\kappa_1) - \mathsf{P}(\kappa)}, \tag{71}$$

where

$$\mathfrak{Q}(\kappa;\zeta) = \frac{1}{2\pi i}\sum_s \zeta(s)q(s)\int_{\mathfrak{L}} \frac{dz}{z}\, e^{-\kappa z}\frac{\epsilon e^{z\lambda(s)}}{1+\epsilon e^{z\lambda(s)}}\, e^{Y(z;\lambda)}. \tag{72}$$

The integral in (72) may be evaluated by the saddle point method under the same circumstances as that for boson fields. (See Sec. 4.) This gives

$$\mathfrak{Q}(\kappa;\zeta) \approx \sum_s \zeta(s)q(s)\frac{\epsilon\exp[-\theta_\kappa\lambda(s)]}{1+\epsilon\exp[-\theta_\kappa\lambda(s)]}\,\mathsf{P}(\kappa), \tag{73}$$

where the saddle point $z = -\theta_\kappa$ is given by

$$\kappa = \int \frac{\lambda(s)\,d\omega(s)}{\exp[\theta_\kappa\lambda(s)] + \epsilon}. \tag{74}$$

If κ_1 and κ are sufficiently close in value, the saddle points for $\mathfrak{Q}(\kappa_1;\lambda)$ and $\mathfrak{Q}(\kappa;\lambda)$ are the same; then one obtains from (71)

$$\left(\Phi_{v,\kappa}, \sum_s \zeta(s)\mathcal{N}(s)\Phi_{v,\kappa}\right)_\epsilon^{\mathrm{F}} \approx \int \frac{\zeta(s)\,d\omega(s)}{\exp[\theta_\kappa\lambda(s)] + \epsilon}. \tag{75}$$

Thus giving for the expected number of fermions occupying the value s, when the energy of the field is on the energy shell $\kappa = \sum_s \lambda(s)\nu(s)$, the value

$$(\Phi_{v,\kappa}, \mathcal{N}(s)\Phi_{v,\kappa})_\epsilon^{\mathrm{F}} \approx d\omega(s)/\exp[\theta_\kappa\lambda(s)] + \epsilon. \tag{76}$$

V. CLASSICAL LIMIT OF QUANTUM STATES

In the previous sections, the spaces $\mathfrak{F}_\epsilon^{\mathrm{B}}$, and $\mathfrak{F}_\epsilon^{\mathrm{F}}$ of functionals appropriate to Bose–Einstein and Fermi–Dirac statistics, respectively, were introduced. It will be seen in what follows that the space $\mathfrak{F}_\omega$, appropriate to Boltzmann statistics, is the limiting case of $\mathfrak{F}_\epsilon^{\mathrm{B}}$ and $\mathfrak{F}_\epsilon^{\mathrm{F}}$ as $\epsilon \to 0$ if the quantum variable s has no point eigenvalue. Since $\hbar \to 0$ implies the above limit, one has that as $\hbar \to 0$ *every* quantum state, described by a myriotic field, approaches the *same* classical state. More precisely, let $\phi(\nu)$ be the reduced representer of the state Φ in $\mathfrak{F}_\epsilon^{\mathrm{B}}$ or $\mathfrak{F}_\epsilon^{\mathrm{F}}$, in the limit $\epsilon \to 0$; if s has no point eigenvalue, one obtains the same state Φ, with reduced representer $\phi(\nu)$, but in $\mathfrak{F}_\omega$.

The projection F, which was interpreted by multiplication by the functional $F(\nu)$ defined by (65), may be defined precisely so as to be applied to ideal elements. Let $\mathfrak{R}$ be the finite part of the partition $\mathfrak{T}$ and $\mathfrak{T}'$ be a refinement of $\mathfrak{T}$. Let the subscript k' denote the cells $C_{k'}$ of $\mathfrak{T}'$ which lie in $\mathfrak{R}$. Define the functional

$$\begin{aligned} F'_{\mathfrak{R}}(\nu) &= 1 \quad \nu_{k'} = 0 \quad \text{or 1 for each } k', \\ &= 0 \quad \text{otherwise.} \end{aligned} \tag{77}$$

Let $\phi(\nu)$ be a functional compatible in the second manner with some partition $\mathfrak{T}''$. Since any two partitions have a common refinement and a function compatible with a given partition is also compatible with a refinement of that partition, one may suppose, without loss of generality, that $\mathfrak{T}''$ is a refinement of $\mathfrak{T}'$. Then $F'_{\mathfrak{R}}(\nu)\phi(\nu)$ is well defined and is compatible in the second manner with $\mathfrak{T}''$. Consider a sequence of refinements of the partition $\mathfrak{T}$; then, since $\mathfrak{T}'$ is a refinement of $\mathfrak{T}$,

$$F_{\mathfrak{R}}F_{\mathfrak{R}'} = F_{\mathfrak{R}}. \tag{78}$$

The operators $F_{\mathfrak{R}'}$ corresponding to this succession of refinements of $\mathfrak{T}$ forms a nonincreasing sequence of projection and by a theorem of von Neumann converge to a limit projection. Finally, one considers a sequence of regions $\mathfrak{R}^\sigma$, with $\sigma = 1, 2, 3, \cdots$, which tend to cover the whole s-space. For $\mathfrak{R}^\tau$ contained in $\mathfrak{R}^\sigma$, one has

$$F_{\mathfrak{R}^\sigma}F_{\mathfrak{R}^\tau} = F_{\mathfrak{R}^\tau}. \tag{79}$$

As in the above case, the sequence of projections $F_{\mathfrak{R}^\sigma}$ forms a nonincreasing sequence of projections which converge to a limit projection F and is denoted by multiplication by the functional $F(\nu)$.

Therefore, the projection F is defined precisely in the Hilbert spaces $\mathfrak{F}_\epsilon^{\mathrm{F}}$, $\mathfrak{F}_\epsilon^{\mathrm{B}}$, and $\mathfrak{F}_\omega$ of functionals compatible in the second manner.

Consider the state obtained, in both Hilbert spaces $\mathfrak{F}_\epsilon^{\mathrm{F}}$ and $\mathfrak{F}_\epsilon^{\mathrm{B}}$, by applying the projection F to the equidistribution state Φ_v. The norm of this F-equidistribution state will be of considerable value later on in establishing the classical limit of quantum states.

Suppose the point eigenvalues of the quantum variable s has no limit point. Denote these eigenvalues by $s^{(\rho)}$, $\rho = 1, 2, 3, \cdots$, and by W_ρ, the weight of the cell consisting of the point $s^{(\rho)}$

Let the partition $\mathfrak{T}'$, a refinement of $\mathfrak{T}$, be so chosen that each eigenvalue $s^{(\rho)}$ contained in $\mathfrak{R}$, the finite part of $\mathfrak{T}$, forms a cell of $\mathfrak{T}'$. Let the cells $C_{k'}$, with weight ω'_k, refer to the cells of $\mathfrak{T}'$ which lie in $\mathfrak{R}$ and contain no eigenvalue. Consider first the case of boson fields; then, from (9) and (77),

$$\begin{aligned} (F'_{\mathfrak{R}}(\nu), F'_{\mathfrak{R}}(\nu))_\epsilon^{\mathrm{B}} &= \prod_\rho^{\mathfrak{R}} (1 + W_\rho) \exp\left(\frac{W_\rho}{\epsilon} \ln(1-\epsilon)\right) \\ &\quad \times \prod_k{}' (1 + \omega'_k) \exp\left(\frac{\omega_{k'}}{\epsilon} \ln(1-\epsilon)\right). \end{aligned} \tag{80}$$

The product $\prod_\rho^{\mathfrak{R}}$ refers to the eigenvalues $s^{(\rho)}$ in $\mathfrak{R}$ and the product $\prod'_k$ to all the cells $C_{k'}$ in $\mathfrak{R}$. The second term in the product in (80) becomes, as one chooses finer refinements,

$$\begin{aligned} &\prod_k{}' (1 + \omega'_k) \exp[(\omega_{k'}/\epsilon)\ln(1-\epsilon)] \\ &\quad = \exp\left(\epsilon^{-1} \sum_k{}' \omega'_k \ln(1-\epsilon^2)\right). \end{aligned} \tag{81}$$

Now $\sum'_k \omega'_k = \omega(\mathfrak{R}) - \sum_\rho^{\mathfrak{R}} W_\rho$ is the contribution to the total weight $\omega(\mathfrak{R}) = \int_{\mathfrak{R}} d\omega(s) < \infty$ from all the cells in $\mathfrak{R}$ excluding the point eigenvalues and $\sum'_k \omega'_{\mathfrak{R}} \leq F(\mathfrak{R}) < \infty$. For the limit $(F_{\mathfrak{R}}(\nu), F_{\mathfrak{R}}(\nu))_\epsilon^{\mathrm{B}}$ of $(F'_{\mathfrak{R}}(\nu), \omega'_{\mathfrak{R}}(\nu))_\epsilon^{\mathrm{B}}$, one has

$$\begin{aligned} (F_{\mathfrak{R}}(\nu), F_{\mathfrak{R}}(\nu))_\epsilon^{\mathrm{B}} &= \exp\left(\frac{\omega(\mathfrak{R})}{\epsilon}\ln(1-\epsilon^2)\right) \\ &\quad \times \prod_\rho^{\mathfrak{R}} (1 + W_\rho) \exp\left(\frac{-W_\rho}{\epsilon}\ln(1+\epsilon)\right), \\ &\qquad 0 \leq \epsilon \leq 1. \end{aligned} \tag{82}$$

Similarly, for the case of fermion fields, (66) and (77) give

$$\begin{aligned} (F_{\mathfrak{R}}(\nu), F_{\mathfrak{R}}(\nu))_\epsilon^{\mathrm{F}} &= \prod_\rho^{\mathfrak{R}} (1 + W_\rho) \exp\left(\frac{-W_\rho}{\epsilon}\ln(1+\epsilon)\right), \\ &\qquad 0 \leq \epsilon \leq \infty. \end{aligned} \tag{83}$$

The method used above in derivings (82) and (83) is somewhat different than that used by Friedrichs in obtaining the corresponding result for the Maxwell–Boltzmann case. In fact, the above limiting process leads to a different result for the Maxwell-Boltzmann case from that obtained by Friedrichs. For the Maxwell–Boltzmann case, one has

$$\begin{aligned} (F_{\mathfrak{R}}(\nu), F_{\mathfrak{R}}(\nu))_\epsilon^{\mathrm{M-B}} &= \exp\left[\left(-1 + \frac{1}{\epsilon}\ln(1+\epsilon)\right)\omega(\mathfrak{R})\right] \\ &\quad \times \prod_\rho^{\mathfrak{R}} (1 + W_\rho) \exp\left(\frac{-W_\rho}{\epsilon}\ln(1+\epsilon)\right), \\ &\qquad 0 \leq \epsilon \leq \infty. \end{aligned} \tag{84}$$

Our result (84) reduces to that given by Friedrichs only in the limit $\epsilon \to 0$.

From the projective nature of the operator F it is clear that the quantities given by (82), (83), and (84) must be less than unity. That this is so is easy to verify. However, Friedrichs' method of evaluating these quantities would lead, in the absence of point eigenvalues, to a value greater than unity for the Fermi–Dirac case.

The parameters ϵ of (82) and (83) are given, for nonrelativistic kinematics, by

$$1 = \frac{4\pi}{h^3}(2mk)^{\frac{3}{2}} \frac{V}{N} T^{\frac{3}{2}} \int_0^\infty \frac{x^2\, dx}{\epsilon^{-1} e^{x^2} \pm 1}, \tag{85}$$

where V, N, and T represent the volume, number of particles, and temperature, respectively, of the noninteracting equilibrium state in the space $\mathfrak{F}_\epsilon^{\mathrm{F}}$ or $\mathfrak{F}_\epsilon^{\mathrm{B}}$. The upper sign refers to the Fermi–Dirac case and the lower sign to the Bose–Einstein case. For the Maxwell–Boltzmann case, ϵ is given by

$$N = \epsilon V (mkT/2\pi\hbar^2)^{\frac{3}{2}}. \tag{86}$$

In fact, in the limit $\epsilon \to 0$ *both* parameters ϵ given by (85) approach the result given by (86).

Consider the expressions (82), (83), and (84) in the limit when ϵ approaches zero with $\omega(\mathfrak{R}) < \infty$. One finds

$$\begin{aligned}(F_{\mathfrak{R}}(\nu), F_{\mathfrak{R}}(\nu))_{\epsilon=0}^{\mathrm{M-B}} &= (F_{\mathfrak{R}}(\nu), F_{\mathfrak{R}}(\nu))_{\epsilon=0}^{\mathrm{F}} \\ &= (F_{\mathfrak{R}}(\nu), F_{\mathfrak{R}}(\nu))_{\epsilon=0}^{\mathrm{B}} \\ &= \prod_\rho^{\mathfrak{R}} (1 + W_\rho) \exp(-W_\rho). \end{aligned} \tag{87}$$

If $\mathfrak{R}$ covers the whole s-space, this becomes

$$(F(\nu), F(\nu))_{\epsilon=0} = \prod_\rho (1 + W_\rho) \exp(-W_\rho), \tag{88}$$

which is less than unity in the presence of point eigenvalues. Hence, in the absence of point eigenvalues, one has that $F_{\mathfrak{R}}(\nu)\phi(\nu) = \phi(\nu)$ for the functional $\phi(\nu) \equiv 1$. From this result one can prove that $F_{\mathfrak{R}}(\nu)\phi(\nu) = \phi(\nu)$ for every boson, Maxwell-Boltzmann, or fermion functional $\phi(\nu)$, that is, the projector F is the identity in the limit $\hbar \to 0$ if the quantum variable s has no point eigenvalue.

It will be sufficient to have $F_{\mathfrak{R}}\phi(\nu) = \phi(\nu)$ for all functionals $\phi(\nu)$ of a dense subset in $\mathfrak{F}_\epsilon^{\mathrm{B}}$ or $\mathfrak{F}_\epsilon^{\mathrm{F}}$. A dense subset is given by the compatible functionals which are different from zero for only a given occupation $\nu_1 = \nu_1^0$, $\nu_2 = \nu_2^0, \cdots, \phi^{\mathfrak{T}_0}(\nu_0) = \phi^0$. Without loss of generality, ϕ^0 may be chosen to be unity. In what follows the case of boson fields is considered. The situation for fermion and Maxwell–Boltzmann fields goes through with slight alterations.

Let $\phi_0(\nu)$ be such a functional and suppose $\mathfrak{T}^0$ is a refinement of the partition $\mathfrak{T}$ which has finite part $\mathfrak{R}$. Let $\mathfrak{T}'$ be a refinement of $\mathfrak{T}$ and $F'_{\mathfrak{R}}$, the operator defined by (77). Then,

$$\begin{aligned}(\|(1 - F'_{\mathfrak{R}})\phi_0\|_\epsilon^{\mathrm{B}})^2 &= \sum_{\nu'}{}' |\phi_0(\nu)|^2 \prod_s \frac{[\nu'(s) + g'(s) - 1]!}{\nu'(s)!\,[g'(s) - 1]!} \epsilon^{\nu'(s)} e^{g'(s)\ln(1-\epsilon)}. \end{aligned} \tag{89}$$

The prime in the summation symbol indicates that one should omit all occupations numbers $\nu_1', \nu_2', \cdots$ for which each ν_k' is either zero or one. Thus,

$$(\|(1 - F'_{\mathfrak{R}})\phi_0\|_\epsilon^{\mathrm{B}})^2 \le \sum_{\nu'}{}' \prod_s \frac{[\nu'(s) + g'(s) - 1]!}{\nu'(s)!\,[g'(s) - 1]!} \epsilon^{\nu'(s)} e^{g'(s)\ln(1-\epsilon)} \tag{90}$$

or

$$\|(1 - F'_{\mathfrak{R}})\phi_0\|_\epsilon^{\mathrm{B}} \le \|(1 - F'_{\mathfrak{R}})1\|_\epsilon^{\mathrm{B}}. \tag{91}$$

Since the refinement $\mathfrak{T}'$ can be made arbitrarily fine, one has that

$$\|(1 - F_{\mathfrak{R}})\phi_0\|_\epsilon^{\mathrm{B}} \le \|(1 - F_{\mathfrak{R}})1\|_\epsilon^{\mathrm{B}}. \tag{92}$$

Now,

$$\begin{aligned}(\|(1 - F_{\mathfrak{R}})1\|_\epsilon^{\mathrm{B}})^2 &= (\|1\|_\epsilon^{\mathrm{B}})^2 - (\|F_{\mathfrak{R}}1\|_\epsilon^{\mathrm{B}})^2 \\ &= 1 - (\|F_{\mathfrak{R}}1\|_\epsilon^{\mathrm{B}})^2 \to 0 \end{aligned} \tag{93}$$

as $\epsilon \to 0$ because of (88), in the absence of point eigenvalues. Thus, from the dense nature of the subset of functionals $\phi_0(\nu)$, the statement $F_{\mathfrak{R}}\phi(\nu) = \phi(\nu)$ is proved for every boson functional $\phi(\nu)$ as $\hbar \to 0$, in the absence of point eigenvalues.

The conclusion that in the limit $\hbar \to 0$ the state in $\mathfrak{F}_\epsilon^{\mathrm{B}}$ (or $\mathfrak{F}_\epsilon^{\mathrm{F}}$) with the representer given by the functional $\phi(\nu)$ gives the same result as that given by the functional $\phi(\nu)$ in $\mathfrak{F}_\epsilon^{\mathrm{M-B}}$ follows readily from the above. Now, from (9), (66), and (77), in the absence of point eigenvalues,

$$\begin{aligned}(F_{\mathfrak{R}}\Phi_1, \Phi_2)_\epsilon^{\mathrm{F}} &= \exp[-\epsilon^{-1}\ln(1 - \epsilon^2)\omega(\mathfrak{R})](F_{\mathfrak{R}}\Phi_1, \Phi_2)_\epsilon^{\mathrm{B}} \end{aligned} \tag{94}$$

for arbitrary states Φ_1 and Φ_2. Hence, in the limit $\epsilon \to 0$, since $F_{\mathfrak{R}}\phi(\nu) = \phi(\nu)$, one has that

$$(\Phi_1, \Phi_2)_{\epsilon=0}^{\mathrm{F}} = (\Phi_1, \Phi_2)_{\epsilon=0}^{\mathrm{B}}. \tag{95}$$

Therefore, all the physical results of the theory approach the same classical result. Note that the order of the limiting processes $\epsilon \to 0$ and $\mathfrak{R}$ covering the whole s-space cannot be interchanged in (82) and (84). Thus, the result of Friedrichs that for the Maxwell–Boltzmann case the values of $\nu(s)$ might have been restricted to $\nu(s) = 0$ and $\nu(s) = 1$ for all s except for point eigenvalues is only true here in the limit $\hbar \to 0$. Note, also, that Planck's constant does not appear when evaluating physical quantities in the Maxwell–Boltzmann case, for example, the expected number of particles at the value s on the energy shell $\sum_s \nu(s)\lambda(s) = \kappa$, but it does appear in expression (84) where the projector F occurs.

VI. NONSEPARABILITY OF THE HILBERT SPACE

The Hilbert space of all compatible and ideal occupation functionals $\phi(\nu)$, with inner product defined by (9) [or (66)], will be denoted by $\mathfrak{F}_\epsilon^{\mathrm{B}}$ (or $\mathfrak{F}_\epsilon^{\mathrm{F}}$). The subscript ϵ, with $0 \leq \epsilon < 1$, emphasizes the dependence of the inner product on this parameter. Consider the Hilbert space $\mathfrak{F}_{\epsilon'}^{\mathrm{B}}$ with $\epsilon' \neq \epsilon$ and $0 \leq \epsilon' < 1$. In what follows it will be shown that for myriotic fields the spaces $\mathfrak{F}_\epsilon^{\mathrm{B}}$ and $\mathfrak{F}_{\epsilon'}^{\mathrm{B}}$ are orthogonal. Hence, one obtains a sequence of Hilbert spaces, each orthogonal to all the others, parametrized by the continuous variable ϵ. This representing a nonseparable Hilbert space.

Consider the cell $\mathcal{C}$ in such a way that it contains all bounded cells of the partition $\mathcal{T}$ with which the functional $\phi(\nu)$ is compatible. One has that $W(\mathcal{C}) = \int_C d\omega(s) < \infty$ and $W(\mathcal{C})$ approaches infinity when the cell $\mathcal{C}$ tends to cover the whole s-space. Now,

$$(\Phi, \Phi)_{\epsilon'}^{\mathrm{B}} = \sum_\nu |\phi(\nu)|^2 \prod_s (\epsilon')^{\nu(s)} e^{g(s)\ln(1-\epsilon')} \frac{[\nu(s) + g(s) - 1]!}{\nu(s)!\,[g(s) - 1]!} = \left(\Phi, \left(\frac{\epsilon'}{\epsilon}\right)^{\mathcal{N}(\mathcal{C})} \exp\left[\frac{W(\mathcal{C})}{\epsilon} \ln\left(\frac{1-\epsilon'}{1-\epsilon}\right)\right]\Phi\right)_\epsilon^{\mathrm{B}}, \quad (96)$$

where the operator

$$\mathcal{N}(\mathcal{C}) = \int_C A^+(s)A^-(s)\, dm(s) \quad (97)$$

corresponds to the number of particles in the cell $\mathcal{C}$. Expression (96) suggests introducing the operator

$$T = (\epsilon'/\epsilon)^{\frac{1}{2}\mathcal{N}(\mathcal{C})} \exp\{[W(\mathcal{C})/2\epsilon] \ln[(1-\epsilon')/(1-\epsilon)]\}, \quad (98)$$

which transforms the state represented by the functional $\phi(\nu)$ in $\mathfrak{F}_\epsilon^{\mathrm{B}}$ to the *same* state in $\mathfrak{F}_{\epsilon'}^{\mathrm{B}}$. Actually, the operator T maps elements of the space $\mathfrak{F}_\epsilon^{\mathrm{B}}$ with representer $\phi(\nu)$ into elements of the same space but with representer

$$(\epsilon'/\epsilon)^{\frac{1}{2}\nu(\mathcal{C})} \exp\{[W(\mathcal{C})/2\epsilon] \ln[(1-\epsilon')/(1-\epsilon)]\}\phi(\nu),$$

with $\nu(\mathcal{C}) = \sum_{s\in\mathcal{C}} \nu(s)$. Since, by assumption, $(\Phi, \Phi)^{\mathrm{B}} < \infty$, therefore, one has that $(\Phi, \Phi)_{\epsilon'}^{\mathrm{B}} < \infty$ for $0 \leq \epsilon' < 1$. It follows from (96) and (98) that

$$(\Phi, T\Phi)_\epsilon^{\mathrm{B}} = (\Phi, \Phi)_{(\epsilon\epsilon')^{\frac{1}{2}}} \exp\left([W(\mathcal{C})/\epsilon] \times \ln\{[(1-\epsilon')(1-\epsilon)]^{\frac{1}{2}}/[1-(\epsilon'\epsilon)^{\frac{1}{2}}]\}\right), \quad (99)$$

which tends to zero as the cell $\mathcal{C}$ covers the whole of s-space since

$$0 < [(1-\epsilon')(1-\epsilon)]^{\frac{1}{2}}/[1-(\epsilon'\epsilon)^{\frac{1}{2}}] < 1$$

for

$$0 < \epsilon < 1 \quad \text{and} \quad 0 < \epsilon' < 1.$$

By the Schwarz inequality and result (99),

$$(\Phi_1, T\Phi_2)_\epsilon^{\mathrm{B}} \to 0 \quad \text{as} \quad W(\mathcal{C}) \to \infty \quad \text{for} \quad 0 < \epsilon < 1 \quad (100)$$

for arbitrary functionals $\phi_1(\nu)$ and $\phi_2(\nu)$ in $\mathfrak{F}_\epsilon^{\mathrm{B}}$. Therefore, the operator T takes every vector of $\mathfrak{F}_\epsilon^{\mathrm{B}}$ out of this space and into the orthogonal space $\mathfrak{F}_{\epsilon'}^{\mathrm{B}}$.

Similar results hold for the cases of Maxwell–Boltzmann and Fermi–Dirac statistics. For instance, for the Maxwell–Boltzmann case treated by Friedrichs

$$(\Phi, \Phi)_\omega = \sum_\nu |(\phi(\nu))|^2 \prod_s \frac{[d\omega(s)]^{\nu(s)}}{\nu(s)!} e^{-d\omega(s)} < \infty. \quad (101)$$

Suppose the weight function is modified by a simple nonzero multiplicative factor so that $d\omega'(s) = C\, d\omega(s)$. The new scalar product is, evidently,

$$(\Phi, \Phi)_{C\omega} = \sum_\nu |\phi(\nu)|^2 \prod_s \frac{[d\omega'(s)]^{\nu(s)} e^{-d\omega'(s)}}{\nu(s)!} < \infty, \quad (102)$$

for $0 < C < \infty$. But,

$$(\Phi, \Phi)_{C\omega} = (\Phi, C^{\mathcal{N}(\mathcal{C})} e^{-CW(\mathcal{C})+W(\mathcal{C})}\Phi)_\omega. \quad (103)$$

Introduce the operators

$$T = C^{\frac{1}{2}\mathcal{N}(\mathcal{C})} e^{\frac{1}{2}[-CW(\mathcal{C})+W(\mathcal{C})]}. \quad (104)$$

Hence, by (103) and (104),

$$(\Phi, T\Phi)_\omega = e^{-W(\mathcal{C})(\frac{1}{2}+\frac{1}{2}C-\sqrt{C})}(\Phi, \Phi)_{(C\omega)^{\frac{1}{2}}}, \quad (105)$$

which approaches zero as the cell $\mathcal{C}$ covers the whole of s-space, since $\frac{1}{2} + \frac{1}{2}C - \sqrt{C} > 0$ for $0 < C \neq 1$.

[1] I. E. Segal, Ann. Math. **48**, 930 (1947).
[2] R. Haag and D. Kastler, J. Math. Phys. **5**, 848 (1964).
[3] R. Haag, N. M. Hugenholtz, and M. Winnink, Commun. Math. Phys. **5**, 215 (1967).
[4] S. Doplicher, D. Kastler, and D. W. Robinson, Commun. Math. Phys. **3**, 1 (1966); D. Ruelle, *ibid.* **3**, 133 (1966); D. Kastler and D. W. Robinson, *ibid.* **3**, 151 (1966).

[5] M. Alexanian, J. Math. Phys. **9**, 725, 734 (1968).

[6] See, for instance, R. Kurth, *Axiomatics of Classical Statistical Mechanics* (Pergamon, New York, 1960), Chap. V.

[7] K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields* (Interscience, New York, 1953), in particular, Part IV.

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[9] In Ref. 5, a macroscopic equilibrium state is the equivalence class of microscopic equilibrium states with the same values for the macroscopic variables. [See (10) in Ref. 5.]

[10] A functional $f(\nu)$ is compatible in the first manner with the partition $\mathcal{T}$ if it depends only on the values ν_k, $k = 1, 2, \cdots$, and ν_* and the functional vanishes unless $\nu_* = 0$. Note that for functionals compatible in the first manner the ϵ converging factor is no longer needed. However, its use in the definition of the inner product will be continued.

[11] This result holds for temperatures above the condensation temperature. For lower temperatures an added term, corresponding to the zero momentum state, may be necessary.

[12] For myriotic fields, $\sum_s g(s) = \infty$, the exponential factor in (66) is essential for the existence of an equidistribution state.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Dispersion Relations, Froissart–Gribov Transforms, and Distributions

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(Received 21 September 1970)

We construct a family of distribution spaces $\mathcal{K}'_\lambda$. Each $\mathcal{K}'_\lambda$ completely characterizes the (tempered) distributions (i) which are the discontinuity of functions holomorphic in a cut plane with given boundedness properties and (ii) the Froissart–Gribov transforms of which are holomorphic in a half-plane with given asymptotic behavior. The main results are stated in two reciprocal theorems. Such a reciprocity shows the adequacy of our spaces $\mathcal{K}'_\lambda$. Some mathematical properties of these ones are given after introducing the proper test function spaces $\mathcal{K}_\lambda$. In particular, we prove a representation theorem for the distributions in $\mathcal{K}'_\lambda$.

1. INTRODUCTION AND RESULTS

In elementary particle physics, one constantly has to deal with the following three objects:

(1) a scattering amplitude $F(z)$ which usually is an analytic function of z (the cosine of the scattering angle) in a complex cut plane;

(2) an absorptive amplitude $\Delta(x)$ which, within a factor $2i$, is the discontinuity of $F(z)$ through the cut;

(3) partial wave amplitudes $f(l)$, which are connected to $\Delta(x)$ by the so-called Froissart–Gribov transformation[1] [see, further on, Eq. (1.1)].

It is well known that when $\Delta(x)$, defined say on[2] $[z_0, +\infty]$, is a function which behaves like x^λ at infinity, we have the following:

(i) It is possible to construct a function $F(z)$ holomorphic in $\mathsf{C}[z_0, +\infty]$ with the discontinuity $2i\Delta(x)$, which behaves like z^λ at infinity in the complex z-plane;

(ii) The Froissart–Gribov transform $f(l)$ of $\Delta(x)$ is holomorphic in the complex half-plane $\operatorname{Re} l > \lambda$.

We want to emphasize the fact that if $\Delta(x)$ (always bounded in modulus by Cx^λ, where C is a constant) oscillates at infinity, it may happen that there exists a function $F(z)$ which behaves at infinity like z^μ with $\mu < \lambda$. At the same time $f(l)$ will be analytic in the larger domain $\operatorname{Re} l > \mu$. This shows that one cannot give a reciprocal statement for (i) and (ii): If $F(z)$ behaves like z^λ or if $f(l)$ is holomorphic in $\operatorname{Re} l > \lambda$, nothing can be said about the behavior of $|\Delta(x)|$ when x goes to infinity.

Secondly, the discontinuity through the cut of a given function $F(z)$ analytic in $\mathsf{C}[z_0, +\infty]$ is not necessarily a function: It may be a distribution (or even a more complicated object like a hyperfunction). In axiomatic quantum field theory, the absorptive parts generally are distributions. Thus we cannot restrict ourselves to amplitudes $F(z)$ the discontinuity of which are functions, and we will allow $\Delta(x)$ to be a distribution (which from now on we shall denote Δ_x).

The purpose of this paper is to solve the following two problems:

(1) If $F(z)$ is a holomorphic function in $\mathsf{C}[z_0, +\infty]$, bounded in modulus by $C\,|z|^\lambda$ in any direction of the complex z plane but possibly in the direction of the positive real axis, with a discontinuity $2i\Delta_x$ which is a distribution, what can be said about Δ_x?

(2) Let $f(l)$ be the Froissart–Gribov transform of a distribution Δ_x; that is to say,

$$f(l) = \langle \Delta_x, Q_l(x) \rangle, \tag{1.1}$$

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Secondly, the discontinuity through the cut of a given function $F(z)$ analytic in $\mathsf{C}[z_0, +\infty]$ is not necessarily a function: It may be a distribution (or even a more complicated object like a hyperfunction). In axiomatic quantum field theory, the absorptive parts generally are distributions. Thus we cannot restrict ourselves to amplitudes $F(z)$ the discontinuity of which are functions, and we will allow $\Delta(x)$ to be a distribution (which from now on we shall denote Δ_x).

The purpose of this paper is to solve the following two problems:

(1) If $F(z)$ is a holomorphic function in $\mathsf{C}[z_0, +\infty]$, bounded in modulus by $C\,|z|^\lambda$ in any direction of the complex z plane but possibly in the direction of the positive real axis, with a discontinuity $2i\Delta_x$ which is a distribution, what can be said about Δ_x?

(2) Let $f(l)$ be the Froissart–Gribov transform of a distribution Δ_x; that is to say,

$$f(l) = \langle \Delta_x, Q_l(x) \rangle, \tag{1.1}$$

where $Q_l(x)$ is the Legendre function of the second kind and, as usual, $\langle \Delta_x, \varphi(x) \rangle$ denotes the scalar product of the distribution Δ_x with the test function $\varphi(x)$. Knowing that $f(l)$ is holomorphic in the half-plane $\mathrm{Re}\, l > \lambda$, what can be said about the distribution Δ_x?

In order to make clear the results we have obtained, we shall start summarizing them right now, postponing the different proofs to the following sections.

The study of the two problems formulated above will lead us to construct spaces $\mathcal{K}'_\lambda$ of tempered distributions on the real axis, such that the answers we are looking for can be formulated in two theorems. Before defining the spaces $\mathcal{K}'_\lambda$, we shall state these theorems:

Theorem 1: Let Δ_x be a distribution which

(A1) belongs to $\mathcal{K}'_\lambda$ with $\lambda \geq -1$ and

(A2) has its support contained in $[z_0, +\infty]$. Then there exists a function $F(z)$

(B1) holomorphic in $\mathrm{C}[z_0, +\infty]$ with the discontinuity $2i\Delta_x$ and

(B2) bounded in the cut plane by

$$|F(z)| < \text{const} \times (1 + |z|)^{\lambda+\epsilon}/|\theta|^{p(\epsilon)},$$

where ϵ is any positive number (as small as one wants), θ is the phase of z ($-\pi < \theta \leq \pi$), and $p(\epsilon)$ a nonnegative number which eventually may indefinitely increase when ϵ approaches zero. Reciprocally, let $F(z)$ be a function enjoying properties (B1) and (B2) with $\lambda \geq -1$. Then its discontinuity satisfies (A1) and (A2).

Let us make some comments about this first theorem:

(1) The presence of the factor $1/|\theta|^{p(\epsilon)}$ in the bound (B2) ensures that the boundary value of $F(z)$ on the two sides of the cut (and thus the discontinuity) is a distribution.[3] Moreover, when θ is fixed $\neq 0$, that is to say, in any complex direction different from the direction of the positive real axis, $|F(z)|$ is bounded by $C(1 + |z|)^{\lambda+\epsilon}$ for any strictly positive ϵ. But, in the direction of the positive real axis, $|F(z)|$ is allowed to grow much faster, and its rate of growth is no longer connected to λ.[4]

(2) The bound (B2) is the kind of bound which emerges from axiomatic field theory.[5] It allows the writing down of dispersion relations with a finite number of subtractions.

(3) As consequences of the reciprocal character of Theorem 1: First, if Δ_x does not belong to $\mathcal{K}'_\lambda$, there is no function $F(z)$ with the discontinuity $2i\Delta_x$ which satisfies a bound of the form (B2); second, if $F(z)$, holomorphic in $\mathrm{C}[z_0, +\infty]$, does not satisfy (B2), its discontinuity does not belong to $\mathcal{K}'_\lambda$.

The reciprocal character of Theorem 1 ensures that the spaces $\mathcal{K}'_\lambda$ are the good ones to be considered (at least when $\lambda \geq -1$). Let us remark that neither the spaces $\mathcal{O}'_\lambda$ introduced by Bremermann and Durand in a similar context[6] nor the various ones studied by Gel'fand and Shilov[7] are convenient in that respect.

The restriction $\lambda \geq -1$ is essential. It makes Theorem 1 only a partial answer to our problem. We shall come back to that point later on, when we know the content of $\mathcal{K}'_\lambda$.

Now comes the second theorem:

Theorem 2: Let Δ_x be a distribution which enjoys properties (A1) and (A2) of Theorem 1. Then its Froissart–Gribov transform $f(l)$ is

(C1) holomorphic in the half-plane $\mathrm{Re}\, l > \lambda$ and

(C2) bounded by

$$|f(l)| < P_\epsilon(|l|)[z_0 + (z_0^2 - 1)^{\frac{1}{2}}]^{-\mathrm{Re}\, l} \quad \text{for} \quad \mathrm{Re}\, l \geq \lambda + \epsilon,$$

where ϵ is any positive number and $P_\epsilon(|l|)$ is a polynomial in $|l|$, the degree of which depends on ϵ and may eventually indefinitely increase when ϵ approaches zero. Reciprocally, let $f(l)$ be a function satisfying (C1) and (C2) with $\lambda \geq -1$. Then it is the Froissart–Gribov transform of a distribution which enjoys properties (A1) and (A2) and which is given by

$$\Delta_x = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} dl (2l + 1) f(l) P_l(x), \quad \xi > \lambda. \tag{1.2}$$

Some comments about this second theorem are in order:

(1) The bound (C2) means that, in the half-plane $\mathrm{Re}\, l > \lambda$, $|f(l)|$ exponentially decreases at infinity in all directions but the direction of the imaginary axis where $|f(l)|$ is allowed to grow polynomially in $|l|$.[8]

(2) The first part of Theorem 2 is trivial. It is the extension to the distributions of $\mathcal{K}'_\lambda$ of a well-known result proved by Froissart.[1] On the contrary, to our knowledge, the reciprocal statement is new.

(3) The third comment we made after Theorem 1 keeps all its value here.

(4) The exact mathematical meaning of the inversion formula (1.2) in terms of test functions will be given in Sec. 4.

So far we said nothing about the spaces $\mathcal{K}'_\lambda$. To describe them, we first introduce the spaces $\mathcal{J}'_\lambda$. They are such that any distribution Δ_x which belongs to $\mathfrak{J}'_\lambda$ [and satisfies (A2)] has the following representation:

$$\Delta_x = x^{\lambda+1} D^p[(\log x)^q x^{p-1} \bar{\Delta}(x)], \qquad (1.3)$$

where p and q are nonnegative integers and $\bar{\Delta}(x)$ is a continuous and bounded function of x (D is the symbol of derivation in the sense of distributions).

The representation (1.3) is valid for any value of λ. However, when $\lambda \geq -1$, Eq. (1.3) can be replaced by

$$\Delta_x = D^p[(\log x)^q x^{\lambda+p} \tilde{\Delta}(x)], \qquad (1.4)$$

where $\tilde{\Delta}(x)$ has the same properties as $\bar{\Delta}(x)$.

We note that, for any value of λ, the distributions Δ_x in $\mathfrak{J}'_\lambda$ are tempered: the $\mathfrak{J}'_\lambda$ are subspaces of $\mathcal{S}'$, the space of tempered distributions.[9] Moreover, if $\lambda_1 < \lambda_2$, then $\mathfrak{J}'_{\lambda_1}$ is contained in $\mathfrak{J}'_{\lambda_2}$: $\mathfrak{J}'_{\lambda_1} \subset \mathfrak{J}'_{\lambda_2} \subset \mathcal{S}'$.

Now comes the definition of $\mathcal{K}'_\lambda$: It is the intersection of all the spaces $\mathfrak{J}'_\mu$ for μ strictly larger than λ,

$$\mathcal{K}'_\lambda = \bigcap_{\mu > \lambda} \mathfrak{J}'_\mu . \qquad (1.5)$$

A given distribution Δ_x which belongs to $\mathcal{K}'_\lambda$ has a representation of the type (1.3) [or (1.4) when $\lambda \geq -1$] in each $\mathfrak{J}'_\mu$, with parameters p_μ and q_μ and a function $\bar{\Delta}_\mu(x)$ [or $\tilde{\Delta}_\mu(x)$] which depend on μ. In particular, it may happen that p_μ indefinitely increases when μ approaches λ (in Sec. 2 we shall exhibit a distribution which has that property). This phenomenon is the origin of the possible indefinite increase of $p(\epsilon)$ in the bound (B2) and of the degree of $P_\epsilon(|l|)$ in the bound (C2), when ϵ approaches zero.

Let us make some comments about these definitions:

(1) According to Eq. (1.4), the distribution

$$\Delta_x = D \sin e^x = e^x \cos e^x$$

belongs to $\mathfrak{J}'_{-1}$. It is indeed a function, and we see that its modulus is not bounded at infinity by any power of $|x|$. At the same time, it oscillates more and more rapidly when $|x|$ increases. This has to be put close to what we said at the beginning of the introduction. We realized that, in order to have reciprocal statements in Theorems 1 and 2, we had to be able to take into account oscillations in the absorptive parts: These oscillations are completely described by the representations (1.3) and (1.4).

(2) When regularizing Δ_x by an infinitely differentiable function $\alpha(x)$, the oscillations of Δ_x kill its fast increase at infinity. One could so hope to recover, for the regularized distribution ${}^\alpha\Delta(x)$, a behavior at infinity at $C\,|x|^\lambda$, if Δ_x belongs to $\mathfrak{J}'_\lambda$. This is not true, as it will be shown in Sec. 2 on an explicit example.

(3) If Δ_x is a positive distribution (like the absorptive part in forward direction), then p is not larger than 2 in formulas (1.3) and (1.4), and the functions between brackets are convex.

(4) Once more we encounter the condition $\lambda \geq -1$. In order to understand this important condition, we have to say a few words about the test functions. The distributions of $\mathfrak{J}'_\lambda$ operate on test functions which belong to a space $\mathfrak{J}_\lambda$, which will be constructed in Sec. 2. What we have to know here is that when $\lambda \geq -1$, $\mathfrak{J}_\lambda$ contains no polynomial in x. On the contrary, when $\lambda < -N$, $N = 1, 2, \cdots$, $\mathfrak{J}_\lambda$ contains all polynomials of degree $\leq N - 1$.

Suppose now that a distribution Δ_x, belonging to $\mathfrak{J}'_\lambda$ for $-(N+1) \leq \lambda < -N$, can be represented according to Eq. (1.4) with p at least equal to N. Then, we immediately conclude that Δ_x satisfies N "sum rules":

$$\langle \Delta_x, x^n \rangle = \langle (\log x)^q x^{\lambda+p} \tilde{\Delta}(x), (-D)^p x^n \rangle = 0 \quad \text{for} \quad n = 0, 1, \cdots, N-1. \qquad (1.6)$$

These "sum rules" are exactly the conditions Δ_x has to satisfy in addition to (A1) and (A2), in order to have Theorem 1 for $\lambda < -1$. However, the representation (1.4) is not valid in general for $\lambda < -1$: This implies that there exist distributions in $\mathfrak{J}'_\lambda$ which do not satisfy any "sum rule." Consequently, to these distributions there correspond no functions $F(z)$ with properties (B1) and (B2). That is the reason why we cannot extend Theorem 1 (and also Theorem 2) to $\lambda < -1$.

This means that the spaces $\mathfrak{J}'_\lambda$ are not convenient for our purpose when $\lambda < -1$. Let us say, however, that it is possible to construct more sophisticated spaces such that Theorems 1 and 2 hold for $\lambda < -1$. This requires some more work, and it is now under investigation.

(5) Finally let us give two examples which illustrate the previous considerations. The first one is $\delta(x - x_1)$. It has the representation

$$\delta(x - x_1) = D^2[(x - x_1)\theta(x - x_1)], \qquad (1.7)$$

where $\theta(x - x_1)$ is the "Heaviside function." The function between brackets in Eq. (1.7) being continuous and bounded by $C\,|x|$, $\delta(x - x_1)$ belongs to $\mathfrak{J}'_{-1}$. Indeed, it belongs to $\mathfrak{J}'_{-\infty}$, as it can be shown easily by using representations of type (1.3).

Its Froissart–Gribov transform is $Q_l(x_1)$, which is holomorphic in $\mathrm{Re}\, l > -1$, in accordance with Theorem 2. $\{Q_l(x_1)$ is indeed holomorphic in $\mathbb{C}[-\infty, -1]$.$\}$ Note that, although $\delta(x - x_1)$ belongs to $\mathfrak{J}'_{-\infty}$, $Q_l(x_1)$ is not holomorphic in $\mathrm{Re}\, l > -\infty$, because $\delta(x - x_1)$ satisfies no "sum rule."

The inversion formula (1.2) gives

$$\delta(x - x_1) = \frac{1}{2\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl(2l + 1)P_l(x)Q_l(x_1), \quad \xi > -1. \quad (1.8)$$

As it will be explained in Sec. 4, the right-hand side of Eq. (1.8) belongs to $\mathcal{J}'_\xi$: It is not a representation of $\delta(x - x_1)$ in $\mathcal{J}'_{-1}$.

The second example is the unitarity kernel of Mandelstam[10]:

$$K_x = \frac{\theta(x - x_1x_2 - [(x_1^2 - 1)(x_2^2 - 1)]^{\frac{1}{2}})}{(x^2 + x_1^2 + x_2^2 - 2xx_1x_2 - 1)^{\frac{1}{2}}}, \quad x_1, x_2 > 1. \quad (1.9)$$

It has the representation

$$K_x = D\left(\theta(x - x_+)\log\frac{(x - x_-)^{\frac{1}{2}} + (x - x_+)^{\frac{1}{2}}}{(x - x_-)^{\frac{1}{2}} - (x - x_+)^{\frac{1}{2}}}\right), \quad (1.10)$$

where

$$x_\pm = x_1x_2 \pm [(x_1^2 - 1)(x_2^2 - 1)]^{\frac{1}{2}}.$$

We notice that the function between brackets in Eq. (1.10) is continuous, and behaves at infinity like $\log x$. Thus K_x belongs to $\mathcal{J}'_{-1}$.

Its Froissart–Gribov transform is[11]

$$\int_{x_+}^{\infty} dx \frac{Q_l(x)}{[(x - x_-)(x - x_+)]^{\frac{1}{2}}} = Q_l(x_1)Q_l(x_2), \quad (1.11)$$

and it is holomorphic in $\mathrm{Re}\, l > -1$. The inversion formula (1.2) gives

$$\frac{\theta(x - x_1x_2 - [(x_1^2 - 1)(x_2^2 - 1)]^{\frac{1}{2}})}{(x^2 + x_1^2 + x_2^2 - 2xx_1x_2 - 1)^{\frac{1}{2}}} = \frac{1}{2\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl(2l + 1)P_l(x)Q_l(x_1)Q_l(x_2), \quad \xi > -1. \quad (1.12)$$

As in formula (1.8), the right-hand side of Eq. (1.12) is indeed a representation of K_x in $\mathcal{J}'_\xi$, and not in $\mathcal{J}'_{-1}$.

Before ending this section, let us sketch the content of the following ones.

Section 2 is devoted to the mathematical study of $\mathcal{J}'_\lambda$ and $\mathcal{K}'_\lambda$ and their test function spaces $\mathcal{J}_\lambda$ and $\mathcal{K}_\lambda$. All of them are given the structure of topological linear spaces. The main result of Sec. 2 is Theorem 3, which gives the representation of the distributions in $\mathcal{J}'_\lambda$. Sections 3 and 4 are devoted respectively to the proofs of Theorems 1 and 2. Some technical points are deferred to four appendices.

2. THE SPACES $\mathcal{J}'_\lambda$ AND $\mathcal{K}'_\lambda$ OF TEMPERED DISTRIBUTIONS

Our first task will be to build our spaces $\mathcal{J}'_\lambda$. The principle of the method will consist to relate them to the tempered distribution space $\mathcal{S}'$ by means of a simple change of variable. To this end, we have to construct the appropriate spaces $\mathcal{J}_\lambda$ of test functions. We define $\mathcal{J}_\lambda$ as the set of all complex-valued, infinitely differentiable functions φ over $\mathbb{R}_x$, such that for all $q > 0$

$$\lim_{|x|\to\infty} (\log |x|)^q\, |x|^{\lambda+p+1}\, D^p\varphi(x) = 0, \quad p = 0, 1, 2, \cdots. \quad (2.1)$$

The linear space $\mathcal{J}_\lambda$ will be endowed with the following topology: A sequence $\{\varphi_i\}$ will converge to 0 in $\mathcal{J}_\lambda$ if $\{[\log(2 + |x|)]^q(1 + |x|)^{\lambda+p+1}D^p\varphi_i(x)\}$ converges to 0 uniformly over $\mathbb{R}$ for all $q, p = 0, 1, \cdots$.

We next consider the space $\mathcal{S}$ of all complex-valued, infinitely differentiable functions Φ with fast decrease over $\mathbb{R}_\tau$ (in the sense of Schwartz[12]) together with the mapping $\mathbb{R}_\tau \to \mathbb{R}_x$ defined by $x = \sinh\tau$. $\mathcal{S}$ being equipped with the standard topology, we have the following.

Lemma 1: (1) The mapping $\tau \to x = \sinh\tau$ induces an isomorphism $H: \varphi \to \Phi$ between $\mathcal{J}_\lambda$ and $\mathcal{S}$ defined by

$$\Phi(\tau) = (\cosh\tau)^{\lambda+1}\varphi(\sinh\tau).^{13} \quad (2.2)$$

(2) The bijection H is a homeomorphism.

Proof: Since the mapping $\tau \to x = \sinh\tau$ is a C^∞-diffeomorphism, in order to prove (1), one only has to show the equivalence of the condition (2.1) with

$$\lim_{|\tau|\to\infty} |\tau|^q\, D_\tau^p\Phi(\tau) = 0, \quad \forall\, q, p = 0, 1, \cdots. \quad (2.3)$$

But from

$$D_\tau^p\Phi(\tau) = [(1 + x^2)^{\frac{1}{2}}D_x]^p[(1 + x^2)^{\frac{1}{2}(\lambda+1)}\varphi(x)]$$

it is easily shown that

$$|\tau|^q\, D_\tau^p\Phi(\tau) = \sum_{p'=0}^{p} \alpha_{pp'}(x)D_x^{p'}\varphi(x), \quad (2.4)$$

where

$$\alpha_{pp'}(x) \underset{|x|\to\infty}{=} O[(\log|x|)^q\, |x|^{\lambda+p'+1}]$$

so that (2.1) $\Rightarrow$ (2.2).

In the same way, (2.2) $\Rightarrow$ (2.1) because

$$(\log|x|)^q\, |x|^{\lambda+p+1}\, D_x^p\varphi(x) = \sum_{p'=0}^{p} \beta_{pp'}(\tau)D_\tau^{p'}\Phi(\tau) \quad (2.5)$$

with

$$\beta_{pp'}(\tau) \underset{|\tau|\to\infty}{=} O[|\tau|^q].$$

Part (2) of the lemma is true if every sequence $\{\varphi_i\}$ converging to 0 in $\mathfrak{J}_\lambda$ generates (via the isomorphism H) a corresponding sequence $\{\Phi_i\}$ converging to 0 in $\mathcal{S}$, and reciprocally. But this is obvious from Eqs. (2.4) and (2.5). QED

Let us now consider, together with the tempered distribution space $\mathcal{S}'$, the topological dual $\mathfrak{J}'_\lambda$ of $\mathfrak{J}_\lambda$.

We can endow the linear spaces $\mathcal{S}'$ and $\mathfrak{J}'_\lambda$ with the strong topology of the dual (i.e., the topology of the uniform convergence in the bounded sets of $\mathcal{S}$ and $\mathfrak{J}_\lambda$ respectively).[14] Then we have an immediate counterpart of Lemma 1.

Lemma 2: (1) The isomorphism H induces an isomorphism $H':\Delta_x \to \Gamma_\tau(\Delta_x \in \mathfrak{J}'_\lambda, \Gamma_\tau \in \mathcal{S}')$ between $\mathfrak{J}'_\lambda$ and $\mathcal{S}'$ defined by

$$\langle \Delta_x, \varphi(x)\rangle = \langle \Gamma_\tau, \Phi(\tau)\rangle, \quad \forall\ \varphi \in \mathfrak{J}_\lambda, \Phi = H(\varphi). \tag{2.6}$$

(2) The bijection H' is a homeomorphism.

The proof is trivial.

Let us notice that, in case the considered distributions actually are functions, Eq. (2.6) takes the form

$$\int dx \Delta(x)\varphi(x) = \int d\tau \Gamma(\tau)\Phi(\tau)$$

and the isomorphism H' reduces to

$$H':\Delta(x) \to \Gamma(\tau) = (\cosh \tau)^{-\lambda}\Delta(\sinh \tau),$$

i.e., a simple change of variable when $\lambda = 0$.

Lemmas 1 and 2 allow us to transfer the well-known algebraic and topological properties of $\mathcal{S}$ (resp. $\mathcal{S}'$) to $\mathfrak{J}_\lambda$ (resp. $\mathfrak{J}'_\lambda$). Thus, each $\mathfrak{J}_\lambda$ is a locally convex, separated, complete, bornological space. Moreover, $\mathfrak{J}_\lambda$ is a denumerably normed space. Therefore, it is a Fréchet space. A denumerable basis of neighborhoods can be defined as

$$\begin{aligned} V_\lambda(Q, P, \epsilon) &= \{\varphi \mid \varphi \in \mathfrak{J}_\lambda, |\log(2 + |x|)^q(1 + |x|)^{\lambda+p+1}D^p\varphi| \\ &\le \epsilon, \forall\ x \in \mathbb{R}, p \le P\}, \quad Q, P = 0, 1, 2, \cdots. \end{aligned} \tag{2.7}$$

On the other hand, each $\mathfrak{J}'_\lambda$ is a locally convex, separated, complete space. Its topology is defined by a nondenumerable basis of neighborhoods. Furthermore, the sets $\{\mathfrak{J}_\lambda\}$ and $\{\mathfrak{J}'_\lambda\}$ are ordered by the following obvious inclusion relations (with the same "variable" x in all spaces $\mathfrak{J}_\lambda$ and $\mathcal{S}$):

$$\mathcal{S} \subset \mathfrak{J}_{\lambda_2} \subset \mathfrak{J}_{\lambda_1}, \quad \mathfrak{J}'_{\lambda_1} \subset \mathfrak{J}'_{\lambda_2} \subset \mathcal{S}', \quad \lambda_1 < \lambda_2. \tag{2.8}$$

Here, $X \subset Y$ means

(i) X is a linear subspace of Y,

(ii) the topology of X is stronger than the topology induced on X by that of Y.

Finally, we see that the family $\{\mathfrak{J}'_\lambda\}$ is a covering of the tempered distribution space $\mathcal{S}'$:

$$\mathcal{S} = \bigcap_{-\infty<\lambda<\infty} \mathfrak{J}_\lambda, \quad \mathcal{S}' = \bigcup_{-\infty<\lambda<\infty} \mathfrak{J}'_\lambda.$$

We now turn to the construction of concrete representations for the distributions belonging to $\mathfrak{J}'_\lambda$. Such representations are easily deduced from the known representations of general tempered distributions by using the isomorphism H'. As we are especially interested in distributions with support bounded at the left (which for convenience we suppose to be contained in $[a, \infty]$ with $a > 1$), we include this restriction in our statement.

Theorem 3: (1) Every distribution $\Delta_x \in \mathfrak{J}'_\lambda$ with supp $\Delta_x \subset [a, \infty]$ has the representation

$$\Delta_x = x^{\lambda+1}D^p[(\log x)^q x^{p-1}\bar{\Delta}(x)], \tag{2.9}$$

where p and q are some integers ≥ 0 and $\bar{\Delta}(x)$ is a complex-valued, bounded, continuous function over $\mathbb{R}$ with supp $\bar{\Delta}(x) \subset [a, \infty]$. Conversely, every distribution Δ_x having the representation (2.9) belongs to $\mathfrak{J}'_\lambda$ with supp $\Delta_x \subset [a, \infty]$.

(2) If $\lambda \ge -1$, the representation (2.9) can be written in the alternative way:

$$\Delta_x = D^p[(\log x)^q x^{\lambda+p}\tilde{\Delta}(x)], \tag{2.10}$$

where $\tilde{\Delta}(x)$ has the same properties as $\bar{\Delta}(x)$.

(3) The functions $\bar{\Delta}(x)$ and $\tilde{\Delta}(x)$ are univocally determined by the distribution Δ_x.

(4) If Δ_x is a positive distribution (i.e., a positive measure), one can put $p = 2$ in formulas (2.9) and (2.10). Then both brackets are convex functions over $\mathbb{R}$.

Proof: We first consider the case $\lambda \ge -1$. If Δ_x has the form (2.10), we get

$$\langle \Delta_x, \varphi(x)\rangle = (-1)^p \int_a^\infty dx \frac{\tilde{\Delta}(x)}{x(\log x)^2}[(\log x)^{q+2}x^{\lambda+p+1}D^p\varphi(x)]$$

so that, according to Eq. (2.1),

$$\langle \Delta_x, \varphi(x)\rangle < C\int_a^\infty \frac{dx}{x(\log x)^2} < \infty, \quad \forall\ \varphi \in \mathfrak{J}_\lambda, \quad a > 1,$$

Moreover

$$\text{supp}\ \varphi \subset \complement[a, \infty] \Rightarrow \langle \Delta_x, \varphi(x)\rangle = 0,$$
$$\{\varphi_i\} \to 0 \Rightarrow \{\langle \Delta_x, \varphi_i(x)\rangle\} \to 0.$$

Thus

$$\Delta_x \in \mathfrak{J}'_\lambda \quad \text{and} \quad \operatorname{supp} \Delta_x \subset [a, \infty].$$

Conversely, let Δ_x be a distribution satisfying these conditions. As we are concerned only with the positive values of x, we can replace at this stage the C^∞-diffeomorphism $\mathbb{R}_\tau \to \mathbb{R}_x$ of the Lemma 1 by the C^∞-diffeomorphism $\mathbb{R}_\tau \to \mathbb{R}_{x+}$ defined by $x = e^\tau$ and the isomorphism H by

$$\Phi(\tau) = e^{(\lambda+1)\tau}\varphi(e^\tau). \tag{2.11}$$

Then, clearly, the Lemmas 1 and 2 are still true with some obvious supplementary conditions on the various spaces involved. Thus

$$H': \Delta_x \to \Gamma_\tau \quad \text{with} \quad \Gamma_\tau \in \mathcal{S}', \quad \operatorname{supp} \Gamma_\tau \subset [\log a, \infty].$$

Now we can use for Γ_τ the well-known representation of tempered distributions,[15]

$$\Gamma_\tau = D_\tau^p[\tau^q \tilde{\Gamma}(\tau)], \tag{2.12}$$

where p and q are some integers ≥ 0 and $\tilde{\Gamma}(\tau)$ a complex-valued, bounded, continuous function over $\mathbb{R}$. Furthermore, from the support property of Γ_τ, it may be assumed [by adding a polynomial of degree $< p$ to $\tau^q\tilde{\Gamma}(\tau)$ if needed] that $\operatorname{supp} \tilde{\Gamma}(\tau) \subset [\log a, \infty]$. Hence, according to Eqs. (2.6), (2.11), and (2.12),

$$\begin{aligned} \langle \Delta_x, \varphi(x)\rangle &= (-1)^p \int_{\log a}^\infty d\tau \tilde{\Gamma}(\tau)\tau^q D_\tau^p[e^{(\lambda+1)\tau}\varphi(e^\tau)] \\ &= \sum_{p'=0}^{p} \gamma_{pp'} \int_a^\infty dx \tilde{\Gamma}(\log x)(\log x)^q x^{\lambda+p'} D_x^{p'}\varphi(x), \\ &\qquad \forall\, \varphi \in \mathfrak{J}_\lambda. \end{aligned}$$

Thus

$$\Delta_x = \sum_{p'=0}^{p} (-1)^{p'} \gamma_{pp'} D^{p'}[(\log x)^q x^{\lambda+p'} \tilde{\Gamma}(\log x)].$$

But, for $\lambda \geq -1$, we have

$$D^{p'}[(\log x)^q x^{\lambda+p'}\tilde{\Gamma}(\log x)] = D^p[(\log x)^{q'} x^{\lambda+p}\tilde{\gamma}(x)], \quad p' \leq p,$$

with $\tilde{\gamma}(x)$ a bounded, continuous function with support in $[a, \infty]$. Indeed, this relation is easily obtained by recurrence if we remark that

$$D^{p'-1}[(\log x)^q x^{\lambda+p'-1}\tilde{\sigma}_{p'-1}(x)] = D^{p'}[(\log x)^{q+1} x^{\lambda+p'}\tilde{\sigma}_{p'}(x)]$$

with

$$\tilde{\sigma}_{p'}(x) = \int_a^x dx' \, \frac{x'^{\lambda+p'-1}}{x^{\lambda+p'}} \frac{(\log x')^q}{(\log x)^{q+1}} \tilde{\sigma}_{p'-1}(x').$$

Then $\tilde{\sigma}_{p'}(x)$ has the properties required for $\tilde{\gamma}(x)$ if $\tilde{\sigma}_{p'-1}(x)$ does (the condition $\lambda \geq -1$ is crucial at this point).

Finally we see that Δ_x has the form (2.10), and the proof of (2) is complete.

Now we can turn to the general case (1). From the first definitions, it is clear that $\Delta_x \in \mathfrak{J}'_\lambda$ if and only if $x^{-\lambda-1}\Delta_x \in \mathfrak{J}'_{-1}$. As the representation (2.10) is valid for $\lambda = -1$, the proof of (1) reduces to that of (2).

In order to show that $\bar{\Delta}(x)$ is unique, it suffices to write (2.9) with two functions $\bar{\Delta}(x)$ and $\bar{\Delta}'(x)$ in the form

$$\Delta_x = x^{\lambda+1}D^p[\rho(x)] = x^{\lambda+1}D^p[\rho'(x)].$$

Hence

$$\delta^{(p)} * (\rho - \rho') = 0.$$

But $\delta^{(p)}$, ρ, $\rho' \in \mathcal{D}'_+$ and, since the convolution algebra in $\mathcal{D}'_+$ has no divisor of 0,[16] we conclude that $\rho - \rho' = 0$ and $\bar{\Delta}(x) = \bar{\Delta}'(x)$.

The unicity of $\tilde{\Delta}(x)$ follows from the same argument, and (3) is proved.

Finally, if Δ_x is a positive distribution, the property (4) arises from the fact that any positive measure is the second derivative of some convex function.[17] The details are given in Appendix A. {Some care is required at this point, because one cannot be sure "*a priori*" that the general representation (2.9) [or (2.10)] really coincides with that one for which $p = 2$.}

QED

Let us remark that parts (1), (2), and (4) of the theorem still hold if one removes all conditions involving the supports [of Δ_x, $\bar{\Delta}(x)$, and $\tilde{\Delta}(x)$] and replaces Eqs. (2.9) and (2.10) by

$$\Delta_x = (1 + |x|)^{\lambda+1}D^p\{[\log(2 + |x|)]^q(1 + |x|)^{p-1}\bar{\Delta}(x)\},$$

$$\Delta_x = D^p\{[\log(2 + |x|)]^q(1 + |x|)^{\lambda+p}\tilde{\Delta}(x)\}.$$

This follows from the fact that every distribution $\Delta_x \in \mathfrak{J}'_\lambda$ can be written as the sum of two distributions belonging to $\mathfrak{J}'_\lambda$ (with support bounded at the left, resp. the right) for which the theorem applies.

It could be expected that the distributions Δ_x belonging to $\mathfrak{J}'_\lambda$, besides their representations, are characterized as well by their asymptotic behavior after regularization (i.e., after convolution of Δ_x with a C^∞ function α with compact support). In fact, such a characterization does not exist: Of course, as the Δ_x are tempered distributions, the functions ${}^\alpha\Delta(x) = \Delta_x * \alpha(x)$, $\alpha \in \mathcal{D}$, are polynomially bounded at infinity, but there is no connection between λ and the degree of that polynomial. This feature appears clearly on the following example:

$$\Delta_x = D^{p-2}x^pD^2\Delta(x)$$

with

$$D^2\Delta(x) = \sum_{n=1}^{\infty}(-1)^n\delta(x - n).$$

Then $\Delta_x \in \mathcal{J}_0'$, $\forall\, p$, but

$$^{\alpha}\Delta(x) = \sum_{n=2}^{\infty}(-1)^n \alpha^{(p-2)}(x-n)n^p.$$

Since α has a compact support, the best bound for the regularized distribution is

$$|^{\alpha}\Delta(x)| < Cx^p.$$

Again, this example shows that the (minimum) value of p appearing in the representation of a distribution Δ_x is connected not only to the local structure of Δ_x (i.e., its order) but also to the oscillatory character of its asymptotic behavior.

However, in the case of positive measures in $\mathcal{J}_\lambda'$, a λ-dependent asymptotic bound can be derived after regularization (see Appendix A), namely,

$$^{\alpha}\Delta(x) \underset{x\to\infty}{=} O[(\log x)^q x^{\lambda+1}],\ \forall\, \alpha \in \mathcal{D}, \quad \text{for some} \quad a > 0. \tag{2.13}$$

Such a bound actually can be saturated. For example,

$$\Delta_x = \sum_{n=1}^{\infty} n^q 2^{n(\lambda+1)}\delta(x-2^n)$$

is a positive measure belonging to $\mathcal{J}_\lambda'$ {it can be written in the form $\Delta_x = x^{\lambda+1}D^2\rho(x)$ with

$$\rho(x) \underset{x\to\infty}{=} O[(\log x)^{q+2}x]\}$$

and

$$\limsup_{x\to\infty} |^{\alpha}\Delta(x)|/(\log x)^q x^{\lambda+1} \geq |\alpha(0)|/(\log 2)^q.$$

For the needs of the following sections, it is convenient to introduce new spaces of distributions involving families of spaces $\mathcal{J}_\lambda'$, in such a way that the inessential logarithms occurring in the latter disappear.

We first consider new spaces of test functions, $\mathcal{K}_\lambda$, algebraically defined by

$$\mathcal{K}_\lambda = \bigcup_{\mu>\lambda} \mathcal{J}_\mu.$$

By virtue of the inclusion relations (2.8), we can write as well

$$\mathcal{K}_\lambda = \bigcup_{n=1}^{\infty} \mathcal{J}_{\lambda+1/n} \tag{2.14}$$

or equivalently

$$\mathcal{K}_\lambda = \Big\{\varphi \mid \varphi \in C^\infty,\ \lim_{|x|\to\infty} |x|^{\lambda+n_\varphi^{-1}+p+1}D^p\varphi = 0, \forall\, p \geq 0, \text{ for some integer } n_\varphi\Big\}.$$

We wish to endow $\mathcal{K}_\lambda$ with the topology of the inductive limit.[18] Indeed this is the strongest locally convex topology over $\mathcal{K}_\lambda$ allowing us to construct the topological dual $\mathcal{K}_\lambda'$ in a canonical way. Thus there will be no difficulty in characterizing the distributions of $\mathcal{K}_\lambda'$ by means of explicit representations deduced from Eqs. (2.9) and (2.10).

Two equivalent bases of neighborhoods for $\mathcal{K}_\lambda$ can be built starting from the neighborhoods (2.7)[18,19]:

$$\mathcal{V}_\lambda(\{P\},\{\epsilon\}) = \mathcal{E}_c\Big(\bigcup_{n=1}^{\infty} V_{\lambda+1/n}(O, P_n, \epsilon_n)\Big), \tag{2.15}$$

$$\overline{\mathcal{V}}_\lambda(\{P\},\{\epsilon\}) = \bigcup_{n=1}^{\infty}\Big(\bigoplus_{m=1}^{n} V_{\lambda+1/m}(O, P_m, \epsilon_m)\Big), \tag{2.16}$$

where $\{P\}$ design any sequence of nonnegative integers and $\{\epsilon\}$ any sequence of positive numbers. We have used the notation $\mathcal{E}_c$ = convex envelope, and

$$\bigoplus_m E_m = \Big\{\varphi \mid \varphi = \sum_m \varphi_m,\ \varphi_m \in E_m\Big\}.$$

It should be emphasized that $\mathcal{K}_\lambda$ is *not* a *strict* inductive limit of the spaces $\mathcal{J}_{\lambda+1/n}$, for the topology of $\mathcal{J}_{\lambda+1/(n-1)}$ is strictly stronger than the topology induced on $\mathcal{J}_{\lambda+1/(n-1)}$ by that of $\mathcal{J}_{\lambda+1/n}$. In other words, there exists a neighborhood of O in $\mathcal{J}_{\lambda+1/(n-1)}$ which does not contain any intersection $V_{\lambda+1/n} \cap \mathcal{J}_{\lambda+1/(n-1)}$. In fact, it turns out that

$$V_{\lambda+1/(n-1)}(Q,P,\epsilon) \not\supset V_{\lambda+1/n}(Q',P',\epsilon') \cap \mathcal{J}_{\lambda+1/(n-1)}, \quad \forall\, Q, Q', P, P', \epsilon, \epsilon'$$

for simple functions can be exhibited, which enter in $V_{\lambda+1/n} \cap \mathcal{J}_{\lambda+1/(n-1)}$ but not in $V_{\lambda+1/(n-1)}$.

According to Eqs. (2.15) or (2.16), each $\mathcal{K}_\lambda$ is a locally convex, separated space having a nondenumerable basis of neighborhoods. Moreover, $\mathcal{K}_\lambda$ is a bornological space, as an inductive limit of Fréchet spaces.

On the other hand, $\mathcal{K}_\lambda$ seems to be neither complete nor semireflexive (this latter property, which would imply the former, does not follow from the reflexivity of the $\mathcal{J}_{\lambda+1/n}$ because we do not have a strict inductive limit). $\mathcal{K}_\lambda$ does not seem even to be a quasi-complete space, though we have not been able to produce a full proof of this fact.

Now we can assert that the topological dual of $\mathcal{K}_\lambda$ is given by

$$\mathcal{K}_\lambda' = \bigcap_{n=1}^{\infty} \mathcal{J}_{\lambda+1/n}'. \tag{2.17}$$

As a matter of fact, every distribution contained in the intersection (2.17) being continuous over each $\mathcal{J}_{\lambda+1/n}$ (equipped with its own topology) is continuous over their inductive limit, too. Conversely, every continuous linear functional over $\mathcal{K}_\lambda$ has to be continuous over each $\mathcal{J}_{\lambda+1/n}$, and consequently belongs to $\bigcap_{n=1}^{\infty} \mathcal{J}_{\lambda+1/n}'$.

The space $\mathcal{K}'_\lambda$, endowed with the strong topology of the dual, is a locally convex, separated space having a nondenumerable basis of neighborhoods. It is a complete space since $\mathcal{K}_\lambda$ is a bornological space.

Let us notice the following inclusion relations [which have the same meaning as in Eq. (2.8)]:

$$\mathcal{J}_{\lambda_3} \subset \mathcal{K}_{\lambda_2} \subset \mathcal{K}_{\lambda_1} \subset \mathcal{J}_{\lambda_1}, \quad \mathcal{J}'_{\lambda_1} \subset \mathcal{K}'_{\lambda_1} \subset \mathcal{K}'_{\lambda_2} \subset \mathcal{J}'_{\lambda_3}, \quad \lambda_1 < \lambda_2 < \lambda_3. \tag{2.18}$$

That $\mathcal{J}'_\lambda$ is strictly contained in $\mathcal{K}'_\lambda$ is exhibited by the distribution

$$\Delta_x = \theta(x - e)x^\lambda e^{(\log\log x)^2}, \tag{2.19}$$

which belongs to $\mathcal{K}'_\lambda$ but not to $\mathcal{J}'_\lambda$.

Considering finally the representation problem, we see from Eq. (2.17) that every $\Delta_x \in \mathcal{K}'_\lambda$ has a representation of the type (2.9) or (2.10) *when it operates on* $\mathcal{J}_\mu$, $\mu > \lambda$. However, as it was already pointed out in the Introduction, nothing prevents the parameters p and q from being dependent on μ in Eqs. (2.9) and (2.10) (in fact, the parameter q is irrelevant here since the logarithmic factor is removable when μ is varying). Clearly p can always be chosen as a nonincreasing, integer-valued function of μ which is allowed to grow indefinitely when $\mu \to \lambda$.

To summarize, Theorem 3 becomes a representation theorem valid for distributions $\Delta_x \in \mathcal{K}'_\lambda$ if we replace Eqs. (2.9) and (2.10) by

$$\Delta_x = x^{\lambda+1+1/n} D^{p_n}[x^{p_n - 1}\tilde{\Delta}_n(x)], \tag{2.9'}$$

$$\Delta_x = D^{p_n}[x^{\lambda+p_n+1/n}\tilde{\Delta}_n(x)], \quad \lambda \geq -1. \tag{2.10'}$$

Here, $\{p_n\}$ is a nondecreasing (eventually unbounded) sequence of positive integers, the index $n = 1, 2, \cdots$ referring to the test function space $\mathcal{J}_{\lambda+1/(n-1)}$ where Δ_x is operating.

For the sake of clarity, we shall give an example where the use of an unbounded sequence $\{p_n\}$ is unavoidable. The distribution

$$\Delta_x = \theta(x)\sum_{n=1}^{\infty}\frac{x^{1/n}}{n^2}\sin(x^{1/n^2}) \tag{2.20}$$

obviously belongs to $\mathcal{J}'_1$ [the right-hand side is $O(x)$]. Actually, it is possible to show that $\Delta_x \in \mathcal{J}'_{1/4N}$, $N = 1, 2, \cdots$, $\Delta_x \notin \mathcal{J}'_0$, and that Δ_x, *as an element of* $\mathcal{J}'_{1/4N}$, has for "best" representation (i.e., with minimal p)

$$\Delta_x = D^N[x^{N+1/4N}\tilde{\Delta}_N(x)] \tag{2.21}$$

with $\tilde{\Delta}_N(x)$ a bounded, continuous function with support $[0, \infty]$, such that $\limsup |\tilde{\Delta}_N(x)| > 0$ as $x \to \infty$.

In order to prove Eq. (2.21), let us write the distribution (2.20) in the form

$$\Delta_x = \sum_{n=1}^{\infty}\frac{1}{n^2}\Delta_n(x). \tag{2.22}$$

Then it can be shown by successive integrations that $\Delta_n(x)$ has the family of representations

$$\Delta_n(x) = D^p[x^{p+(1/n)-p/n^2}\tilde{\Delta}_{n,p}(x)], \quad p = 0, 1, \cdots, \tag{2.23}$$

where the functions $\tilde{\Delta}_{n,p}(x)$ have the properties required above for $\tilde{\Delta}_N(x)$.

Now, for given N, the formula (2.21) will follow from Eqs. (2.22) and (2.23) if one can find a $p = p(N)$ such that

$$p + (1/n) - p/n^2 \leq p + 1/4N, \quad n = 1, 2, \cdots.$$

This leads us to the optimal choice

$$p(N) = \max_{n\geq 1} n(1 - n/4N) = N.$$

Then

$$\Delta_n(x) = D^N[x^{N+1/4N}\tilde{\Delta}_{n,N}(x)]$$

with

$$\limsup_{x\to\infty} |\tilde{\Delta}_{n,N}(x)| = \begin{cases} \limsup_{x\to\infty} |\tilde{\Delta}_{2N,N}(x)| > 0, & n = 2N, \\ 0, & n \neq 2N, \end{cases}$$

so that

$$\limsup_{x\to\infty} |\tilde{\Delta}_N(x)| > 0.$$

Moreover, it is easy to convince oneself of the uniform convergence over $\mathbb{R}_+$ of the various series involved.

As a result, $\Delta_x \in \mathcal{K}'_0$ and the representation (2.10') applies with $p_n = n/4$, $n = 4, 8, \cdots$, but it does not apply with $p_n < n/4$.

Needless to say, such a peculiar behavior has no character of generality: It did not occur in our previous example (2.12), for which, however, we had $\Delta_x \in \mathcal{K}'_\lambda$ and $\Delta_x \notin \mathcal{J}'_\lambda$. In fact, the case $p_n \to \infty$ never happens for positive measures, according to part (4) of Theorem 3.

As a conclusion to this section, let us turn to the problem of the convolution in the spaces $\mathcal{J}_\lambda$ and $\mathcal{J}'_\lambda$. Some useful properties of this operation are contained in the following two lemmas, the proof of which will be given in Appendix B.

Lemma 3: Let $\{\Delta_x^{(i)}\}$ be a (finite) set of distributions $\Delta_x^{(i)} \in \mathcal{J}'_{\lambda_i}$, $\lambda_i + 1 \geq 0$, all their supports being bounded on the same side. Define λ by

$$\lambda + 1 = \sum_i (\lambda_i + 1) \geq 0.$$

Then the convolution product $(*_i \Delta^{(i)})_x$ exists and belongs to $\mathfrak{J}'_\lambda$. It is commutative and associative, and has its support bounded on the same side as the $\Delta_x^{(i)}$.

Lemma 4: Let $\{\Delta_x^{(i)}\}$ be a (finite) set of distributions $\Delta_x^{(i)} \in \mathfrak{J}'_{\lambda_i}$, $\lambda_i + 1 \geq 0$, all their supports being bounded on the right. Let $\varphi(x)$ be a test function $\in \mathfrak{J}_\mu$, with a support bounded on the left, and $\alpha(x)$ a bounded C^∞ function, also with a support bounded on the left and equal to 1 for x larger than a given number. If

$$\nu + 1 \equiv \mu + 1 - \sum_i (\lambda_i + 1) \geq 0,$$

then the convolution product $(*_i \Delta_x^{(i)} * \varphi)(x)$ exists and is commutative and associative, and $\alpha(x) \times (*_i \Delta^{(i)} * \varphi)(x)$ belongs to $\mathfrak{J}_\nu$.

As an immediate consequence of Lemma 4, one has the following.

Corollary: Let $\{\Delta_x^{(i)}\}$ be a (finite) set of distributions $\Delta_x^{(i)} \in \mathfrak{J}'_{\lambda_i}$, $\lambda_i + 1 \geq 0$, and $\varphi(x)$ a test function belonging to $\mathfrak{J}_\mu$, all these objects with supports bounded on the same side. If $\mu + 1 \geq \sum_i (\lambda_i + 1)$, then

$$\left\langle \left(\mathop{*}_{i=1}^{N} \Delta^{(i)} \right)_x, \varphi(x) \right\rangle = \left\langle \left(\mathop{*}_{i=2}^{N} \Delta^{(i)} \right)_x, (\check{\Delta}^{(1)} * \varphi)(x) \right\rangle, \tag{2.24}$$

where $\check{\Delta}_x^{(1)}$ is deduced from $\Delta_x^{(1)}$ by changing x into $-x$.

3. DISPERSION RELATIONS

We now are in a position to put our distributions Δ_x in correspondence with analytic functions by means of Cauchy integrals. Let us first remark that for $z \in \mathbb{C}$, $\operatorname{Im} z \neq 0$,

$$\alpha(x)/x^m(x - z) \in \mathfrak{J}_\lambda \quad \text{for any integer} \quad m \geq [\lambda + 1],$$

$\alpha(x)$ being C^∞ function with support $[a, \infty]$, such that $\alpha(x) = 1$ for $x \geq b > a$, $a > 0$.

Thus, expressions like $\langle \Delta_x, \alpha(x)/x^m(x - z) \rangle$ are meaningful as long as $\Delta_x \in \mathfrak{J}'_\lambda$. Moreover, if

$$\operatorname{supp} \Delta_x \subset [z_0, \infty],$$

we can always choose $b < z_0$, so that the previous expressions do not depend on the function $\alpha(x)$. In this way, taking for m the smallest admissible value, we are led to the natural generalization of the Cauchy integral for distributions:

$$F(z) = \pi^{-1} z^n \langle \Delta_x, \alpha(x)/x^n(x - z) \rangle, \quad n = [\lambda + 1]. \tag{3.1}$$

This equation is nothing but a dispersion relation with n subtractions (at the origin) for the function $F(z)$, if we identify the distribution $2i\Delta_x \in \mathfrak{J}'_\lambda$ with the "discontinuity" of $F(z)$ through the (positive) real axis. On the other hand, n is the minimum number of necessary subtractions if $\Delta_x \notin \mathfrak{J}'_{\lambda-1}$. In the following, these considerations will be given a precise meaning when $\lambda \geq -1$. Of course, the results will apply (and are of interest only) if the support of Δ_x is not compact (otherwise $\lambda = -\infty$).

Let us notice that, given z in $\mathbb{C}[z_0, +\infty]$, supp $\alpha(x)$ can always be chosen in such a way that Eq. (3.1) makes sense. As $F(z)$ does not depend on the accessory function $\alpha(x)$, this latter will be omitted in the following.

Furthermore, as the proofs of the subsequent propositions are almost straightforward (and often modified versions of standard proofs; cf., for example, Ref. 4), we shall generally be content with only sketching them.

Theorem 4: Let Δ_x be a distribution which belongs to $\mathfrak{J}'_\lambda$, $\lambda \geq -1$, and such that $\operatorname{supp} \Delta_x \subset [z_0, \infty]$, $z_0 > 1$. It has the representation (2.10) with

$$\operatorname{supp} \tilde{\Delta}(x) \subset [z_0, \infty].$$

Then, the function $F(z)$ defined by Eq. (3.1) is holomorphic in $\mathbb{C}[z_0, \infty]$ and bounded by

$$|F(z)| < C(1 + |z|)^\lambda [\log (2 + |z|)]^{q+1} \times \begin{cases} |\theta|^{-p}, & p \geq 1, \\ \log (4/|\theta|), & p = 0, \end{cases} \tag{3.2}$$

where

$$z = |z| e^{i\theta}, \quad -\pi < \theta \leq \pi.$$

Proof: The holomorphy of $F(z)$ for $z \in \mathbb{C}[z_0, \infty]$ is a direct consequence of the continuity of the linear functional Δ_x and of the holomorphy in z of the test function considered. In order to prove the bound (3.2), we insert the representation (2.10) into Eq. (3.1). This gives

$$F(z) = \sum_{m=0}^{p} C_{pm} F_m(z),$$

where

$$F_m(z) = z^n \int_{z_0}^{\infty} dx \tilde{\Delta}(x) (\log x)^q \frac{x^{\lambda+m-n}}{(x - z)^{m+1}}.$$

Then, splitting up the integration path in three parts, $(z_0, |z|/2)$, $(|z|/2, |z|)$, and $(|z|, \infty)$, we easily find suitable bounds in $|z|$ for the three corresponding pieces. We finally obtain

$$|F_m(z)| < C\, |z|^\lambda\, [\log (2 + |z|)]^{q+1} \times \int_{\frac{1}{2}}^{2} \frac{dt}{[(t - \cos \theta)^2 + \sin^2 \theta]^{(m+1)/2}},$$

$$m = 0, 1, \cdots, p.$$

Now, it is an elementary task to show that the last integral is $O(\theta^{-m})$ for $m \geq 1$ and $O(\log|\theta|)$ for $m = 0$. This leads to Eq. (3.2). QED

Let us notice that, as long as one only looks for a bound of $F(z)$ in $|z|$ free from logarithmic factors and for *fixed* $\theta \neq 0$, it suffices to show that the set of test functions $|z|^{n-\lambda-\epsilon}/x^n(x - |z|\, e^{i\theta})$ is a bounded set in $\mathfrak{J}_\lambda$ when $|z|$ goes from 0 to ∞. Would we not have the explicit representation of Δ_x at our disposal, it would be much less trivial to obtain a bound of the type (3.2) where some kind of "uniformity" in θ is preserved.

We now want to derive a reciprocal of Theorem 4. It is well known that the boundary value for $\operatorname{Im} z \to 0+$ (or $\operatorname{Im} z \to 0-$) of a function $F(z)$ holomorphic in $\mathbb{C}[-\infty, \infty]$, polynomially bounded at infinity, and regular enough in the vicinity of the real axis, generates a tempered distribution. More precisely, the discontinuity of $F(z)$ through the real axis can be defined as the distribution $2iA_x \in \mathcal{S}'$ such that

$$\langle A_x, \varphi(x)\rangle = \frac{1}{2i}\lim_{y\to 0+}\int_{-\infty}^{\infty} dx[F(x+iy) - F(x-iy)]\varphi(x), \quad \forall\ \varphi \in \mathcal{S}.$$

In the case we are interested in, as we insist on recovering distributions which belong to our spaces $\mathfrak{J}'_\lambda$, we have to adopt a somewhat different definition of the discontinuity $2iA_x$, which indeed is in the very nature of the problem.

Let $F(z)$ be given by Eq. (3.1) with $\Delta_x \in \mathfrak{J}'_\lambda$, $\operatorname{supp}\Delta_x \subset [z_0, \infty]$. We define its discontinuity $2iA_x$ through the real axis by

$$\langle A_x, \varphi(x)\rangle = \frac{1}{2i}\lim_{\theta\to 0+}\int_0^{\infty} dr[F(re^{i\theta}) - F(re^{-i\theta})]\varphi(r), \quad \forall\ \varphi \in \mathfrak{J}_\lambda. \tag{3.3}$$

That the integral of the right-hand side exists $\forall\ \theta \neq 0$ is an immediate consequence of the bound (3.2). That it generates a distribution $A_x \in \mathfrak{J}'_\lambda$ when $\theta \to 0+$ is ensured by the following proposition.

Lemma 5: The discontinuity $2iA_x$ of the function $F(z)$ is nothing but the distribution $2i\Delta_x$.

Proof: From Eqs. (3.1)–(3.3), we get

$$\langle A_x, \varphi(x)\rangle = \frac{1}{\pi}\lim_{\theta\to 0+}\int_0^{\infty} dr\langle\Delta_{x'}, \psi_{r,\theta}(x')\rangle, \tag{3.4}$$

where

$$\psi_{r,\theta}(x') = \frac{x'\sin(n\theta) - r\sin[(n-1)\theta]}{x'^n(x'^2 - 2x'r\cos\theta + r^2)} \times r^n\varphi(r) \in \mathfrak{J}_{n-\epsilon} \subset \mathfrak{J}_\lambda, \quad \forall\ r, \theta > 0.$$

Let us put

$$\Phi_\theta(x') = \int_0^\infty dr\psi_{r,\theta}(x') = \int_0^\infty dt\,\frac{\sin(n\theta) - t\sin[(n-1)\theta]}{t^2 - 2t\cos\theta + 1}\,\varphi(tx'). \tag{3.5}$$

Then, using Eq. (2.1) in order to get bounds on $D^p_{x'}\varphi(tx')$, we easily see that

$$D^p\Phi_\theta(x') \underset{|x'|\to\infty}{=} O[(\log|x'|)^{-q}\,|x'|^{-\lambda-p-1}], \quad \forall\ \theta > 0, \quad q, p = 0, 1, \cdots.$$

Since now $\Phi_\theta(x') \in \mathfrak{J}_\lambda$, the continuity of $\Delta_{x'}$ allows us to write Eq. (3.4) in the form

$$\langle A_x, \varphi(x)\rangle = \pi^{-1}\lim_{\theta\to 0+}\langle\Delta_{x'}, \Phi_\theta(x')\rangle.$$

Next, it can be shown from Eq. (3.5) that $\Phi_\theta(x')$ converges to $\pi\varphi(x')$ in the topology of $\mathfrak{J}_\lambda$ when $\theta \to 0+$. This implies, again via the continuity of $\Delta_{x'}$,

$$\langle A_x, \varphi(x)\rangle = \langle\Delta_{x'}, \varphi(x')\rangle, \quad \forall\ \varphi \in \mathfrak{J}_\lambda,$$

and the proof is complete. QED

We can now state our main theorem.

Theorem 5: Let $F(z)$ be a holomorphic function in $\mathbb{C}[z_0, \infty]$ which satisfies the bound (3.2). Then its discontinuity through the real axis [in the sense of Eq. (3.3)] is a distribution $2iA_x \in \mathfrak{J}'_\lambda$, and $\operatorname{supp} A_x \subset [z_0, \infty]$.

To establish it, we need the following lemma, the proof of which is postponed to Appendix C.

Lemma 6: Let $F_{(m)}(z)$ be a primitive of order m of the function $F(z)$ and $\rho(r)$ the function over $\mathbb{R}_+$ defined by

$$\rho(r) = (2i)^{-1}\lim_{\theta\to 0+}[F_{(p+1)}(re^{i\theta}) - F_{(p+1)}(re^{-i\theta})]. \tag{3.6}$$

Then [with $F_{(0)}(z) = F(z)$]

(1) $|F_{(m)}(z)| < C(1 + |z|)^{\lambda+m}[\log(2 + |z|)]^{q+2}$
$$\times \begin{cases} |\theta|^{-p+m}, & m = 0, \cdots, p-1 \text{ and } p \geq 1 \\ \log(4/|\theta|), & m = p \\ 1, & m = p+1 \end{cases}$$

(2) $\rho(r)$ is continuous over $\mathbb{R}_+$,

(3) $\operatorname{supp}\rho(r) \subset [z_0, \infty]$,

(4) $\rho(r) \underset{r\to\infty}{=} O[r^{\lambda+p+1}(\log r)^{q+2}]$.

Proof of the theorem: We start from the identity valid $\forall\ \varphi \in \mathfrak{J}_\lambda$:

$$\int_0^\infty dr[F(re^{i\theta}) - F(re^{-i\theta})]\varphi(r)$$
$$= (-1)^{p+1}\int_0^\infty dr[F_{(p+1)}(re^{i\theta}) - F_{(p+1)}(re^{-i\theta})]D^{p+1}\varphi(r). \tag{3.7}$$

It results from $(p + 1)$ integrations by parts, taking into account the bounds (1) of Lemma 6 at each step.

According to Eqs. (3.3) and (3.7),

$$\langle A_x, \varphi(x)\rangle = \frac{(-1)^{p+1}}{2i}\lim_{\theta\to 0+}\int_0^\infty dr \times [F_{(p+1)}(re^{i\theta}) - F_{(p+1)}(re^{-i\theta})]D^{p+1}\varphi(r).$$

Now, it suffices to use Eq. (3.6) together with the properties (3) and (4). Because of the absolute convergence of integrals, we can reverse the order of limit and integration, so that

$$\langle A_x, \varphi(x)\rangle = (-1)^{p+1}\int_{z_0}^\infty dr\rho(r)D^{p+1}\varphi(r).$$

Hence

$$A_x = D^{p+1}\rho(x), \tag{3.8}$$

and the conclusion follows from the properties (2)-(4) of Lemma 6 together with Theorem 3.

Collecting Theorems 4 and 5, Lemma 3, and the definition of the spaces $\mathcal{K}'_\lambda$ given in Sec. 2, we are led immediately to Theorem 1 of Sec. 1.

Let us remark that in Eq. (3.8), there is one more differentiation than in Eq. (2.10). This means that in case the function $F(z)$ in the hypothesis of Theorem 5 actually is generated by a distribution $\Delta_x \in \mathfrak{J}'_\lambda$ [and consequently satisfies the bound (3.3)], something has been lost in the above construction of A_x $(= \Delta_x)$. Thus, in a sense, we have not complete reciprocity. This is unavoidable unless we refine the bound (3.2). But this seems to be properly feasible only if we simultaneously add some regularity properties to the function $\tilde{\Delta}(x)$ of Eq. (2.10) (such as Hölder continuity), which is beyond the scope of this paper.

To conclude this section, let us quote a consequence of previous results, which is by no means surprising but yet demands to be proved because of our particular definition of the "discontinuity."

Corollary: Any function $F(z)$ which is holomorphic in $[z_0, \infty]$, has a given discontinuity $2i\Delta_x \in \mathcal{K}'_\lambda$ through the real axis, and satisfies the bound (B2) of Theorem 1 is determined up to an arbitrary polynomial of degree $[\lambda]$.

Proof: It is sufficient to show that if $\Delta_x = 0$, then $F(z)$ is such a polynomial.

Take a fixed ϵ in the bound (B2). From Eq. (3.8) and the unicity property (3) of Theorem 3,

$$\Delta_x = 0 \Rightarrow \rho(x) = 0.$$

Now, since

$$\lim_{\theta\to 0+} F_{(p+1)}(re^{i\theta}) \quad \text{and} \quad \lim_{\theta\to 0-} F_{(p+1)}(re^{i\theta})$$

are continuous functions over $\mathbb{R}_+$ [see Appendix C, Eq. (C4)ff.], $F_{(p+1)}(z)$ is an entire function (see Ref. 3). But then, according to property (1) of Lemma 6, it is a polynomial of degree $\leq \lambda + p + 1 + \epsilon$. Thus $F(z) = D^{p+1}F_{(p+1)}(z)$ is a polynomial of degree $[\lambda]$ since ϵ is arbitrarily small. QED

4. THE FROISSART-GRIBOV TRANSFORMATION

To prove Theorem 2, use could be made of an auxiliary function $F(z)$ as defined by Theorem 1 in terms of Δ_x and related to $f(l)$ by its Legendre polynomial expansion $F(z) = \pi^{-1}\sum_l (2l + 1)f(l)P_l(z)$. Then one would be led to perform a Sommerfeld-Watson transformation[20] on that expansion, in order to make full use of Theorem 1.

Here we shall rather follow another line of reasoning: we shall use a trick already proposed by Froissart,[1] which is to get rid of the Legendre function of the second kind $Q_l(x)$ by expressing it as an Abel transform (see Appendix D)[21]:

$$Q_l(x) = q_l(x) * \theta(-x)/\sqrt{-x}. \tag{4.1}$$

$q_l(x)$ is the following function:

$$q_l(x) = \begin{cases} 0, & x \leq 1, \\ 1/[2(x^2 - 1)]^{\frac{1}{2}}[x + (x^2 - 1)^{\frac{1}{2}}]^{l+\frac{1}{2}}, & x > 1. \end{cases} \tag{4.2}$$

Now consider a distribution $\Delta_x \in \mathfrak{J}'_\mu$, with a support contained in $[z_0, +\infty]$. We first notice that $\theta(x)/\sqrt{x} \in \mathfrak{J}'_{-\frac{1}{2}}$ and that $q_l(x) \in \mathfrak{J}_{\mathrm{Re}\, l+\frac{1}{2}-\epsilon}$, $\forall\ \epsilon > 0$. Then by virtue of Eq. (2.24), under the condition $-1 \leq \mu \leq \mathrm{Re}\, l - \epsilon$, one has

$$f(l) = \langle \Delta_x, [\theta(-x)/\sqrt{-x}] * q_l(x)\rangle$$
$$= \langle \Delta_x * [\theta(x)/\sqrt{x}], q_l(x)\rangle,$$

and the distribution

$$^A\Delta_x \equiv \Delta_x * \theta(x)/\sqrt{x} \tag{4.3}$$

belongs to $\mathfrak{J}'_{\mu+\frac{1}{2}}$. Let us define the distribution Γ_τ such that, for any test function $\varphi(x) \in \mathfrak{J}_{\mu+\frac{1}{2}}$,

$$\langle {}^A\Delta_x, \varphi(x)\rangle = \langle \Gamma_\tau, \sinh \tau\varphi(\cosh \tau)\rangle. \tag{4.4}$$

According to Lemma 2 (here, the mapping $z = \cosh \tau$ is not the one of Lemma 2, but the result still holds), $e^{-(\mu+\frac{1}{2})\tau}\Gamma_\tau$ is a tempered distribution. Furthermore, from the expression (4.2) of $q_l(x)$, one obtains

$$f(l) = (1/\sqrt{2})\langle \Gamma_\tau, e^{-(l+\frac{1}{2})\tau}\rangle, \qquad (4.5)$$

which makes $f(l)$ the Laplace transform of Γ_τ. Thus we have decomposed the Froissart–Gribov transformation into a product of three transformations:

(1) the Abel transformation (4.3),
(2) the isomorphism ${}^A\Delta_x \to \Gamma_\tau$ defined by (4.4),
(3) the Laplace transformation (4.5).

As $e^{-(\mu+\frac{1}{2})\tau}\Gamma_\tau$ is tempered, $f(l)$ is holomorphic in $\operatorname{Re} l > \mu$.[22] Moreover, from the support property (A2) of Δ_x, one easily deduces that $\operatorname{supp} \Gamma_\tau \subset [\arg\cosh z_0, +\infty]$. Consequently, $f(l)$ is bounded by[23]

$$|f(l)| < P_\mu(|l|) \exp[-(\arg\cosh z_0) \operatorname{Re} l] < P_\mu(|l|)[z_0 + (z_0^2 - 1)^{\frac{1}{2}}]^{-\operatorname{Re} l}, \qquad (4.6)$$

where $P_\mu(|l|)$ is a polynomial in $|l|$, the degree of which is precisely the number of derivations in the representation of Δ_x in $\mathfrak{J}'_\mu$.

Reciprocally, let $f(l)$ be holomorphic in $\operatorname{Re} l > \mu$ and bounded by (4.6). Then it is the Laplace transform (4.5) of a distribution Γ_τ such that $e^{-(\mu+\frac{1}{2}+\epsilon)}\Gamma_\tau$ is tempered $\forall\, \epsilon$, and with a support contained in $[\arg\cosh z_0, +\infty]$.[23] Equation (4.4) defines in terms of Γ_τ a distribution ${}^A\Delta_x$, the support of which is contained in $[z_0, +\infty]$ and which by virtue of Lemma 2 belongs to $\mathfrak{J}'_{\mu+\frac{1}{2}+\epsilon}$, $\forall\, \epsilon > 0$. Now Eq. (4.3), considered as a convolution equation in Δ_x, has a unique solution given by[21,24]

$$\Delta_x = \pi^{-1}\delta'_x * [\theta(x)/\sqrt{x}] * {}^A\Delta_x. \qquad (4.7)$$

According to Lemma 3, $[\theta(x)/\sqrt{x}] * {}^A\Delta_x$ belongs to $\mathfrak{J}'_{\mu+1+\epsilon}$. Then $\Delta_x \in \mathfrak{J}'_{\mu+\epsilon}$, $\forall\, \epsilon > 0$, and by using Eq. (2.24) one easily shows that $f(l)$ is the Froissart–Gribov transform of Δ_x.

Now suppose that Δ_x [always with the same support property (A2)] belongs to $\mathcal{K}'_\lambda$, that is to say to $\mathfrak{J}'_\mu$, $\forall\, \mu > \lambda$. Then, from the above arguments, $f(l)$ obviously enjoys properties (C1) and (C2). Reciprocally, such a function $f(l)$ is the Froissart–Gribov transform of a distribution Δ_x which belongs to $\mathfrak{J}'_\mu$, $\forall\, \mu > \lambda$, and thus also to $\mathcal{K}'_\lambda$, with a support contained in $[z_0, +\infty]$.

To complete the proof of Theorem 2, we have to prove Eq. (1.2). It will not be difficult, because each one of the three transformations which compose the Froissart–Gribov transformation can be easily inverted.

First of all, the inverse Laplace transform of $f(l)$ is[22]

$$\Gamma_\tau = \frac{\sqrt{2}}{2\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl e^{(l+\frac{1}{2})\tau} f(l), \quad \xi > \lambda. \qquad (4.8)$$

We already know that, because of the bound C_2 on $f(l)$, the support of Γ_τ is contained in

$$[\arg\cosh z_0, +\infty].$$

Then for positive τ

$$0 = \frac{\sqrt{2}}{2\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl e^{-(l+\frac{1}{2})\tau} f(l), \quad \xi > \lambda.$$

This enables us to give Γ_τ a new expression which will be useful in the following:

$$\Gamma_\tau = \frac{\sqrt{2}}{\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl \sinh(l + \tfrac{1}{2})\tau f(l), \quad \xi > \lambda. \qquad (4.9)$$

Equations (4.7), (4.4), and (4.9) define Δ_x in terms of $f(l)$. More precisely, let $\varphi(x)$ be a test function belonging to $\mathfrak{J}_\mu$, $\mu > \lambda$:

$$\begin{aligned}\langle \Delta_x, \varphi(x)\rangle &= -\pi^{-1}\langle[\theta(x)/\sqrt{x}] * {}^A\Delta_x, \varphi'(x)\rangle \\ &= -\pi^{-1}\langle {}^A\Delta_x, [\theta(-x)/\sqrt{-x}] * \varphi'(x)\rangle \\ &\qquad \text{by virtue of Eq. (2.24)}^{25} \\ &= -\pi^{-1}\langle \Gamma_\tau, \sinh\tau\psi(\cosh\tau)\rangle \\ &\qquad \text{by virtue of Eq. (4.4),}\end{aligned}$$

where, according to Lemma 4, the test function $\psi(x) \equiv [\theta(-x)/\sqrt{-x}] * \varphi'(x)$ belongs to $\mathfrak{J}_{\mu+\frac{1}{2}}$. Next, by definition of the integral (4.9),

$$\begin{aligned}-\frac{1}{\pi}\langle \Gamma_\tau, \sinh\tau\psi(\cosh\tau)\rangle &= \frac{1}{2\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl f(l) \\ &\quad \times \left\langle \frac{-2\sqrt{2}}{\pi}\sinh(l + \tfrac{1}{2})\tau, \sinh\tau\psi(\cosh\tau)\right\rangle.\end{aligned}$$

Coming back to the variable x, we can write the scalar product in the right-hand side as $\langle -\tilde{\omega}_l(x), \psi(x)\rangle$, where

$$\tilde{\omega}_l(x) = (2^{\frac{3}{2}}/\pi)\{[x + (x^2 - 1)^{\frac{1}{2}}]^{l+\frac{1}{2}} - [x - (x^2 - 1)^{\frac{1}{2}}]^{l+\frac{1}{2}}\}.$$

From the definition of $\psi(x)$ and according to Eq. (2.24),

$$\begin{aligned}-\langle \tilde{\omega}_l(x), \psi(x)\rangle &= \langle \delta'_x * [\theta(x)/\sqrt{x}] * \tilde{\omega}_l(x), \varphi(x)\rangle \\ &= \langle [\theta(x)/\sqrt{x}] * D\tilde{\omega}_l(x), \varphi(x)\rangle.\end{aligned}$$

The last equality comes from the associativity of the above double convolution product. Now

$$\frac{\theta(x)}{\sqrt{x}} * D\tilde{\omega}_l(x) = (2l+1)\frac{\sqrt{2}}{\pi} \times \frac{[x+(x^2-1)^{\frac{1}{2}}]^{l+\frac{1}{2}} + [x-(x^2-1)^{\frac{1}{2}}]^{l+\frac{1}{2}}}{(x^2-1)^{\frac{1}{2}}} * \frac{\theta(x)}{\sqrt{x}},$$

and the right-hand side of this equation is nothing but $(2l+1)P_l(x)$, where $P_l(x)$ is the Legendre function of the first kind (see Appendix D). Finally, collecting all these results, we get

$$\langle\Delta_x, \varphi(x)\rangle = \frac{1}{2\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl(2l+1)f(l)\langle P_l(x), \varphi(x)\rangle, \quad \xi > \lambda. \quad (4.10)$$

Let us note that $P_l(x)$ belongs to $\mathfrak{J}'_{\mathrm{Re}\,l}$. Thus $\langle P_l(x), \varphi(x)\rangle$ is meaningful if and only if $\mu \geq \mathrm{Re}\, l = \xi$, that is to say, $\varphi(x) \in \mathfrak{J}_\xi$. Furthermore,

$$(2l+1)\langle P_l(x), \varphi(x)\rangle = -(2^{\frac{1}{2}}/\pi)\langle e^{(l+\frac{1}{2})\tau} - e^{-(l+\frac{1}{2})\tau}, \sinh\tau\psi(\cosh\tau)\rangle. \quad (4.11)$$

The right-hand side is the sum of two terms (coming from $e^{\pm(l+\frac{1}{2})\tau}$) which, considered as functions of $\mathrm{Im}\,(l+\frac{1}{2})$, are, within constant factors, the Fourier transforms of

$$\chi_\pm(\tau) = e^{\pm(\xi+\frac{1}{2})\tau}\sinh\tau\psi(\cosh\tau).$$

But with $\psi(x)$ belonging to $\mathfrak{J}_{\mu+\frac{1}{2}}$, it results from Lemma 1 that $\chi_\pm(\tau)$ are fastly decreasing in τ when $\mu \geq \xi$. As a consequence $\langle P_l(x), \varphi(x)\rangle$ is also fastly decreasing in the variable[26] Im l and, due to the polynomial bound of $f(l)$ in Im l, the integral over l in Eq. (4.10) converges absolutely (and exponentially).

The formula (4.10) realizes the inversion of the Froissart–Gribov transformation. It can be written

$$\Delta_x = \frac{1}{2\pi i}\int_{\xi-i\infty}^{\xi+i\infty} dl(2l+1)f(l)P_l(x), \quad \xi > \lambda. \quad (4.12)$$

The right-hand side can be applied only on test functions belonging to $\mathfrak{J}_\xi$: It is indeed a representation of Δ_x in $\mathfrak{J}'_\xi$. As ξ can approach λ as close as one wants, Eq. (4.12) provides us with a set of representations of Δ_x in $\mathcal{K}'_\lambda$.

ACKNOWLEDGMENTS

We are much indebted to Dr. A. Connes for very interesting discussions. One of us (G. A.) is grateful to Professor C. Bloch for the hospitality extended to him at Saclay.

APPENDIX A

We give here (i) a detailed proof of the part (4) of Theorem 3 and (ii) the derivation of the asymptotic bound (2.13).

(i) Let Δ_x be a positive measure $\in \mathfrak{J}'_\lambda$, $\lambda \geq -1$, with supp $\Delta_x \subset [a, \infty]$. We have

$$H': \Delta_x \to \Gamma_\tau$$

with

$$\Gamma_\tau \in \mathcal{S}' \cap {}^+\mathcal{C}', \quad \mathrm{supp}\,\Gamma_\tau \subset [\log a, \infty], \quad (A1)$$

$${}^+\mathcal{C}' = \text{space of positive measures over } \mathbb{R}_\tau.$$

Then, according to a theorem of Schwartz,[17] $\Gamma_\tau = D\rho(\tau)$, where $\rho(\tau)$ is a nondecreasing function with support contained in $[\log a, \infty]$.

Thus, for $\Phi(\tau) \in \mathcal{S}$,

$$\langle\Gamma_\tau, \Phi(\tau)\rangle = -\int_{\log a}^\infty d\tau\rho(\tau)D\Phi(\tau). \quad (A2)$$

Since $\Gamma_\tau \in \mathcal{C}'$, we have also, for $\Phi(\tau) \in \mathcal{C}$,

$$\langle\Gamma_\tau, \Phi(\tau)\rangle = \int_{\log a}^\infty d\mu(\tau)\Phi(\tau). \quad (A3)$$

Moreover, according to another theorem[27] of Schwartz, property (A1) implies that μ is a tempered positive measure, i.e., such that

$$\int_{\log a}^T d\mu(\tau) < CT^q \quad \text{for some integer } q. \quad (A4)$$

Now, let $\chi(\tau)$ be a nonnegative C^∞ function bounded by 1 such that

$$\chi(\tau) = \begin{cases} 1 & \text{for } \tau \in [\log a, T] \\ 0 & \text{for } \tau \in \complement[\log a - \Delta, T+\Delta]. \end{cases}$$

As $\chi(\tau) \in \mathcal{S} \cap \mathcal{C}$, Eqs. (A2) and (A3) apply, giving respectively

$$\langle\Gamma_\tau, \chi(\tau)\rangle = \int_T^{T+\Delta} d\tau\rho(\tau)[-D\chi(\tau)] \geq \rho(T),$$

$$\langle\Gamma_\tau, \chi(\tau)\rangle = \int_{\log a}^{T+\Delta} d\mu(\tau)\chi(\tau) \leq \int_{\log a}^{T+\Delta} d\mu(\tau),$$

so that, from Eq. (A4),

$$\rho(\tau) < C\tau^q.$$

Then, using Eqs. (2.6), (2.11), and (A2), we get

$$\langle\Delta_x, \varphi(x)\rangle = -\int_a^\infty dx\sigma(x)D\varphi(x) \quad \forall\, \varphi \in \mathfrak{J}_\lambda, \quad (A5)$$

where

$$\sigma(x) = \rho(\log x)x^{\lambda+1} + \int_a^x dx'\rho(\log x')x'^\lambda \underset{x\to\infty}{=} O[(\log x)^{q+1}x^{\lambda+1}]. \quad (A6)$$

We finally obtain the desired result by a further integration by parts in Eq. (A5).

(ii) Let us take $\alpha \in \mathfrak{D}$ with supp $\alpha \subset [b, c]$. From Eqs. (A5) and (A6),

$$^{\alpha}\Delta(x) = \Delta_x * \alpha(x) = \langle \Delta_y, \alpha(x-y)\rangle = -\int_{x-c}^{x-b} dy\sigma(y)\alpha'(x-y),$$

$$|^{\alpha}\Delta(x)| < \sup_{b\le y\le c} \alpha'(y)\int_{x-c}^{x-b} dy\sigma(y) < C(\log x)^{q+1}x^{\lambda+1},$$

which leads to Eq. (2.13). QED

APPENDIX B

This appendix is devoted to the study of the convolution product in the spaces $\mathfrak{J}_\lambda$ and $\mathfrak{J}'_\lambda$. Of course, we want to define this product in such a way that it coincides with the convolution product in $\mathfrak{D}$ and $\mathfrak{D}'$. We first start with the following:

Proposition: Let Δ_x be a distribution in $\mathfrak{J}'_\lambda$, $\lambda + 1 \geq 0$, with its support bounded on the right (say contained in $[-\infty, -a]$, $a > 1$) and $\alpha(x)$ a function as defined in Lemma 4. Then the transformation $\varphi(x) \to \alpha(x)\langle\Delta_y, \varphi(x-y)\rangle$ is a continuous linear mapping of $\mathfrak{J}_\mu$ into $\mathfrak{J}_{\mu-(\lambda+1)}$, if $\mu \geq \lambda$.

Proof: Let $\varphi(x) \in \mathfrak{J}_\mu$. The scalar product $\psi(x) \equiv \langle\Delta_y, \varphi(x-y)\rangle$ exists if $\mu \geq \lambda$, and the support of $\psi(x)$ is the whole real axis. We want first to prove that $\psi(x)$ is a C^∞ function which behaves like the functions belonging to $\mathfrak{J}_\nu$ [with $\nu = \mu - (\lambda + 1)$] when x tends to $+\infty$. When x goes to $-\infty$, $\psi(x)$ is not well behaved. Then, if one multiplies $\psi(x)$ by $\alpha(x)$, the result will belong to $\mathfrak{J}_\nu$.

From Theorem 3, Δ_x has the representation (note the change of notation):

$$\Delta_x = D^p\tilde{\Delta}(x),$$

where $\tilde{\Delta}(x)$ is a continuous function with its support contained in $[-\infty, -a]$ and

$$|\tilde{\Delta}(x)| \leq C\,|x|^{\lambda+p}(\log|x|)^q. \quad \text{(B1)}$$

Then

$$\psi(x) = \int_{-\infty}^{-a} dy\tilde{\Delta}(y)\varphi^{(p)}(x-y).$$

Let us differentiate r times with respect to x under the integral sign the right-hand side of this equation. An elementary calculation shows that the resulting integral is absolutely convergent, which proves that $\psi(x) \in C^\infty$. More precisely, using for $\tilde{\Delta}(x)$ the bound (B1) and for $\varphi^{(k)}(x)$ the bound

$$|\varphi^{(k)}(x)| \leq C/(1+|x|)^{\mu+k+1}[\log(2+|x|)]^s \quad \text{for any } s,$$

one easily finds that for x sufficiently large

$$|\psi^{(r)}(x)| \leq \frac{C}{x^{\mu-\lambda+r}(\log x)^{s-q-2}}\int_a^\infty \frac{dy}{y\log^2 y}.$$

This inequality proves the announced behavior of $\psi(x)$.

To prove the continuity of the mapping $\varphi(x) \to \alpha(x)\psi(x)$, it is sufficient to consider a sequence $\{\varphi_n(x)\}$ converging to zero in $\mathfrak{J}_\mu$, that is to say, such that

$$|\varphi_n^{(k)}(x)| \leq \epsilon_{n,k,s}/(1+|x|)^{\mu+k+1}[\log(2+|x|)]^s, \quad \forall\, s,$$

with, for any fixed k and s, $\epsilon_{n,k,s} \to 0$ when $n \to \infty$.

Then, as previously, one easily shows that

$$|\psi_n^{(r)}(x)| \leq C\epsilon_{n,p+r,s}/(1+|x|)^{\mu-\lambda+r}[\log(2+|x|)]^{s-q-2}$$

from which it is not difficult to deduce that the sequence $\{\psi_n(x)\}$ converges to zero in $\mathfrak{J}_{\mu-(\lambda+1)}$. QED

When $\varphi(x) \in \mathfrak{D}$, $\psi(x)$ coincides with the usual convolution product: $\psi(x) = (\Delta * \varphi)(x)$ (regularized distribution). So, when $\varphi \in \mathfrak{J}_\mu$, we will still call $\psi(x)$ the convolution product $(\Delta * \varphi)(x)$.

We now prove Lemma 3. We first define the convolution product $(*_{i=1}^N \Delta^{(i)})_x$ by

$$\left\langle \left(\mathop{*}_{i=1}^{N} \Delta^{(i)}\right)_x, \varphi(x)\right\rangle = \langle\Delta_{x_1}^{(1)}, \langle\Delta_{x_2}^{(2)}, \cdots, \langle\Delta_{x_N}^{(N)}, \varphi(x_1+x_2+\cdots+x_N)\rangle\cdots\rangle\rangle \quad \text{(B2)}$$

From the above proposition, the right-hand side of this equation is defined when $\mu + 1 \geq \sum_i (\lambda_i + 1)$, through a succession of continuous linear mappings

$$\mathfrak{J}_\mu \to \mathfrak{J}_{\mu-(\lambda_N+1)} \to \cdots \to \mathfrak{J}_{\mu-\sum_{i=1}^N(\lambda_i+1)} \to \mathbb{C},$$

which proves that $(*_{i=1}^N \Delta^{(i)})_x$ is a distribution in $\mathfrak{J}'_\lambda$ with

$$\lambda + 1 = \sum_{i=1}^{N}(\lambda_i + 1).$$

By (B2), the product $(*_{i=1}^N \Delta^{(i)})_x$ is not obviously commutative and associative. That it is indeed commutative and associative results from the following facts:

(1) It coincides with the usual convolution product when $\varphi(x) \in \mathfrak{D}$;

(2) the convolution product in $\mathfrak{D}'$ is commutative and associative[28];

(3) $\mathfrak{D}$ is dense in $\mathfrak{J}_\mu$.

Property (1) is obvious, and the proof of the third one is left to the reader. Finally, the support property of the product trivially results from its definition (B2).

Now Lemma 4 appears as an immediate consequence of the above proposition and Lemma 3. The proposition is indeed nothing but Lemma 4 in the case where there is only one distribution $\Delta_x^{(i)}$.

The proof of corollary (2.24) goes as follows: Consider the set of N distributions $\Delta_x^{(i)} \in \mathfrak{J}'_{\lambda_i}$, $\lambda_i + 1 \geq 0$, and the test function $\varphi(x) \in \mathfrak{J}_\mu$, all these objects having their supports contained, say, in $[a, +\infty]$. Define the distributions $\check{\Delta}_x^{(i)}$ deduced from $\Delta_x^{(i)}$ by changing x into $-x$. Under the condition

$$\mu + 1 \geq \sum_{i=1}^{N} (\lambda_i + 1),$$

one has successively

$$\left\langle \left(\mathop{*}_{i=1}^{N} \Delta^{(i)} \right)_x, \varphi(x) \right\rangle = \left(\mathop{*}_{i=1}^{N} \check{\Delta}^{(i)} * \varphi \right)(0)$$

$$= \left[\left(\mathop{*}_{i=2}^{N} \check{\Delta}^{(i)} \right) * (\check{\Delta}^{(1)} * \varphi) \right](0)$$

by virtue of Lemma 4

$$= \left\langle \left(\mathop{*}_{i=2}^{N} \Delta^{(i)} \right)_x, (\check{\Delta}^{(1)} * \varphi)(x) \right\rangle.$$

APPENDIX C: PROOF OF LEMMA 6

For $m = 0$, the property (1) is nothing but the bound (3.2) (with $q \to q + 1$).

Suppose now that this property holds for some $m < p$, $p \geq 1$, and choose $\theta_0 > 0$. We have

$$F_{(m+1)}(re^{i\theta}) = F_{(m+1)}(0) + \int_0^r dr' e^{i\theta_0} F_{(m)}(r'e^{i\theta_0}) + \int_{\theta_0}^{\theta} d\theta' re^{i\theta'} F_{(m)}(re^{i\theta'}).$$

But

$$|F_{(m)}(r'e^{i\theta_0})| < C(1 + r')^{\lambda+m}[\log(2 + r')]^{q+2}, \quad r' \in [0, \infty[,$$

$$|F_{(m)}(re^{i\theta'})| < C(1 + r)^{\lambda+m}[\log(2 + r)]^{q+2}\theta'^{-p-m}, \quad \theta' \in]0, \pi].$$

Thus, $\forall\, r \geq 0$, $0 < \theta \leq \pi$, we get

$$|F_{(m+1)}(re^{i\theta})| \leq |F_{(m+1)}(0)| + \int_0^r dr' \, |F_{(m)}(r'e^{i\theta_0})| + r\int_{\theta_0}^{\theta} d\theta' \, |F_{(m)}(re^{i\theta'})|$$
$$< C(1 + r)^{\lambda+m+1}[\log(2 + r)]^{q+2} \times \begin{cases} \theta - p + m + 1, & m + 1 < p, \\ \log(4/\theta), & m + 1 = p, \end{cases} \tag{C1}$$

and a similar result for $-\pi < \theta < 0$, so that the property (1) is true also for $(m + 1)$ and, by induction, for all $m = 0, 1, \cdots, p$. Next,

$$F_{(p+1)}(re^{i\theta}) = F_{(p+1)}(re^{i\theta_0}) + \int_{\theta_0}^{\theta} d\theta' re^{i\theta'} F_{(p)}(re^{i\theta'}), \tag{C2}$$

which implies, as above,

$$|F_{(p+1)}(re^{i\theta})| < C(1 + r)^{\lambda+p+1}[\log(2 + r)]^{q+2} \times \int_{\theta_0}^{\theta} d\theta' \log\frac{4}{\theta'}.$$

Hence

$$|F_{(p+1)}(z)| < C(1 + |z|)^{\lambda+p+1}[\log(2 + |z|)]^{q+2}, \tag{C3}$$

which concludes the proof of property (1).

Now, from the absolute convergence of the integral appearing in the left-hand side of Eq. (C2) for all θ, we deduce that both limits

$$\lim_{\theta \to 0\pm} F_{(p+1)}(re^{i\theta})$$

exist $\forall\, r \geq 0$ and generate two functions over $\mathbb{R}_+$ verifying the bound (C3). Inserting this bound into Eq. (3.6), one obtains the property (4).

The continuity of $\rho(r)$ follows from a similar argument. According to Eqs. (C2) and (C1), we have, for fixed $r_1 \geq 0$, $r_2 = r_1 + \Delta r$, and $0 < \theta < \theta_0$,

$$|F_{(p+1)}(r_2e^{i\theta}) - F_{(p+1)}(r_1e^{i\theta})|$$
$$\leq |F_{(p+1)}(r_2e^{i\theta_0}) - F_{(p+1)}(r_1e^{i\theta_0})| + \int_{\theta}^{\theta_0} d\theta' \, |r_2F_{(p)}(r_2e^{i\theta'}) - r_1F_{(p)}(r_1e^{i\theta'})|$$
$$< o(r_1, \theta_0; \Delta r) + a(r_1)\int_{\theta}^{\theta_0} d\theta' \log\frac{4}{\theta'}$$
$$< o(r_1, \theta_0; \Delta r) + b(r_1)\theta_0 \log\frac{4}{\theta_0}, \tag{C4}$$

where

$$\lim_{\Delta r \to 0} o(r_1, \theta_0; \Delta r) = 0, \quad \forall\, r_1, \theta_0. \tag{C5}$$

As the last member of Eq. (C4) no longer depends on θ, this inequality remains true in the limit $\theta \to 0+$. Therefore,

$$|\rho(r + \Delta r) - \rho(r)| < o(r, \theta_0; \Delta r) + b(r)\theta_0 \log(4/\theta_0), \quad \forall\, r \geq 0,\ \theta_0 > 0. \tag{C6}$$

Since θ_0 is arbitrarily small, the continuity property (2) results from Eqs. (C5) and (C6).

Finally, the support property (3) is an immediate consequence of the holomorphy of $F_{(p+1)}(z)$ in $\mathbb{C}[z_0, \infty]$. QED

APPENDIX D: INTEGRAL REPRESENTATIONS OF $P_l(x)$ AND $Q_l(x)$

When $\tau > 0$ and Re $(l + 1) > 0$, one has[29]

$$P_l(\cosh \tau) = \frac{\sqrt{2}}{\pi}\int_0^{\tau} d\tau' \frac{\cosh (l+\frac{1}{2})\tau'}{(\cosh \tau - \cosh \tau')^{\frac{1}{2}}},$$

$$Q_l(\cosh \tau) = \frac{1}{\sqrt{2}}\int_{\tau}^{\infty} d\tau' \frac{e^{-(l+\frac{1}{2})\tau'}}{(\cosh \tau' - \cosh \tau)^{\frac{1}{2}}}.$$

By the change of variable $x = \cosh \tau$, these representations become

$$P_l(x) = \int_1^x \frac{dx'}{(x-x')^{\frac{1}{2}}}\, p_l(x'), \tag{D1}$$

$$Q_l(x) = \int_x^{\infty} \frac{dx'}{(x'-x)^{\frac{1}{2}}}\, q_l(x'), \tag{D2}$$

where

$$p_l(x) = \begin{cases} 0, & x \le 1, \\ \dfrac{1}{\pi\sqrt{2}} \dfrac{[x+(x^2-1)^{\frac{1}{2}}]^{l+\frac{1}{2}} + [x-(x^2-1)^{\frac{1}{2}}]^{l+\frac{1}{2}}}{(x^2-1)^{\frac{1}{2}}}, & x > 1, \end{cases}$$

$$q_l(x) = \begin{cases} 0, & x \le 1, \\ \dfrac{1}{[2(x^2-1)]^{\frac{1}{2}}[x+(x^2-1)^{\frac{1}{2}}]^{l+\frac{1}{2}}}, & x > 1. \end{cases}$$

In Eqs. (D1) and (D2), $P_l(x)$ and $Q_l(x)$ appear as Abel transforms. Precisely, one can write

$$P_l(x) = p_l(x) * [\theta(x)/\sqrt{x}], \tag{D3}$$

$$Q_l(x) = q_l(x) * [\theta(-x)/\sqrt{-x}]. \tag{D4}$$

Note that

$$P_l(x) \in \mathfrak{J}'_{\mathrm{Re}\, l}, \quad Q_l(x) \in \mathfrak{J}_{\mathrm{Re}\, l-\epsilon}, \quad \forall\, \epsilon > 0.$$

[1] M. Froissart, Phys. Rev. **123**, 1053 (1961); V. N. Gribov, Zh. Eksp. Teor. Fiz. [Sov. Phys. JETP **14**, 478, 1395 (1962)].

[2] For simplicity, we shall assume that $F(z)$ has no left-hand cut and is holomorphic in the complex z plane cut from z_0 to $+\infty$, with $z_0 > 1$. Then $\Delta(x)$ is defined on $[z_0, +\infty]$. We shall denote the cut plane by $C[z_0, +\infty]$. Moreover, all through this paper, we shall never be concerned with the dependence of $F(z)$ in an energy variable.

[3] We remind the reader that a necessary and sufficient condition for $F(z)$ to have a discontinuity which is a distribution is that when z approaches a point x on the cut, $|F(z)|$ be bounded by some power of the inverse of the distance of z to the cut (the power may depend on x). See, for example, R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics and All That* (Benjamin, New York, 1964), Chap. 2.

[4] The dependence of $p(\epsilon)$ on ϵ, and the possibility that $p(\epsilon)$ indefinitely increases when ϵ goes to zero, are related to a property of the distributions in $\mathcal{K}'_\lambda$. This will be discussed later on.

[5] H. Epstein, V. Glaser, and A. Martin, Commun. Math. Phys. **13**, 257 (1969).

[6] H. J. Bremermann and L. Durand III, J. Math. Phys. **2**, 240 (1961); H. J. Bremermann, *Distribution, Complex Variables and Fourier Transforms* (Addison-Wesley, Reading, Mass., 1965), Chap. 6.

[7] I. M. Gel'fand and G. E. Shilov, *Generalized Functions* (Academic, New York, 1968), Vols. 2 and 3.

[8] Concerning the dependence on ϵ of $p_\epsilon(l)$, see Footnote 4.

[9] L. Schwartz, *Théorie des distributions* (Hermann, Paris, 1966), Chap. VII.

[10] S. Mandelstam, Phys. Rev. **112**, 1344 (1958).

[11] See, for example, L. Robin, *Fonctions sphériques de Legendre et fonctions sphéroidales* (Gauthier-Villars, Paris, 1958), Chap. VI, Eq. (130).

[12] Reference 9, Chap. VII, Paragraph 3.

[13] The choice of the factor $(\cosh \tau)^{\lambda+1}$ is by no means unique. Only its asymptotic behavior is prescribed, and we have taken the most convenient form ensuring the validity of the statement.

[14] N. Bourbaki, *Eléments de mathématiques, Espaces vectoriels topologiques* (*Livre V*) (Hermann, Paris, 1953–1955), Chap. IV, Paragraph 3.

[15] Reference 9, Chap. VII, Theorem VI.

[16] Reference 9, Chap. VI, Theorem XIV.

[17] Reference 9, Chap. II, Paragraph 4.

[18] Reference 14, Chap. II, Paragraph 2, No. 4.

[19] L. V. Kantorivich and G. P. Akilov, *Functional Analysis in Normed Spaces* (Pergamon, New York, 1964), Chap. XI, Paragraph 5.6.

[20] T. Regge, Nuovo Cimento **14**, 951 (1959).

[21] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford U.P., Oxford, 1948), Chap. XI, Paragraph 14.

[22] Reference 9, Chap. VIII.

[23] Reference 9, p. 310, Remarque 2.

[24] Reference 9, Chap. VI, Paragraph 10.

[25] The reader will verify that each time we invoke Lemmas 3 and 4 or Corollary (2.24), the conditions for their validity are fulfilled.

[26] Reference 9, Chap. VII, Theorem XII.

[27] Reference 9, Chap. VII, Theorem VII.

[28] Reference 9, Chap. VI, Theorem XIII.

[29] H. Bateman, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Chap. III, Paragraph 3.7.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Classification of the Harrison Metrics*

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(Received 7 July 1970)

Harrison's 40 space–time metrics have been checked to see if they represent vacuum solutions. Four of them are found to be nonvacuum. The Petrov classification is found for all the metrics, and those of type D are placed in their (invariantly defined) Kinnersley classes.

I. INTRODUCTION

In 1959 Harrison published 30 exact solutions of the Einstein vacuum field equations.[1] Twenty of these solutions are nondegenerate in the sense that they appear to depend on three variables. Since these metrics are exceedingly complicated, very little work has been done with them.

One of the present authors has developed a computer system called ALAM for carrying out algebraic manipulation.[2,3] ALAM was used to carry out all the calculations described in Secs. II and IV. In Sec. II Harrison's solutions are outlined and the results of a direct check to see whether they correspond to vacuum solutions are given. Section III describes an algorithm for determining the Petrov type of a metric, and Sec. IV gives the Petrov classification of Harrison's metrics. In Sec. V, the type D metrics are placed in their invariantly defined Kinnersley[4] classes.

II. HARRISON'S SOLUTIONS OF THE VACUUM FIELD EQUATIONS

In his paper[1] Harrison seeks exact three variable solutions of the Einstein vacuum field equations $R_{\mu\nu} = 0$, for a diagonal metric of the "linked-pair" form

$$g_{\mu\nu} = \delta_{\mu\nu} e_\nu A_\nu^2(x^0, x^1) B_\nu^2(x^0, x^3) \qquad (1)$$

(where Greek indices run from 0 to 3 and $e_0 = 1$ and $e_1 = e_2 = e_3 = -1$, which is the opposite signature to that used by Harrison). He calls solutions which apparently cannot be reduced to functions of two variables "nondegenerate," and those which can "degenerate."[5] We shall adhere to this terminology in this paper. He finds 18 nondegenerate solutions which he labels

I-B-1 to I-B-4,

II-A-1 to II-A-7,

II-B-1 to II-B-3,

II-C-1 to II-C-4,

where I and II refer to the functional form of the metrics and not to their Petrov type. He also includes 12 degenerate solutions labeled

III-1 to III-12.

We have relabeled I-A-1 and I-A-2 by III-11 and III-12, respectively, since they are degenerate (see Appendix A).

The solutions contain parameters which are either arbitrary (λ and l) or which can independently take on the values ± 1 (the ϵ's), and eight of them contain functions each of which is a solution of a first-order ordinary differential equation. However, we have found that, if a particular metric tensor is to remain real, then, since all factors raised to nonintegral powers must be positive, the ϵ's may have to satisfy certain restrictions:

(i) II-A-2, II-A-3, II-B-1, II-C-2; no solutions exist for $\epsilon_2 = -1$;

(ii) II-A-4, II-A-5, II-C-3; $x_3 \gtrless 0$ requires that $\epsilon_1 = \pm 1$;

(iii) II-B-2; $x_0 \gtrless 0$ requires that $\epsilon_2 = \pm 1$.

For convenience, we have omitted the parameter l which, in each case, merely multiplies the metric by a constant conformal factor which does not affect any of the analysis.

Harrison points out that ten additional metrics may be obtained by replacing any appearance of $\sinh\theta$, where θ is a function of the coordinates, by $\cosh\theta$ or e^θ. The three possibilities $\sinh\theta$, $\cosh\theta$, and e^θ are labeled (a), (b), and (c), respectively in this paper.

ALAM was used to calculate the Ricci tensor in order to check directly whether these 40 metrics actually represent vacuum solutions. In fact, four metrics, I-B-1(b), I-B-1(c), I-B-2, and III-6, were found to be nonvacuum, whereas the remainder are indeed vacuum (see Table II, Sec. IV). The mixed components of the energy–momentum tensors for the nonvacuum metrics are given in Appendix B. Harrison obtained sixteen of the metrics directly by solving the vacuum field equations, and thirteen others were generated from these by complex coordinate transformations. In his thesis[6] Harrison claims that I-B-2 was obtained in this manner, but, since I-B-2 is not a vacuum metric, no such transformation can exist.

III. AN ALGORITHM FOR DETERMINING PETROV TYPE

The Weyl tensor $C_{\mu\nu\rho\sigma}$ defines a symmetric spinor Ψ_{ABCD} by the equivalence

$$C_{\mu\nu\rho\sigma} \leftrightarrow \Psi_{ABCD}\epsilon_{\dot{W}\dot{X}}\epsilon_{\dot{Y}\dot{Z}} + \Psi_{\dot{W}\dot{X}\dot{Y}\dot{Z}}\epsilon_{AB}\epsilon_{CD} \quad (2)$$

where ϵ_{AB} is the Levi-Civita alternating symbol in two dimensions.[7] Every symmetric spinor can be decomposed canonically into a symmetrized product of principal 1-spinors

$$\Psi_{ABCD} = \alpha_{(A}\beta_B\gamma_C\delta_{D)} \quad \text{say}, \quad (3)$$

the α_A, β_A, γ_A, and δ_A thus determining the principal null directions of $C_{\mu\nu\rho\sigma}$. The necessary and sufficient condition for an arbitrary spinor ζ^A to be a principal spinor of Ψ_{ABCD} is

$$\Psi_{ABCD}\zeta^A\zeta^B\zeta^C\zeta^D = 0. \quad (4)$$

The Petrov classification is given by the multiplicity of the roots of this equation.

Expanding (4) out into components and, provided that $\Psi_0 \not\equiv 0$, dividing by $(\zeta^1)^4$, we obtain

$$\Psi_0 z^4 + 4\Psi_1 z^3 + 6\Psi_2 z^2 + 4\Psi_3 z + \Psi_4 = 0, \quad (5)$$

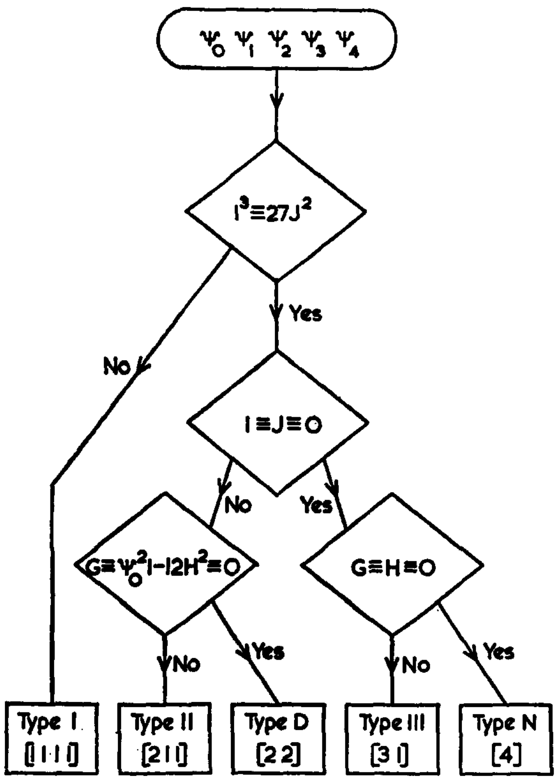

FIG. 1. Flow diagram for determining the Petrov type from the Ψ's.

TABLE I. The case $\Psi_0 \equiv \Psi_4 \equiv 0$, where $D \equiv 9\Psi_2^2 - 16\Psi_1\Psi_3$.

$\Psi_1 \equiv 0$	$\Psi_2 \equiv 0$	$\Psi_3 \equiv 0$		0
		$\Psi_3 \not\equiv 0$		III
	$\Psi_2 \not\equiv 0$	$\Psi_3 \equiv 0$		D
		$\Psi_3 \not\equiv 0$		II
$\Psi_1 \not\equiv 0$	$\Psi_2 \equiv 0$	$\Psi_3 \equiv 0$		III
		$\Psi_3 \not\equiv 0$		I
	$\Psi_2 \not\equiv 0$	$\Psi_3 \equiv 0$		II
		$\Psi_3 \not\equiv 0$	$D \equiv 0$	II
			$D \not\equiv 0$	I

where $z = \zeta^0/\zeta^1$ and Ψ_0, Ψ_1, Ψ_2, Ψ_3, and Ψ_4 are the Newman–Penrose scalars[8] defined in terms of the Weyl tensor and a null tetrad $(l^\alpha, n^\alpha, m^\alpha, \bar{m}^\alpha)$ by

$$\begin{aligned}
\Psi_0 &= -C_{\alpha\beta\gamma\delta}l^\alpha m^\beta l^\gamma m^\delta,\\
\Psi_1 &= -C_{\alpha\beta\gamma\delta}l^\alpha n^\beta l^\gamma m^\delta,\\
\Psi_2 &= -\tfrac{1}{2}C_{\alpha\beta\gamma\delta}(l^\alpha n^\beta l^\gamma n^\delta - l^\alpha n^\beta m^\gamma \bar{m}^\delta),\\
\Psi_3 &= C_{\alpha\beta\gamma\delta}l^\alpha n^\beta n^\gamma \bar{m}^\delta,\\
\Psi_4 &= -C_{\alpha\beta\gamma\delta}n^\alpha \bar{m}^\beta n^\gamma \bar{m}^\delta.
\end{aligned}$$

Equation (5) is a quartic with algebraic expressions as coefficients.

Defining

$$\begin{aligned}
I &\equiv \Psi_0\Psi_4 - 4\Psi_1\Psi_3 + 3\Psi_2^2,\\
J &\equiv \begin{vmatrix} \Psi_0 & \Psi_1 & \Psi_2 \\ \Psi_1 & \Psi_2 & \Psi_3 \\ \Psi_2 & \Psi_3 & \Psi_4 \end{vmatrix},\\
G &\equiv \Psi_0^2\Psi_3 - 3\Psi_0\Psi_1\Psi_2 + 2\Psi_1^3,\\
H &\equiv \begin{vmatrix} \Psi_0 & \Psi_1 \\ \Psi_1 & \Psi_2 \end{vmatrix},
\end{aligned}$$

we see that the necessary and sufficient conditions for (5) to have

(i) at least two equal roots is $I^3 \equiv 27J^2$,
(ii) at least three equal roots is $I \equiv J \equiv 0$,
(iii) four equal roots is $G \equiv H \equiv I \equiv 0$,
(iv) two pairs of equal roots is

$$G \equiv \Psi_0^2 I - 12H^2 \equiv 0.$$

The algorithm for determining the Petrov type can be conveniently displayed in the form of a flow diagram (Fig. 1).

If $\Psi_0 \equiv 0$, but $\Psi_4 \not\equiv 0$, we divide the expanded form of (4) by $(\zeta^0)^4$ instead to obtain a quartic in (ζ^1/ζ^0). We then interchange Ψ_0 with Ψ_4 and Ψ_1 with Ψ_3 in the definitions of I, J, G, and H and in condition (iv), and the algorithm proceeds as before. If, however, both Ψ_0 and Ψ_4 vanish identically, then, although the above algorithm still applies, the work may be simplified considerably; the classification for this case is summarized in Table I.

IV. THE PETROV CLASSIFICATION OF HARRISON'S METRICS

In the last section we presented an algorithm for determining the Petrov type of a metric. Since an algorithm is an unambiguous procedure for a mechanizable solution of a problem, it is susceptible to being programmed for a computer. Such a program was written in ALAM. The program evaluates the Weyl tensor and, for a given null tetrad, the Newman–Penrose scalars, and then proceeds to apply the algorithm. Since the metrics are diagonal, it is straightforward to construct an orthonormal tetrad (we chose unit vectors along the coordinates lines) and hence to construct a null tetrad in the usual way.

By this procedure, we determined the Petrov type, at every point, of all the algebraically special Harrison metrics. However, the calculation for the remaining metrics in many cases proved to be too complicated for ALAM. We therefore proceeded in the following manner. From Sec. III, the condition for a metric to be algebraically special is

$$I^3 \equiv 27J^2. \tag{6}$$

This relationship is an identity, and, if we can find some value or values of the coordinates for which the left-hand side is different from the right-hand side, then we may conclude that the corresponding metric is of Petrov type I since the identity is violated. A metric cannot change to a higher type on a closed subset, but may change to a lower type. It is therefore possible that these metrics become algebraically special on some subspaces of lower dimension.[9] For some metrics it was sufficient to test for violation of the identity (6) on a subspace, whereas for the more complicated metrics it was necessary to test at a point. Of course, care had to be taken to choose values of the coordinates for which the expressions in (6) were real and finite. With this technique, all the remaining metrics were classified. The results are given in Table II.

V. THE TYPE D METRICS

Fourteen of Harrison's metrics are of type D. Kinnersley[4] has recently found all type D vacuum solutions and classified them invariantly, and so it is of interest to find the Kinnersley class to which each of these Harrison metrics belong. Kinnersley chooses coordinates (u, r, x, y) such that one of the principal null directions is $l^\mu = \delta^\mu_1$, and he makes r an affine parameter along l^μ. To find the required coordinate transformation, we choose one of the principal null directions of each Harrison metric and found the corresponding transformation to l^μ. This, coupled with the fact that $g_{01} = 1$ in Kinnersley's form of the metrics, gives the complete r-dependence of the

TABLE II. Classification of the Harrison metrics.

Nondegenerate metrics				Degenerate metrics			
	Vacuum?				Vacuum?		
Metric	Yes	No	Petrov type	Metric	Yes	No	Petrov type
I-B-1(a)	√		I	III-1	√		D
I-B-1(b)		√	I	III-2	√		D
I-B-1(c)		√	I	III-3	√		D
I-B-2		√	I	III-4(a)	√		D
I-B-3	√		I	III-4(b)	√		D
I-B-4	√		I	III-4(c)	√		O
II-A-1	√		I	III-5	√		I
II-A-2	√		I	III-6		√	I
II-A-3	√		I	III-7(a)	√		D
II-A-4	√		I	III-7(b)	√		D
II-A-5	√		I	III-7(c)	√		D
II-A-6	√		I	III-8	√		D
II-A-7	√		I	III-9(a)	√		D
II-B-1	√		I	III-9(b)	√		D
II-B-2	√		I	III-9(c)	√		D
II-B-3	√		I	III-10	√		D
II-C-1	√		I	III-11	√		I
II-C-2	√		I	III-12(a)	√		I
II-C-3	√		I	III-12(b)	√		I
II-C-4	√		I	III-12(c)	√		D

TABLE III. The Kinnersley classification of the type D metrics.

Metric	Transformation to Kinnersley's form	Kinnersley class
III-1	$x_0 = r,\ \ x_1 = x,\ \ x_2 = \frac{1}{2}r^2 - u,\ \ x_3 = y.$	I (NUT[a]; $\mu_0 = \rho_0 = 0$)
III-2	$x_0 = \ln u^2,\ \ x_1 = (\lambda^2 r/x^2) - (2\lambda x/u),\ \ x_2 = \ln(x/\lambda u^2),\ \ x_3 = y$	IV.B ($C = 0$)
III-3	$x_0 = (2r/x^2) + u,\ \ x_1 = (1 + \gamma^2 x^4)^{\frac{1}{2}}/4\gamma,\ \ x_2 = (2r/x^2) - u,\ \ x_3 = \tan^{-1}(\gamma x^2),$ $\gamma = [4(1-y)]^{-1}$	IV.B ($C = 0$)
III-4(a)	$x_0 = u[(r^2/2u) + 1]^{\frac{1}{2}},\ \ x_1 = 2x,\ \ x_2 = 2y,\ \ x_3 = \ln[(r^2/2u) + 1]^{\frac{1}{2}}$	I (NUT[a]; $\mu_0 = \rho_0 = 0$)
III-4(b)	$x_0 = u[(r^2/2u) - 1]^{\frac{1}{2}},\ \ x_1 = 2x,\ \ x_2 = 2y,\ \ x_3 = \ln[(r^2/2u) - 1]^{\frac{1}{2}}$	I (NUT[a]; $\mu_0 = \rho_0 = 0$)
III-7(a)	$x_0 = \cosh^{-1}[(ur/x^2) + 1],\ \ x_1 = \frac{1}{2}\ln\tanh\frac{1}{2}\cosh^{-1}[(ur/x^2) + 1] - \ln u^{\frac{1}{2}},$ $x_2 = y,\ \ x_3 = [1 - (2x)^{-1}]^{\frac{1}{2}}$	IV.B ($C = \frac{1}{2}$)
III-7(b)	$x_0 = \sinh^{-1}[(r\sigma/2x^2) + \rho],\ \ x_1 = \tan^{-1}(e^{x_0}) - \tan^{-1}\rho,\ \ x_2 = y,$ $x_3 = [1 - (2x)^{-1}]^{\frac{1}{2}}$ ($\sigma = 3u^2 + 2^{\frac{5}{2}}u + 3,\ \rho = 3u + 2^{\frac{1}{2}}$)	IV.B ($C = \frac{1}{2}$)
III-7(c)	$x_0 = \ln(r/2x^2),\ \ x_1 = -(x^2/r) - u,\ \ x_2 = y,\ \ x_3 = [1 - (2x)^{-1}]^{\frac{1}{2}}$	IV.B ($C = \frac{1}{2}$)
III-8	$x_0 = \cos^{-1}[1 - (ur/x^2)],\ \ x_1 = \frac{1}{2}\ln\tan\frac{1}{2}\cos^{-1}[1 - (ur/x^2)] + \ln u^{\frac{1}{2}},\ \ x_2 = y,$ $x_3 = [(2x)^{-1} - 1]^{\frac{1}{2}}$	IV.B ($C = -\frac{1}{2}$)
III-9(a)	$x_0 = -u + r + \frac{1}{2}\ln(1 - 2r),\ \ x_1 = \frac{1}{2}y,\ \ x_2 = x,\ \ x_3 = [(2r)^{-1} - 1]^{\frac{1}{2}}$	II.B ($a = l = 0$)
III-9(b)	same as for III-9(a)	II.C ($a = l = 0$)
III-9(c)	same as for III-9(a)	II.D ($a = l = 0$)
III-10	$x_0 = t,\ \ x_1 = \frac{1}{2}\phi,\ \ x_2 = \theta,\ \ x_3 = [1 - (2r)^{-1}]^{\frac{1}{2}}$	I (Schwarzschild)
III-12(c)	$y_0 = \lambda^4 u^2,\ \ y_1 = x/(\lambda^5 u^2),\ \ y_2 = y,\ \ y_3 = (r/x^2) - (2x/\lambda u)$	IV.B ($C = 0$)

[a] NUT refers to the metrics of E. Newman, L. Tamburino, and T. Unti, J. Math. Phys. 4, 915 (1963).

transformation. Finally, we used the remainder of the tensor transformation law on the metric together with inspection of possible candidates at each stage of the integration.

The results are given in Table III. Of the 14 metrics only eight were found to be distinct. In Appendix C we give the corresponding Kinnersley metrics with their principal null directions and Killing solutions.

VI. SUMMARY

The 40 Harrison metrics include four nonvacuum solutions of which three are nondegenerate and one is degenerate. All the nondegenerate metrics and five degenerate metrics (including the nonvacuum one) are type I. The remaining fifteen consist of one type O solution and the rest type D. Of the 14 type D metrics one is Schwarzschild, three are NUT (with $\mu_0 = \rho_0 = 0$), seven cover the three cases of Kinnersley class IV.B, and the remaining three are Kinnersley class II.B, II.C, and II.D (all with $a = l = 0$). Altogether there are 21 vacuum solutions which are type I and are thus candidates for physically realistic exact radiative solutions.

Of course, with the exception of Schwarzschild and possibly NUT, there still remains the task of obtaining a physical realization of the Harrison metrics. It is hoped that, with the arrival of computing systems for help in routine algebra, this task may soon be accomplished.

ACKNOWLEDGMENTS

We should like to thank Professor F. A. E. Pirani for discussions during the course of this work. One of us (R. A. R.-C.) acknowledges the receipt of a Research Studentship given by the Science Research Council of Great Britain.

APPENDIX A

Presented below are (i) the transformations which reduce III-11, III-12(a), III-12(b), and III-12(c) to functions of two variables, together with (ii) the transformed metric. The first three are type I, but they become algebraically special on the hypersurfaces given in (iii).

III-11:

(i) $y_0 = x_0, \quad y_1 = x_1 \sin x_3,$

$y_2 = x_2, \quad y_3 = x_1 \cos x_3;$

(ii) $ds^2 = \lambda^2 y_0 y_1^3 \, dy_0^2 - y_1^{\frac{3}{2}} y_0^2 \, dy_1^2 - y_1^{-1} y_0^{-1} \, dy_2^2 - y_1^{\frac{3}{2}} y_0^2 \, dy_3^2;$

(iii) $675\lambda^4 y_0^2 + 432 y_1 - 652\lambda^2 y_0 y_1^{\frac{1}{2}} = 0.$

III-12(a):

(i) $y_0 = x_0 \cosh x_3, \quad y_1 = x_1,$

$y_2 = x_2, \quad y_3 = x_0 \sinh x_3;$

(ii) $ds^2 = y_1^2 y_3^{\frac{3}{2}} \, dy_0^2 - \lambda^2 y_1 y_3^2 \, dy_1^2 - y_1^{-1} y_3^{-1} \, dy_2^2 - y_1^2 y_3^{\frac{3}{2}} \, dy_3^2;$

(iii) $675\lambda^4 y_1^2 + 432 y_3 + 652\lambda^2 y_1 y_3^{\frac{1}{2}} = 0.$

III-12(b):

(i) $y_0 = x_0 \cosh x_3, \quad y_1 = x_1,$

$y_2 = x_2, \quad y_3 = x_0 \sinh x_3;$

(ii) $ds^2 = y_1^2 y_0^{\frac{3}{2}} \, dy_0^2 - \lambda^2 y_1 y_0^3 \, dy_1^2 - y_1^{-1} y_0^{-1} \, dy_2^2 - y_1^2 y_0^{\frac{3}{2}} \, dy_3^2;$

(iii) $675\lambda^4 y_1^2 + 432 y_0 - 652\lambda^2 y_1 y_0^{\frac{1}{2}} = 0.$

III-12(c):

(i) $y_0 = x_0 e^{x_3}, \quad y_1 = x_1, \quad y_2 = x_2, \quad y_3 = x_0 e^{-x_3};$

(ii) $ds^2 = y_1^2 y_0^{\frac{3}{2}} \, dy_0 \, dy_3 - \lambda^2 y_1 y_0^3 \, dy_1^2 - y_1^{-1} y_0^{-1} \, dy_2^2.$

APPENDIX B

With our sign conventions, from the nonvacuum field equations $T^\mu_\nu = \kappa G^\mu_\nu$, the mixed components of the energy-momentum tensor T^μ_ν for the four nonvacuum metrics are

$$T^\mu{}_\nu = \operatorname{diag} \kappa(\rho, p_1, p_2, p_3),$$

where we have the following:

I-B-1(b): $\rho = 2p_2 = -2p_3 = 4(\cosh x_3)^{-1} \times (x_1 + x_0)^{-2-\alpha}(x_0 - x_1)^{\alpha-2}, \quad p_1 = 0;$

I-B-1(c): $\rho = 2p_2 = -2p_3 = 2e^{-x_3}(x_1 + x_0)^{-2-\alpha} \times (x_0 - x_1)^{\alpha-2}, \quad p_1 = 0;$

I-B-2: $\rho = 0, \quad 2p_3 = -2p_2 = -p_1 = 4(\sin x_3)^{-1}(x_1 + x_0)^{\alpha-2} \times (x_1 - x_0)^{-2-\alpha};$

III-6: $\rho = \frac{1}{24}\Omega[2(\beta + 7) - 6x_3^{2+\frac{1}{2}\beta} - \epsilon_2 x_3(3 + 4\beta)],$

$p_1 = \frac{1}{12}\Omega[(7 + \beta) - 3x_3^{2+\frac{1}{2}\beta}],$

$p_2 = \frac{1}{24}\Omega[\epsilon_2 x_3(25 + 14\beta) - 2x_3^{2+\frac{1}{2}\beta}(4\beta + 7)],$

$p_3 = \frac{1}{12}\Omega[1 - x_3^{2+\frac{1}{2}\beta}].$

Here

$$\Omega = x_3^{\frac{1}{2}\beta}(x_3 - \epsilon_2)^{-\frac{1}{2}}(x_3 + \epsilon_2)^{-\frac{3}{2}-\beta}(x_0 + \tfrac{1}{3}\sqrt{3}x_1)^{-3-\beta},$$
$$\alpha = \pm\sqrt{2}, \quad \beta = \pm\sqrt{3}, \quad \epsilon_2 = \pm 1.$$

TABLE IV. Kinnersley's metrics for Harrison's type D solutions.

I (NUT; $\mu_0 = \rho_0 = 0$)	$ds^2 = (m/r)\, du^2 + 2\, du\, dr - r^2\, dx^2 - r^2\, dy^2$ $l^\mu = (0, 1, 0, 0), \quad n^\mu = (1, m/r, 0, 0)$ $\xi^\mu = (\alpha_1, 0, -\alpha_2 y + \alpha_3, \alpha_2 x + \alpha_4)$
II.B ($a = l = 0$)	$ds^2 = -(1 + 2m/r)\, du^2 + 2\, du\, dr - r^2\, dx^2 - r^2 \sinh^2 x\, dy^2$ $l^\mu = (0, 1, 0, 0), \quad n^\mu = (1, \frac{1}{2}(1 + 2m/r), 0, 0)$ $\xi^\mu = (\alpha_1, 0, \alpha_2 \cos y - \alpha_3 \sin y, -\alpha_2 \sin y \coth x - \alpha_3 \cos y \coth x + \alpha_4)$
II.C ($a = l = 0$)	$ds^2 = -(1 + 2m/r)\, du^2 + 2\, du\, dr - r^2\, dx^2 - r^2 \cosh^2 x\, dy^2$ $l^\mu = (0, 1, 0, 0), \quad n^\mu = (1, \frac{1}{2}(1 + 2m/r), 0, 0)$ $\xi^\mu = (\alpha_1, 0, \alpha_2 e^{-y} - \alpha_3 e^{y}, \alpha_2 e^{-y} \tanh x + \alpha_3 e^{y} \tanh x + \alpha_4)$
II.D ($a = l = 0$)	$ds^2 = -(1 + 2m/r)\, du^2 + 2\, du\, dr - r^2\, dx^2 - r^2 e^{2x}\, dy^2$ $l^\mu = (0, 1, 0, 0), \quad n^\mu = (1, \frac{1}{2}(1 + 2m/r), 0, 0)$ $\xi^\mu = (\alpha_1, 0, -\alpha_2 - \alpha_3 y, \alpha_2 y + \alpha_3(\frac{1}{2}y^2 - \frac{1}{2}e^{-2x}) + \alpha_4)$
IV ($C = \pm\frac{1}{2}, 0$)	$ds^2 = -(2Cr^2/x^2)\, du^2 + 2\, du\, dr - (4r/x)\, du\, dx - \frac{1}{2}\xi^{-2}\, dx^2 - 2\xi^2\, dy^2, \quad \xi = [C + (m/x)]^{\frac{1}{2}}$ $l^\mu = (0, 1, 0, 0), \quad n^\mu = (1, Cr^2/x^2, 0, 0)$ $C = \pm\frac{1}{2}, \quad \xi^\mu = (-\frac{1}{2}\alpha_1 u^2 - \alpha_2 u + \alpha_3, \alpha_1(ur + x^2/2C) + \alpha_2 r, 0, \alpha_4)$ $C = 0, \quad \xi^\mu = (-\alpha_1 u + \alpha_2, \alpha_1 r + \alpha_3 x^2, 0, \alpha_4)$

APPENDIX C

We present in Table IV the Kinnersley metrics found in Sec. V together with their principal null directions l^μ and n^μ and four-parameter group of motions ξ^μ (where α_1, α_2, α_3, and α_4 are the parameters).

* This research has been sponsored in part by the Aerospace Research Laboratories through the European Office of Aerospace Research, OAR, U.S. Air Force.

[1] B. K. Harrison, Phys. Rev. 116, 1285 (1959).
[2] R. A. d'Inverno, Computer J. 12, 124 (1969).
[3] R. A. d'Inverno, thesis, London University, 1970.
[4] W. Kinnersley, J. Math. Phys. 10, 1195 (1969).
[5] More precisely degenerate corresponds to the existence of an isometry group containing at least a two-parameter Abelian subgroup. We have not checked the possibility that some of the nondegenerate solutions may, in fact, be degenerate in this sense.
[6] B. K. Harrison, thesis, Princeton University, 1959.
[7] For an account of the two component spinor calculus and the Petrov classification, see F. A. E. Pirani, *Brandeis Summer Institute in Theoretical Physics, Lectures on General Relativity (1964)*, edited by S. Deser and K. W. Ford (Prentice-Hall, Englewood Cliff, N.J. 1965), Vol. 1, Chap. 3, and R. Penrose. Ann. Phys. 10, 171 (1960).
[8] E. Newman and R. Penrose, J. Math. Phys. 3, 566 (1962).
[9] See Appendix A, for example.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Representations of States of Infinite Systems in Statistical Mechanics*

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(Received 8 January 1971)

This paper deals with the representation of states of infinite systems in classical statistical mechanics in terms of probability densities, correlation functions, and zero-density correlation functions. The class of states considered includes equilibrium states treated previously by Ruelle, and is believed to contain low-density nonequilibrium states as well. The theory is based on Carter's exponential construction for measure spaces, the representations being in terms of functions on the exponential (i.e., union of symmetrized direct powers) of one-particle phase space. The main result, which establishes the connections between these three representations, essentially extends a result of Ruelle, but is based on $\mathfrak{L}_1$-convergence rather than uniform convergence on compacts.

1. INTRODUCTION

Consider a mechanical system consisting of variably many indistinguishable particles in a phase space $R \times E^3$. By a finite system we mean one in which the region R of configuration space is bounded and at most finitely many particles are present. An infinite system is one in which R has infinite measure and infinitely many particles are present, but with only finitely many in each bounded subregion. As pointed out by several authors,[1] the mechanical state of a finite system is most appropriately represented by a finite unordered sequence in X, an unordered sequence being an equivalence class of ordered sequences under rearrangement. A special sequence 0 is included, to represent the state in which no particles are present. As explained in Sec. 2 below, these unordered sequences form a measure space X_e, aptly called the "exponential" of X, whose measure ξ_e is the "exponential" of Lebesgue measure ξ. The instantaneous statistical state of a finite system is thus represented by a probability measure for X_e. Similarly,[2] the statistical state of an infinite system corresponds to a probability measure for the space X_ϵ of unordered infinite sequences in X having only finitely many components in each bounded subregion of R.

Most states considered in statistical mechanics have simpler representations in terms of functions on X_e. A function $f(x)$ on X_e is equivalent to a sequence of functions $f_0(0), f_1(x_1), f_2(x_1, x_2), \cdots$, where $f_0(0)$ is a constant and, for $n > 0$, $f_n(x_1, \cdots, x_n)$ is a symmetric function of n variables $x_i \in X$. Integration on X_e is characterized by

$$\int f(x)\, d\xi_e(x) = f_0(0) + \sum_{n=1}^{\infty} \frac{1}{n!} \int f_n(x_1, \cdots, x_n)\, dx_1 \cdots dx_n. \quad (1.1)$$

For a finite system, a probability measure on X_e which is absolutely continuous with respect to ξ_e is represented by a probability density w, satisfying $\int w\, d\xi_e = 1$. The corresponding zero-density correlation function[3,4]

$$\eta(x) = w(x)/w(0) \quad (1.2)$$

is defined whenever there is a positive probability that no particles are present $[w(0) \neq 0]$. It also serves to

APPENDIX C

We present in Table IV the Kinnersley metrics found in Sec. V together with their principal null directions l^μ and n^μ and four-parameter group of motions ξ^μ (where α_1, α_2, α_3, and α_4 are the parameters).

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[2] R. A. d'Inverno, Computer J. **12**, 124 (1969).

[3] R. A. d'Inverno, thesis, London University, 1970.

[4] W. Kinnersley, J. Math. Phys. **10**, 1195 (1969).

[5] More precisely degenerate corresponds to the existence of an isometry group containing at least a two-parameter Abelian subgroup. We have not checked the possibility that some of the nondegenerate solutions may, in fact, be degenerate in this sense.

[6] B. K. Harrison, thesis, Princeton University, 1959.

[7] For an account of the two component spinor calculus and the Petrov classification, see F. A. E. Pirani, *Brandeis Summer Institute in Theoretical Physics, Lectures on General Relativity* (*1964*), edited by S. Deser and K. W. Ford (Prentice-Hall, Englewood Cliff, N.J. 1965), Vol. 1, Chap. 3, and R. Penrose. Ann. Phys. **10**, 171 (1960).

[8] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

[9] See Appendix A, for example.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Representations of States of Infinite Systems in Statistical Mechanics*

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(Received 8 January 1971)

This paper deals with the representation of states of infinite systems in classical statistical mechanics in terms of probability densities, correlation functions, and zero-density correlation functions. The class of states considered includes equilibrium states treated previously by Ruelle, and is believed to contain low-density nonequilibrium states as well. The theory is based on Carter's exponential construction for measure spaces, the representations being in terms of functions on the exponential (i.e., union of symmetrized direct powers) of one-particle phase space. The main result, which establishes the connections between these three representations, essentially extends a result of Ruelle, but is based on $\mathfrak{L}_1$-convergence rather than uniform convergence on compacts.

1. INTRODUCTION

Consider a mechanical system consisting of variably many indistinguishable particles in a phase space $R \times E^3$. By a finite system we mean one in which the region R of configuration space is bounded and at most finitely many particles are present. An infinite system is one in which R has infinite measure and infinitely many particles are present, but with only finitely many in each bounded subregion. As pointed out by several authors,[1] the mechanical state of a finite system is most appropriately represented by a finite unordered sequence in X, an unordered sequence being an equivalence class of ordered sequences under rearrangement. A special sequence 0 is included, to represent the state in which no particles are present. As explained in Sec. 2 below, these unordered sequences form a measure space X_e, aptly called the "exponential" of X, whose measure ξ_e is the "exponential" of Lebesgue measure ξ. The instantaneous statistical state of a finite system is thus represented by a probability measure for X_e. Similarly,[2] the statistical state of an infinite system corresponds to a probability measure for the space X_ϵ of unordered infinite sequences in X having only finitely many components in each bounded subregion of R.

Most states considered in statistical mechanics have simpler representations in terms of functions on X_e. A function $f(x)$ on X_e is equivalent to a sequence of functions $f_0(0), f_1(x_1), f_2(x_1, x_2), \cdots$, where $f_0(0)$ is a constant and, for $n > 0$, $f_n(x_1, \cdots, x_n)$ is a symmetric function of n variables $x_i \in X$. Integration on X_e is characterized by

$$\int f(x)\, d\xi_e(x) = f_0(0) + \sum_{n=1}^{\infty} \frac{1}{n!} \int f_n(x_1, \cdots, x_n)\, dx_1 \cdots dx_n. \quad (1.1)$$

For a finite system, a probability measure on X_e which is absolutely continuous with respect to ξ_e is represented by a probability density w, satisfying $\int w\, d\xi_e = 1$. The corresponding zero-density correlation function[3,4]

$$\eta(x) = w(x)/w(0) \quad (1.2)$$

is defined whenever there is a positive probability that no particles are present [$w(0) \neq 0$]. It also serves to represent the state, since

$$w(x) = \eta(x) \Big/ \int \eta \, d\xi_e. \qquad (1.3)$$

The grand canonical equilibrium state, for example, is given by

$$\eta(x) = e^{-\theta H(x) - \tau l(x)}, \qquad (1.4)$$

where H is the system Hamiltonian with $H(0) = 0$ and $l(x)$ is the "length" of X. Often the correlation function ρ may be used to represent the state, being related to w by

$$\rho(x) = \int w(xy) \, d\xi_e(y), \qquad (1.5)$$

$$w(x) = \int (-1)^{l(y)} \rho(xy) \, d\xi_e(y). \qquad (1.6)$$

Equations (1.5) and (1.6) are compact forms of

$$\begin{aligned} \rho_n(x_1, \cdots, x_n) &= w_n(x_1, \cdots, x_n) \\ &\quad + \sum_{k=0}^{\infty} \frac{1}{k!} \int w_{n+k}(x_1, \cdots, x_n, y_1, \cdots, y_k) \\ &\quad \times dy_1 \cdots dy_k, \end{aligned}$$

$$\begin{aligned} w_n(x_1, \cdots, x_n) &= \rho_n(x_1, \cdots, x_n) \\ &\quad + \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int \rho_{n+k}(x_1, \cdots, x_n, y_1, \cdots, y_k) \\ &\quad \times dy_1 \cdots dy_k. \end{aligned}$$

To represent the state S of an infinite system by functions on X_e, let $\{R_n\}$ be an increasing sequence of bounded measurable subregions with limit R, and let $X_n = R_n \times E^3$ be the corresponding sequence of phase spaces. It is known[5] that the state S is determined by the corresponding sequence of induced states on the finite systems occupying the R_n, obtained by observing only those particles in R_n. The induced state for R_n may be represented by a probability measure P_n for X_e, rather than $(X_n)_e$, obtained by (arbitrarily) removing all the particles outside X_n. If each P_n is absolutely continuous, the state S is represented by the corresponding sequence of probability densities w_n. The only condition on the w_n is compatibility (see Sec. 4 below). If the induced states on R_n have correlation functions $\tilde{\rho}_n$, defined on $(X_n)_e$, the compatibility condition ensures that these functions may be chosen so as to have a common extension ρ to X_e. In this case S is represented by the single "correlation function" ρ.

The most common way of representing equilibrium states is by the "zero-density correlation function" (1.4). Ruelle[6] has shown, for a class of infinite systems in sufficiently low-density equilibrium states, that this function determines S as follows: The function

$$\eta^{(n)}(x) = \begin{cases} \eta(x) & \text{if } \; x \in (X_n)_e \\ 0 & \text{otherwise} \end{cases} \qquad (1.7)$$

is the zero-density correlation function of a state having no particles outside X_n. Let ρ_n be the corresponding correlation function, given by (1.3) and (1.5). Then $\rho_n(x)$ converges (uniformly on compacts) to the correlation function $\rho(x)$ of a state S. Our main result, Theorem 5.1, establishes a similar representation for a class of zero-density correlation functions, which contains Ruelle's as a subclass but which is not limited to the equilibrium case. It is also shown that each of these states is represented by a sequence of probability densities w_n as above. Further connections between these representations are established, including the fact that the functions w_n determine η through

$$\eta(x) = \lim_{n \to \infty} [w_n(x)/w_n(0)]. \qquad (1.8)$$

2. SOME MATHEMATICAL PRELIMINARIES

We denote the set of all nonnegative integers by N. For each $n \in N$, let $X^{\cdot n}$ be the nth direct power of X. When $n = 0$, $X^{\cdot n}$ is the singleton set $\{\varnothing\} = \{0\}$. The union of $X^{\cdot n}$ for all $n \in N$ is denoted by $X_e^{\cdot}$.

Two ordered sequences x, y are equivalent if they have the same length and one is a rearrangement of the other. The equivalence classes are called unordered sequences in X. Each unordered sequence x has a length $l(x)$, equal to the common length of its members. The set of all unordered sequences in X is denoted by X_e or $\exp X$.

An unordered sequence of length n in X may be written as a formal product

$$x = x_1 \cdots x_n,$$

where the order of factors is irrelevant.[7] When $n = 0$, we write $x = 0$. By collecting equal factors, the product can also be written in the form

$$x = t_1^{r_1} \cdots t_m^{r_m},$$

where $t_1, \cdots, t_m$ are the distinct factors of x and $r_1, \cdots, r_m$ are the corresponding multiplicities.

There is a natural binary operation on X_e defined as follows: If $x = x_1 \cdots x_m$ and $y = y_1 \cdots y_n$, then

$$xy = x_1 \cdots x_m y_1 \cdots y_n.$$

This in turn induces an operation on the class of all subsets of X_e, called the symmetric product, given by

$$AB = \{xy : x \in A, y \in B\}.$$

Let $\mathcal{A}$ be the family of all complex-valued functions defined on X_e. On $\mathcal{A}$ we introduce a "star product" corresponding to a similar product used by Ruelle[8] and Schwartz.[9] To this end we first define partitions of an unordered sequence, and their indices: Let $x \in X_e$ and let n be a positive integer. An n partition of x is an n-tuple of unordered sequences $(x_1, \cdots, x_n)$ such that $x = x_1 \cdots x_n$. The set of all n partitions x will be denoted by $P_n(x)$. The index of an unordered sequence $x = t_1^{r_1} \cdots t_m^{r_m}$ is

$$I(x) = r_1! \cdots r_m!$$

and the index of an n partition $(x_1, \cdots, x_n)$ of x is

$$I(x_1, \cdots, x_n) = I(x)/I(x_1) \cdots I(x_n).$$

Now the star product $\phi * \Psi$, with $\phi, \Psi \in \mathcal{A}$, is defined by

$$\phi * \Psi(x) = \sum \{I(x_1, x_2)\phi(x_1)\Psi(x_2):(x_1, x_2) \in P_2(x)\}.$$

This product is clearly commutative, associative, distributive over addition, and homogeneous in the sense that

$$c(\phi * \Psi) = (c\phi) * \Psi = \phi * (c\Psi).$$

Also, there is an identity 1^* given by

$$1^*(x) = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{otherwise} \end{cases}.$$

Each member ϕ of $\mathcal{A}$ has a unique inverse if $\phi(0) \neq 0$, since the equation $\phi * \Psi(x) = 1^*(x)$ can be solved by recursion for $\Psi(x)$, with increasing values of $I(x)$.[10]

For each $x \in X_e$, we define a linear operator $D_x:\mathcal{A} \to \mathcal{A}$ by the equation

$$D_x\phi(y) = \phi(xy).$$

This corresponds to a similar operator used by Ruelle.[8] Notice that $D_xD_y = D_{xy}$ for all $x, y \in X_e$. When $x = 0$, D_x is the identity.

We shall follow the terminology of Ref. 2 in the treatment of exponential measure spaces. Thus, a measurable space for a set X is a σ-algebra $\mathfrak{X}$ of subsets of X; a measure space for X is a σ-finite measure ξ defined on such a σ-algebra. The subspaces of $\mathfrak{X}$ are the σ-algebras $\mathfrak{X} \cap A$ induced on the measurable sets $A \in \mathfrak{X}$; the subspaces of ξ are the restrictions of ξ to the subspaces of $\mathfrak{X}$. Thus the subspaces are in one-to-one correspondence with the measurable sets, and all relations and operations (disjointness, unions, etc.) for measurable sets carry over to the corresponding relations on the subspaces of $\mathfrak{X}$ or ξ.

For each positive integer n, $\mathfrak{X}^{\cdot n}$ denotes the nth direct power of $\mathfrak{X}$, and $\xi^{\cdot n}$ denotes the nth direct power of ξ. When $n = 0$, $\mathfrak{X}^{\cdot n} = \{\varnothing, \{0\}\}$ and $\xi^{\cdot 0}$ is the measure defined on $\mathfrak{X}^{\cdot 0}$ by $\xi^{\cdot 0}(\{0\}) = 1$. The "measure-theoretic union" of direct powers of $\mathfrak{X}$,

$$\mathfrak{X}_e^{\cdot} = \left\{\sum_{n=0}^{\infty} A_n : A_n \in \mathfrak{X}^{\cdot n} \text{ for each } n\right\},$$

is a σ-algebra of subsets of $X_e^{\cdot}$. The set function $\xi_e^{\cdot}$ defined on $\mathfrak{X}_e^{\cdot}$ by

$$\xi_e^{\cdot}(E) = \sum_{n=0}^{\infty} \frac{1}{n!} \xi^{\cdot n}(E \cap X^{\cdot n})$$

is a σ-finite measure. The quotient spaces of $\mathfrak{X}_e^{\cdot}$ and $\xi_e^{\cdot}$ under the natural projection $p:X_e^{\cdot} \to X_e$ are called the exponentials of $\mathfrak{X}$ and ξ, written $\exp \mathfrak{X}$ and $\exp \xi$, or alternatively $\mathfrak{X}_e$ and ξ_e. The following theorem,[11] which motivates the exponential terminology, is central to the development of our theory.

Theorem 2.1 (Exponential decomposition law): Let α, β be a disjoint pair of subspaces of ξ. Then the concatenation function $(x, y) \to xy$ is an isomorphism of the product space $\exp \alpha \times \exp \beta$ onto $\exp (\alpha + \beta)$.

As a corollary to this result, we have the following.

Theorem 2.2: Let α, β be a disjoint pair of subspaces of ξ corresponding to $A, B \in \mathfrak{X}$, respectively, and let $\gamma = \alpha + \beta$. Then, for every γ_e-integrable function ϕ,

$$\int_{(A+B)_e} \phi(z)\, d\gamma_e(z) = \int_{A_e}\int_{B_e} \phi(xy)\, d\alpha_e(x)\, d\beta_e(y)$$

or, equivalently,

$$\int_{(A+B)_e} \phi(z)\, d\xi_e(z) = \int_{A_e}\int_{B_e} \phi(xy)\, d\xi_e(x)\, d\xi_e(y).$$

Now let $\mathcal{M}$ be the set of all $\mathfrak{X}_e$-measurable functions and $\mathfrak{L}_1$ be the set of all ξ_e-integrable functions. One shows easily that $\mathcal{M}$ is closed under the star product, the corresponding inverse operation, and the D_x operation.[4] Furthermore, we have the following "known" result.[12]

Theorem 2.3: If ϕ_1, ϕ_2 are ξ_e-integrable, then so is $\phi_1 * \phi_2$. Moreover,

(i) $$\int \phi_1 * \phi_2\, d\xi_e = \left(\int \phi_1\, d\xi_e\right)\left(\int \phi_2\, d\xi_e\right),$$

(ii) $$\int |\phi_1 * \phi_2|\, d\xi_e \leq \left(\int |\phi_1|\, d\xi_e\right)\left(\int |\phi_2|\, d\xi_e\right).$$

3. THE SUBSPACE $\mathcal{N}$ AND OPERATOR T

For a precise mathematical discussion of the relationship between probability densities and correlation functions, we introduce a special subspace $\mathcal{N}$

of $\mathfrak{L}_1$ as follows: Let $z^l\phi$ denote the pointwise product $(z^l\phi)(x) = z^{l(x)}\phi(x)$. Then $\mathcal{N}$ is the set of all functions $\phi \in \mathcal{M}$ such that, for each complex number z and all $x \in X_e$, the function $z^l D_x\phi$ belongs to $\mathfrak{L}_1$. As suggested by the relations (1.5) and (1.6), we define linear operators T and U on $\mathcal{N}$ by the equations

$$T\phi(x) = \int D_x\phi \, d\xi_e, \tag{3.1}$$

$$U\phi(x) = \int (-1)^{l(y)} D_x\phi(y) \, d\xi_e(y). \tag{3.2}$$

Our next theorem implies that if a probability density w belongs to $\mathcal{N}$, then the corresponding correlation function $\rho = Tw$ also belongs to $\mathcal{N}$ and $w = U\rho$.

Theorem 3.1: The operator T maps $\mathcal{N}$ one-to-one onto $\mathcal{N}$, and its inverse is U.

Proof: Since $(T\phi) \circ p$ is $\mathfrak{X}_e$-measurable, $T\phi$ and $D_xT\phi$ belong to $\mathcal{M}$. From the construction of the exponential measure, the integral $\int |z^{l(y)} D_x(T\phi)(y)| \, d\xi_e$ can be written as

$$\sum_{k=0}^{\infty} \frac{|z|^k}{k!} \int_{X^{\cdot k}} \left| \sum_{j=0}^{\infty} \frac{1}{j!} \int_{X^{\cdot j}} (D_x\phi) \circ p(y_1, \cdots, y_k, w_1, \cdots, w_j) \, d\xi^{\cdot j} \right| d\xi^{\cdot k}.$$

Rearranging and using the binomial theorem, we have

$$\int |z^{l(y)} D_x(T\phi)(y)| \, d\xi_e \le \int (1 + |z|)^{l(y)} |D_x\phi(y)| \, d\xi_e,$$

which implies that $T\phi \in \mathcal{N}$. Similar calculations show that $TU\phi = UT\phi = \phi$.

We shall need the following properties of $\mathcal{N}$.

Theorem 3.2: (i) If $\phi \in \mathcal{N}$, then $D_x\phi \in \mathcal{N}$ for all $x \in X_e$. (ii) If $\phi, \Psi \in \mathcal{N}$, then $\phi * \Psi \in \mathcal{N}$.

Proof: Part (i) is trivial. To prove (ii), first show by induction on $l(x)$ that

$$D_x(\phi * \Psi) = \sum \{I(u, v) D_u\phi * D_v\Psi : (u, v) \in P_2(x)\},$$

where $\phi, \Psi \in \mathcal{A}$, and $x \in X_e$. Since $z^l(\phi * \Psi) = (z^l\phi) * (z^l\Psi)$, the result now follows from Theorem 2.3.

4. INDUCED PROBABILITY DENSITIES AND THE EXTENSION PROPERTY OF CORRELATION FUNCTIONS

Consider a random experiment whose outcomes are unordered sequences in a set X and whose events are members of a σ-algebra $\mathfrak{X}_e$. Let Y be a measurable subset of X and Z be its complement in X. Suppose we are only interested in observing what happens in Y without regard to what happens elsewhere. Then the original experiment induces a new experiment whose outcomes are points in Y_e and whose events are members of the σ-algebra $\mathfrak{Y}_e$, with $\mathfrak{Y} = \mathfrak{X} \cap Y$. Each unordered sequence $x \in X_e$ can be factored uniquely into a product yz of unordered sequences $y \in Y_e$ and $z \in Z_e$ (see Theorem 2.1). If $x = yz$ represents an outcome of the original experiment, then y represents the corresponding outcome of the induced experiment. An event $A \in \mathfrak{Y}_e$ occurs if and only if, in the above factorization, $y \in A$. Thus:

(1) An event A in the induced experiment has the same interpretation as the event AZ_e in the original experiment.

(2) If P_X is the probability measure on $\mathfrak{X}_e$ corresponding to the original experiment, then the probability measure P_Y for the induced experiment is given by

$$P_Y(A) = P_X(AZ_e). \tag{4.1}$$

In the case where P_X is absolutely continuous with respect to the exponential measure ξ_e, we obtain the following, using Theorem 2.2.

Theorem 4.1: Let P_Y be an induced probability measure of P_X as above. If P_X is absolutely continuous with respect to ξ_e, with probability density w_X, then P_Y is absolutely continuous with respect to the restriction of ξ_e to $\mathfrak{Y}_e$, and its probability density is given a.e. on Y_e by

$$w_Y(x) = \int_{Z_e} w_X(xy) \, d\xi_e(y). \tag{4.2}$$

The probability density w_Y is called the induced probability density of w_X, and Eq. (4.2) is the "compatibility condition" between these densities.

Now let $\mathcal{N}_X$ and $\mathcal{N}_Y$ be the subspaces of $\mathfrak{L}_1(X_e)$ and $\mathfrak{L}_1(Y_e)$ corresponding to the subspace $\mathcal{N}$ introduced in Sec. 3. Then we have the following, again using Theorem 2.3.

Theorem 4.2: Let w_X be a probability density belonging to $\mathcal{N}_X$. Then the induced probability density

$$w_Y(y) = \int_{Z_e} D_y w_X \, d\xi_e$$

belongs to $\mathcal{N}_Y$.

Consider next the correlation functions ρ_X, ρ_Y corresponding to a compatible pair of densities w_X, w_Y. It is intuitively clear from the physical interpretation of correlation functions that ρ_X should be equal to ρ_Y a.e. on Y_e. Indeed, taking w_X, w_Y to be members of $\mathcal{N}_X$, $\mathcal{N}_Y$, respectively, and

$$\rho_X = T_X w_X, \quad \rho_Y = T_Y w_Y \tag{4.3}$$

where T_X and T_Y are the operators on $\mathcal{N}_X$ and $\mathcal{N}_Y$ corresponding to the operator T of Sec. 3, we have the following.

Theorem 4.3: Let w_X and w_Y be probability densities on X_e and Y_e belonging to $\mathcal{N}_X$ and $\mathcal{N}_Y$, respectively. Let ρ_X and ρ_Y be the correlation functions given by Eq. (4.3). Then w_X and w_Y are related by Eq. (4.2) if and only if ρ_Y is the restriction of ρ_X to Y_e.

Proof: Since $Z_e \subset X_e$, the function ϕ defined on Y_e by

$$\phi(y) = \int_{Z_e} w_X(yz)\, d\xi_e(z)$$

satisfies $\phi \le (T_X w_X) \mid Y_e = \rho_X \mid Y_e$, and hence $\phi \in \mathcal{N}_Y$. Applying Theorem 2.2 to the integral $T_X w_X$, we obtain $\rho_X \mid Y_e = T_Y \phi$, or equivalently

$$\phi = U_Y(\rho_X \mid Y_e),$$

and the theorem follows.

Finally, if $w_Y \in \mathcal{N}_Y$ is a probability density on Y_e and $\rho_Y = T_Y w_Y$ is the corresponding correlation function, it is often convenient to work with the extensions w_Y^E, ρ_Y^E of these functions to X_e, given by

$$\phi^E(x) = \begin{cases} \phi(x) & \text{if } x \in Y_e \\ 0 & \text{otherwise} \end{cases}.$$

Clearly, w_Y^E is a probability density belonging to $\mathcal{N}_X$, corresponding to an experiment in which no particles occur in Z, and ρ_Y^E is the corresponding correlation function; $\rho_Y^E = T_X w_Y^E$.

5. INFINITE SYSTEMS AND THE LIMIT THEOREM

The study of equilibrium statistical mechanics suggests that zero-density correlation functions η may be used as representatives for a more general class of infinite states, with probability densities and correlation functions determined essentially as in Sec. 1. We now introduce a class $\mathcal{K}$ of functions η which do represent states in this way, and establish the connections between these various representations. As in Sec. 1, let $\{X_n : n \in N\}$ be an increasing sequence of measurable sets, whose union is X. Throughout the discussion we use the following notational convention. For each $\phi \in \mathcal{A}$, $n \in N$, $\phi^{(n)}$ denotes the product $\chi_n \phi$, where χ_n is the characteristic function of $(X_n)_e$. Then $\mathcal{K}$ consists of all functions $\eta \in \mathcal{M}$ such that

(i) $\eta \ge 0$ and $\eta(0) = 1$,

(ii) for each $n \in N$, the function $\eta^{(n)} \in \mathcal{N}$,

(iii) the integral $\int |\eta^{-1} * D_x \eta|\, d\xi_e$ exists for all $x \in X_e$ and is bounded above by a function $g(x)$ such that $g^{(n)} \in \mathcal{N}$ for all $n \in N$.

It is shown in Ref. 4, Sec. 4.2, that those equilibrium states considered by Ruelle[6] belong to $\mathcal{K}$.

Associated with each $\eta \in \mathcal{K}$, we have the following functions:

(a) The sequence of probability densities

$$v_n = \left(\int \eta^{(n)}\, d\xi_e\right)^{-1} \eta^{(n)}$$

which belong to $\mathcal{N}$ by condition (ii) on $\mathcal{K}$.

(b) The corresponding sequence of correlation functions

$$\rho_n = T v_n$$

which belong to $\mathcal{N}$ by Theorem 3.1.

(c) The function ρ defined by

$$\rho(x) = \int \eta^{-1} * D_x \eta\, d\xi_e,$$

which will turn out to be the correlation function for the infinite system. We will show that each $\rho^{(n)}$ belongs to $\mathcal{N}$ (see the notational convention above).

(d) The sequence of functions

$$w_n = U\rho^{(n)},$$

which will turn out to be the family of compatible probability densities for the infinite system. These functions belong to $\mathcal{N}$ by Theorem 3.1.

(e) The probability densities $v_{m,n}$ induced by v_n when $n \ge m$,

$$v_{m,n}(x) = \chi_m(x) \int_{(X_n \sim X_m)_e} D_x v_n\, d\xi_e,$$

which belong to $\mathcal{N}$ by Theorem 4.2 and the remark at the end of Sec. 4. We will show that $v_{m,n}$ approaches the probability density w_m for the infinite system as $n \to \infty$. Throughout the remainder of this section, the symbols v_n, ρ_n, ρ, $v_{m,n}$, and w_n will refer to the functions just defined.

Theorem 5.1: Let $\eta \in \mathcal{K}$. Then, as $n \to \infty$,

(i) ρ_n converges pointwise to ρ, $v_{m,n}$ converges pointwise to w_m, $w_n/w_n(0)$ converges pointwise to η,

(ii) for each $m \in N$ and $x \in X_e$,

$$\int |D_x \rho_n^{(m)} - D_x \rho^{(m)}|\, d\xi_e \to 0,$$

$$\int |D_x v_{m,n} - D_x w_m|\, d\xi_e \to 0,$$

$$\int |D_x w_n^{(m)}/w_n(0) - D_x \eta^{(m)}|\, d\xi_e \to 0.$$

Furthermore, the sequence of functions $\{w_m : m \in N\}$ forms a family of compatible probability densities.

The proof is contained in the following list of propositions:

(1) Let $\phi \in \mathcal{A}$ and $\phi(0) \neq 0$. Then for each $n \in N$, $(\phi^{(n)})^{-1} = (\phi^{-1})^{(n)}$ and

$$(\phi^{(n)})^{-1} * D_x\phi^{(n)} = \chi_n(x)(\phi^{-1} * D_x\phi)^{(n)}.$$

(2) For each $n \in N$,

$$\rho_n(x) = \chi_n(x)\int (\eta^{-1} * D_x\eta)^{(n)}\, d\xi_e.$$

Proof: By definition,

$$\rho_n(x) = \left(\int \eta^{(n)}\, d\xi_e\right)^{-1} \int D_x\eta^{(n)}\, d\xi_e.$$

The second integral may be written in the form

$$\int \eta^{(n)} * (\eta^{(n)})^{-1} * D_x\eta^{(n)}\, d\xi_e$$

which, by (1), is equal to

$$\chi_n(x)\int \eta^{(n)} * (\eta^{-1} * D_x\eta)^{(n)}\, d\xi_e.$$

The result now follows from condition (iii) on $\mathcal{H}$ and Theorem 2.3.

(3) As $n \to \infty$, ρ_n converges pointwise to ρ and, for all $m \in N$, $x \in X_e$,

$$\int |D_x\rho_n^{(m)} - D_x\rho^{(m)}|\, d\xi_e \to 0.$$

Proof: Taking n sufficiently large that $\chi_n(x) = 1$, we have, by (2),

$$\rho_n(x) - \rho(x) = \int (\chi_n - 1)(\eta^{-1} * D_x\eta)\, d\xi_e,$$

which approaches zero by the Lebesgue dominated convergence theorem. It follows that ρ is measurable and that $D_x\rho_n$ converges pointwise to $D_x\rho$. Again by (2),

$$|D_x\rho_n^{(m)}(y)| \leq \chi_m(xy)\int |\eta^{-1} * D_{xy}\eta|\, d\xi_e,$$

whence, by condition (iii) on $\mathcal{H}$, $|D_x\rho^{(m)}| \leq D_xg^{(m)}$. By Theorem 3.2, $D_xg^{(m)}$ belongs to $\mathcal{N}$ and (3) follows by the dominated convergence theorem.

(4) For all $m, n \in N$ with $m \leq n$, $U\rho_n^{(m)} = v_{m,n}$.

Proof: Taking $Y = \dot{X}_m$ and $w_X = v_n$, we have, in the notation of Sec. 4, $\rho_Y^{\mathrm{E}} = \rho_n^{(m)}$ and $w_Y^{\mathrm{E}} = v_{m,n}$. Thus $\rho_n^{(m)} = Tv_{m,n}$, which is equivalent to

$$U\rho_n^{(m)} = v_{m,n}.$$

(5) As $n \to \infty$, $v_{m,n}$ converges pointwise to w_m and, for each $x \in X_e$,

$$\int |D_xv_{m,n} - D_xw_m|\, d\xi_e \to 0.$$

Proof: By (4),

$$\begin{aligned}|v_{m,n}(x) - w_m(x)| &= \left|\int (-1)^{l(y)}D_x\rho_n^{(m)}(y)\, d\xi_e(y) - \int (-1)^{l(y)}D_x\rho^{(m)}(y)\, d\xi_e(y)\right| \\ &\leq \int |D_x\rho_n^{(m)}(y) - D_x\rho^{(m)}(y)|\, d\xi_e(y),\end{aligned}$$

which approaches zero by (3). Again by (4) and (2),

$$\begin{aligned}|D_xv_{m,n}(y)| &= \left|\int (-1)^{l(y)}\rho_n^{(m)}(xyz)\, d\xi_e(z)\right| \\ &\leq \int \chi_m(xyz)\left|\int (\eta^{-1} * D_{xyz}\eta)^{(n)}\, d\xi_e\right| d\xi_e(z) \\ &\leq \int g^{(m)}(xyz)\, d\xi_e(z) = D_xTg^{(m)}(y).\end{aligned}$$

Since $D_xTg^{(m)} \in \mathcal{N}$, the result follows.

(6) The sequence $\{w_m : m \in N\}$ forms a family of probability densities, which are compatible in the sense that if $m \leq n$, then

$$w_m(x) = \chi_m(x)\int_{(X_n\sim X_m)_e} D_xw_n\, d\xi_e.$$

Proof: It follows from (5) that $w_m \geq 0$. Since $\rho^{(m)} = Tw_m$, we have

$$\int w_m\, d\xi_e = Tw_m(0) = \rho^{(m)}(0) = \int 1^*\, d\xi_e = 1.$$

Thus w_m is a probability density. By Theorem 4.3 these densities are compatible.

(7) As $n \to \infty$, $w_n/w_n(0)$ converges pointwise to η and, for each $x \in X_e$,

$$\int |D_xw_n^{(m)}/w_n(0) - D_x\eta^{(m)}|\, d\xi_e \to 0.$$

Proof: By definition,

$$v_{m,n}(x) = \chi_m(x)\left(\int_{(X_n)_e} \eta^{(n)}\, d\xi_e\right)^{-1} \int_{(X_n\sim X_m)_e} D_x\eta^{(n)}\, d\xi_e.$$

By (1) and Theorem 2.3,

$$\int_{(X_n\sim X_m)_e} D_x\eta^{(n)}\, d\xi_e = \chi_n(x)\left(\int_{(X_n\sim X_m)_e} \eta^{(n)}\, d\xi_e\right) \times \left(\int_{(X_n\sim X_m)_e} \eta^{-1} * D_x\eta\, d\xi_e\right).$$

Since

$$\int_{(X_n\sim X_m)_e} 1^*\, d\xi_e = \xi_e(\{0\}) = 1,$$

it follows that

$$\frac{v_{m,n}(x)}{v_{m,n}(0)} = \chi_m(x)\int_{(X_n\sim X_m)_e} \eta^{-1} * D_x\eta \, d\xi_e.$$

In the limit $n \to \infty$, this becomes

$$\frac{w_m(x)}{w_m(0)} = \chi_m(x)\int_{(X\sim X_m)_e} \eta^{-1} * D_x\eta \, d\xi_e.$$

Here $(X \sim X_m)_e$ is decreasing with m to the set $\{0\}$; hence

$$\lim_{m\to\infty} [w_m(x)/w_m(0)] = (\eta^{-1} * D_x\eta)(0).$$

By condition (i) on $\mathcal{K}$, this is $\eta(x)$. The rest now follows from the inequality

$$\left|\frac{D_x w_n^{(m)}(y)}{w_n(0)}\right| \leq X_m(xy)\int |\eta^{-1} * D_{xy}\eta| \, d\xi_e \leq D_x g^{(m)}(y).$$

* This paper is based on part of the doctoral dissertation of C. Y. Shen (Ref. 4). Work supported by U.S. National Science Foundation, under Grants Nos. GP 6144 and GP 7474.

† Present address: Department of Mathematics, Simon Fraser University, Burnaby 2, British Columbia.

[1] See, for example, J. E. Moyal, Acta Math. **108**, 1 (1962), T. E. Harris, Z. Wahrscheinlichkeitstheorie **10**, 102 (1968), or Ref. 2.

[2] D. S. Carter and P. M. Prenter, "Exponential Spaces and Counting Processes," Z. Wahrscheinlichkeitstheorie (to be published).

[3] So named because it is the correlation function for a limiting conditional experiment in which no particles are present except as represented by x; see Ref. 4, Sec. 3.1.

[4] C. Y. Shen, "Probability Densities and Correlation Functions in Statistical Mechanics," Department of Mathematics, Oregon State University, Technical Report No. 35, 1967. See Theorems 2.7.1, 2.7.2, and 2.7.3.

[5] See Ref. 2, Sec. 8.

[6] D. Ruelle, Ann. Phys. **25**, 109 (1963).

[7] See Ref. 2, Sec. 1.

[8] D. Ruelle, Rev. Mod. Phys. **36**, 580 (1964).

[9] J. Schwartz, Statistical Mechanics, Lecture notes, Courant Institute of Mathematical Sciences, New York University, 1957.

[10] An exact formula for the inverse is given in Ref. 4, Eq. 2.4.4.

[11] See Ref. 2, Proposition 6.6.

[12] See Refs. 9 and 4, Theorem 2.7.4.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Periodic Solutions of a Nonlinear Differential Equation

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(Received 13 November 1970)

Periodic solutions of the nonlinear differential equation $\ddot{x} + f(x) = 0$ are investigated. The qualitative characteristics of the solution are explored and several theorems about the basic nature of the solution are presented. The solution is then obtained in terms of a Fourier series and numerical calculations are carried out to fifth-order accuracy. The dependence of the frequency of the solution on the amplitude is studied. As an example, the solution is applied to the problem of obtaining the orbit of a charged particle moving in a radial electric field.

I. INTRODUCTION

The type of differential equation treated in this paper is a second-order, ordinary nonlinear differential equation (NLDE) for a one-dimensional, conservative system. Only periodic solutions are considered since, for a conservative system, these are the only bounded solutions.

Before presenting the method of solution developed in this paper, it is useful to consider the capabilities and limitations of some of the well-established methods of solution. Closed-form solutions are not considered since they are very much the exception rather than the rule. Instead, the emphasis is placed on approximation methods which allow the solution to be determined to some desired degree of accuracy.

The first method considered, and perhaps the most familiar, is that of single-parameter perturbation theory. This method depends on the facts that the solutions of a reduced form (usually linear) of the original NLDE are known and that the difference between the NLDE and the reduced form is, in some sense, small. This difference, the perturbation, is then multiplied by some parameter, say ϵ, assumed to be small, if such a parameter is not initially present. By using this parameter and the solution to the reduced differential equation, a power series solution is obtained which approximately satisfies the original NLDE. When the perturbation is sufficiently small, one or two corrective terms usually give the solution to the desired accuracy. One of the limitations of the perturbation method is that ϵ is required to be sufficiently small; otherwise the power series expansion does not converge. Another difficulty occurs if periodic solutions are desired—namely, the treatment of nonperiodic terms in the power series expansion when they occur.[1] A particular variation of the it follows that

$$\frac{v_{m,n}(x)}{v_{m,n}(0)} = \chi_m(x)\int_{(X_n\sim X_m)_e} \eta^{-1} * D_x\eta \, d\xi_e.$$

In the limit $n \to \infty$, this becomes

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Here $(X \sim X_m)_e$ is decreasing with m to the set $\{0\}$; hence

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By condition (i) on $\mathcal{H}$, this is $\eta(x)$. The rest now follows from the inequality

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The first method considered, and perhaps the most familiar, is that of single-parameter perturbation theory. This method depends on the facts that the solutions of a reduced form (usually linear) of the original NLDE are known and that the difference between the NLDE and the reduced form is, in some sense, small. This difference, the perturbation, is then multiplied by some parameter, say ϵ, assumed to be small, if such a parameter is not initially present. By using this parameter and the solution to the reduced differential equation, a power series solution is obtained which approximately satisfies the original NLDE. When the perturbation is sufficiently small, one or two corrective terms usually give the solution to the desired accuracy. One of the limitations of the perturbation method is that ϵ is required to be sufficiently small; otherwise the power series expansion does not converge. Another difficulty occurs if periodic solutions are desired—namely, the treatment of nonperiodic terms in the power series expansion when they occur.[1] A particular variation of the perturbation method, due to Lindstedt,[2] is sometimes called renormalization.[3] In this approach a power series expansion, in terms of the perturbation parameter ϵ, is developed for the displacement and frequency since the frequency is generally dependent on the amplitude of the motion. By constraining the solution to be periodic, conditions are established from which the power series coefficients for the frequency are determined.

A second method is the asymptotic method ($\epsilon \to 0$) of Krylov and Bogoliubov.[4,5] Similar to the perturbation theory described above, this method assumes that periodic solutions to a reduced linear form of the NLDE are known. The solution to the NLDE is then represented as a power series expansion in terms of the perturbation parameter. To complete the development, the amplitude and phase of the solution to the reduced LDE are allowed to vary in time and, along with the perturbing function, are represented as power series in terms of the perturbation parameter. By grouping like order terms of these expansions, a set of differential equations results which can be solved recursively to yield successively higher-order approximations to the exact solution as $\epsilon \to 0$. Finally, an appropriate constraint is imposed to assure that only periodic solutions are obtained. This method is actually a refinement, by Bogoliubov, of the original method which is similar to the variation of parameters technique applied to ordinary LDE. Because of its similarity to perturbation theory, the asymptotic method suffers from the same difficulty and cannot be applied for large ϵ.

When the perturbing function is not sufficiently small, a third approach is to develop the solution in an asymptotic series expansion instead of a power series expansion. Such a solution has been developed for the autonomous, nonlinear van der Pol differential equation by Dorodnitsin.[6] One difficulty with the method is that several solutions may need to be developed and joined by a type of analytic continuation.

Another approach, along the same lines as those mentioned above, uses the Laplace transform. Again a constraint must be imposed to assure that only periodic solutions are obtained.[7]

All of the above methods have a common deficiency. Their expansions are for a single perturbing term or function. If several independent perturbing functions occur, then the above methods must be extended to a multiterm perturbation theory. Such a theory has been developed and applied to two problems in elastostatics.[8] However, the solutions developed are nonperiodic solutions and are of no utility to us here. Although it is probably possible to develop a multiterm perturbation theory for periodic solutions, a different alternative is pursued in obtaining solutions to the NLDE treated in this paper.

The approach selected for obtaining solutions to the NLDE involves basically two parts. First, the general characteristics and form of the solution are obtained by applying functional and dimensional arguments and using the fact that periodic solutions are known to exist. Second, by using the theoretical work as a foundation and guide, the NLDE is reduced to a set of simultaneous nonlinear algebraic equations. The solution to these equations, by iteration, yields the complete expressions for the Fourier coefficients and the frequency.

In Sec. II we present the qualitative characteristics of the DE to be considered, the analytical form of the DE, and the assumed periodic solutions.

In Sec. III we develop the quantitative characteristics of the solution through functional and dimensional arguments and state and prove several theorems regarding the solutions.

In Sec. IV we obtain and solve the algebraic equations required to determine the numerical constants of the solution.

In Sec. V we apply the solution to the motion of a charged particle moving in a cylindrically symmetric electric field; we then present the numerical results to illustrate the applicability and behavior of the general solution.

II. QUALITATIVE CONSIDERATIONS

This paper is confined to a consideration of differential equations of the form

$$\ddot{x} + f(x) = 0, \tag{1}$$

which can be thought of as representing the one-dimensional motion of a particle. The qualitative nature of the motion is made clear if a potential function is introduced by means of

$$f(x) = \frac{d\psi}{dx}. \tag{2}$$

The system is conservative and has the first integral

$$\mathcal{E} = \tfrac{1}{2}\dot{x}^2 + \psi(x) = \text{const.} \tag{3}$$

We will examine the periodic solutions in the vicinity of a stable equilibrium point which, for simplicity, we take to be at $x = 0$. Figure 1 illustrates a possible potential function. The potential function is assumed to possess a Taylor series expansion which we express as

$$\psi = \tfrac{1}{2}\alpha x^2 + \tfrac{1}{3}\beta x^3 + \tfrac{1}{4}\gamma x^4 + \tfrac{1}{5}\delta x^5 + \tfrac{1}{6}\epsilon x^6. \tag{4}$$

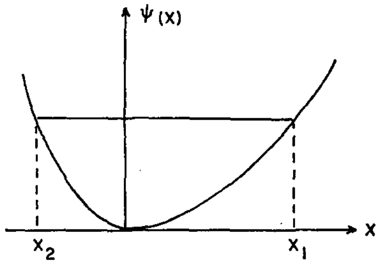

FIG. 1. Typical potential function.

The differential equation is then

$$\ddot{x} + \alpha x + \beta x^2 + \gamma x^3 + \delta x^4 + \epsilon x^5 = 0. \quad (5)$$

The end result of our calculations will be to produce an approximate solution which is sufficiently accurate to justify the inclusion of all terms in (5). The end result is based on the assumption that the higher terms in (5) are less important than the lower terms. Nevertheless, the basic idea of the method really depends on only one assumption, namely that the solutions are periodic. The procedure can easily be modified to treat a differential equation of the form

$$\ddot{x} + \alpha x + \epsilon x^5 = 0, \quad (6)$$

where ϵ is large and α is small or even zero.

Given some energy, the particle moves back and forth between turning points x_1 and x_2 as illustrated in Fig. 1. Qualitatively the motion resembles Fig. 2 where x is plotted against ωt, ω being the circular frequency of the motion. Such a motion can be represented by a Fourier series:

$$x = b_0 + \sum_{n=1}^{\infty} (b_n \cos n\omega t + a_n \sin n\omega t). \quad (7)$$

There is no loss in generality if it is assumed that the initial velocity of the particle is zero. The NLDE (5) has the property of invariance under time reversal, meaning that the solution as illustrated in Fig. 2 is symmetric about $\omega t = \pi$. The solution is therefore representable as

$$x = b_0 + \sum_{n=1}^{\infty} b_n \cos n\omega t. \quad (8)$$

The restriction of zero initial velocity can be removed

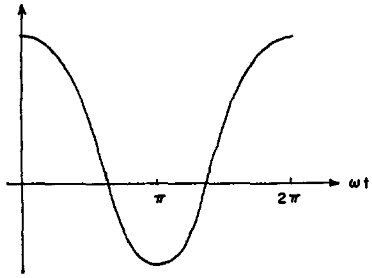

FIG. 2. Periodic oscillations of a particle released from rest.

by writing, in place of (8),

$$x = b_0 + \sum_{n=1}^{\infty} b_n \cos n(\omega t - \phi). \quad (9)$$

If the potential function $\psi(x)$ is assumed to be continuous, it follows that both $x(t)$ and its first derivative are continuous. The Fourier series (8) therefore converges uniformly and absolutely for all t.

III. GENERAL PROPERTIES OF THE SOLUTION

Since in (8) we have already assumed that the initial velocity is zero, there is only one parameter remaining which must be fixed by the initial displacement. This parameter is chosen to be the coefficient b_1 of the leading term in the Fourier series. All other parameters, namely the coefficients b_0, b_2, b_3, $\cdots$, the frequency ω, the energy, and the turning points x_1 and x_2, must be expressible in terms of b_1, and it is one of the goals of this paper to exhibit this functional dependence explicitly.

Theorem 1: The coefficients $b_n(b_1)$ are even or odd functions of b_1 according as n is even or odd.

Proof: Let two particles be released simultaneously, one at the turning point x_1, the other at x_2, both turning points corresponding to the same energy. The two motions will be as illustrated in Fig. 3 and can be represented as

$$x(t) = b_0(b_1) + b_1 \cos \omega t + \sum_{n=2}^{\infty} b_n(b_1) \cos n\omega t, \quad (10)$$

$$x'(t) = b_0'(b_1') + b_1' \cos \omega t + \sum_{n=2}^{\infty} b_n'(b_1') \cos n\omega t. \quad (11)$$

From Fig. 3, one easily sees that the solutions (10) and (11) are related in a simple way:

$$x'(\omega t + \pi) = x(\omega t). \quad (12)$$

Therefore

$$b_0'(b_1') - b_1' \cos \omega t + \sum_{n=2}^{\infty} (-1)^n b_n'(b_1') \cos n\omega t$$
$$= b_0(b_1) + b_1 \cos \omega t + \sum_{n=2}^{\infty} b_n(b_1) \cos n\omega t. \quad (13)$$

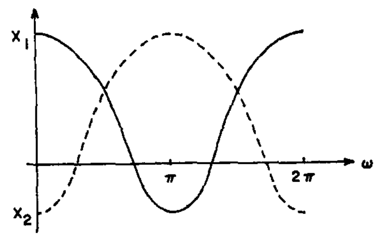

FIG. 3. Periodic oscillations of two particles of the same energy released at opposite turning points.

Term-by-term comparison shows that

$$b_1' = -b_1, \tag{14}$$

$$(-1)^n b_n'(-b_1) = b_n(b_1). \tag{15}$$

The functional dependence of the coefficients on b_1 must ultimately be determined by substituting the Fourier series into the NLDE, and, since (10) and (11) are identical in form, the dependence of b_n' on b_1' must be the same as the dependence of b_n on b_1. This allows us to remove the prime in (15):

$$(-1)^n b_n(-b_1) = b_n(b_1). \tag{16}$$

Theorem 2: The frequency is an even function of b_1.

Proof: The solutions (10) and (11) both correspond to the same energy and, of course, have the same frequency:

$$\omega(b_1') = \omega(b_1) = \omega(-b_1). \tag{17}$$

Theorem 3: The turning points are functionally related by means of

$$x_2(b_1) = x_1(-b_1). \tag{18}$$

Proof: The turning points are found by setting $\omega t = 0$ and $\omega t = \pi$ in (10):

$$x_1 = b_0 + b_1 + b_2 + b_3 + \cdots,$$
$$x_2 = b_0 - b_1 + b_2 - b_3 + \cdots. \tag{19}$$

The result follows by an application of (16).

Theorem 4: The energy of the particle is an even function of b_1.

Proof: The total energy is related to the turning points by means of

$$\mathcal{E} = \psi[x_1(b_1)] = \psi[x_2(b_1)] = \psi[x_1(-b_1)]. \tag{20}$$

Thus

$$\mathcal{E}(b_1) = \mathcal{E}(-b_1). \tag{21}$$

In a linear system, the energy is proportional to the square of the amplitude which is a special case of (21).

The coefficients $b_0, b_2, b_3, \cdots$ as well as the frequency are assumed to be continuous, differentiable functions of b_1. They can therefore be expanded in power series which are expressed as

$$b_n = g_{n0} + g_{n1}b_1 + g_{n2}b_1^2 + \cdots, \tag{22}$$

where the coefficients g_{ij} can depend only on the parameters $\alpha, \beta, \gamma, \cdots$ of the NLDE (5) and numerical factors.

We now prove the following theorem.

Theorem 5: The series for b_n begins with the term b_1^n when $\alpha \neq 0$, while b_0 is of the order b_1^2. The theorem does not hold if $\alpha = 0$ as we will show by an example later.

Proof: We first show that the even coefficients have no constant term and the odd coefficients have no linear term. If $\alpha \neq 0$, the solution in the limit $b_1 \to 0$ is

$$x = b_1 \cos \omega t. \tag{23}$$

If the linear and constant terms were present in the coefficients b_n as given by (22), the solution would take the limiting form

$$x = b_1(\cos \omega t + g_{31} \cos 3\omega t + \cdots)$$
$$+ g_{00} + g_{20} \cos 2\omega t + g_{40} \cos 4\omega t + \cdots \tag{24}$$

in violation of (23).

We now show that the coefficients $b_4, b_6, \cdots$ have no second-order terms. We already know that $b_3, b_5, \cdots$ can have no terms of order lower than b_1^3. The DE accurate to second order is

$$\ddot{x} + \alpha x + \beta x^2 = 0. \tag{25}$$

If the solution (8) is substituted into (25) and all terms of higher order than b_1^2 are discarded, the result is

$$\alpha b_0 + (\alpha - \omega^2)b_1 \cos \omega t + (\alpha - 4\omega^2)b_2 \cos 2\omega t$$
$$+ (\alpha - 16\omega^2)b_4 \cos 4\omega t + \text{higher even harmonics}$$
$$+ \tfrac{1}{2}b_1^2\beta(1 + \cos 2\omega t) = 0. \tag{26}$$

Since the coefficients of each harmonic must vanish, $b_4, b_6, \cdots$ are all zero to second order.

If we now write down the DE accurate to third order and proceed in exactly the same manner, this time retaining all terms to order b_1^3, we find that $b_5, b_7, \cdots$ have no terms proportional to b_1^3. What happens is that the nonlinear terms βx^2 and γx^3 never contribute harmonics of any higher order than the order of the terms being retained. This will be true as we extend the proof to higher and higher orders. The reason is that when products of the form $\cos^r m\theta \times \cos^s n\theta$ are expanded into harmonic series, the highest harmonic is always $\cos(rm + ns)\theta$. Theorem 5 is therefore established.

It is possible to predict what the actual dependence of the factors g_{ij} in (22) is on the parameters $\alpha, \beta, \gamma, \delta$, and ϵ of the NLDE (5). If x is assumed to have dimensions of length L and t dimensions of time T, then b_n must also have dimensions of length for consistency. Since each parameter involves T^{-2}, the same number of parameters (sum of exponents) must appear in the numerator and denominator of the g_{ij}, which are assumed to be algebraic functions of α, β, γ, δ, and ϵ. Such quantities are expressed in (27)–(30):

$$L^{-1}: \ \beta/\alpha, \tag{27}$$

$$L^{-2}: \ \gamma/\alpha, \beta^2/\alpha^2, \tag{28}$$

$$L^{-3}: \ \delta/\alpha, \beta^3/\alpha^3, \beta\gamma/\alpha^2, \tag{29}$$

$$L^{-4}: \ \epsilon/\alpha, \gamma^2/\alpha^2, \beta^4/\alpha^4, \beta\delta/\alpha^2, \beta^2\gamma/\alpha^3. \tag{30}$$

Quantities absent from (27), for example, are γ/β, δ/γ, ϵ/δ; similar quantities are also absent from (28)–(30). If we require that all solutions to (5) reduce to that of the simple harmonic oscillator for $\alpha \neq 0$, then only terms with powers of α in the denominator are acceptable since all g_{ij} must go to zero as β, γ, $\delta, \cdots \to 0$ in any manner. Thus, by using only the quantities (27)–(30) and the requirement of dimensional consistency, we obtain the following functional forms for the g_{ij} and the b_n:

$$g_{02} = c_{01}\beta/\alpha, \tag{31}$$

$$g_{04} = c_{02}\delta/\alpha + c_{03}\beta^3/\alpha^3 + c_{04}\beta\gamma/\alpha^2, \tag{32}$$

$$g_{22} = c_{21}\beta/\alpha, \tag{33}$$

$$g_{24} = c_{22}\delta/\alpha + c_{23}\beta^3/\alpha^3 + c_{24}\beta\gamma/\alpha^2, \tag{34}$$

$$g_{33} = c_{31}\gamma/\alpha + c_{32}\beta^2/\alpha^2, \tag{35}$$

$$g_{35} = c_{33}\epsilon/\alpha + c_{34}\gamma^2/\alpha^2 + c_{35}\beta^4/\alpha^4 + c_{36}\beta\delta/\alpha^2 + c_{37}\beta^2\gamma/\alpha^3, \tag{36}$$

$$g_{44} = c_{41}\delta/\alpha + c_{42}\beta^3/\alpha^3 + c_{43}\beta\gamma/\alpha^2, \tag{37}$$

$$g_{55} = c_{51}\epsilon/\alpha + c_{52}\gamma^2/\alpha^2 + c_{53}\beta^4/\alpha^4 + c_{54}\beta\delta/\alpha^2 + c_{55}\beta^2\gamma/\alpha^3. \tag{38}$$

The list has been extended to include terms which are of order b_1^5. The constants c_{ij} are numerical factors and do not depend in any way on the parameters of the NLDE or on the initial conditions. We therefore arrive at the general form which the Fourier series representation of the periodic solutions of (5) must take. All terms up to fifth order have been retained. It is clear how to proceed if higher-order terms are required.

The frequency of the motion can be expressed as

$$\omega^2 = \alpha[1 + g_{12}b_1^2 + g_{14}b_1^4 + \cdots], \tag{39}$$

where

$$g_{12} = c_{12}\gamma/\alpha + c_{13}\beta^2/\alpha^2, \tag{40}$$

$$g_{14} = c_{14}\epsilon/\alpha + c_{15}\gamma^2/\alpha^2 + c_{16}\beta^4/\alpha^4 + c_{17}\beta\delta/\alpha^2 + c_{18}\beta^2\gamma/\alpha^3. \tag{41}$$

It is many times asserted that the linear system can be corrected by the inclusion of the second-order term βx^2 in (5). Equation (40) reveals that this is not correct as far as the frequency is concerned. Both β and γ appear in (40) and often in practice the two terms in which they occur are of the same order of magnitude. Thus, if (5) is obtained by means of a Taylor series expansion of some potential function, it is really necessary to include the third-order term γx^3 in order that the expression (39) for the frequency be accurate to second order in b_1. Similarly, the fifth-order term is required in the NLDE in order that the frequency be accurate to fourth order.

IV. DETERMINATION OF THE SOLUTION

The numerical constants c_{ij} must be found by formally substituting the Fourier series solution into the NLDE. The results of Sec. III permit this task to be accomplished in a simplified fashion. Since the expressions for g_{ij} are valid for any choices of α, β, $\gamma, \cdots$ (except $\alpha = 0$), they are valid in particular if $\beta = \gamma = \delta = 0$. We therefore consider the NLDE

$$\ddot{x} + \alpha x + \epsilon x^5 = 0. \tag{42}$$

A simplification results in this case because the potential function is *symmetric*, meaning that the solution will be of the form

$$x = b_1 \cos \omega t + b_3 \cos 3\omega t + b_5 \cos 5\omega t + \cdots. \tag{43}$$

To fifth order in b_1,

$$x^5 = b_1^5 \cos^5 \omega t = b_1^5(\tfrac{5}{8} \cos \omega t + \tfrac{5}{16} \cos 3\omega t + \tfrac{1}{16} \cos 5\omega t). \tag{44}$$

If (43) is substituted into (42) and the coefficients of like harmonics equated to zero, the result is the system of algebraic equations

$$(\alpha - \omega^2)b_1 + \tfrac{5}{8}\epsilon b_1^5 = 0, \tag{45}$$

$$(\alpha - 9\omega^2)b_3 + \tfrac{5}{16}\epsilon b_1^5 = 0, \tag{46}$$

$$(\alpha - 25\omega^2)b_5 + \tfrac{1}{16}\epsilon b_1^5 = 0. \tag{47}$$

Equation (45) is solved for the frequency to get

$$\omega^2 = \alpha[1 + \tfrac{5}{8}(\epsilon/\alpha)b_1^4]. \tag{48}$$

Since b_3 is of order b_1^3 and b_5 is of order b_1^5, the approximation $\omega^2 = \alpha$ is sufficient in (46) and (47). We find

$$b_3 = \tfrac{5}{128}(\epsilon/\alpha)b_1^5, \tag{49}$$

$$b_5 = \tfrac{1}{384}(\epsilon/\alpha)b_1^5. \tag{50}$$

Comparison of the above results with (36), (38), and (41) reveals that

$$c_{33} = \tfrac{5}{128}, \quad c_{51} = \tfrac{1}{384}, \quad c_{14} = \tfrac{5}{8}. \tag{51}$$

All of the remaining constants can be found by a similar consideration of the two DE

$$\ddot{x} + \alpha x + \beta x^2 + \gamma x^3 = 0, \tag{52}$$

$$\ddot{x} + \alpha x + \beta x^2 + \delta x^4 = 0. \tag{53}$$

We recover here a kind of *superposition principle* for nonlinear DE's in the sense that the solutions of (42), (52), and (53) can be combined to obtain the solution of the more general equation (5). Equations (52) and (53) are admittedly more complicated than (42) but are quite tractable and we have succeeded in computing all numerical constants. These are displayed in Table I. In substituting the solution (8) into the NLDE, the various power of x are computed accurate to fifth order in b_1 and the resulting expressions are written out in terms of harmonic series by using appropriate trigonometric identities.[9] For Eq. (52) the resulting algebraic equations are

$$\alpha b_0 + \beta(\tfrac{1}{2}b_1^2 + b_0^2 + \tfrac{1}{2}b_2^2) + \gamma(\tfrac{3}{2}b_1^2 b_0 + \tfrac{3}{4}b_1^2 b_2) = 0, \tag{54}$$

$$b_1(\alpha - \omega^2) + \beta(2b_1b_0 + b_1b_2 + b_2b_3) + \gamma(\tfrac{3}{4}b_1^2 + \tfrac{3}{4}b_1^2 b_3 + 3b_1b_0^2 + 3b_1b_0b_2 + \tfrac{3}{2}b_1b_2^2) = 0, \tag{55}$$

$$b_2(\alpha - 4\omega^2) + \beta(\tfrac{1}{2}b_1^2 + 2b_0b_2 + b_1b_3) + \gamma(\tfrac{3}{2}b_1^2 b_0 + \tfrac{3}{2}b_1^2 b_2) = 0, \tag{56}$$

$$b_3(\alpha - 9\omega^2) + \beta(b_1b_2 + b_1b_4 + 2b_0b_3) + \gamma(\tfrac{1}{4}b_1^3 + \tfrac{3}{2}b_1^2 b_3 + 3b_1b_0b_2 + \tfrac{3}{4}b_1b_2^2) = 0, \tag{57}$$

$$b_4(\alpha - 16\omega^2) + \beta(\tfrac{1}{2}b_2^2 + b_1b_3) + \gamma\tfrac{3}{4}b_1^2 b_2 = 0, \tag{58}$$

$$b_5(\alpha - 25\omega^2) + \beta(b_1b_4 + b_2b_3) + \gamma(\tfrac{3}{4}b_1^2 b_3 + \tfrac{3}{4}b_1b_2^2) = 0. \tag{59}$$

These equations are solved by iteration by first considering the third-order equations obtained by neglecting all fourth- and fifth-order terms such as b_0^2, $b_1b_0^2$, etc.[9]

Let us consider briefly the possibility of solving (42) even if $\alpha = 0$. Investigation of the potential function shows that the solutions are periodic if $\epsilon > 0$. If we assume that b_3 and b_5 are of decreasing magnitude, then (44) remains valid as the leading term in x^5. Equations (45), (46), and (47) then remain valid, and their solution is

$$\omega^2 = \tfrac{5}{8}\epsilon b_1^4, \quad b_3 = \tfrac{1}{18}b_1, \quad b_5 = \tfrac{1}{250}b_1. \tag{60}$$

The coefficients are indeed of decreasing order of magnitude as one might expect from general considerations of the convergence of Fourier series. Theorem 5 is no longer valid since now b_3 and b_5 are actually *linear* in b_1. The higher coefficients $b_7, b_9, \cdots$ are also linear in b_1, and their inclusion in the calculation would therefore produce modifications (hopefully small) in the numerical coefficients appearing in (60). This is not so for the c_{ij} appearing in the solution for $\alpha \neq 0$. They are precise numbers and, once found, are not modified by extending the calculation to higher orders in b_1. Numerical values are summarized in Table I.

V. APPLICATION

If a charged particle moves in the space between two charged concentric cylindrical electrodes, the equation of motion for its orbit is

$$\frac{d^2x}{d\theta^2} + x - \frac{x_0^2}{x} = 0, \tag{61}$$

where $x = 1/r$ and $r_0 = 1/x_0$ is the radius of its stable circular orbit assuming that the force is one of attraction toward the inner electrode. The variables r and θ are polar coordinates. If the function which appears

TABLE I. Values of c_{ij}.

i \ j	1	2	3	4	5	6	7	8	
0	$-\frac{1}{2}$	$-\frac{3}{8}$	$-\frac{19}{72}$	$\frac{5}{8}$	—	—	—	—	b_0
1	1	$\frac{3}{4}$	$-\frac{5}{6}$	$\frac{5}{8}$	$\frac{3}{128}$	$-\frac{335}{864}$	$-\frac{7}{4}$	$\frac{143}{96}$	ω
2	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{59}{432}$	$-\frac{31}{96}$	—	—	—	—	b_2
3	$\frac{1}{32}$	$\frac{1}{48}$	$\frac{5}{128}$	$-\frac{21}{1024}$	$\frac{79}{2304}$	$-\frac{3}{320}$	$-\frac{43}{768}$	—	b_3
4	$\frac{1}{120}$	$\frac{1}{432}$	$\frac{1}{96}$	—	—	—	—	—	b_4
5	$\frac{1}{384}$	$\frac{1}{1024}$	$\frac{5}{20736}$	$\frac{11}{2880}$	$\frac{5}{2304}$	—	—	—	b_5

in (61) is expanded in a Taylor series about $x = x_0$, the result is

$$\left(\frac{d^2x}{d\theta^2}\right) + 2(x - x_0) - r_0(x - x_0)^2 + r_0^2(x - x_0)^3 - r_0^3(x - x_0)^4 + r_0^4(x - x_0)^5 = 0, \quad (62)$$

where $0 < x < 2x_0$ is the range over which the expansion converges. We identify

$$\alpha = 2, \quad \beta = -r_0, \quad r = r_0^2, \quad \delta = -r_0^3, \quad \epsilon = r_0^4. \quad (63)$$

The following solution is easily constructed:

$$\begin{aligned} r_0/r = {} & 1 + 0.2500(r_0b_1)^2 + 0.064\,25(r_0b_1)^4 \\ & + (r_0b_1)\cos\omega\theta \\ & - [0.083\,33(r_0b_1)^2 + 0.019\,68(r_0b_1)^4]\cos 2\omega\theta \\ & + [0.010\,42(r_0b_1)^3 + 0.021\,20(r_0b_1)^5]\cos 3\omega\theta \\ & - 0.001\,85(r_0b_1)^4\cos 4\omega\theta \\ & + 0.002\,79(r_0b_1)^5\cos 5\omega\theta, \end{aligned} \quad (64)$$

$$\omega^2 = 2[1 + 0.166\,67(r_0b_1)^2 + 0.042\,82(r_0b_1)^4]. \quad (65)$$

Here, ω is not the frequency but $\omega\theta = \pi$ gives the angular displacement between the turning points of the orbit. In computing the second term in (65) note that

$$\begin{aligned} g_{12} &= c_{12}(\gamma/\alpha) + c_{13}(\beta^2/\alpha^2) \\ &= \tfrac{3}{8}r_0^2 - \tfrac{5}{24}r_0^2. \end{aligned} \quad (66)$$

Thus the third-order term in the NLDE is actually more important than the second-order term as far as computing ω^2 correct to order b_1^2!

If the initial conditions are such that $r_0b_1 = 0.5$,

$$\begin{aligned} r_0/r = {} & 1 + 0.0665 + 0.5000\cos\omega\theta \\ & - 0.0220\cos 2\omega\theta + 0.0026\cos 3\omega\theta \\ & - 0.0001\cos 4\omega\theta + 0.0001\cos 5\omega\theta, \end{aligned} \quad (67)$$

$$\omega^2 = 2.0887. \quad (68)$$

The minimum value of r (inner turning point) results if $\theta = 0$. This gives the maximum value of x:

$$x_{\max} = 1.547x_0. \quad (69)$$

For values of x much larger than this, the Taylor series in (62) does not converge very rapidly; in fact it becomes divergent at $x = 2x_0$. We see, however, that the Fourier series (67) is rapidly convergent and gives a good representation of the orbit.

* In partial fulfillment of the requirements of the Master of Science Degree.

[1] R. Bellman, *Perturbation Techniques in Mathematics, Physics, and Engineering* (Holt, New York, 1964), p. 56.
[2] N. Minorsky, *Nonlinear Oscillations* (Van Nostrand, Princeton, N.J., 1962), p. 224.
[3] R. Bellman, Ref. 1, p. 57.
[4] N. Minorsky, Ref. 2, p. 329.
[5] N. Bogoliubov and Y. A. Mitropolsky, *Asymptotic Methods in the Theory of Non-Linear Oscillations* (Hindustan, India, 1961).
[6] N. Bogoliubov, Ref. 5.
[7] L. A. Pipes, *Applied Mathematics for Engineers and Physicists* (McGraw-Hill, New York, 1958).
[8] J. L. Nowinski and I. A. Ismail, "Application of a Multi-Parameter Perturbation Method to Elastostatics," in *Developments in Theoretical and Applied Mechanics*, edited by W. A. Shaw (Pergamon, Oxford, 1965), Vol. 2, pp. 35–45.
[9] T. C. Bradbury, *Theoretical Mechanics* (Wiley, New York, 1968).

Invariant Imbedding and the Variational Treatment of Fredholm Integral Equations with Displacement Kernels*

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(Received 30 July 1970)

Fredholm integral equations with displacement kernels play a significant role in such areas as radiative transfer and optimal filtering. Frequently, these equations are studied by using the fact that their solutions minimize certain quadratic functionals, which opens the way to the employment of the Rayleigh–Ritz method. The aim presented in this paper is radically different. It is shown that the minimizer of the quadratic functional satisfies a Cauchy problem, no use being made of the integral equation. This notion is of analytic interest and computational utility.

I. INTRODUCTION

Consider the quadratic functional in v,

$$Q(v) = \int_0^x v^2(t)\,dt - \int_0^x\int_0^x k(|t-y|)v(t)v(y)\,dt\,dy, \quad x > 0, \quad (1)$$

where

$$k(r) = \int_0^1 e^{-r/z}w(z)\,dz, \quad r > 0. \quad (2)$$

Further assume that $Q(v)$ is positive definite. We wish to find the function $v = u$, $0 \le t \le x$, which minimizes the functional

$$F = Q(v) - 2\int_0^x g(t)v(t)\,dt. \quad (3)$$

The traditional approach[1] is to introduce the variation $\epsilon\eta(t)$,

$$v = u + \epsilon\eta, \quad (4)$$

substitute in Eq. (3), and conclude that the first variation vanishes:

$$0 = \int_0^x \eta(t)\Big(u(t) - \int_0^x k(|t-y|)u(y)\,dy - g(t)\Big)\,dt. \quad (5)$$

Use of the fundamental lemma of the calculus of variations then provides the Euler equation

$$u(t) - \int_0^x k(|t-y|)u(y)\,dy - g(t) = 0, \quad (6)$$

which is a Fredholm integral equation of the second kind. (It occurs in the theories of radiative transfer,[2] optimal filtering,[3] and elsewhere.) Our aim is quite different. We wish to derive a Cauchy problem for the optimizer u, without using the Euler equation (6). In Ref. 4, Eq. (6) was used. This is of analytic interest and of computational utility. Presumably our method can be extended to give a new treatment of a much larger class of variational problems than is treated here.

II. DERIVATION

Observe that the optimizer depends upon x and write

$$u = u(t, x), \quad 0 \le t \le x. \quad (7)$$

Bellman[5] has used this imbedding to study the resolvent kernel using dynamic programming. Differentiate both sides of Eq. (5) with respect to x to obtain

$$0 = \eta(x)\Big(u(x,x) - \int_0^x k(x-y)u(y,x)\,dy - g(x)\Big) + \int_0^x \eta(t)\Big(u_x(t,x) - k(x-t)u(x,x) - \int_0^x k(|t-y|)u_x(y,x)\,dy\Big)\,dt. \quad (8)$$

In view of the arbitrariness of the function η, it follows that the optimizer u satisfies the two equations

$$u(x,x) = g(x) + \int_0^x k(x-y)u(y,x)\,dy, \quad x > 0 \quad (9)$$

and

$$u_x(t,x) = k(x-t)u(x,x) + \int_0^x k(|t-y|)u_x(y,x)\,dy, \quad 0 \le t \le x, \quad (10)$$

for x sufficiently small. These are the equations with which we shall work.

Introduce the function Φ as the solution of the integral equation

$$\Phi(t,x) = k(x-t) + \int_0^x k(|t-y|)\Phi(y,x)\,dy, \quad 0 \le t \le x. \quad (11)$$

It follows that

$$u_x(t,x) = \Phi(t,x)u(x,x), \quad 0 \le t \le x, \quad (12)$$

which is one of the basic differential equations. The representation for the kernel k given in Eq. (2) suggests introducing the function

$$J = J(t, x, z), \quad (13)$$

as the solution of the integral equation

$$J(t, x, z) = e^{-(x-t)/z} + \int_0^x k(|t-y|)J(y, x, z)\,dy,$$
$$0 \le t \le x, \quad 0 \le z \le 1. \quad (14)$$

It is seen directly that

$$\Phi(t, x) = \int_0^1 J(t, x, z)w(z)\,dz. \quad (15)$$

Differentiation of both sides of Eq. (14) with respect to x yields the relation

$$J_x(t, x, z) = -z^{-1}e^{-(x-t)/z} + k(x-t)J(x, x, z) + \int_0^x k(|t-y|)J_x(y, x, z)\,dy. \quad (16)$$

This is viewed as an integral equation for the function J_x. According to Eqs. (11) and (14) its solution is

$$J_x(t, x, z) = -z^{-1}J(t, x, z) + J(x, x, z)\Phi(t, x), \quad t \le x. \quad (17)$$

In view of Eq. (15), Eq. (17) is a differential equation for the function J; x is the independent variable, and t and z are parameters. The function $J(x, x, z)$ must now be considered.

In Eq. (14) replace t by $x - t$ to obtain the equation

$$J(x-t, x, z) = e^{-t/z} + \int_0^x k(|x-t-y|)J(y, x, z)\,dy. \quad (18)$$

Then introduce a new variable of integration by replacing y by $x - y$, which yields the integral equation

$$J(x-t, x, z) = e^{-t/z} + \int_0^x k(|t-y|)J(x-y, x, z)\,dy. \quad (19)$$

Through differentiation with respect to x, it is seen that

$$\frac{d}{dx}J(x-t, x, z) = k(x-t)J(0, x, z) + \int_0^x k(|t-y|)\frac{d}{dx}J(x-y, x, z)\,dy. \quad (20)$$

According to Eq. (11) the solution of this integral equation for the function $(d/dx)J(x-t, x, z)$ is

$$\frac{d}{dx}J(x-t, x, z) = J(0, x, z)\Phi(t, x). \quad (21)$$

Introduce the functions X and Y by means of the definitions

$$X(x, z) = J(x, x, z), \quad (22)$$

$$Y(x, z) = J(0, x, z). \quad (23)$$

By putting $t = 0$ in Eqs. (21) and (17) and using Eq. (15), it is seen that the differential equations for the functions X and Y are

$$X_x(x, z) = Y(x, z)\int_0^1 Y(x, z')w(z')\,dz', \quad (24)$$

$$Y_x(x, z) = -z^{-1}Y(x, z) + X(x, z)\int_0^1 Y(x, z')w(z')\,dz', \quad x > 0. \quad (25)$$

From the definitions of the functions X and Y and the integral equation (14) for the function J, it follows that the initial conditions at $x = 0$ are

$$X(0, z) = 1, \quad (26)$$

$$Y(x, z) = 1. \quad (27)$$

The functions X and Y are determined from the Cauchy problem in Eqs. (24)–(27). For a fixed value of t and $x > t$, the function $J(t, x, z)$ is determined by the differential equation (17), the relation (15), and the initial condition at $x = t$,

$$J(t, x, z)\big|_{x=t} = X(t, z), \quad 0 \le z \le 1. \quad (28)$$

Next we return to the second factor in the right side of Eq. (12), $u(x, x)$. According to Eq. (9) this may be written

$$\begin{aligned} u(x, x) &= g(x) + \int_0^x k(x-y)u(y, x)\,dy \\ &= g(x) + \int_0^x \int_0^1 e^{-(x-y)/z}w(z)\,dz\,u(y, x)\,dy \\ &= g(x) + \int_0^1 w(z)\,dz \int_0^x e^{-(x-y)/z}u(y, x)\,dy. \end{aligned} \quad (29)$$

By introducing the function e,

$$e(z, x) = \int_0^x e^{-(x-y)/z}u(y, x)\,dy, \quad 0 \le v \le 1, \quad 0 \le x, \quad (30)$$

we see that

$$u(x, x) = g(x) + \int_0^1 e(z, x)w(z)\,dz. \quad (31)$$

Now a differential equation for the function e is to be obtained. Differentiation of both sides of Eq. (30) yields

$$\begin{aligned} e_x(z, x) &= u(x, x) - z^{-1}e(z, x) + \int_0^x e^{-(x-y)/z}u_x(y, x)\,dy \\ &= -z^{-1}e(z, x) + u(x, x) \times \left(1 + \int_0^x e^{-(x-y)/z}\Phi(y, x)\,dy\right). \end{aligned} \quad (32)$$

It remains to evaluate the integral in the last equation. Through cross multiplication of Eqs. (11) and (14), integration, and cancellation of the double integrals, it follows that

$$\int_0^x e^{-(x-y)/z}\Phi(y, x)\, dy = \int_0^x J(y, x, z)k(x - y)\, dy. \quad (33)$$

From Eq. (14) it is seen that

$$\int_0^x J(y, x, z)k(x - y)\, dy = J(x, x, z) - 1, \quad (34)$$

or

$$\int_0^x e^{-(x-y)/z}\Phi(y, x)\, dy = X(x, z) - 1. \quad (35)$$

Equation (32) becomes the desired differential equation

$$e_x(z, x) = -z^{-1}e(z, x) + X(x, z) \times \left(g(x) + \int_0^1 e(z', x)w(z')\, dz'\right). \quad (36)$$

The initial condition on e at $x = 0$ is

$$e(z, 0) = 0, \quad (37)$$

which follows from Eq. (30). The derivation of the Cauchy problem is now complete.

III. THE CAUCHY METHOD[4]

The method for determining the value of $u(t, c)$ for a given value of t and for c sufficiently small is as follows. The functions X, Y, and e are determined on the interval $0 \leq x \leq t$ by means of the Cauchy problem

$$X_x(x, z) = Y(x, z)\int_0^1 Y(x, v)w(v)\, dv, \quad X(0, z) = 1, \quad (38)$$

$$Y_x(x, z) = -z^{-1}Y(x, z) + X(x, z) \times \int_0^1 Y(x, v)w(v)\, dv, \quad Y(0, z) = 1, \quad (39)$$

$$e_x(z, x) = -z^{-1}e(z, x) + X(x, z) \times \left(g(x) + \int_0^1 e(v, x)w(v)\, dv\right), \quad e(z, 0) = 0, \quad (40)$$

for

$$0 \leq z \leq 1. \quad (41)$$

At $x = t$ the differential equations for the functions J and u are adjoined:

$$J_x(t, x, z) = -z^{-1}J(t, x, z) + X(x, z) \times \int_0^1 J(t, x, v)w(v)\, dv, \quad 0 \leq z \leq 1, \quad (42)$$

and

$$u_x(t, x) = \left(g(x) + \int_0^1 e(v, x)w(v)\, dv\right) \times \int_0^1 J(t, x, v)w(v)\, dv. \quad (43)$$

The initial conditions on these functions at $x = t$ are

$$J(t, t, z) = X(t, z) \quad (44)$$

and

$$u(t, t) = g(t) + \int_0^1 e(v, t)w(v)\, dv. \quad (45)$$

The integration of the equations for the functions X, Y, e, J, and u is carried out from $x = t$ to $x = c$, at which point the value of $u(t, c)$ is determined.

In effect, the function u is determined at a fixed value of t for all x for which $c \geq x \geq t$. In view of the nonlinear nature of the differential equations, the solution may become infinite for a finite value of x, which necessitates the restriction on the size of x.

IV. DISCUSSION

The numerical integration of the initial value problem described in the previous section can be carried out by replacing the integrals by finite sums using Gaussian quadrature formulas. This reduces the differential–integral equations to a system of ordinary differential equations. In practice this has worked extremely well.[6,7]

It would be highly desirable to prove that the function u, produced as the solution of the initial value problem, does satisfy the Euler equation (6) and, further, that it does minimize the quadratic functional F.

Traditionally, approximate solutions of the Fredholm integral equation (6) are obtained by applying the Rayleigh–Ritz method to the minimization of the functional F. The analysis presented here opens up many new interesting possibilities by using combinations of the two.

* This research is supported by the United States Air Force under Project Rand.

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[1] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1953), Vol. 1.
[2] V. V. Sobolev, *A Treatise on Radiative Transfer* (Van Nostrand, Princeton, N.J., 1963).
[3] D. Middleton, *Topics in Communication Theory* (McGraw-Hill, New York, 1965).
[4] H. H. Kagiwada and R. E. Kalaba, RAND Corporation Report RM-5186-PR, 1966.
[5] R. E. Bellman, Proc. Am. Math. Soc. **8**, 435 (1957).
[6] R. E. Bellman, H. H. Kagiwada, R. E. Kalaba, and S. Ueno, J. Math. Anal. Appl. **12**, 541 (1965).
[7] J. Buell, H. H. Kagiwada, R. E. Kalaba, A. McNabb, and A. Schumitzky, J. Quant. Spectr. Radiative Transfer **8**, 1481 (1968).

Radiative Transfer in Spherical Shell Atmospheres with Radial Symmetry*

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(Received 30 July 1970)

In recent years, the need to allow for the effect of curvature on the formation of spectral lines has been recognized not only in the fields of planetary and stellar atmospheric physics but also in the field of neutron transport in spherical reactors. This paper is of interest in these and related fields. Initial value systems are obtained for the scattering and transmission functions and emergent intensities for inhomogeneous, anisotropically scattering spherical media both with internal and external sources and with various types of cores.

1. INTRODUCTION

In recent years, the need to allow for the effect of curvature on the formation of spectral lines has been recognized, not only in the fields of planetary and stellar atmospheric physics, but also in the field of neutron transport in spherical reactors.[1–3]

The approximate solution of the transfer equation in spherical geometry has been discussed by several authors.[4–17] Invariant imbedding equations governing the reflection functions in spherical homogeneous shell atmospheres with isotropic scattering were obtained rigorously from the transfer equations without referring to the symbolic delta function of Dirac in the formulation of the problem.[18,19] Heaslet and Warming[20] have reduced the exact solution of the spherical transport equation to that of the transport equation in slab geometry; this approach is valid in the homogeneous isotropic case.

By extension of the numerical approach used in the radiative transfer theory in slab geometry,[21,22] the numerical solution of the spherical shell and cylindrical transport problems has been obtained.[23,24] Also, the particle-counting technique has been applied to the diffuse reflection from homogeneous cylindrical regions.[25] Recently this approach has been extended to the diffuse transmission of light from a central source through an inhomogeneous spherical shell with isotropic scattering.[26]

This paper, making use of the invariant imbedding technique, derives rigorously the integro-differential equations for the scattering and transmission functions and intensity in inhomogeneous, anisotropically scattering media from the transfer equations in the following problems:

(i) an externally illuminated spherical shell atmosphere with a reflecting inner surface;

(ii) a spherical shell atmosphere surrounding a perfect black core;

(iii) a spherical shell atmosphere surrounding a vacuum core with a central point source;

(iv) a spherical shell atmosphere with internal sources of radiation.

In astrophysical contexts, the above problems correspond to

(i) Chandrasekhar's radiation problem in spherical geometry,

(ii) Schuster's problem in the theory of line formation by a scattering spherical shell atmosphere,

(iii) the diffuse transmission of light from a central star by a spherical nebula in the field of ultraviolet radiation,

(iv) the formation of absorption lines by an absorbing and scattering spherical shell atmosphere.

These problems will be treated in Secs. 2–5, respectively. The equations obtained in this paper are exact and, we believe, new. Some of them were obtained with the aid of the probabilistic method.[27]

2. AN EXTERNALLY ILLUMINATED SPHERICAL SHELL ATMOSPHERE WITH A REFLECTING INNER SURFACE

The Equation of Transfer and the Boundary Value Problem

Consider an inhomogeneous, anisotropically scattering, source-free spherical shell atmosphere bounded by the concentric spherical surfaces with radii x and y, $0 < y < x$. The inner surface reflects radiation isotropically according to the Lambert law with a constant surface albedo A. Radiation which is not reflected at the surface is absorbed there.

Let conical flux of radiation of πF per unit area normal to itself be uniformly incident on the outer surface at inclination $\cos^{-1} u$, $0 < u \leq 1$, to the inward-directed radius vector. Assume that the radiation field is radially symmetric; then the intensity and source function are independent of the azimuth. We shall consider the intensity in the total radiation field, where

total intensity = diffuse intensity
+ intensity of reduced
incident radiation.

Let r be the radial coordinate, $y \leq r \leq x$. The intensity in the total radiation field at r directed toward the outer surface is denoted $I(r, +v)$ and the intensity of the inward-directed radiation is $I(r, -v)$, where $0 < v \leq 1$. As usual, v is the cosine of the angle measured from the outward-directed radius vector if the radiation is propagating in an outgoing direction, or from the inward-directed radius vector if the radiation is propagating inwards.

The equation of transfer for the total radiation field is

$$v\frac{\partial I}{\partial r}(r, v) + \frac{1-v^2}{r}\frac{\partial I}{\partial v} + \alpha(r)I = \tfrac{1}{2}\sigma(r)\int_{-1}^{+1} p(r; v, v')I(r, v')\,dv', \quad (1)$$

where $\alpha(r)$ and $\sigma(r)$ are, respectively, the volume attenuation and scattering coefficients and the azimuth independent phase function $p(r; v, v')$ is given in terms of the standard phase function for single scattering $p(r; v, \varphi; v', \varphi')$ by the relation

$$p(r; v, v') = (2\pi)^{-1}\int_0^{2\pi} p(r; v, \varphi; v', \varphi')\,d\varphi'. \quad (2)$$

The local reciprocity principle is satisfied. The function $p(r, v, v')$ is normalized to 2 on the unit sphere. The boundary conditions satisfied by the total intensity are

$$I(x, -v) = \tfrac{1}{2}F\delta(v - u) \quad (3)$$

and

$$I(y, +v) = 2A\int_0^1 I(y, -v')v'\,dv' + \tfrac{1}{2}Fe^{-\tau(x,y,u)}\delta(v)\,d(u, u_c), \quad (4)$$

where $0 \leq v \leq 1$, $d(u, u_c)$ is the Kronecker delta function, and $u_c = [1 - (y/x)^2]^{\frac{1}{2}}$.

Refer to Fig. 1 and define the distance

$$x_1 = x(1 - u^2)^{\frac{1}{2}}. \quad (5)$$

In the case $y < x_1$, the length x_1 is the shortest distance OC between the photon path AD and the center O. It is noted that, at some general point B along AD at radial distance r, the path makes an angle whose cosine is u^* with the radius vector, where u^* is given by the formula

$$u^* = u^*(r) = [1 - (x/r)^2(1 - u^2)]^{\frac{1}{2}}. \quad (6)$$

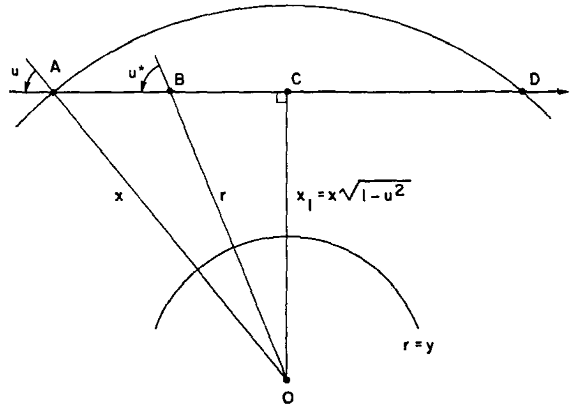

FIG. 1.

The optical distance along the path AB is

$$\tau(x, r, u) = \int_{ru^*}^{xu} \alpha(z)\,ds(z), \quad (7)$$

where

$$s(z) = [z^2 - x^2(1 - u^2)]^{\frac{1}{2}}. \quad (8)$$

The intensity of the reduced incident radiation in the ingoing direction BC at point B is therefore

$$\frac{F}{2}\frac{u}{u^*}\left(\frac{x}{r}\right)^2 e^{-\tau(x,r,u)}\delta(v - u^*), \quad (9)$$

for $r \geq x_1 \geq y$, and $u^* > 0$, because of the deterministic change in state.

We now introduce the new intensity function $I^*(r, v)$ as follows:

$$I(r, -v) = I^*(r, -v) + \frac{F}{2}\frac{u}{u^*}\left(\frac{x}{r}\right)^2 e^{-\tau(x,r,u)}\delta(v - u^*)h(r - x_1), \quad (10)$$

$$I(r, +v) = I^*(r, +v), \quad (11)$$

where

$$h(q) = 0, \quad q < 0; \qquad = 1, \quad q \geq 0, \quad (12)$$

for $0 < v \leq 1$, $y \leq r \leq x$. Note that, when $r < x_1$, the total radiation field contains only the diffuse contribution. Then $I(r, v) = I^*(r, v)$ for all v, $-1 \leq v \leq 1$. When $r \geq x_1$, however, reduced incident radiation is present. It is included in the definition of the outgoing intensity $I^*(r, +v)$, but it is *not* included in the ingoing intensity function $I^*(r, -v)$, where $0 < v \leq 1$. This definition of the function $I^*(r, v)$ is made so that the scattering and transmission functions soon to be introduced give, respectively, the *total* intensity of radiation emerging from the outer surface

$$I^*(x, +v) = (F/4v)S(x, y; v, u), \quad (13)$$

and the ingoing *diffuse* intensity at the inner surface

$$I^*(y, -v) = (F/4v)T(x, y; v, u). \quad (14)$$

This is not unlike the convention in the plane-parallel case.

From the above equations it is readily seen that the function $I^*(r, v)$ satisfies the equation

$$v \frac{\partial I^*}{\partial r}(r, v) + \frac{1 - v^2}{r}\frac{\partial I^*}{\partial v} + \alpha(r)I^* = J(r, v), \quad (15)$$

where

$$J(r, v) = \tfrac{1}{2}\sigma(r)\int_{-1}^{+1} p(r; v, v')I^*(r, v')\, dv' + \tfrac{1}{4}F\sigma(r)\frac{u}{u^*}\left(\frac{x}{r}\right)^2 \times e^{-\tau(x,r,u)}p(r; v, -u)h(r - x_1), + \tfrac{1}{2}Fe^{-\tau(x,y,u)}\delta(v)\, d(u, u_c) \quad (16)$$

and it satisfies the boundary conditions

$$I^*(x, -v) = 0, \quad (17)$$

$$I^*(y, +v) = 2A\int_0^1 I^*(y, -v')v'\, dv' + FA\frac{u^2}{u^*}\left(\frac{x}{y}\right)^2 e^{-\tau(x,y,u)}h(y - x_1). \quad (18)$$

The Initial Value Problem for the Intensity of the Reflected Radiation

In a manner similar to that used in slab geometry,[1] it is assumed that the law of reflection of radiation by a spherical shell is given by the equation

$$I(r, +v) = \frac{1}{2v}\int_0^1 S(r, y; v, v')I(r, -v')\, dv'. \quad (19)$$

This defines the scattering function $S(r, y; v, v')$, $0 \le v, v' \le 1$. On inserting Eqs. (10) and (11) into Eq. (19), we find

$$I^*(r, +v) = \frac{F}{4v}\frac{u}{u^*}\left(\frac{x}{r}\right)^2 e^{-\tau(x,r,u)}S(r, y; v, u^*)h(r - x_1) + \frac{1}{2v}\int_0^1 S(r, y; v, v')I^*(r, -v')\, dv'. \quad (20)$$

Equation (20) corresponds to the first law of diffuse reflection in slab geometry [Ref. 1, Sec. 50, Eq. (5)].

In the limit $r = x$, Eq. (20) becomes

$$I(x, +v) = I^*(x, +v) = (F/4v)S(x, y; v, u), \quad (21)$$

with the use of Eqs. (6), (7), and (17). The angular distribution of the total radiation emerging from the outer surface is directly expressed in terms of the scattering function.

Differentiate Eq. (20) with respect to r, use Eqs. (6)–(8), pass to the limit $r = x$, and make use of the boundary condition of Eq. (17) to obtain

$$\left[\frac{dI^*}{dr}(r, +v)\right]_{r=x} = \frac{F}{4v}\left(-\frac{1 - u^2}{u^2 x}S(x, y; v, u) - \frac{1 + v^2}{v^2 x}S + \frac{\alpha(x)}{u}S + \frac{\partial S}{\partial x} + \frac{1 - v^2}{vx}\frac{\partial S}{\partial v} + \frac{1 - u^2}{ux}\frac{\partial S}{\partial u}\right) + \frac{1}{2v}\int_0^1 S(x, y; v, v')\left[\frac{dI^*}{dr}(r, -v')\right]_{r=x} dv'. \quad (22)$$

Equation (15) yields

$$\left[\frac{dI^*}{dr}(r, +v)\right]_{r=x} = \frac{1}{v}\left(-\alpha(x)\frac{F}{4v}S(x, y; v, u) + J(x, +v)\right), \quad (23)$$

$$\left[\frac{dI^*}{dr}(r, -v)\right]_{r=x} = -\frac{1}{v}J(x, -v), \quad (24)$$

where, by Eq. (16),

$$J(x, v) = \tfrac{1}{4}F\sigma(x)p(x; v, -u) + \tfrac{1}{2}[\tfrac{1}{4}F\sigma(x)]\int_0^1 p(x; v, v')S(x, y; v', u)\frac{dv'}{v'}. \quad (25)$$

Substitution of Eqs. (23)–(25) in Eq. (22) provides us with the desired functional equation

$$\frac{\partial S}{\partial x}(x, y; v, u) + \frac{1 - v^2}{vx}\frac{\partial S}{\partial v} + \alpha(x)\left(\frac{1}{v} + \frac{1}{u}\right)S + \frac{1 - u^2}{ux}\frac{\partial S}{\partial u} - \frac{v^2 + u^2}{v^2u^2x}S = \sigma(x)\left(p(x; v, -u) + \tfrac{1}{2}\int_0^1 p(x; v, v')S(x, y; v', u)\frac{dv'}{v'} + \tfrac{1}{2}\int_0^1 S(x, y; v, u')p(x; -u', -u)\frac{du'}{u'} + \tfrac{1}{4}\int_0^1\int_0^1 S(x, y; v, u')p(x; -u', v') \times S(x, y; v', u)\frac{du'}{u'}\frac{dv'}{v'}\right). \quad (26)$$

The boundary condition of Eq. (18) leads to the *initial* condition on the function S when the thickness of the atmosphere is zero, i.e., when $x = y$:

$$S(x, y; v, u)|_{x=y} = 4Avu + 2v\delta(v - u)\, d(u, u_c)|_{x\to y}. \quad (27)$$

In the case of an inhomogeneous shell with isotropic scattering, Eq. (26) reduces to that given in Ref. 26.

The Initial Value Problem for the Intensity of the Diffusely Transmitted Radiation

The next task shall be to determine the intensity $I(y, -v)$ of the radiation diffusely transmitted to the inner surface in the direction $-v$ due to the incident rays. An initial value problem for the transmission function $T(x, y; v, u)$ is to be derived.

Let the intensity of the total transmitted radiation be expressed as

$$I(y, -v) = I(r, -v^*) \frac{v^*}{v}\left(\frac{r}{y}\right)^2 e^{-\tau(r,y,v)} h(y - r_1) + \frac{1}{2v}\int_0^1 T(r, y; v, v') I(r, -v')\, dv', \quad (28)$$

where $I(r, -v)$ is given by Eq. (10); the optical path length is

$$\tau(r, y, v) = \int_{yv}^{rv^*} \alpha(z)\, ds(z), \quad (29)$$

where

$$v^* = v^*(r) = [1 - (y/r)^2(1 - v^2)]^{\frac{1}{2}}, \quad (30)$$

$$s(z) = [z^2 - y^2(1 - v^2)]^{\frac{1}{2}}, \quad (31)$$

and

$$r_1 = r(1 - v^{*2})^{\frac{1}{2}}. \quad (32)$$

The first term on the right-hand side of Eq. (28) represents the direct transmission of the total intensity of radiation in the direction $-v$, $0 < v \leq 1$, and the second term arises from the diffuse transmission of the inward-directed radiation by the spherical shell atmosphere of thickness $(r - y)$ below.

By combining Eq. (28) with Eq. (10), the law of *diffuse* transmission may be written

$$\begin{aligned} I^*(y, -v) &+ \frac{F}{2}\frac{u}{u^0}\left(\frac{x}{y}\right)^2 e^{-\tau(x,y,u)}\delta(v - u^0)h(y - x_1) \\ &= \left[I^*(r, -v^*) + \frac{F}{2}\frac{u}{u^*}\left(\frac{x}{r}\right)^2 \times e^{-\tau(x,r,u)}\delta(v - u^*)h(r - x_1)\right] \\ &\times \frac{v^*}{v}\left(\frac{r}{y}\right)^2 e^{-\tau(r,y,v)}h(y - r_1) \\ &+ \frac{F}{4v}\frac{u}{u^*}\left(\frac{x}{r}\right)^2 e^{-\tau(x,r,u)}T(r, y; v, u^*)h(r - x_1) \\ &+ \frac{1}{2v}\int_0^1 T(r, y; v, v')I^*(r, -v')\, dv', \end{aligned} \quad (33)$$

where

$$u^0 = [1 - (x/y)^2(1 - u^2)]^{\frac{1}{2}}. \quad (34)$$

The intensity of the diffusely transmitted radiation is

$$I^*(y, -v) = (F/4v)T(x, y; v, u). \quad (35)$$

Differentiation of Eq. (33) with respect to r, use of Eqs. (29)–(31), passage to the limit $r = x$, and use of Eq. (24) lead to the integro-differential equation for the transmission function

$$\begin{aligned} &\frac{\partial T}{\partial x}(x, y; v, u) + \frac{1 - v^2}{vx}\frac{\partial T}{\partial v} + \frac{1 - u^2}{ux}\frac{\partial T}{\partial u} + \frac{\alpha(x)}{u}T - \frac{v^2 + u^2}{v^2u^2x}T \\ &= \sigma(x)\Big[e^{-\tau(x,y,v)}\frac{v^*}{v}\left(\frac{x}{y}\right)^2 p(x; -v^*, -u) \\ &+ e^{-\tau(x,y,v)}\frac{v^*}{v}\left(\frac{x}{y}\right)^2 \tfrac{1}{2}\int_0^1 p(x; -v^*, v')S(x, y; v', u)\frac{dv'}{v'} \\ &+ \tfrac{1}{2}\int_0^1 T(x, y; v, u')p(x; -u', -u)\frac{du'}{u'} \\ &+ \tfrac{1}{4}\int_0^1\int_0^1 T(x, y; v, u')p(x; -u', v') \times S(x, y; v', u)\frac{du'}{u'}\frac{dv'}{v'}\Big], \end{aligned} \quad (36)$$

where

$$\tau(x, y, v) = \int_{yv}^{xu} \alpha(z)\, ds(z), \quad (37)$$

$$v^* = v^*(x) = [1 - (y/x)^2(1 - v^2)]^{\frac{1}{2}}. \quad (38)$$

The initial condition is

$$T(x, y; v, u)\big|_{x=y} = 0. \quad (39)$$

3. A SPHERICAL SHELL ATMOSPHERE SURROUNDING A PERFECT BLACK CORE

The Boundary Value Problem

Consider an inhomogeneous, anisotropically scattering, source-free spherical shell atmosphere bounded by the surfaces $r = x$ and $r = y$, $0 < y < x$, with a perfect black core which is an emitter and a perfect absorber. In the terminology of astrophysics, an anisotropically scattering spherical shell atmosphere surrounds the spherical photospheric surface which emits radiation in the outward direction in a known manner. In the plane-parallel perfectly scattering atmosphere, this problem is called the Schuster problem of the theory of line formation.

Let conical flux of radiation of πF per unit area normal to itself be incident uniformly on the inner surface in the outgoing direction $+u$, $0 < u \leq 1$. The boundary value problem for the total intensity, appropriate to this case, is given by the equation of transfer, Eq. (1), together with the boundary conditions

$$I(x, -v) = 0, \tag{40}$$

$$I(y, +v) = \tfrac{1}{2}F\delta(v - u), \tag{41}$$

where $0 < v \leq 1$.

The function $I^*(r, v)$ is introduced by means of the relations

$$I(r, -v) = I^*(r, -v), \tag{42}$$

$$I(r, +v) = I^*(r, +v) + \frac{F}{2}\frac{u}{u_*}\left(\frac{y}{r}\right)^2 e^{-\tau(y,r,u)}\delta(v - u_*), \tag{43}$$

where $0 < v \leq 1$,

$$u_* = u_*(r) = [1 - (y/r)^2(1 - u^2)]^{\frac{1}{2}}, \tag{44}$$

$$\tau(y, r, u) = \int_{yu}^{ru_*} \alpha(z)\, ds(z), \tag{45}$$

$$s(z) = [z^2 - y^2(1 - u^2)]^{\frac{1}{2}}. \tag{46}$$

The boundary value problem for $I^*(r, v)$ is given by Eq. (15), where the source function is

$$J(r, v) = \tfrac{1}{2}\sigma(r)\int_{-1}^{+1} p(r; v, v')I^*(r, v')\, dv' + \tfrac{1}{4}F\sigma(r)\frac{u}{u_*}\left(\frac{y}{r}\right)^2 e^{-\tau(y,r,u)}p(r; v, u_*), \tag{47}$$

and the boundary conditions are

$$I^*(x, -v) = 0, \tag{48}$$

$$I^*(y, +v) = 0, \tag{49}$$

for $0 < v \leq 1$.

The Initial Value Problem for the Intensity of Emergent Radiation Due to a Uniformly Emitting Core

We shall find an invariant imbedding equation governing the transmission function $T_e(y, x; v, u)$ for this case. The outgoing diffuse intensity at r is expressed as the sum of the diffuse transmission of the incident radiation and the reflection by the spherical shell atmosphere of thickness $(r - y)$ of the ingoing radiation at r:

$$I^*(r, +v) = (F/4v)T_e(y, r; v, u) + (2v)^{-1}\int_0^1 S_e(r, y; v, u')I^*(r, -u')\, du'. \tag{50}$$

This transmission function gives the diffuse intensity of the radiation emerging from the outer surface of the shell due to multiple scattering of radiation emitted by the blackbody source:

$$I^*(x, +v) = (F/4v)T_e(y, x; v, u). \tag{51}$$

Equation for function S_e is the same as that discussed previously. In fact, one of the reasons we considered the problem of diffuse reflection due to external conical flux of radiation is that the scattering function is needed in the functional equations for the problems of the blackbody core and internal radiation sources.

On differentiating Eq. (50) with respect to r, passage to the limit $r = x$, and use of Eq. (48), we have

$$\begin{aligned}\frac{\partial T_e}{\partial x}(y, x; v, u) &+ \frac{1 - v^2}{vx}\frac{\partial T_e}{\partial v} + \alpha(x)\frac{T_e}{v} - \frac{1 - v^2}{v^2 x}T_e \\ &= \sigma(x)\Bigg[\frac{u}{u_*}\left(\frac{y}{x}\right)^2 p(x; v, u_*)e^{-\tau(y,x,u)} \\ &+ \frac{1}{2}\int_0^1 p(x; v, v')T_e(y, x; v', u)\frac{dv'}{v'} \\ &+ \frac{1}{2}\frac{u}{u_*}\left(\frac{y}{x}\right)^2 e^{-\tau(y,x,u)} \\ &\times \int_0^1 S(x, y; v, u')p(x; -u', u_*)\frac{du'}{u'} \\ &+ \frac{1}{4}\int_0^1\int_0^1 S(x, y; v, u')p(x; -u', v') \\ &\times T_e(y, x; v', u)\frac{du'}{u'}\frac{dv'}{v'}\Bigg],\end{aligned} \tag{52}$$

where

$$u_* = u_*(x) = [1 - (y/x)^2(1 - u^2)]^{\frac{1}{2}}, \tag{53}$$

which is the required integro-differential equation. The function S_e satisfies Eq. (26), and the initial conditions are

$$S_e(x, y; v, u)|_{x=y} = 2v\delta(v - u)\, d(u, u_c)|_{x\to y}, \tag{54}$$

$$T_e(y, x; v, u)|_{x=y} = 0. \tag{55}$$

Equation (55) is a consequence of the boundary condition (49). Equation (54) is the result of putting $A = 0$ in Eq. (27).

Intensity of Emergent Radiation Due to an Angular Distribution of Sources at the Core

The intensity of radiation emerging from the outer surface of the spherical shell atmosphere due to multiple scattering of radiation emitted by the black core, when the intensity of the emitted radiation depends on the direction, can be readily expressed in terms of the function $T_e(y, x; v, u)$. Let $I^{(s)}(y, +w)$ be the intensity distribution of light emitted at the radiating surface at $r = y$, $0 < w \leq 1$. Then the emergent radiation can be considered as arising from the direct and diffuse transmission of the emitted radiation. Hence,

$$I(x, +v) = I^{(s)}(y, +w)\frac{w}{v}\left(\frac{y}{x}\right)^2 e^{-\tau(y,x,w)} + \frac{1}{2v}\int_0^1 T_e(y, x; v, w')I^{(s)}(y, w')\,dw', \quad (56)$$

where

$$w = [1 - (x/y)^2(1 - v^2)]^{\frac{1}{2}}. \quad (57)$$

In slab geometry, the greatest astrophysical interest is attached to the case of a linear function in w for $I^{(s)}(y, +w)$. An interesting inverse problem would be the estimation of the distribution of sources, $I^{(s)}(y, +w)$, based on observations of the emergent radiation.

4. A SPHERICAL SHELL ATMOSPHERE SURROUNDING A VACUUM CORE WITH A CENTRAL POINT SOURCE

The Boundary Value Problem

Consider an inhomogeneous, anisotropically scattering, spherical shell atmosphere bounded by the surface $r = x$ and $r = y$, $0 < y < x$, surrounding a vacuum core with a point source of radiation at the center. There is no scattering or absorbing material in the core. It is assumed that the central point source emits radiation isotropically. In other words, a constant flux of radiation is normally incident on the inner surface $r = y$. In astrophysical contexts, this is the problem of the diffuse transmission of light from a central star through a spherical planetary nebula in the field of ultraviolet as well as Lyman-alpha radiation, allowing for the Milne boundary conditions (the diffuse flux across the inner surface vanishes).

The boundary value problem for the total intensity is given by Eq. (1) together with the boundary conditions

$$I(x, -v) = 0, \quad (58)$$

$$I(y, +v) = I(y, -v) + \tfrac{1}{2}F\delta(v - 1). \quad (59)$$

The function $I^*(r, v)$ is introduced according to the relations [cf. Eqs. (42) and (43)]

$$I(r, -v) = I^*(r, -v), \quad (60)$$

$$I(r, +v) = I^*(r, +v) + \frac{F}{2}\left(\frac{y}{r}\right)^2 e^{-\tau(y,r)}\delta(v - 1), \quad (61)$$

where

$$\tau(y, r) = \int_y^r \alpha(r)\,dr. \quad (62)$$

The source function is expressed as

$$J(r, v) = \tfrac{1}{2}\sigma(r)\int_{-1}^{+1} p(r; v, v')I^*(r, v')\,dv' + \tfrac{1}{2}F\sigma(r)(y/r)^2 p(r; v, 1)e^{-\tau(y,r)}. \quad (63)$$

The function $I^*(r, v)$ satisfies differential Eq. (15) and boundary conditions

$$I^*(x, -v) = 0, \quad (64)$$

$$I^*(y, +v) = I^*(y, -v). \quad (65)$$

The Initial Value Problem

We introduce the transmission and scattering functions appropriate to this case. The outgoing diffuse intensity at r is expressed as [cf. Eq. (50)]

$$I^*(r, +v) = (F/4v)T_V(y, r; v) + (2v)^{-1}\int_0^1 S_V(r, y; v, u')I^*(r, -u')\,du', \quad (66)$$

the sum of the energy diffusely transmitted from the central source to r, and the reflection by the spherical shell within radius r of the ingoing radiation at r. The transmission function T_V differs from T_e because of the nature of the source as well as the type of core. The scattering function S_V differs from the function S because of the vacuum core. In other words, the quantity

$$(F/4v)S_V(x, y; v, u)$$

gives the intensity of the total emergent radiation for the boundary value problem given by Eqs. (15), (17), and

$$I^*(y, +v) = I^*(y, -v). \quad (67)$$

The function $S_V(x, y; v, u)$ satisfies the same integro-differential equation as does the function $S(x, y; v, u)$, namely Eq. (26). The initial condition is different:

$$S_V(x, y; v, u)|_{x=y} = 2v\delta(v - u). \quad (68)$$

The emergent intensity due to the central source is

$$I^*(x, +v) = (F/4v)T_V(y, x; v). \quad (69)$$

The function $T_V(y, x; v)$ satisfies the integro-differential equation

$$\frac{\partial T_V}{\partial x}(y, x; v) + \frac{1 - v^2}{vx}\frac{\partial T_V}{\partial v} + \alpha(x)\frac{T_V}{v} - \frac{1 - v^2}{v^2 x}T_V$$
$$= \sigma(x)\Bigg[\left(\frac{y}{x}\right)^2 p(x; v, 1)e^{-\tau(y,x)} + \frac{1}{2}\int_0^1 p(x; v, v')T_V(y, x; v')\frac{dv'}{v'} + \frac{1}{2}\left(\frac{y}{x}\right)^2 e^{-\tau(y,x)}\int_0^1 S_V(x, y; v, u')p(x; -u', 1)\frac{du'}{u'}$$
$$+ \frac{1}{4}\int_0^1\int_0^1 S_V(x, y; v, u')p(x; -u', v') \times T_V(y, x; v')\frac{du'}{u'}\frac{dv'}{v'}\Bigg]. \quad (70)$$

The initial condition on T_V is

$$T_V(y, x; v)\big|_{x=y} = 0. \tag{71}$$

In the case of isotropic scattering, Eq. (70) reduces to that given in Ref. 26.

The intensity of the total radiation transmitted through the inhomogeneous spherical shell atmosphere with anisotropic scattering is

$$I(x, +v) = (F/4v)T_V(y, x; v) + \tfrac{1}{2}F(y/x)^2 e^{-\tau(y,x)}\delta(v-1). \tag{72}$$

5. A SPHERICAL SHELL ATMOSPHERE WITH INTERNAL SOURCES OF RADIATION

The Boundary Value Problem

Consider an inhomogeneous, anisotropically scattering spherical shell atmosphere, whose outer and inner radii are x and y, respectively, $0 < y < x$. There are internal emitting sources of radiation with $g(r, v)\,dv\,d\varphi =$ the energy emitted at r in the direction cosine interval $(v, v + dv)$ per unit volume, per unit time, in the element of solid angle $dv\,d\varphi$, $-1 < v < 1$. It is assumed that the indicatrix of scattering and the radiation field are independent of φ, the azimuth. The inner core is a Lambert reflector with albedo A.

The boundary value problem for the intensity $I(r, v)$ is given by Eqs. (1) with the additional term $g(r, v)$ on the right-hand side, (4), and

$$I(x, -v) = 0. \tag{73}$$

There is no distinction between the total and diffuse intensities in this situation.

The Initial Value Problem for the Intensity of Emergent Radiation

The principle of invariant imbedding for the outgoing intensity at r is expressed in the form

$$I(r, +v) = \hat{I}(r, +v) + \frac{1}{2v}\int_0^1 S(r, y; v, v')I(r, -v')\,dv'. \tag{74}$$

Here $\hat{I}(r, +v)$ represents the outgoing intensity of radiation at level r that would be present if there were no medium from x to r. This equation relates $I(r, +v)$, the outgoing radiation at r for a shell of outer radius x to $\hat{I}(r, +v)$, the corresponding radiation for a shell of outer radius r. The second term is due to the multiple scattering in the shell of outer radius r of radiation which is incident at r. The function S is discussed in Sec. 2.

By differentiation, passage to the limit $r = x$ and use of the boundary condition (73), we obtain the desired equation for the emergent intensity $I(x, +v)$,

$$\begin{aligned}\frac{\partial I}{\partial x}(x, +v) &+ \frac{1-v^2}{vx}\frac{\partial I}{\partial v}(x, +v) + \frac{\alpha(x)}{v}I(x, +v)\\ &= \frac{1}{v}\left(g(x, +v) + \frac{\sigma(x)}{2}\int_0^1 p(x; v, v')I(x, +v')\,dv'\right)\\ &+ \frac{1}{2v}\int_0^1 S(x, y; v, u')\left(g(x, -u')\right.\\ &\left.+ \frac{\sigma(x)}{2}\int_0^1 p(x; -u', v')I(x, +v')\,dv'\right)\frac{du'}{u'}.\end{aligned} \tag{75}$$

The function S satisfies the integro-differential equation (26) and the initial condition of Eq. (27). The initial condition on $I(x, +v)$, when $x = 0$, is

$$I(x, +v)\big|_{x=y} = 0, \tag{76}$$

obtained by use of the boundary condition of Eq. (4). For slab geometry, corresponding equations are found in Ref. 28.

Note added in proof: Recently, Eq. (26) was obtained independently by several authors with the aid of the invariance principles [cf. A. Uesugi and J. Tsujita, Publ. Astr. Soc. Japan **21,** 370 (1969); R. C. Allen, Jr., L. F. Shampine, and G. Milton Wing, DASA-2421, University of New Mexico, Albequerque, N. Mex. (1970)], whereas the system of equations for the total reflection function considered by Bellman *et. al.*[24,25] was commented on as admitting two solutions [cf. G. B. Rybicki, J. Computational Phys. **6,** 131 (1970)]. It was also shown that Eqs. (52) and (70) coincide with those given by the probabilistic method from the Milne-type integral equation [cf. T. K. Leong and K. K. Sen, Publ. Astr. Soc. Japan **21,** 167 (1969)]. Furthermore, when the attenuation coefficient varies as the inverse power of radial distance, the Milne integral equation of the source function in spherical shell atmosphere was rigorously solved by an extension of Pincherle-Goursat kernel method [cf. T. K. Leong and K. K. Sen, Publ. Astr. Soc. Japan **23,** 99 (1971)]. In addition, Bellman's new gradient technique was extended to the numerical computation of the source functions of radiation in spherical and the spherical shell media [cf. J. Gruschinske and S. Ueno, Publ. Astr. Soc. Japan **22,** 365 (1970); J. Quant. Spectr. Radiative Transfer (to be published)].

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[1] S. Chandrasekhar, *Radiative Transfer* (Oxford U.P., London, 1950).
[2] I. Busbridge, *The Mathematics of Radiative Transfer* (Cambridge U.P., London, 1960).
[3] V. V. Sobolev, *A Treatise on Radiative Transfer* (Van Nostrand, Princeton, N.J., 1963).

[4] D. Barbier and G. W. Curtis, Ann. Astrophys. **19**, 129 (1956).
[5] V. I. Barkov, Opt. Spektrosk. **14**, 537 (1963) [Opt. Spectrosc. **14**, 285 (1963)].
[6] I. N. Minin and V. V. Sobolev, Astron. Zh. **40**, 496 (1963) [Sov. Astron. AJ **7**, 379 (1963)].
[7] I. N. Minin and V. V. Sobolev, Kosmich. Issled. **1**, 227 (1963) [Cosmic Res. **1**, 190 (1963)].
[8] I. N. Minin and V. V. Sobolev, Kosmich. Issled. **2**, 610 (1964) [Cosmic Res. **2**, 529 (1964)].
[9] V. V. Sobolev and I. N. Minin, Iskusstv. Sputniki Zemli **14**, 7 (1962) [Planet. Space Sci. **11**, 657 (1963)].
[10] V. V. Sobolev, Astron. Zh. **37**, 3 (1960) [Sov. Astron. AJ **4**, 1 (1960)]; **39**, 632 (1962) [**6**, 497 (1963)].
[11] H. K. Sen, Astrophys. J. **110**, 276 (1949).
[12] R. D. Chapman, Astrophys. J. **143**, 61 (1966).
[13] J. Lenoble and Z. Sekera, Proc. Natl. Acad. Sci. (U.S.) **47**, 372 (1961).
[14] I. N. Minin, Astron. Zh. **41**, 662 (1964) [Sov. Astron. AJ **8**, 528 (1965)].
[15] S. J. Wilson and K. K. Sen, Can. J. Phys. **43**, 432 (1965).
[16] S. J. Wilson and K. K. Sen, Ann. Astrophys. **28**, 348 (1965).
[17] S. J. Wilson and K. K. Sen, Ann. Astrophys. **28**, 855 (1965).
[18] P. B. Bailey, J. Math. Anal. Appl. **8**, 144 (1964).
[19] P. B. Bailey and G. M. Wing, J. Math. Anal. Appl. **8**, 170 (1964).
[20] M. A. Heaslet and R. F. Warming, J. Quant. Spectr. Radiative Transfer **5**, 669 (1965).
[21] R. E. Bellman, R. E. Kalaba, and M. C. Prestrud, *Invariant Imbedding and Radiative Transfer in Slabs of Finite Thickness* (Elsevier, New York, 1963).
[22] R. E. Bellman, H. H. Kagiwada, R. E. Kalaba, and M. C. Prestrud, *Invariant Imbedding and Time-Dependent Transport Processes* (Elsevier, New York, 1964).
[23] R. E. Bellman and R. E. Kalaba, Proc. Natl. Acad. Sci. (U.S.) **54**, 1293 (1965).
[24] R. E. Bellman, H. H. Kagiwada, and R. E. Kalaba, J. Computational Phys. **1**, 245 (1966).
[25] R. E. Bellman and R. E. Kalaba, Proc. Natl. Acad. Sci. (U.S.) **43**, 514 (1957).
[26] R. E. Bellman, H. H. Kagiwada, R. E. Kalaba, and S. Ueno, J. Math. Phys. **9**, 909 (1968).
[27] T. K. Leong and K. K. Sen, Ann. Astrophys. **31**, 467 (1968).
[28] R. E. Bellman, H. H. Kagiwada, R. E. Kalaba, and S. Ueno, Icarus **7**, 365 (1967); **11**, 417 (1969).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Contributions of Spin-J Baryon Poles to $\pi N \rightarrow \pi N$ and $\pi N \rightarrow \gamma N$ Amplitudes*

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(Received 7 July 1970)

Contributions of baryon poles of spin J to the $\pi N \rightarrow \pi N$ and $\pi N \rightarrow \gamma N$ amplitudes have been calculated using the Wigner–Bargmann formalism. An ambiguity arising from off-the-mass-shell continuation of the propagator has been discussed and a continuation which gives pure spin-J behavior of the propagator for timelike propagator momentum has been given. Moreover, it has been shown that the parts of the amplitudes (with timelike propagator momentum) containing the highest power of the cosine of the scattering angle are free of this ambiguity.

I. INTRODUCTION

In view of the interest being taken in the Van Hove model, the contribution of arbitrary spins to the scattering amplitudes have gained some importance. Blankenbecler[1] and Sugar[2] have considered boson poles of spin J in the scattering of bosons, and recently Carlitz and Kislinger[3] have given the term having the highest power in the cosine of the scattering angle θ coming from the baryon pole of spin J in the $\pi N \rightarrow \pi N$ scattering amplitude. In the following work we derive complete expressions for the contributions of baryon poles of spin J to the $\pi N \rightarrow \pi N$ and $\pi N \rightarrow \gamma N$ scattering amplitude. For the $\pi N \rightarrow \pi N$ case we have considered the direct u-channel diagram [Fig. 1(A)] as well as the crossed diagram [Fig. 1(B)] and have used an effective Lagrangian with $\leftrightarrow$ over the derivatives $\partial_{\mu_1}\partial_{\mu_2}\cdots$. A similar effective Lagrangian has been used in Ref. 2. Carlitz and Kislinger's result is for the pole in the u-channel and corresponds to calculating Fig. 1(A) without the $\leftrightarrow$ over the derivatives in the effective Lagrangian and also replacing M_J^2 by $-f^2$ in the numerators of spin-1 propagators

$$\Lambda_{\mu\nu}(f) = \left(\delta_{\mu\nu} + \frac{f_\mu f_\nu}{M_J^2}\right)$$

which enter in the spin-J propagator and thus eliminating the spin-zero part from the $\Delta_{\mu\nu}(f)$. We find that even after this elimination the helicity amplitudes in the center-of-mass frame $T_A(\lambda', \lambda)$ do not contain a pure $d^{J'}_{\lambda'\lambda}(\theta)$ angular dependence. The reason for this is that the Dirac part of the propagator for this amplitude containing the factor $(1 \pm (\sqrt{u}/M_J)\gamma_4)$ is off the mass shell and if we replace M_J by $\sqrt{-f^2} = \sqrt{u}$, we do obtain a pure $d^J_{\lambda'\lambda}(\theta)$ behavior. However, for the purpose of reggeization without parity doubling,[3] the M_J in $(1 \pm (\sqrt{\mu}/M_J)\gamma_4)$ is necessary

[4] D. Barbier and G. W. Curtis, Ann. Astrophys. **19**, 129 (1956).
[5] V. I. Barkov, Opt. Spektrosk. **14**, 537 (1963) [Opt. Spectrosc. **14**, 285 (1963)].
[6] I. N. Minin and V. V. Sobolev, Astron. Zh. **40**, 496 (1963) [Sov. Astron. AJ **7**, 379 (1963)].
[7] I. N. Minin and V. V. Sobolev, Kosmich. Issled. **1**, 227 (1963) [Cosmic Res. **1**, 190 (1963)].
[8] I. N. Minin and V. V. Sobolev, Kosmich. Issled. **2**, 610 (1964) [Cosmic Res. **2**, 529 (1964)].
[9] V. V. Sobolev and I. N. Minin, Iskusstv. Sputniki Zemli **14**, 7 (1962) [Planet. Space Sci. **11**, 657 (1963)].
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[16] S. J. Wilson and K. K. Sen, Ann. Astrophys. **28**, 348 (1965).
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[18] P. B. Bailey, J. Math. Anal. Appl. **8**, 144 (1964).
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[20] M. A. Heaslet and R. F. Warming, J. Quant. Spectr. Radiative Transfer **5**, 669 (1965).
[21] R. E. Bellman, R. E. Kalaba, and M. C. Prestrud, *Invariant Imbedding and Radiative Transfer in Slabs of Finite Thickness* (Elsevier, New York, 1963).
[22] R. E. Bellman, H. H. Kagiwada, R. E. Kalaba, and M. C. Prestrud, *Invariant Imbedding and Time-Dependent Transport Processes* (Elsevier, New York, 1964).
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[24] R. E. Bellman, H. H. Kagiwada, and R. E. Kalaba, J. Computational Phys. **1**, 245 (1966).
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[26] R. E. Bellman, H. H. Kagiwada, R. E. Kalaba, and S. Ueno, J. Math. Phys. **9**, 909 (1968).
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[28] R. E. Bellman, H. H. Kagiwada, R. E. Kalaba, and S. Ueno, Icarus 7, 365 (1967); **11**, 417 (1969).

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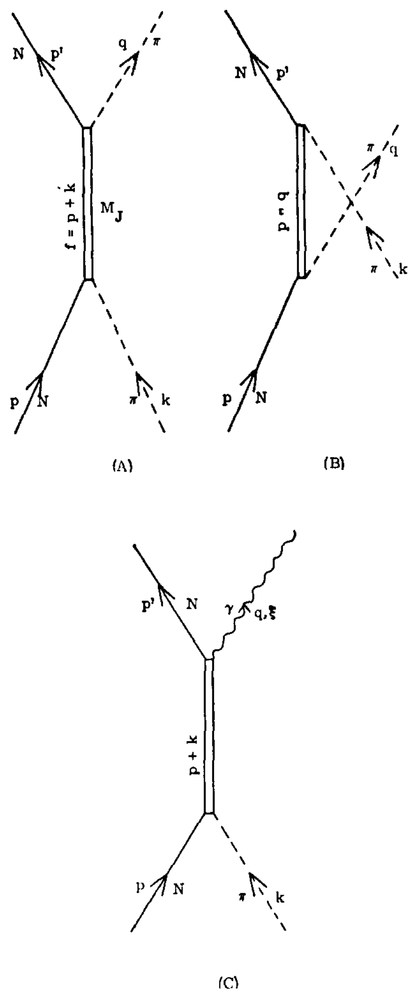


FIG. 1. Feynman diagrams for $\pi N \to \pi N$ scattering process with the propagator corresponding to a particle of spin J and mass M_J. Figures 1(A) and 1(B) are, respectively, the direct and the crossed diagrams for this process. Figure 1(C) is the Feynman diagram for $\pi N \to \gamma N$ scattering process with the propagator corresponding to a particle with spin J and mass M_J.

and so we keep this M_J as it is. A slightly different continuation which is equivalent to replacing M_J by $\sqrt{-f^2}$ in another factor of the Dirac part of the propagator does give a pure $d^J_{\lambda'\lambda}(\theta)$ behavior. These two ways of continuation may be said to introduce an ambiguity. However, the part of T_A containing the highest power $l = J - \frac{1}{2}$ of $\cos\theta$ (used in Ref. 3) will be seen to be independent of this ambiguity.

Instead of the generalized Rarita–Schwinger formalism used in Refs. 1–3, we have employed the Wigner–Bargmann formalism and it gives the propagator directly in terms of the rotation matrices.

II. PROPAGATOR ON THE MASS SHELL

Let P_μ and P'_μ be two arbitrary 4-vectors and f_μ be a 4-vector on the shell of the spin-J particle

$$f_\lambda f_\lambda = -M_J^2. \tag{1}$$

For $\pi N \to \pi N$ scattering process through an intermediate particle of spin J and mass M_J, we will have to calculate the quantity

$$\begin{aligned} T_{\alpha\alpha'}(P,f,P') &= P_{\mu_1}P_{\mu_2}\cdots P_{\mu_l} \\ &\times \Big((C^{-1}\gamma_{\mu_1})_{\beta_1\beta_2}(C^{-1}\gamma_{\mu_2})_{\beta_3\beta_4}\cdots(C^{-1}\gamma_{\mu_l})_{\beta_{3l-1}\beta_{2l}}\frac{1}{2^l} \\ &\times \sum_{\sigma=-J}^{+J} U^{(\sigma)}_{\alpha\beta_1\beta_2\cdots\beta_{2l}}(f)\bar{U}^{(\sigma)}_{\alpha'\beta_1'\beta_2'\cdots\beta_{2l}}(f) \\ &\times (\gamma_{\nu_1}C)_{\beta_1'\beta_2'}(\gamma_{\nu_2}C)_{\beta_3'\beta_4'}\cdots(\gamma_{\nu_l}C)_{\beta_{2l-1}'\beta_{2l}'}\Big) \\ &\times P'_{\nu_1}P'_{\nu_2}\cdots P'_{\nu_l} \end{aligned} \tag{2a}$$

where the integer l is related to J by

$$J = l + \tfrac{1}{2}. \tag{2b}$$

The expression within the braces in (2a) is actually the numerator of the Rarita–Schwinger propagator used in Refs. 1 and 2. The propagator momentum f is on the mass shell and $U^{(\sigma)}_{\alpha\beta_1\beta_2,\cdots,\beta_{2l}}(f)$ is the Wigner–Bargmann positive-energy wavefunction describing the particles with spin J and mass M_J. The Rarita–Schwinger free field operator is related to the Wigner–Bargmann free field operator by[4]

$$\begin{aligned} \psi_\alpha^{\mu_1\mu_2\cdots\mu_l}(x) &= \frac{1}{\sqrt{2^l}}(C^{-1}\gamma_{\mu_1})_{\beta_1\beta_2} \\ &\times (C^{-1}\gamma_{\mu_2})_{\beta_3\beta_4}\cdots(C^{-1}\gamma_{\mu_l})_{\beta_{2l-1}\beta_{2l}}\psi_{\alpha\beta_1\beta_2\cdots\beta_{2l}}(x), \end{aligned} \tag{3}$$

and a similar relation holds for the momentum wavefunctions. $U^{(\sigma)}(f)$ is obtained by applying a $2J$-fold Kronecker product of the Lorentz boost operators

$$L(f) = e^{\frac{1}{2}\gamma_5\underline{\sigma}\cdot\check{\underline{f}}\tanh^{-1}f/f_0} \tag{4a}$$

$$= \frac{f_0 + M_J + \gamma_5\underline{\sigma}\cdot\underline{f}}{(2M_J(f_0+M_J))^{\frac{1}{2}}} \tag{4b}$$

on $U^{(\sigma)}(0)$ which is the completely symmetrized $2J$-fold Kronecker product of the Dirac spinors

$$u^1 = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \quad u^2 = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}. \tag{4c}$$

The normalized $U^{(\sigma)}(0)$, where σ is the spin component along the third axis, is given by[5]

$$U^{(\sigma)}(0) = [{}^{2J}C_{J-\sigma}]^{-\frac{1}{2}}\sum_P u^1 \times u^2 \times \cdots \times u^1. \tag{4d}$$

$\sum_P$ stands for all the ${}^{2J}C_{J-\sigma}$ distinct permutations of the $2J$ Dirac spinors u^1 and u^2. The four Dirac matrices γ_μ are Hermitian and we use the representation in which $\underline{\gamma} = -\rho_2 \times \sigma$, $\gamma_4 = \rho_3 \times I$. C^{-1} is the charge conjugation matrix $-\rho_1 \times i\sigma_2 = \gamma_5 i\sigma_2$.

The commutator $[\psi(x), \bar{\psi}(x')]$ can be calculated by using the momentum space expansions of $\psi(x)$, $\bar{\psi}(x')$. The numerator in the momentum integral comes out to be

$$\sum_{\sigma=-J}^{+J} U^{(\sigma)}(f)\bar{U}^{(\sigma)}(f).$$

Following Blankenbecler and Sugar, we take this to be the numerator of the propagator for the pole diagrams.[6] The factors $C^{-1}\gamma_\mu$ and $\gamma_\nu C$ and P_μ and P'_ν in (2a) come from the derivative coupling. The same numerator is obtained if we use the dispersion relation approach and put in a single-particle intermediate state of spin J in the imaginary part.

In order to reduce the right-hand side of (2a) to the desired form, the Lorentz transformations are taken out of $U^{(\sigma)}(f)$ and $\bar{U}^{(\sigma)}(f)$:

$$U^{(\sigma)}_{\alpha\beta_1\cdots\beta_{2l}}(f) = L_{\alpha\lambda}(f)L_{\beta_1\lambda_1}(f) \times L_{\beta_2\lambda_2}(f)\cdots L_{\beta_{2l}\lambda_{2l}}(f)U^{(\sigma)}_{\lambda\lambda_1\lambda_2\cdots\lambda_{2l}'}(0). \quad (5)$$

Apart from $L_{\alpha\lambda}(f)$, two consecutive Lorentz transformations combine with one $C^{-1}\gamma\cdot P$ in (2a) to give

$$\begin{aligned} L_{\beta_1\lambda_1}(f)(C^{-1}\gamma\cdot P)_{\beta_1\beta_2}L_{\beta_2\lambda_2}(f) &= [L^T(f)C^{-1}\gamma\cdot PL(f)]_{\lambda_1\lambda_2} \\ &= [C^{-1}L^{-1}(f)\gamma\cdot PL(f)]_{\lambda_1\lambda_2} \\ &= [C^{-1}\gamma\cdot\mathbf{P}]_{\lambda_1\lambda_2}. \end{aligned} \quad (6a)$$

$\mathbf{P}_\mu$ is the transformed 4-vector defined by

$$\mathbf{P}_\mu = P_\nu a_{\nu\mu}(f), \quad (6b)$$

where $a_{\mu\nu}(f)$ is the pure Lorentz transformation given by[7]

$$a_{ij}(f) = \delta_{ij} + \breve{f}_i\breve{f}_j\frac{(f_0 - M_J)}{M_J},$$
$$a_{4i}(f) = \frac{if_i}{M_J} = -a_{i4}(f), \quad a_{44} = \frac{f_0}{M_J}. \quad (7)$$

$a_{\mu\nu}(f)$ takes f_ν to its rest frame and

$$L(f)\gamma_4L^{-1}(f) = \frac{\gamma\cdot f}{iM_J}; \quad (8a)$$

$a_{\mu\nu}(f)$ are orthogonal,

$$a_{\mu\lambda}(f)a_{\mu\nu}(f) = \delta_{\lambda\nu}, \quad (8b)$$

and summed over the space indices give

$$a_{i\lambda}(f)a_{i\nu}(f) = \delta_{\lambda\nu} + \frac{f_\lambda f_\nu}{M_J^2}, \quad (8c)$$

which is just the numerator of the spin-1 propagator.

Returning to (6), we note that

$$[P_\mu a_{\mu\nu}(f)C^{-1}\gamma_\nu]_{\lambda_1\lambda_2} = [P_\mu a_{\mu j}C^{-1}\gamma_i + P_\mu a_{\mu 4}C^{-1}\gamma_4]_{\lambda_1\lambda_2}, \quad (9a)$$

$\lambda_1\lambda_2$ are contracted with the indices of the rest spinors of the form (4); the contribution of the second term on the right-hand side in (9) therefore vanishes. $C^{-1}\gamma_j$ can be written $i\gamma_4C^{-1}\sigma_j$ where C^{-1} is the Dirac matrix

$$C^{-1} = i\sigma_2. \quad (9b)$$

γ_4 gets absorbed by the rest spinors, and (9) becomes equivalent to $(iC^{-1}\underline{\sigma}\cdot\underline{\mathbf{P}})\lambda_1\lambda_2$; $\mathbf{P}_j$ is the transformed 3-vector given by

$$P_\mu a_{\mu j}(f) = \mathbf{P}_j. \quad (10a)$$

Similarly the Lorentz transformations contracted from

$$\bar{U}^{(\sigma)}(f) = U^\dagger(f)\gamma_4\times\gamma_4\times\cdots\times\gamma_4 \quad (11a)$$

are combined with $\gamma\cdot P'C$ and are equivalently written as $-i\underline{\sigma}\cdot\underline{\mathbf{P}}'C$ with

$$\mathbf{P}_j = P'_\mu a_{\mu j}(f). \quad (10b)$$

Considering all such factors, we get

$$\begin{aligned} T_{\alpha\alpha'} = L_{\alpha\lambda}(f)L^{-1}_{\lambda'\alpha'}(f) &\times (C^{-1}\underline{\sigma}\cdot\underline{\mathbf{P}})_{\lambda_1\lambda_2}(C^{-1}\underline{\sigma}\cdot\underline{\mathbf{P}})_{\lambda_3\lambda_4}\cdots(C^{-1}\underline{\sigma}\cdot\underline{\mathbf{P}})_{\lambda_{2l-1}\lambda_{2l}} \\ &\times \sum_\sigma U^{(\sigma)}_{\lambda\lambda_1\lambda_2\cdots\lambda_{2l}}(0)\bar{U}^{(\sigma)}_{\lambda'\lambda_1'\lambda_2'\cdots\lambda_{2l}'}(\underline{\sigma}\cdot\underline{\mathbf{P}}'C)_{\lambda_1'\lambda_2'} \\ &\times (\underline{\sigma}\cdot\mathbf{P}'C)_{\lambda_3'\lambda_4'}\cdots(\underline{\sigma}\cdot\mathbf{P}'C)_{\lambda_{2l-1}'\lambda_{2l}'}. \end{aligned} \quad (11b)$$

The scattering process will be considered to take place in the x_1x_3 plane, P and P' and f will depend linearly on the two ingoing and two outgoing momenta, and so we may assume $\underline{P}$, $\underline{P}'$, and $\underline{f}$ to lie in the x_1x_3 plane. The transformed momenta $\underline{\mathbf{P}}$ and $\underline{\mathbf{P}}'$ are then easily shown to lie in the x_1x_3 plane. Let $\underline{\mathbf{P}}$ and $\underline{\mathbf{P}}'$ make angles φ and φ' with the x_3 axis, respectively; then

$$\begin{aligned} (C^{-1}\underline{\sigma}\cdot\underline{\mathbf{P}})_{\lambda_1\lambda_2} &= [C^{-1}R(\varphi)\sigma_3\mathbf{P}R^\dagger(\varphi)]_{\lambda_1\lambda_2} \\ &= \mathbf{P}[R^{\dagger T}(\varphi)C^{-1}\sigma_3R^\dagger(\varphi)]_{\lambda_1\lambda_2} \\ &= \mathbf{P}(C^{-1}\sigma_3)_{\tau_1\tau_2}R^\dagger_{\tau_1\lambda_1}(\varphi(R^\dagger_{\tau_1\lambda_2} \\ &= \mathbf{P}(C^{-1}\sigma_3)_{\tau_1\tau_2}[R^\dagger(\varphi)\times R^\dagger(\varphi)]_{\tau_1\tau_2,\lambda_1\lambda_2}. \end{aligned} \quad (12a)$$

The rotation matrix $R(\varphi)$ has the usual form $e^{-i\sigma_2\varphi/2}$. Similarly

$$(\underline{\sigma}\cdot\underline{\mathbf{P}}'C)_{\lambda_1'\lambda_2'} = [R(\varphi')\times R(\varphi')]_{\lambda_1'\lambda_2',\tau_1'\tau_2'}(\sigma_3C)_{\tau_1'\tau_2'}. \quad (12b)$$

We now apply the Fierz identity for the matrices σ_i and obtain[5]

$$\begin{aligned} &(C^{-1}\sigma_3)_{\tau_1\tau_2}(\sigma_3C)_{\tau_1'\tau_2'} \\ &= (C^{-1}\sigma_3)_{\tau_2\tau_1}(\sigma_3C)_{\tau_2'\tau_1'} \\ &= \tfrac{1}{2}[\delta_{\tau_2'\tau_2}(C^{-1}\sigma_3 \mid \sigma_3C)_{\tau_1\tau_1'} + (\sigma_j)_{\tau_2'\tau_2}(C^{-1}\sigma_3\sigma_j\sigma_3C)_{\tau_1\tau_1'}] \end{aligned} \quad (13a)$$

$$= \tfrac{1}{2}[1\times 1 + \sigma_j\times\sigma_j - 2\sigma_3\times\sigma_3]_{\tau_1'\tau_2',\tau_1\tau_2} \equiv Q_{\tau_1'\tau_2',\tau_1\tau_2}. \quad (13b)$$

Taking into account all such factors and combining them in Kronecker products, we are able to write $T_{\alpha\alpha'}$ in the form

$$T_{\alpha\alpha'}(P,f,P') = \frac{\mathbf{P}^l\mathbf{P}'^l}{2^l}\sum_{\sigma=-J}^{J}\bar{U}^{(\sigma)}_{\lambda'\cdots}(0)R(\varphi') \times R(\varphi')\times\cdots\times R(\varphi')Q\times Q\times\cdots\times QR^\dagger(\varphi) \times R^\dagger(\varphi)\times\cdots\times R^\dagger(\varphi)U^{(\sigma)}_{\lambda\cdots}(0)L_{\alpha\lambda}(f)L^{-1}(f)_{\lambda'\alpha'}. \tag{14}$$

In $U^{(\sigma)}_{\lambda\cdots}$ the dots are placed for the indices in which the $2l$-fold Kronecker products of $R^\dagger(\varphi)$ act. The number of Q's is l and each Q contains two spinor indices as its rows and columns. We know that a $2J\,(=2l+1)$-fold Kronecker product of $R^\dagger(\varphi)$ acting on the spin-J wavefunctions $U^{(\sigma)}$ gives[4] $\sum_{\sigma'} d^J_{\sigma'\sigma}(\varphi)U^{(\sigma')}$. We therefore introduce one $R^\dagger(\varphi)$ and $R(\varphi')$ by writing

$$U^{(\sigma)}_{\lambda\cdots} = R_{\lambda\tau}(\varphi)R^\dagger_{\tau\delta}(\varphi)U^{(\sigma)}_{\delta\cdots} \tag{15a}$$

and

$$\bar{U}^{(\sigma)}_{\lambda'\cdots} = \bar{U}^{(\sigma)}_{\delta'\cdots}(0)R_{\delta'\tau'}(\varphi')R^\dagger_{\tau'\lambda'}(\varphi'), \tag{15b}$$

and obtain the $2J$-fold Kronecker product

$$[R^\dagger(\varphi)\times R^\dagger(\varphi)\times\cdots\times R^\dagger(\varphi)]_{\tau\cdots,\delta\cdots} = e^{iJ_2\varphi}_{\tau\cdots,\delta\cdots} \tag{15c}$$

as a factor. The J_i are the total spin operators

$$J_i = \tfrac{1}{2}(\sigma_i\times 1\times 1\times\cdots\times 1 + 1\times\sigma_i\times 1\cdots\times 1 + \cdots + 1\times 1\times\cdots\times 1\times\sigma_i). \tag{16}$$

Similarly a factor $e^{-iJ_2\varphi'}$ is obtained. Now, since

$$e^{iJ_2\varphi}_{\tau\cdots,\delta\cdots}\cdot U^{(\sigma)}_{\delta\cdots} = \sum_{\sigma'=-J}^{J} d^J_{\sigma\sigma'}(\varphi)U^{(\sigma')}_{\tau\cdots}, \tag{17}$$

(14) becomes

$$T_{\alpha\alpha'}(P,f,P') = \frac{(\mathbf{PP}')^l}{2^l}\sum_{\sigma\sigma'\sigma''}\bar{U}^{(\sigma'')}_{\tau'\cdots}Q\times Q\times\cdots\times QU^{(\sigma')}_{\tau\cdots} \cdot d^J_{\sigma\sigma'}(\varphi)d^J_{\sigma\sigma''}(\varphi')[L(f)R(\varphi)]_{\alpha\tau}[R^\dagger(\varphi')L^{-1}(f)]_{\tau'\alpha'}. \tag{18}$$

Defining

$$S_i = \tfrac{1}{2}(1\times\sigma_i + \sigma_i\times 1), \tag{19a}$$

we get

$$\sigma_i\times\sigma_i = 2S^2 - 3\cdot 1\times 1. \tag{19b}$$

Operating between the completely symmetrical spinors formed from u^1 and u^2, S^2 has the eigenvalue $1(1+1)=2$ and hence $\sigma_i\times\sigma_i$ in each Q can be replaced by 1×1 and Q in (18) and is then given by[5]

$$Q = 1\times 1 - \sigma_3\times\sigma_3, \tag{20a}$$

Q has the property

$$Qu^1\times u^1 = Qu^2\times u^2 = 0,\quad Qu^1\times u^2 = 2u^1\times u^2,\quad Qu^2\times u^1 = 2u^2\times u^1. \tag{20b}$$

Using these equations and referring to the form (4d) of $U^{(\sigma)}(0)$, we easily see that in the summation over σ' and σ'' in (18) only $\sigma' = \pm\frac{1}{2}$ and $\sigma'' = \pm\frac{1}{2}$ terms will survive and even from these $U^{(\pm\frac{1}{2})}$ only the parts

$$\frac{1}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}u^{1,2}\times(u^1\times u^2+u^2\times u^1)\times(u^1\times u^2+u^2\times u^1)\times\cdots\times(u^1\times u^2+u^2\times u^1) \equiv \frac{1}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}u^{1,2}\times V \tag{21}$$

will give contributions, since

$$\bar{V}V = 2^l \tag{22}$$

and, writing[8,9]

$$\varphi - \varphi' = \boldsymbol{\theta}, \tag{23}$$

we have

$$\sum d^J_{\sigma\tau}(\varphi')d^J_{\sigma k}(\varphi) = d^J_{\tau k}(\varphi-\varphi') = d^J_{\tau k}(\boldsymbol{\theta}), \tag{24a}$$

$$d^J_{-\tau,-k}(\boldsymbol{\theta}) = (-1)^{\tau-k}d^J_{\tau,k}(\boldsymbol{\theta}). \tag{24b}$$

A simple calculation shows that (18) can be written in the form

$$T_{\alpha\alpha'}(p,f,p') = \frac{(\mathbf{PP}')^l}{2^l}\frac{2^l2^l}{(2J)!}(J-\tfrac{1}{2})!\,(J+\tfrac{1}{2})! \times[d^J_{\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})L(f)R(\varphi)(u^1\bar{u}^1+u^2\bar{u}^2)R^\dagger(\varphi')L^{-1}(f) + d^J_{-\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})L(f)R(\varphi)(u^1\bar{u}^2-u^2\bar{u}^1)R^\dagger(\varphi')L^{-1}(f)]. \tag{25}$$

To simplify this expression further, we note that

$$L(f)R(\varphi)(u^1\bar{u}^1+u^2\bar{u}^2)R^\dagger(\varphi')L^{-1}(f) = L(f)R(\varphi)\frac{1+\gamma_4}{2}R^\dagger(\varphi')L^{-1}(f) = L(f)\frac{1+\gamma_4}{2}(\cos\tfrac{1}{2}\boldsymbol{\theta} - i\sigma_2\sin\tfrac{1}{2}\boldsymbol{\theta})L^{-1}(f). \tag{26}$$

Since a γ_4 can be taken out of $\frac{1}{2}(1+\gamma_4)$ and attached to $-i\sigma_2$ term in (25) and as f lies in the x_1x_3 plane, $L(f)$ commutes with $\sigma_2\gamma_4$, giving

$$L(f)\sigma_2\gamma_4L^{-1}(f) = \sigma_2\gamma_4. \tag{27}$$

Also, $\frac{1}{2}(1+\gamma_4)$ transformed by $L(f)$ gives the positive-energy projection operator

$$L(f)\tfrac{1}{2}(1+\gamma_4)L^{-1}(f) = \frac{1}{2}\left(1+\frac{\gamma\cdot f}{iM_j}\right) \tag{28a}$$

$$\equiv \Lambda^\dagger(f). \tag{28b}$$

Hence (26) reduces to

$$\Lambda^\dagger(f)[\cos\tfrac{1}{2}\boldsymbol{\theta} - i\gamma_4\sigma_2\sin\tfrac{1}{2}\boldsymbol{\theta}]. \tag{28c}$$

Similarly, since

$$u^1\bar{u}^2 - u^2\bar{u}^1 = i\sigma_2\gamma_4\,\tfrac{1}{2}(1+\gamma_4), \tag{29}$$

the second bracket in (25) reduces to

$$\Lambda^\dagger(f)(\cos\tfrac{1}{2}\boldsymbol{\theta} - i\sigma_2\gamma_4\sin\tfrac{1}{2}\boldsymbol{\theta}). \tag{30}$$

Therefore

$$\begin{aligned} T_{\alpha\alpha'}(P,f,P') &= (\mathbf{PP}')^l 2^l \frac{(J-\frac{1}{2})!\,(J+\frac{1}{2})!}{(2J)!} \\ &\times [d^J_{\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})\Lambda^\dagger(f)(\cos\tfrac{1}{2}\boldsymbol{\theta} - i\sigma_2\gamma_4\sin\tfrac{1}{2}\boldsymbol{\theta}) \\ &+ d^J_{-\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})\Lambda^\dagger(f)(i\sigma_2\gamma_4\cos\tfrac{1}{2}\boldsymbol{\theta} + \sin\tfrac{1}{2}\boldsymbol{\theta})]_{\alpha\alpha'}. \end{aligned} \tag{31}$$

Via the expressions[9] for $d^J_{\pm\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})$ and the following recursion relation for the Legendre polynomials,

$$P'_{l+1}(\cos\boldsymbol{\theta}) - \cos\boldsymbol{\theta}P'_l(\cos\boldsymbol{\theta}) = (l+1)P_l(\cos\boldsymbol{\theta}), \tag{32}$$

a simpler form for $T_{\alpha\alpha'}$ is obtained[10]:

$$\begin{aligned} T_{\alpha\alpha'}(P,f,P') &= (\mathbf{PP}')^l 2^l \frac{(l)!\,(l+1)!}{(2l+1)!} \\ &\cdot \left[\Lambda^\dagger(f)P_l(\cos\boldsymbol{\theta}) + \Lambda^\dagger(f)i\sigma_2\gamma_4\sin\boldsymbol{\theta}\,\frac{P'_l(\cos\boldsymbol{\theta})}{l+1}\right]_{\alpha\alpha'}. \end{aligned} \tag{33a}$$

(31) and (32) are the forms useful for the $\pi N \to \pi N$ scattering process. $\mathbf{P}_i$ and $\mathbf{P}'_i$ are the Lorentz-transformed vectors given by (10). Their magnitudes and the angle $\boldsymbol{\theta}$ between them are given by

$$\begin{aligned} \mathbf{P}^2 = \mathbf{P}_i\mathbf{P}_i &= P_\mu a_{\mu i}(f)P_\nu a_{\nu i}(f) \\ &= P_\mu\left(\delta_{\mu\nu} + \frac{f_\mu f_\nu}{M_J^2}\right)P_\nu, \end{aligned} \tag{33b}$$

$$\mathbf{P}'^2 = P'_\mu\left(\delta_{\mu\nu} + \frac{f_\mu f_\nu}{M_J^2}\right)P'_\nu, \tag{33c}$$

$$\mathbf{PP}'\cos\boldsymbol{\theta} = P_\mu\left(\delta_{\mu\nu} + \frac{f_\mu f_\nu}{M_J^2}\right)P'_\nu. \tag{33d}$$

III. $\pi N \to \pi N$ SCATTERING PROCESS

In this section we calculate the Born terms for the scattering process

$$\pi(k) + N(p) \to \pi(q) + N(p').$$

k, q are the pion momenta and p, p' are the nucleon momenta. Let m and μ be the masses of the nucleon and the pion, respectively. We use the effective Lagrangian

$$\begin{aligned} \mathcal{L} &= g_{JN\pi}[\bar{\varphi}_\alpha(x)\overleftrightarrow{\partial}_{\mu_1}\overleftrightarrow{\partial}_{\mu_2}\cdots\overleftrightarrow{\partial}_{\mu_l}\varphi(x)] \\ &\times \left\{\frac{1}{\sqrt{2}^l}(C^{-1}\gamma_{\mu_1})_{\beta_1\beta_2}(C^{-1}\gamma_{\mu_2})_{\beta_3\beta_4}\cdots(C^{-1}\gamma_{\mu_l})_{\beta_{2l-1},\beta_{2l}} \right. \\ &\left. \times\ \psi_{\alpha\beta_1\beta_2\cdots\beta_2}(x)\right\} + \text{H.C.} \end{aligned} \tag{34}$$

$\bar{\varphi}_\alpha(x)$, $\varphi(x)$, and $\psi_{\alpha\beta_1\beta_2\cdots\beta_{2l}}(x)$ are the nucleon, pion, and the spin-J baryon fields, respectively. The expression within the braces is the Rarita–Schwinger field for the baryon. An effective Lagrangian similar to this one has been used in Ref. 2. Using (34) we obtain for the amplitude corresponding to the crossed diagram [Fig. 1(B)]

$$T_B = \bar{u}_\alpha(p')T_{\alpha\alpha'}(P,f,P')u_{\alpha'}(p)\frac{g^2_{JN\pi}}{(p'-k)^2 + M_J^2}, \tag{35}$$

with

$$\begin{aligned} P &= (p'+k), \\ p' &= (p+q), \\ f &= (p'-k) = (p-q). \end{aligned} \tag{36}$$

For the conservation of momentum

$$p + k = p' + q \tag{37}$$

and in the c.m. frame in which we calculate the amplitudes

$$\begin{aligned} \underline{p} &= -\underline{k}, \\ \underline{p}' &= -\underline{q}, \\ p_0 &= p'_0 = (q^2+m^2)^{\frac{1}{2}}, \\ k_0 &= q_0 = (q^2+\mu^2)^{\frac{1}{2}}, \end{aligned} \tag{38}$$

$q = |\underline{q}|$ is the c.m. momentum. We consider the scattering process to take place in the x_1x_3 plane. $\underline{p}$ is along the x_3 axis and $\underline{p}'$ makes the scattering angle θ with the x_3 axis. Let us introduce the Mandelstam variables

$$\begin{aligned} u &= -(p+k)^2 = -(p'-q)^2, \\ t &= -(p-q)^2 = -(p'-k)^2, \end{aligned} \tag{39}$$

and also define

$$\lambda_J = \frac{(m^2-\mu^2)^2}{M_J^2}. \tag{40}$$

In the c.m. frame, $\sqrt{u}$ is the energy of collision $= (p_0+k_0)$. Via (36) for P and P', the transformed quantities are obtained from (33):

$$\begin{aligned} \mathbf{P}'^2 = \mathbf{P}^2 &= \lambda_J - u + 2q^2(1-\cos\theta), \\ \cos\boldsymbol{\theta} &= \frac{1}{\mathbf{P}^2}\mathbf{P}_j P'_j = \frac{\lambda_J - u - 2q^2(1-\cos\theta)}{\lambda_J - u + 2q^2(1-\cos\theta)}, \\ \sin\boldsymbol{\theta} &= \frac{1}{\mathbf{P}^2}[8(\lambda_J-u)\cdot q^2(1-\cos\theta)]^{\frac{1}{2}}. \end{aligned} \tag{41}$$

Hence T_B is given explicitly in terms of the scattering angle by

$$T_B = g_{JN\pi}^2 \cdot D_l u(p') \times \left\{\frac{1}{2}\left(1 + \frac{\gamma\cdot(p-q)}{iM_J}\right)[\lambda_J - u + 2q^2(1-\cos\theta)]^l \cdot P_l\left(\frac{\lambda_J - u - 2q^2(1-\cos\theta)}{\lambda_J - u + 2q^2(1-\cos\theta)}\right) + \frac{1}{2}\left(1 + \frac{\gamma\cdot(p-q)}{iM_J}\right) i\sigma_2\gamma_4 \cdot [\lambda_J - u + 2q^2(1-\cos\theta)]^{l-1} \cdot \frac{1}{l+1} P_l'\left(\frac{\lambda_J - u - 2q^2(1-\cos\theta)}{\lambda_J - u + 2q^2(1-\cos\theta)}\right) \cdot [8(\lambda_J - u)q^2(1-\cos\theta)]^{\frac{1}{2}}\right\} u(p)\frac{1}{-t+M_J^2}, \tag{42}$$

where we have used the abbreviation

$$D_l = \frac{(l)!\,(l+1)!}{(2l+1)!}\,2^l. \tag{43}$$

Expanding the Legendre polynomial, we find that the term with the highest power of $\cos\theta$ in

$$[\lambda_J - u + 2q^2(1-\cos\theta)]^l P_l \times \left(\frac{\lambda_J - u - 2q^2(1-\cos\theta)}{\lambda_J - u + 2q^2(1-\cos\theta)}\right) \tag{44a}$$

is

$$(-1)^l q^{2l} \cos^l\theta. \tag{44b}$$

The second term in (42) has $l-1$ as the highest power of $\cos\theta$ in the numerator.

For the u-channel pole, i.e., Fig. 1(A), we have

$$\begin{aligned} P_\mu &= p_\mu' - q_\mu, \\ P_\mu' &= p_\mu - k_\mu, \\ f_\mu &= p_\mu + k_\mu = p_\mu' + q_\mu, \\ \underline{f} &= 0. \end{aligned} \tag{45a}$$

Again we obtain from (33)

$$\mathbf{P}'^2 = \mathbf{P}^2 = 4q^2 - (p_0 - k_0)^2 + \lambda_J, \tag{45b}$$

and so P^2, P'^2 are independent of θ. Also

$$\cos\boldsymbol{\theta} = \frac{1}{\mathbf{P}^2}[4q^2\cos\theta - (p_0-k_0)^2 + \lambda_J],$$

$$\sin\boldsymbol{\theta} = \frac{1}{\mathbf{P}^2}\{[4q^2(1+\cos\theta) - 2(p_0-k_0)^2 + 2\lambda_J] \cdot 4q^2(1-\cos\theta)\}^{\frac{1}{2}}. \tag{46}$$

With these values of $\mathbf{P}^2$, $\mathbf{P}'^2$, $\cos\boldsymbol{\theta}$, and $\sin\boldsymbol{\theta}$, the matrix element for the diagram [1(A)] can be written as

$$T_A = \bar{u}(p')\left\{P^{2l}\cdot D_l\left[\frac{1}{2}\left(1 + \frac{\gamma_4\sqrt{u}}{M_J}\right)P_l(\cos\boldsymbol{\theta}) + \frac{1}{2}\left(1 + \frac{\gamma_4\sqrt{u}}{M_J}\right) i\sigma_2\gamma_4 \sin\boldsymbol{\theta} P_l'(\cos\boldsymbol{\theta})\cdot\frac{1}{l+1}\right]\right\} \times u(p)\frac{g_{JN\pi}^2}{-u+M_J^2}. \tag{47}$$

Since $P'^2 = P^2$ is independent of θ, $\cos\theta$ dependence is contained only in $P_l(\cos\boldsymbol{\theta})$ and $P_l'(\cos\boldsymbol{\theta})$, and again the first term in (47) contains the lth power of $\cos\theta$. If the external masses are equal, i.e., $m = \mu$, the spin zero parts in the spin-1 propagators vanish, and from (45) and (46) we see that $\cos\boldsymbol{\theta} = \cos\theta$, $\mathbf{P}'^2 = \mathbf{P}^2 = 4q^2$. In this case the propagator in T_A should contain only the spin J part.

The propagator momentum for diagram [1(A)], being equal to $p + k$, is timelike, and so the little group of the Poincaré group is SU_2 and we can associate a definite spin with the propagator. Via the Lagrangian (34) (without the arrows $\leftrightarrow$ over the ∂_μ's), $P_\mu = q_\mu$, $P_\nu' = k_\nu$; since $\underline{f} = 0$ for the diagram [1(A)] with the c.m. system, $\mathbf{P}$ and $\mathbf{P}'$ are again free of $\cos\theta$, and a result somewhat similar to (42), with P^2, P'^2, $\cos\boldsymbol{\theta}$ given by (41), is obtained. However, if we replace M_J^2 by $-f_\mu f_\mu$ in Eq. (8c) and thus eliminate the spin zero part, $\mathbf{P}$, $\mathbf{P}'$, and $\cos\boldsymbol{\theta}$ are then given by

$$\begin{aligned} \mathbf{P}' &= \mathbf{P} = q, \\ \cos\boldsymbol{\theta} &= \cos\theta. \end{aligned} \tag{48}$$

For the exchange of natural parity sequence $J^P = \frac{1}{2}^+, \frac{3}{2}^-, \frac{5}{2}^+, \cdots$ of fermion resonances $a\gamma_5$ should be introduced in the effective Lagrangian (34). This means that $\bar{u}(p')$ and $u(p)$ in (47) should be replaced by $\bar{u}(p')\gamma_5$ and $\gamma_5 u(p)$, respectively. The net effect is that the signs of γ_4 in (47) are changed. With these changes the result for T_A is

$$T_A = \frac{g_{JN\pi}^2}{-u+M_J^2} D_l q^{2l}\bar{u}(p')\left[\frac{1}{2}\left(1 - \frac{\gamma_4\sqrt{u}}{M_J}\right)P_l(\cos\theta) - \frac{1}{2}\left(1 - \frac{\gamma_4\sqrt{u}}{M_J}\right)i\sigma_2\gamma_4\sin\theta P_l'(\cos\theta)\frac{1}{l+1}\right]u(p). \tag{49}$$

This is the complete form of Carlitz and Kislinger's result,[3] who have given only the first term in (49) with the factors depending on $l = J = \frac{1}{2}$ absorbed in the coupling constant.

As already mentioned, the propagator for diagram A of Fig. 1 should contain only spin-J parts. This could be true if we can show the helicity amplitude $T_A(\lambda', \lambda)$ (when λ' and λ are the helicities of the initial and final nucleons) has the angular dependence of the form $d^J_{\lambda',\lambda}(\theta)$. Using the form (31) for $T_{\alpha\alpha'}$ and the values (48) for $\mathbf{P}$, $\mathbf{P}'$, and $\cos\boldsymbol{\theta}$, we obtain

$$\begin{aligned}T_A(\lambda',\lambda) &= \bar{u}^{(\lambda')}(p')T(q,p+k,k)\\ &= \frac{g^2_{JN\pi}}{-u^2+M_J^2}D_l q^{2l}\bar{u}(p')\frac{1}{2}\left(1-\frac{\gamma_4\sqrt{u}}{M_J}\right)\\ &\quad\times\{d^J_{\frac{1}{2},\frac{1}{2}}(\theta)\cdot[\cos\tfrac{1}{2}\theta - i\sigma_2\gamma_4\sin\tfrac{1}{2}\theta]\\ &\quad + d^J_{-\frac{1}{2},\frac{1}{2}}(\theta)i\sigma_2\gamma_4[\cos\tfrac{1}{2}\theta - i\sigma_2\gamma_4\sin\theta]\}u^{(\lambda)}(p).\end{aligned} \tag{50}$$

The helicity spinors $u^{(\lambda)}(p)$ and $\bar{u}^{(\lambda')}(p')$ are given by

$$\begin{aligned}u^{(\lambda)}(p) &= e^{\frac{1}{2}\gamma_5\sigma_3\tanh^{-1}(p/p_0)},\quad u^{(\lambda)}(0)\\ \bar{u}^{(\lambda')}(p') &= \bar{u}^{(\lambda')}(0)e^{-\frac{1}{2}\gamma_5\sigma_3\tanh^{-1}(p'/p_0')}e^{i\sigma_2\theta/2}.\end{aligned} \tag{51}$$

The rest spinors $u^{(\lambda)}$ are quantized along the third axis and were previously written as u^1 and u^2. In (50) $e^{i\sigma_2\theta/2}$ commutes with $\frac{1}{2}(1-\gamma_4(\sqrt{u})/M_J)$ and would cancel out the θ-dependent operator $e^{-i\sigma_2\gamma_4\theta/2}$ if it had not contained the γ_4 matrix. The presence of the γ_4 in $e^{-i\sigma_2\gamma_4\theta/2}$ destroys the purely $d^j_{\lambda'\lambda}(\theta)$ form of angular dependence, and so we find that the present off-the-mass-shell continuation of the propagator does not give a purely spin-J contribution. We also note that the γ_4 in (50) cannot be absorbed in $1-\gamma_4\sqrt{u}/M_J$ since $f_0=\sqrt{u}=p_0+k_0$ is off the mass shell, i.e., $f_0=\sqrt{u}\neq M_J$.

However, there is a continuation of the propagator which gives the purely $d^J_{\lambda'\lambda}(\theta)$ behavior for $T_A(\lambda',\lambda)$. Instead of taking $a\gamma_4$ out of $(1+\gamma_4)/2$ in (25) and attaching it to the $i\sigma_2$, we calculate $L(f)i\sigma_2L^{-1}(f)$ directly. Since $\underline{f}$ lies in the x_1x_3 plane, $L(f)$ contains $\gamma_5\sigma_1$ and $\gamma_5\sigma_3$ matrices which commute with $i\sigma_2$, and we have

$$L(f)i\sigma_2L^{-1}(f) = L^2(f)i\sigma_2 = \frac{f_0+\gamma_5\underline{\sigma}\cdot\underline{f}}{M_J}i\sigma_2 \tag{52a}$$

$$= \frac{f_0+\gamma_5\underline{\sigma}\cdot\underline{f}}{(-f^2)^{\frac{1}{2}}}i\sigma_2 \tag{52b}$$

$$= \frac{\gamma\cdot f}{iM_J}\gamma_4 i\sigma_2. \tag{52c}$$

As $\gamma\cdot f/iM_J$ gets absorbed in $\Lambda^\dagger(f)$ in (31), we obtain the previous result if we use (52c). On the other hand, if use is made of (52b) for off-the-mass-shell continuation, then, since for Fig. 1(A) $\underline{f}=0$, $L(f)i\sigma_2L^{-1}(f)\to i\sigma_2$ and $i\sigma_2\gamma_4$ in (49) should be replaced by $i\sigma_2$. The required cancellation takes place, and we obtain

$$\begin{aligned}T_A(\lambda',\lambda) &= \frac{g^2_{JN\pi}}{-u+M_J^2}D_l q^{2l}\bar{u}^{(\lambda')}(0)e^{-\frac{1}{2}\gamma_5\sigma_3\tanh^{-1}(p'/p_0')}\\ &\quad\times\frac{1}{2}\left(1-\frac{\gamma_4\sqrt{u}}{M_J}\right)\\ &\quad\times\{d^J_{\frac{1}{2}\frac{1}{2}}(\theta)+i\sigma_2\,d^J_{-\frac{1}{2},\frac{1}{2}}(\theta)\}e^{\frac{1}{2}\gamma_5\sigma_3\tanh^{-1}(p/p_0)}u^{(\lambda)}(0),\end{aligned} \tag{53}$$

from which we easily get the two independent helicity amplitudes

$$T_A(\tfrac{1}{2},\tfrac{1}{2}) = \frac{g^2_{JN\pi}}{-u+M_J^2}D_l q^{2l}\frac{1}{2}\left(1-\frac{\sqrt{u}}{M_J}\frac{p_0}{m}\right)d^J_{\frac{1}{2},\frac{1}{2}}(\theta), \tag{54a}$$

$$\begin{aligned}T_A(-\tfrac{1}{2},\tfrac{1}{2}) &= -\frac{g^2_{JN\pi}}{-u+M_J^2}D_l q^{2l}\frac{1}{2}\left(\frac{p_0}{m}-\frac{\sqrt{u}}{M_J}\right)d^J_{-\frac{1}{2},\frac{1}{2}}(\theta).\end{aligned} \tag{54b}$$

Carlitz and Kislinger's results is the $P_l(\cos\theta)$ term in T_A given by (49). It does not contain $i\sigma_2\gamma_4$ and is therefore independent of the ambiguity we have discussed above.

IV. SPIN J POLE IN $\pi+N\to N+\gamma$

In this section we calculate the u-channel pole diagram C of Fig. 1 for the photon emission process $\pi N\to N\gamma$. Let $A_\mu(x)$ be the photon field and $\xi_\mu(q)$ be the polarization vector for the photon with momentum q. There are two coupling constants at the photon, nucleon, spin-J baryon vertex.[11] The effective Lagrangian may be written

$$\begin{aligned}\mathcal{L}' &= g_{JN\pi}\bar{\psi}_\alpha^{\mu_1\mu_2\cdots\mu_l}(x)\psi_\alpha(x)\partial_{\mu_1}\partial_{\mu_2}\cdots\partial_{\mu_l}\varphi(x)\\ &\quad + g^{(1)}_{JN\gamma}\bar{\psi}_\alpha(x)\psi_\alpha^{\mu_1\mu_2\mu_3\cdots\mu_l}(x)\partial_{\mu_2}\partial_{\mu_3}\cdots\partial_{\mu_l}A_{\mu_1}(x)\\ &\quad + g^{(2)}_{JN\gamma}(\bar{\psi}(x)\gamma_\mu)_\alpha\psi_\alpha^{\mu_1\mu_2\cdots\mu_l}(x)\partial_{\mu_1}\partial_{\mu_2}\cdots\partial_{\mu_l}A_\mu(x).\end{aligned} \tag{55}$$

The amplitude part containing $g_{JN\pi}g^{(2)}_{JN\gamma}$ will be very similar to T_A and will be written down later. The part involving $g_{JN\pi}g^{(1)}_{JN\gamma}$ after being transformed to the Wigner–Bargmann formalism can be written as

$$\begin{aligned}T_C^{(1)} &= i\frac{g_{JN\pi}g^{(1)}_{JN\gamma}}{-u+M_J^2}\bar{u}_\alpha(p')\Big\{\frac{1}{2^l}(C^{-1}\gamma\cdot\xi(q))_{\beta_1\beta_2}\\ &\quad\times(C^{-1}\gamma\cdot q)_{\beta_3\beta_4}\cdots(C^{-1}\gamma\cdot q)_{\beta_{2l-1}\beta_{2l}}\\ &\quad\times\sum_{\sigma=-J}^{J}U^{(\sigma)}_{\alpha\beta_1\beta_2\cdots\beta_{2l}}(f)\bar{U}^{(\sigma)}_{\alpha\beta_1'\beta_2'\cdots\beta_{2l}'}(\gamma\cdot kC)_{\beta_1'\beta_2'}\\ &\quad\times(\gamma\cdot kC)_{\beta_3'\beta_4'}\cdots(\gamma\cdot kC)_{\beta_{2l-1}'\beta_{2l}'}\Big\}u_{\alpha'}(p).\end{aligned} \tag{56}$$

Let $T(\xi q, f, k)$ denote the expression within the braces in (56). Comparing it with $T(q, f, k)$ given by (2a), we see that one q in $T(q, f, k)$ has been replaced by the photon polarization vector $\xi(q)$. We proceed as before but do not apply the Fierz identity to the pair $[C^{-1}\underline{\sigma}\cdot\underline{\boldsymbol{\xi}}(q)]_{\lambda_1\lambda_2}(\underline{\sigma}\cdot\mathbf{k}C)_{\lambda_1'\lambda_2'}$. We will get an expression corresponding to (14) in which the Kronecker product of R's and Q's will not act on the three indices of $\bar{U}^{\sigma}_{r'\lambda_1'\lambda_2'\cdots}(0)$ and $U^{(\sigma)}_{r\lambda_1\lambda_2\cdots}(0)$. To obtain the rotation operators $e^{iJ_2\theta_k}$ and $e^{iJ_2\theta_q}$, we introduce three rotation operators $R(\theta_q)$ and three $R^\dagger(\theta_a)$ and obtain

$$\begin{aligned} T(\xi q, f, k) = \frac{1}{2^l}\,\mathbf{q}^{l-1}\mathbf{k}^{l-1}&[L(f)R(\boldsymbol{\theta}_q)]_{\alpha\theta}[R^\dagger(\theta_k)L^{-1}(f)]_{\nu\alpha'} \\ &\times [R^\dagger(\boldsymbol{\theta}_k)\underline{\sigma}\cdot\underline{\mathbf{k}}CR^{\dagger T}(\theta_k)]_{\nu_1\nu_2} \\ &\times [R^T(\boldsymbol{\theta}_q)C^{-1}\underline{\sigma}\cdot\underline{\boldsymbol{\xi}}(q)R(\boldsymbol{\theta}_q)]_{\theta_1\theta_2} \\ &\times \sum_\sigma \bar{U}^{(\sigma)}_{\nu'\nu_1'\nu_2'\cdots}\cdot(e^{-iJ_2\boldsymbol{\theta}_k})_{\nu'\nu_1'\nu_2'\cdots,\nu\nu_1\nu_2\cdots} \\ &\times Q\times Q\times\cdots\times Q \\ &\times (e^{+iJ_2\boldsymbol{\theta}_2})_{\theta\theta_1\theta_2\cdots,\delta\delta_1\delta_2\cdots}U^{(\sigma)}_{\delta\delta_1\delta_2\cdots}. \end{aligned} \tag{57}$$

The transformed vectors $\mathbf{q}$, $\mathbf{k}$, and $\boldsymbol{\xi}$ are given by (33). $\boldsymbol{\theta}_q$ and $\boldsymbol{\theta}_k$ are the angles which $\mathbf{q}$ and $\mathbf{k}$ make with the x_3 axis, respectively. Before applying the rotations on U^σ and $\bar{U}^\sigma$, we simplify the factors involving $\underline{\sigma}\cdot\underline{\mathbf{k}}c$ and $\underline{\sigma}\cdot\underline{\boldsymbol{\xi}}$:

$$\begin{aligned} [R^\dagger(\boldsymbol{\theta}_k)\underline{\sigma}\cdot\underline{\mathbf{k}}CR^{\dagger T}(\boldsymbol{\theta}_k)]_{\nu_1\nu_2} &= [R^\dagger(\theta_k)\underline{\sigma}\cdot\underline{\mathbf{k}}R(\boldsymbol{\theta}_k)C]_{\nu_1\nu_2} \\ &= \mathbf{k}(\sigma_3 C)_{\nu_1\nu_2} \\ &= -\mathbf{k}(\sigma_1)_{\nu_1\nu_2} \end{aligned} \tag{58a}$$

and

$$[R^T(\boldsymbol{\theta}_q)C^{-1}\underline{\sigma}\cdot\underline{\xi}R(\boldsymbol{\theta}_q)]_{\theta_1\theta_2} = [CR^\dagger(\theta_q)\underline{\sigma}\cdot\underline{\xi}(q)R(\theta_q)]_{\theta_1\theta_2}. \tag{58b}$$

The Lorentz condition is

$$q_\mu\xi_\mu(q) = 0. \tag{59a}$$

For the transformed vectors $\mathbf{q}$ and $\boldsymbol{\xi}(q)$, we have

$$\begin{aligned} \mathbf{q}_\mu\boldsymbol{\xi}_\mu(q) &= q_\lambda\xi_\nu(q)a_{\lambda\mu}(f)a_{\nu\mu}(f) \\ &= q_\lambda\xi_\nu(q)\delta_{\lambda\nu} = 0. \end{aligned} \tag{59b}$$

On the other hand,

$$\begin{aligned} \underline{\mathbf{q}}\cdot\underline{\boldsymbol{\xi}} &= \mathbf{q}_i\boldsymbol{\xi}_i(q) \\ &= q_\lambda\left(\delta_{\lambda\nu} + \frac{f_\lambda f_\nu}{M_J^2}\right)\xi_\nu(q). \end{aligned} \tag{59c}$$

For the pole diagram C, $\underline{f} = \underline{p} + \underline{k} = 0$, we can also choose the radiation gauge and put

$$\xi_4(q) = 0. \tag{60}$$

Then

$$\underline{\mathbf{q}}\cdot\underline{\boldsymbol{\xi}} = \underline{q}\cdot\underline{\xi} = 0. \tag{61}$$

$\underline{\boldsymbol{\xi}}(q)$ is thus perpendicular to $\underline{\mathbf{q}}$. $\underline{q}$ and $\underline{\mathbf{q}}$ both lie in the x_1x_3 plane. Let

$$\underline{\boldsymbol{\xi}} = \underline{\boldsymbol{\xi}}^\parallel + \underline{\boldsymbol{\xi}}^\perp, \tag{62a}$$

where $\underline{\boldsymbol{\xi}}^\parallel$ lies in the x_1x_3 plane and $\underline{\boldsymbol{\xi}}^\perp$ is along the x_2 axis as shown in Fig. 2. As $\underline{\boldsymbol{\xi}}^\parallel$ is also perpendicular to $\mathbf{q}$, the rotation which transforms $\underline{\sigma}\cdot\underline{\mathbf{q}}$ to $\mathbf{q}\sigma_3$ will transform $\underline{\sigma}\cdot\underline{\xi}^\parallel$ to $\epsilon\boldsymbol{\xi}^\parallel\sigma_1$ with $\epsilon = \pm 1$ depending on the helicity of the photon. Hence

$$\begin{aligned} [C^{-1}R^\dagger(\theta_q)\underline{\sigma}\cdot\underline{\boldsymbol{\xi}}(q)R(\theta_q)]_{\theta_1\theta_2} &= [C^{-1}(\epsilon\sigma_1\boldsymbol{\xi}^\parallel + \sigma_2\boldsymbol{\xi}^\perp)]_{\theta_1\theta_2} \\ &= (\epsilon\sigma_3\boldsymbol{\xi}^\parallel + i\boldsymbol{\xi}^\perp)_{\theta_1\theta_2}. \end{aligned} \tag{62b}$$

Now

$$\begin{aligned} Q\times Q\times\cdots\times Q&e^{+iJ\boldsymbol{\theta}_2}_{\theta\theta_1\theta_2\cdots,\delta\delta_1\delta_2\cdots}U^{(\sigma)}_{\delta\delta_1\delta_2\cdots} \\ &= \sum_{\sigma'} Q\times Q\times\cdots\times Q d^J_{\sigma\sigma'}(\boldsymbol{\theta}_q)U^{(\sigma')}_{\theta\theta_1\theta_2\cdots}. \end{aligned} \tag{63}$$

From the properties of Q [(20b)], we see that only the $U^{(\sigma')}$ with $\sigma' = \pm\frac{3}{2}, \pm\frac{1}{2}$ will give nonzero contribution to (63), and it can be written

$$\begin{aligned} &2^{l-1}\{[d^J_{\sigma\frac{3}{2}}(\boldsymbol{\theta}_q)({}^{2J}C_{J-\frac{3}{2}})^{-\frac{1}{2}}(u^1\times u^1\times u^1)_{\theta\theta_1\theta_2} \\ &+ d^J_{\sigma\frac{1}{2}}(\boldsymbol{\theta}_q)({}^{2J}C_{J-\frac{1}{2}})^{-\frac{1}{2}} \\ &\times(u^1\times u^1\times u^2 + u^1\times u^2\times u^1 + u^2\times u^1\times u^1)_{\theta\theta_1\theta_2} \\ &+ d^J_{\sigma,-\frac{1}{2}}(\boldsymbol{\theta})({}^{2J}C_{J+\frac{1}{2}})^{-\frac{1}{2}} \\ &\times(u^2\times u^2\times u^1 + u^2\times u^1\times u^2 + u^1\times u^2\times u^2)_{\theta\theta_1\theta_2} \\ &+ d^J_{\sigma,-\frac{3}{2}}(\boldsymbol{\theta}_q)({}^{2J}C_{J+\frac{3}{2}})^{-\frac{1}{2}}(u^2\times u^2\times u^2)_{\theta\theta_1\theta_2}] \\ &\times(u^1\times u^2 + u^2\times u^1)\times(u^1\times u^2 + u^2\times u^1) \\ &\times\cdots\times(u^1\times u^2 + u^2\times u^1)\}. \end{aligned} \tag{64}$$

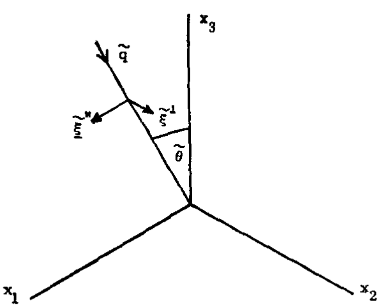
When the indices θ_1 and θ_2 in the above expression are contracted with the indices in $(\epsilon\sigma_3\boldsymbol{\xi} + i\boldsymbol{\xi}^\perp)_{\theta_1\theta_2}$, the first two terms in the coefficients of $d^J_{\sigma,\pm\frac{1}{2}}(\theta_c)$ will not contribute.

On expanding,

$$\bar{U}^{(\sigma)}_{\nu'\nu_1'\nu_2'\cdots}e^{-iJ_2\boldsymbol{\theta}_k}_{\nu'\nu_1'\nu_2'\cdots,\nu\nu_1\nu_2\cdots} = \sum_{\sigma''} d^J_{\sigma\sigma''}(\boldsymbol{\theta}_k)\bar{U}^{(\sigma'')}_{\nu\nu_1\nu_2\cdots}, \tag{65}$$

and calculating (57), we find that only the $\sigma'' = \pm\frac{3}{2}, \pm\frac{1}{2}$ terms in (65) contribute and only that part

FIG. 2. Indication of the directions of the mutually perpendicular vectors $\underline{\mathbf{q}}$, $\underline{\boldsymbol{\xi}}^\parallel$, and $\underline{\boldsymbol{\xi}}^\perp$.



which corresponds to (64) survives. Since $\nu_1\nu_2$ is in (65) and contracted with $\nu_1\nu_2$ in $(\sigma_1)_{\nu_1\nu_2}$, only the first two terms in the coefficients of $d^J_{\sigma,\pm\frac{1}{2}}(\boldsymbol{\theta}_k)$ contribute. A little calculation gives

$$
\begin{aligned}
&T_{\alpha\alpha'}(\xi q, f, k)\\
&= \frac{2\cdot 2^{l-1}2^{l-1}}{2^l}\frac{\mathbf{q}^{l-1}\mathbf{k}^{l-1}}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}[L(f)R(\boldsymbol{\theta}_q)]_{\alpha\theta}\\
&\times [R^\dagger(\boldsymbol{\theta}_k)L^{-1}(f)]_{\nu\alpha'}(\epsilon\sigma_3\boldsymbol{\xi}^{\parallel}+i\boldsymbol{\xi}^{\perp})_{\theta_1\theta_2}\\
&\times\Bigg[\bar{u}^1_\nu\Bigg\{d^J_{\frac{1}{2}\frac{3}{2}}(\boldsymbol{\theta})\cdot\frac{u^1\times u^1\times u^1}{({}^{2J}C_{J-\frac{3}{2}})^{\frac{1}{2}}}\\
&+d^J_{\frac{1}{2}\frac{1}{2}}(\boldsymbol{\theta})\frac{u^2\times u^1\times u^1}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}+d^J_{\frac{1}{2},-\frac{1}{2}}(\boldsymbol{\theta})\frac{u^1\times u^2\times u^2}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}\\
&+d^J_{\frac{1}{2},-\frac{3}{2}}(\boldsymbol{\theta})\frac{u^2\times u^2\times u^2}{({}^{2J}C_{J-\frac{3}{2}})^{\frac{1}{2}}}\Bigg\}_{\theta\theta_1\theta_2}\\
&+\bar{u}^2_\nu\Bigg\{d^J_{-\frac{1}{2},-\frac{3}{2}}(\boldsymbol{\theta})\frac{u^2\times u^2\times u^2}{({}^{2J}C_{J-\frac{3}{2}})^{\frac{1}{2}}}\\
&+d^J_{-\frac{1}{2},-\frac{1}{2}}(\boldsymbol{\theta})\frac{u^1\times u^2\times u^2}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}+d^J_{-\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})\frac{u^2\times u^1\times u^1}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}\\
&+d^J_{-\frac{1}{2},\frac{3}{2}}(\boldsymbol{\theta})\frac{u^1\times u^1\times u^1}{({}^{2J}C_{J-\frac{3}{2}})^{\frac{1}{2}}}\Bigg\}_{\theta\theta_1\theta_2}\Bigg].
\end{aligned}
\tag{66}
$$

In deriving this expression use has been made of (24a) and $\boldsymbol{\theta}=\boldsymbol{\theta}_q-\boldsymbol{\theta}_k$. Via (24b), each term in the second braces can be combined with the corresponding term in the first braces, and, noticing that

$$u^{1,2}_{\theta_1}(\epsilon\sigma_3\boldsymbol{\xi}^{\parallel}+i\xi^{\perp})_{\theta_1\theta_2}u^{1,2}_{\theta_2}=\pm\epsilon\boldsymbol{\xi}^{\parallel}+i\boldsymbol{\xi}^{\perp}, \tag{67}$$

we obtain

$$
\begin{aligned}
&T_{\alpha\alpha'}(\xi q, f, k)\\
&=\frac{2^l}{2}\frac{\mathbf{q}^{l-1}\mathbf{k}^l}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}\Bigg[L(f)R(\boldsymbol{\theta}_q)\cdot\Bigg(\frac{1}{({}^{2J}C_{J-\frac{3}{2}})^{\frac{1}{2}}}d^J_{\frac{1}{2},\frac{3}{2}}(\boldsymbol{\theta})\\
&\times[\epsilon\boldsymbol{\xi}^{\parallel}(u^1\bar{u}^1+u^2\bar{u}^2)+i\boldsymbol{\xi}^{\perp}(u^1\bar{u}^1-u^2\bar{u}^2)]\\
&+\frac{1}{({}^{2J}C_{J-\frac{3}{2}})^{\frac{1}{2}}}d^J_{-\frac{1}{2},\frac{3}{2}}(\boldsymbol{\theta})\\
&\times[\epsilon\boldsymbol{\xi}^{\parallel}(u^1\bar{u}^2-u^2\bar{u}^1)+i\boldsymbol{\xi}^{\perp}(u^1\bar{u}^2+u^2u^1)]\\
&+\frac{1}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}d^J_{\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})\\
&\times[\epsilon\boldsymbol{\xi}^{\parallel}(u^2\bar{u}^1-u^1u^2)+i\boldsymbol{\xi}^{\perp}(u^2u^1+u^1\bar{u}^2)]\\
&+\frac{1}{({}^{2J}C_{J-\frac{1}{2}})^{\frac{1}{2}}}d^J_{-\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})\\
&\times[\epsilon\boldsymbol{\xi}^{\parallel}(u^2\bar{u}^2+u^1\bar{u}^1)+i\boldsymbol{\xi}^{\perp}(u^2\bar{u}^2-u^1\bar{u}^1)]\Bigg)\\
&\times R^\dagger(\boldsymbol{\theta}_k)L^{-1}(f)\Bigg]_{\alpha\alpha'}.
\end{aligned}
\tag{68}
$$

For further reduction of this equation, we note that

$$
\begin{aligned}
u^1\bar{u}^1&=\tfrac{1}{2}(1+\gamma_4)(1+\sigma_3)/2=\Lambda^\dagger(0)(1+\sigma_3)/2,\\
u^2\bar{u}^2&=\Lambda^\dagger(0)(1-\sigma_3)/2,\\
u^1\bar{u}^2&=(\sigma_1+i\sigma_2)/2\Lambda^\dagger(0),
\end{aligned}
\tag{69}
$$

and so are able to write

$$
\begin{aligned}
&\epsilon\boldsymbol{\xi}^{\parallel}(u^1\bar{u}^1+u^2\bar{u}^2)+i\boldsymbol{\xi}^{\perp}(u^1\bar{u}^1-u^2\bar{u}^2)\\
&\quad=\Lambda^\dagger(0)(\epsilon\boldsymbol{\xi}^{\parallel}+i\boldsymbol{\xi}^{\perp}\sigma_3)\\
&\quad=-\Lambda^\dagger(0)i\sigma_2\sigma_3(\epsilon\boldsymbol{\xi}^{\parallel}\sigma_1+\sigma_2\boldsymbol{\xi}^{\perp}).
\end{aligned}
\tag{70}
$$

Also

$$
\begin{aligned}
&R(\boldsymbol{\theta}_q)\sigma_3(\epsilon\boldsymbol{\xi}^{\parallel}\sigma_1+\sigma_2\boldsymbol{\xi}^{\perp})R^\dagger(\boldsymbol{\theta}_k)\\
&=R(\boldsymbol{\theta}_q)\sigma_3R^\dagger(\boldsymbol{\theta}_q)R(\boldsymbol{\theta}_q)(\epsilon\boldsymbol{\xi}^{\parallel}\sigma_1+\sigma_2\boldsymbol{\xi}^{\perp})R^\dagger(\boldsymbol{\theta}_q)R(\boldsymbol{\theta}_q)R^\dagger(\boldsymbol{\theta}_k)\\
&=\frac{1}{\mathbf{q}}\underline{\sigma}\cdot\underline{\mathbf{q}}\underline{\sigma}\cdot\underline{\boldsymbol{\xi}}R(\boldsymbol{\theta}).
\end{aligned}
\tag{71}
$$

Using the above relations and attaching a γ_4 to each $i\sigma_2$, we have

$$
\begin{aligned}
&L(f)R(\boldsymbol{\theta}_q)[\epsilon\boldsymbol{\xi}^{\parallel}(u^1\bar{u}^1+u^2\bar{u}^2)\\
&\quad+i\boldsymbol{\xi}^{\perp}(u^1\bar{u}^1-u^2\bar{u}^2)R^\dagger(\boldsymbol{\theta}_k)L^{-1}(f)\\
&\quad=-\frac{1}{\mathbf{q}}L(f)i\sigma_2\gamma_4\underline{\sigma}\cdot\underline{\mathbf{q}}\Lambda^\dagger(0)\underline{\sigma}\cdot\underline{\boldsymbol{\xi}}e^{-(i/2)\gamma_4\sigma_2\theta}L^{-1}(f)\\
&\quad=-\frac{1}{\mathbf{q}}L(f)i\sigma_2\gamma_4\gamma_5\underline{\gamma}\cdot\underline{\mathbf{q}}\Lambda^\dagger(0)\underline{\gamma}\cdot\underline{\boldsymbol{\xi}}\gamma_5e^{-(i/2)\gamma_4\sigma_2\theta}L^{-1}(f).
\end{aligned}
\tag{72}
$$

Since $L(f)$ commutes with $i\sigma_2\gamma_4$ and from (6a),

$$
\begin{aligned}
L(f)\gamma\cdot\mathbf{q}L^{-1}(f)&=\gamma\cdot q,\\
L(f)\gamma\cdot\boldsymbol{\xi}L^{-1}(f)&=\gamma\cdot\xi,
\end{aligned}
\tag{73}
$$

(72) reduces to

$$-\frac{1}{\mathbf{q}}i\sigma_2\gamma_4\gamma_5(\gamma\cdot q-\mathbf{q}_4)\Lambda^\dagger(f)(\gamma\cdot\xi-\boldsymbol{\xi}^4)\gamma_5e^{-(i/2)\gamma_4\sigma_2\tilde{\theta}}.$$

The three other terms can be treated in a similar fashion, and we obtain on-the-mass-shell propagator part $T'_{\alpha\alpha'}$ for the photo-emission case

$$
\begin{aligned}
&T(\xi q, f, k)\\
&=-\tfrac{1}{2}D_l\mathbf{q}^{l-2}\mathbf{k}^l\Bigg[\Bigg\{d^J_{\frac{1}{2},\frac{3}{2}}(\boldsymbol{\theta})i\sigma_2\gamma_4\gamma_5(\gamma\cdot q-\mathbf{q}_4)\Lambda^\dagger(f)\\
&\times(\gamma\cdot\xi-\boldsymbol{\xi}_4)\gamma_5+d^J_{-\frac{1}{2},\frac{3}{2}}(\boldsymbol{\theta})i\sigma_2\gamma_4\gamma_5(\gamma\cdot q-\mathbf{q}_4)\\
&\times\Lambda^\dagger(f)(\gamma\cdot\xi-\boldsymbol{\xi}_4)\gamma_5\gamma_4i\sigma_2\Bigg\}\left(\frac{l+2}{2}\right)^{\frac{1}{2}}\\
&+d^J_{\frac{1}{2}\frac{1}{2}}(\boldsymbol{\theta})\gamma_5(\gamma\cdot q-\mathbf{q}_4)\Lambda^\dagger(f)(\gamma\cdot\xi-\boldsymbol{\xi}_4)\gamma_5\\
&+d^J_{-\frac{1}{2},\frac{1}{2}}(\boldsymbol{\theta})\gamma_5(\gamma\cdot q-\mathbf{q}_4)\\
&\times\Lambda^\dagger(f)(\gamma\cdot\xi-\boldsymbol{\xi}_4)\gamma_5i\sigma_2\gamma_4\Bigg]e^{-(i/2)\gamma_4\sigma_2\theta}.
\end{aligned}
\tag{74}
$$

$\mathbf{q}$, $\mathbf{k}$, and $\cos\boldsymbol{\theta}$ are given as before by (33) and, since

$$\mathbf{q}_\mu\mathbf{q}_\mu = q_\nu q_\lambda a_{\nu\mu}(f)a_{\lambda\mu}(f) = q_\nu q_\lambda \delta_{\nu\lambda} = 0, \quad (75a)$$

$$\mathbf{q}_4 = i\mathbf{q}_0 = i\mathbf{q}. \quad (75b)$$

Also, since $\boldsymbol{\xi}_\mu(q)\mathbf{q}_\mu = 0$,

$$\boldsymbol{\xi}_4 = \frac{1}{i\mathbf{q}}\,\underline{\mathbf{q}}\cdot\underline{\boldsymbol{\xi}}(q) = \frac{1}{i\mathbf{q}}\left\{q\cdot\xi + \frac{f\cdot\xi f\cdot q}{M_J^2}\right\} = \frac{1}{i\mathbf{q}}\frac{f\cdot\xi f\cdot q}{M_J^2}. \quad (75c)$$

For the amplitude $T_c^{(1)}$, $f = 0$ and, since we employ radiation gauge $\xi_4 = 0$, $\boldsymbol{\xi}_4$ will vanish. We have, therefore,

$$T_C^{(1)} = i\,\frac{g_{JN\pi}g_{JN\gamma}^{(1)}}{-u+M_J^2}\,\bar{u}(p')T(\xi q, p+k, k)u(p), \quad (76)$$

with $T(\xi q, p+k, k)$ given by (74), (75), and (60).

To derive the result corresponding to (49), we equate $\mathbf{q}$, $\mathbf{k}$, $\cos\boldsymbol{\theta}$ to q, k, $\cos\theta = z$, respectively, use the expressions for the d^J matrices given in Ref. 9, and obtain

$$\begin{aligned} T_C^{(1)} = -\frac{1}{2}\frac{g_{JN\pi}g_{JN\gamma}^{(1)}}{-u+M_J^2}D_l\frac{q^{l-2}k^l}{l+1}\bar{u}(p') &\times [\gamma_4 p_0' - m - q(1+\gamma_4)] \\ &\times [i\sigma_2\gamma_4\gamma_5\Lambda^\dagger(p+k)\underline{\gamma}\cdot\underline{\xi}\gamma_5\{(l+2/l)\sin\theta P_l'(z) \\ &+ i\sigma_2\gamma_4[zP_l'(z)(l+2/l) - P_{l+1}'(z)]\} \\ &+ \gamma_5\Lambda^\dagger(p+k)\underline{\gamma}\cdot\underline{\xi}\gamma_5[P_{l+1}'(z) - zP_l'(z) \\ &+ i\sigma_2\gamma_4\sin\theta P_l'(z)]]u(p). \end{aligned} \quad (77)$$

$i\underline{\gamma}\cdot\underline{q} = i\gamma\underline{p}'$ in $i\gamma\cdot q$ has been eliminated by using the Dirac equation. The helicity amplitudes can be obtained from (74) and (76) by noting that the rotation operator $R^\dagger(\theta)$ coming from $\bar{u}^{(\lambda')}(p')$ or going to the right of $\underline{\sigma}\cdot\underline{\xi}$ makes it $\sigma_1 \mp i\sigma_2$, the upper and lower signs standing for helicities $+1$ and -1 of the final state photon, respectively. Then, if we use the continuation which gives $i\sigma_2$ instead of $i\sigma_2\gamma_4$ (as discussed at the end of Sec. III), $R^\dagger(\theta)e^{-i\sigma_2\theta/2} = 1$ and the four independent helicity amplitudes will have the respective $d_{\mu\lambda}^J$ matrices as the only θ-dependent terms. Further, we notice that the polynomials in degree l in $z = \cos\theta$ in $T_C^{(1)}$ given by (77) do not contain γ_4 as factors of $i\sigma_2$ since the γ_4 in $i\sigma_2\gamma_4\gamma_5$ commutes with factors on the right and removes the γ_4 in

$$i\sigma_2\gamma_4[zP_l'(z)(l+2)/2 - P_{l+1}'(z)].$$

Therefore, as in the $\pi N \to \pi N$ case, the part containing the highest degree polynomials $P_{l+1}'(z)$ and $2P_l(z)$ is independent of the ambiguity coming from the two different continuations.

The other term given by the Lagrangian for diagram C involves $g_{JN\pi}g_{JN\gamma}^{(2)}$, has the same propagator as for the $\pi N \to \pi N$ case, and is given by

$$T_C^{(2)} = g_{JN\pi}g_{JN\gamma}^{(2)}D_l q^l k^l \bar{u}(p')\underline{\gamma}\cdot\underline{\xi}\Lambda^\dagger(p+k) \times [P_l(z) - i\sigma_2\gamma_4(1-z^2)^{\frac{1}{2}}P_l'(z)]u(p)\frac{1}{-u+M_J^2}, \quad (78)$$

with

$$\Lambda^\dagger(p+k) = \frac{1}{2}\left(1 + \frac{\gamma_4\sqrt{u}}{M_J}\right). \quad (79)$$

ACKNOWLEDGMENTS

The author is grateful to Professor A. Salam and Professor P. Budini as well as the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste.

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[1] R. Blankenbecler, R. L. Sugar, and J. D. Sullivan, Phys. Rev. **166**, 1515 (1968).

[2] R. Blankenbecler and R. L. Sugar, Phys. Rev. **168**, 1597 (1968).

[3] R. Carlitz and M. Kislinger, Phys. Rev. Letters **24**, 186 (1970).

[4] Lagrangians with $\overleftrightarrow{\partial}$ have also been used in Ref. 2.

[5] Arif-uz-Zaman, Nuovo Cimento **56A**, 493 (1968).

[6] The numerator of the propagator for bosons in Ref. 2 is $\sum \xi^{\mu_1\mu_2\cdots\mu_l}(f)\xi^{\dagger\nu_1\nu_2\cdots\nu_l}(f)$ summed up over all spin components. $\xi^{\mu_1\mu_2\cdots\mu_l}(f)$ is the polarization tensor. Feynman propagators for the Wigner–Bargmann formalism have been discussed by T. W. B. Kibble, Phys. Rev. **139**, 712 (1965).

[7] S. Weinberg, Phys. Rev. **133**, B1318 (1964).

[8] M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957).

[9] M. Jacob and A. C. Wick, Ann. Phys. (N.Y.) **7**, 4041 (1959).

[10] V. A. Alessandrini [Phys. Rev. **172**, 1503 (1968)], working with a Rarita–Schwinger type formalism, has obtained the angular dependence using the results of C. Zemach.

[11] J. C. Rushbrooke, Phys. Rev. **143**, 1345 (1966).

Distribution Functions for an Exactly Soluble Quantum Statistical System*

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(Received 19 August 1970)

Exact expressions are obtained for the distribution functions, in configuration and momentum space, for a system of bosons or spinless fermions interacting via pairwise harmonic forces.

1. INTRODUCTION

In a recent paper[1] it was shown that one could obtain exact expressions for the partition function and energy levels for a system of bosons or fermions interacting via pairwise harmonic oscillator forces. It is the purpose of this paper to show that these results can be extended to include an exact evaluation of both the spatial and momentum distribution functions for such a system.

The study of this model is approached using the methods of quantum statistical mechanics. Because of the strong character of the forces involved, the system we are dealing with is not extensive, i.e., it does not fill the volume available to it but "clumps" together with no unbound states available. One, therefore, has to be careful that a literal interpretation is not placed on the thermodynamic quantities derived. However, the ground state of the system can be studied in detail by taking the zero temperature limit.

2. THE MODEL

The many-body system that we consider has a Hamiltonian

$$H = -\sum_{i=1}^{N} \frac{\partial^2}{\partial \mathbf{x}_i^2} + \frac{\omega^2}{N} \sum_{i<j} (\mathbf{x}_i - \mathbf{x}_j)^2, \tag{1}$$

(with units such that $\hbar^2/2m = 1$).

The structure of a system of bosons or fermions at a temperature T (related to the parameter β via $\beta = 1/kT$) is given completely by a knowledge of the appropriately symmetrized density matrix expressed in coordinate representation

$$\rho_{\text{sym}}^{(N)}(\mathbf{x}_1, \cdots, \mathbf{x}_N; \mathbf{x}_1', \cdots, \mathbf{x}_N'; \beta) = \frac{1}{N!} \sum_p \epsilon_p \rho^{(N)}(\mathbf{x}_1, \cdots, \mathbf{x}_N; \mathbf{x}_p', \cdots, \mathbf{x}_{PN}'; \beta), \tag{2}$$

where the sum is taken over all permutations of the primed variables with the sign $\epsilon_p = 1$ for bosons or an even permutation of fermions and $\epsilon_p = -1$ for an odd permutation of fermions. Here $\rho^{(N)}$ is the N-particle unsymmetrized density matrix, i.e., the solution of the Bloch equation

$$\frac{\partial \rho^{(N)}}{\partial \beta} = H \rho^{(N)} \quad \text{with} \quad \rho^{(N)} \underset{\beta \to 0}{=} \prod \delta(\mathbf{x}_i - \mathbf{x}_i'). \tag{3}$$

The following expression for $\rho^{(N)}$ has been found[1]:

$$\begin{aligned}\rho^{(N)} = {} & (4\pi\beta)^{-\frac{3}{2}}[2\pi \sinh(2\omega\beta)/\omega]^{-\frac{3}{2}(N-1)} \\ & \times \exp\Big(-(\mathbf{X} - \mathbf{X}')^2[1 - 2\omega\beta \operatorname{csch}(2\omega\beta)]/4\beta \\ & - \tfrac{1}{2}\omega \operatorname{csch}(2\omega\beta) \sum_{i=1}^{N} (\mathbf{x}_i - \mathbf{x}_i')^2 \\ & - \frac{\omega}{2N} \tanh(\omega\beta) \sum_{i<j} (\mathbf{r}_{ij}^2 + \mathbf{r}_{ij}'^2)\Big),\end{aligned} \tag{4}$$

where $\mathbf{X} = \sum_i \mathbf{x}_i / N^{\frac{1}{2}}$ and $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$.

Usually, in order to study the structure of an extensive system, we integrate the diagonal element of the symmetrized density matrix over all variables except, say, two or three. This gives the two- or three-particle distribution function. However, the particles of our model form a system of finite extent so it is appropriate to study the structure of this collection of particles by fixing the center-of-mass at the origin and then finding the one- and two-particle distribution functions. For example, we define the one-particle density as

$$n(\mathbf{x}) = \frac{1}{Z_N} \int \cdots \int \rho_{\text{sym}}^{(N)}(\mathbf{x}_1 \cdots \mathbf{x}_N; \mathbf{x}_1 \cdots \mathbf{x}_N; \beta) \times \delta(\mathbf{X}) \sum_i \delta(\mathbf{x} - \mathbf{x}_i)\, d\mathbf{x}_1 \cdots d\mathbf{x}_N, \tag{5}$$

where the normalization factor Z_N is the modified partition function

$$Z_N = \int \cdots \int \rho_{\text{sym}}^{(N)}(\mathbf{x}_1 \cdots \mathbf{x}_N; \beta) \delta(\mathbf{X})\, d\mathbf{x}_1 \cdots d\mathbf{x}_N. \tag{6}$$

It is convenient to calculate first the N-particle Fourier transform of the diagonal element of the density matrix with the center-of-mass fixed at the origin, i.e.,

$$\int\cdots\int \rho_{\text{sym}}^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_N;\beta)\delta(\mathbf{X}) \times \exp\left(i\sum_j \mathbf{k}_j\cdot\mathbf{x}_j\right) d\mathbf{x}_1\cdots d\mathbf{x}_N. \quad (7)$$

We can then obtain the distribution function for an arbitrary number of particles by setting the appropriate number of the $\mathbf{k}_j$ equal to 0 and calculating the inverse Fourier transform. This expression involves the sum over $N!$ terms, each from a different permutation of the particles. The term arising from an arbitrary permutation which can be factorized into a product of cyclic permutations of $M_1, M_2, \cdots, M_r$ variables will have a factor of the form

$$J(\mathbf{k}_1\cdots\mathbf{k}_N) = \int\cdots\int \exp\left(-\sum_{jk} R_{jk}\mathbf{x}_j\cdot\mathbf{x}_k + i\sum_j \mathbf{k}_j\cdot\mathbf{x}_j\right)\delta(X)\, d\mathbf{x}_1\cdots d\mathbf{x}_N, \quad (8)$$

where, from Eq. (4), the matrix R can be expressed as

$$R = \omega\tanh(\omega\beta)(I^{(N)} - B^{(N)}/N) + \tfrac{1}{2}\omega\,\text{csch}\,(2\omega\beta)(A^{(M_1)}\oplus A^{(M_2)}\oplus\cdots\oplus A^{(M_r)}), \quad (9)$$

where $I^{(N)}$ is the $N\times N$ unit matrix, $B^{(N)}$ is an $N\times N$ matrix in which every element is 1, and $A^{(M)}$ represents an $M\times M$ matrix of the form

$$A^{(M)} = \begin{bmatrix} 2 & -1 & 0 & \cdots & -1 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ -1 & 0 & 0 & \cdots & 2 \end{bmatrix} \quad \text{for} \quad M > 2,$$

$$A^{(1)} = [0] \quad \text{and} \quad A^{(2)} = \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix}. \quad (10)$$

In Appendix A, we find an explicit expression for the matrix W for which $(W^+RW)_{jk} = \delta_{jk}\lambda_j$. Thus, if we use the transformation $\mathbf{z}_j = \sum_k W_{jk}\mathbf{x}_k$, Eq. (8) becomes

$$J = \int\cdots\int \exp\left[-\sum_{j=1}^{N-1}\left(z_j^2\lambda_j + i\sum_{l=1}^{N} W_{lj}\mathbf{k}_l\cdot\mathbf{z}_j\right)\right] \times d\mathbf{z}_1\cdots d\mathbf{z}_{N-1}$$
$$= \pi^{\frac{3}{2}(N-1)}\prod_{j=1}^{N-1}\lambda_j^{-\frac{3}{2}}\exp\left(-\tfrac{1}{4}\sum_{jl} K_{jl}\mathbf{k}_j\cdot\mathbf{k}_l\right). \quad (11)$$

Here we have used the fact that $\mathbf{z}_N = \mathbf{X} = \sum_i \mathbf{x}_i/N^{\frac{1}{2}}$ with $\lambda_N = 0$ and have defined

$$K_{jl} = \sum_{k=1}^{N-1} W_{jk}W_{lk}\lambda_k^{-1}. \quad (12)$$

The matrix K has the form (see Appendix B)

$$K = (C^{(M_1)}\oplus C^{(M_2)}\oplus\cdots\oplus C^{(M_r)}) - B^{(N)}/N\omega\tanh(\omega\beta), \quad (13)$$

where

$$C_{jk}^{(M)} = \cosh(M\omega\beta - 2\omega\beta\,|j-k|)/\omega\sinh(M\omega\beta). \quad (14)$$

3. ONE-PARTICLE DENSITY

Using symmetry arguments we can replace the sum over delta functions in the definition [Eq. (5)] of the one-particle density by N times one delta function, i.e., let

$$\sum_i \delta(\mathbf{x}-\mathbf{x}_i) = N\delta(\mathbf{x}-\mathbf{x}_i) = N(2\pi)^{-3}\int \exp(-i\mathbf{k}\cdot\mathbf{x} + i\mathbf{k}\cdot\mathbf{x}_i)\, d\mathbf{k} \quad (15)$$

in the integrand. Thus

$$n(\mathbf{x}) = \frac{N}{Z_N(2\pi)^3}\int d\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{x}}\int\cdots\int d\mathbf{x}_1\cdots d\mathbf{x}_N \times \rho_{\text{sym}}^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_N;\beta)\delta(\mathbf{X})\exp(i\mathbf{k}\cdot\mathbf{x}_i)$$
$$= \frac{(4\pi\beta)^{-\frac{3}{2}}(2\sinh\omega\beta)^3}{Z_N(N-1)!}\sum_p \epsilon_p\prod_{s=1}^{r}[2\sinh(M_s\omega\beta)]^{-3} \times (2\pi)^{-3}\int\exp(-\tfrac{1}{4}k^2K_{ii} - i\mathbf{k}\cdot\mathbf{x})\, d\mathbf{k}. \quad (16)$$

Note that

$$K_{ii} = \kappa_M = [\coth(M\omega\beta) - N^{-1}\coth(\omega\beta)]/\omega \quad (17)$$

depends only on the number of particles, M, in the cycle containing i. The sum over all permutations in Eq. (16) can be written as a double sum by first summing over all permutations in which i is in a cycle of M particles and then summing over M. The number of permutations in which i is in a cycle of M particles is $(N-1)!/(M-1)!$ so that

$$n(\mathbf{x}) = \frac{1}{Z_N}\sum_{M=1}^{N} Z_{N-M}S_M(\pi\kappa_M)^{-\frac{3}{2}}\exp\left(\frac{-x^2}{\kappa_M}\right), \quad (18)$$

where

$$S_M = (\pm 1)^{M+1}[2\sinh(M\omega\beta)]^{-3}, \quad (19)$$

with the upper sign referring to the Bose case and the lower sign to the Fermi case. We can use the fact that

$$N = \int n(\mathbf{x})\, d\mathbf{x} \quad (20)$$

to obtain from Eq. (18) the following simple recurrence relation to evaluate Z_N:

$$Z_N = \frac{1}{N} \sum_{M=1}^{N} Z_{N-M} S_M . \tag{21}$$

In both Eqs. (18) and (21) the initial values

$$Z_0 = [2 \sinh (\omega\beta)]^3 (4\pi\beta)^{-\frac{3}{2}},$$
$$Z_1 = (4\pi\beta)^{-\frac{3}{2}} \tag{22}$$

have to be used.

These recurrence relations provide a convenient method for the numerical evaluation of $n(\mathbf{x})$ and Z_N for relatively small N. Unfortunately, at low temperatures (large β) and large N these recurrence relations become difficult to handle for Fermi systems due to the large cancellations which occur; so it has not been possible to carry through the calculations to study the ground state of Fermi systems larger than nine particles, although there seems to be no difficulty in studying larger Bose systems or Fermi systems at higher temperatures. For all these calculations, the parameter ω was chosen to be 1; this keeps the size of the system of order 1. Figures 1 and 2 show the one-particle density for five bosons and fermions for various values of β. When $\beta > 2$, the system is almost entirely in its ground state. The density profiles for the Fermi case are particularly interesting then in that they show the effect that the Fermi statistical repulsion has in lowering the central density. As the temperature is raised, the higher states start to have an effect. Eventually the shape of both the Fermi and Bose systems reach the same classical Gaussian form at sufficiently high temperatures.

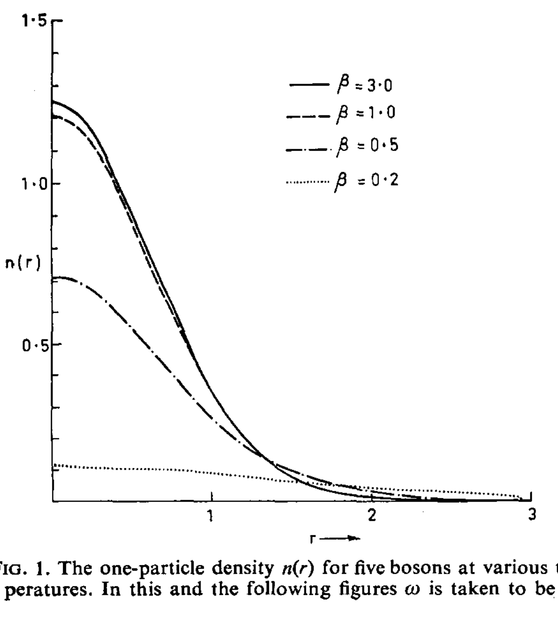

FIG. 1. The one-particle density $n(r)$ for five bosons at various temperatures. In this and the following figures ω is taken to be 1.

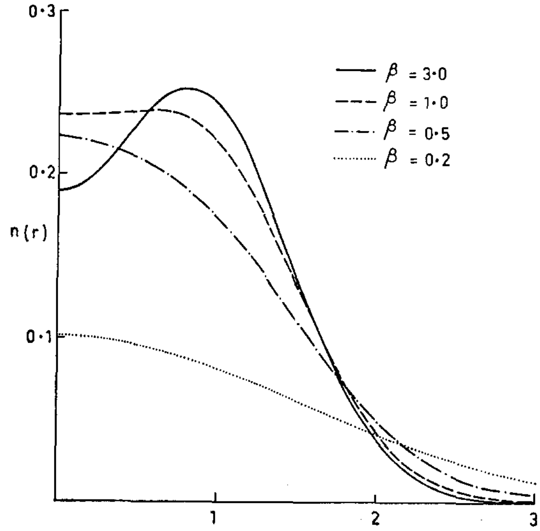

FIG. 2. The one-particle density $n(r)$ for five fermions at various temperatures. Note the effect the Fermi statistical "repulsion" has in depressing the central density when the ground state dominates for large β.

The effect of varying the number of particles for Fermi systems near their ground states is shown in Fig. 3. The way in which the additional particles add to the central density while changing the surface only slightly is most striking. Already, by the time we have nine particles, a structure reminiscent of the nuclear density "oscillations" is becoming apparent. It is perhaps premature to draw any strict parallel between this and the density distribution of nuclei until the effects of spin and isospin are included.

From Eq. (21) and the relation

$$E_N = -\partial \ln Z_N / \partial\beta, \tag{23}$$

between the internal energy E_N (neglecting the center-of-mass contribution) and the partition function, one can obtain the following recurrence relation for E_N:

$$E_N = \frac{1}{NZ_N} \sum_{M=1}^{N} [E_{N-M} + 3M\omega \coth (M\omega\beta)] Z_{N-M} S_M . \tag{24}$$

As an illustration the result of a calculation of E_6 as a function of temperature is shown in Fig. 4. The flat portion of the graphs for low temperatures indicate the region where the ground state dominates. At high temperatures, both the Bose and Fermi results approach the classical expression $E_6 = 15\,kT$ from above; however, this is not apparent on the scale of this figure.

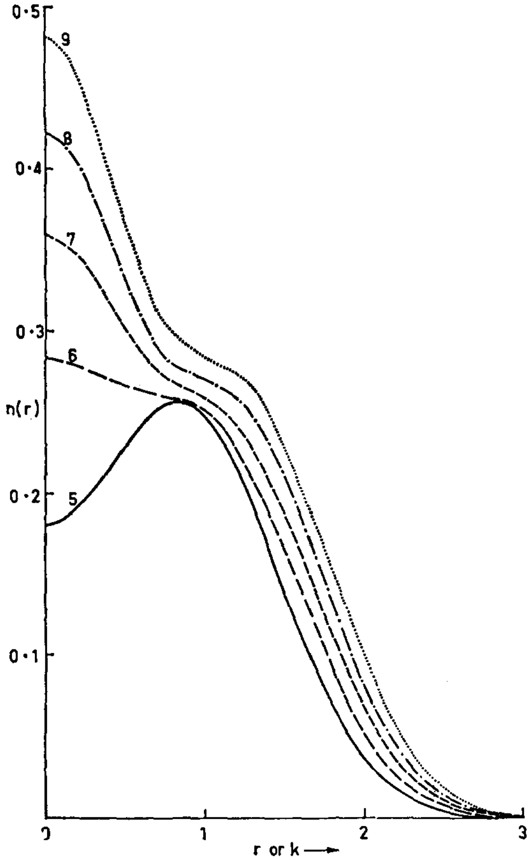

FIG. 3. The one-particle density $n(r)$ for various numbers of fermions at a temperature ($\beta = 2.5$) large enough so that the ground state dominates. The curves also describe the momentum distribution function for these systems (see Sec. 5).

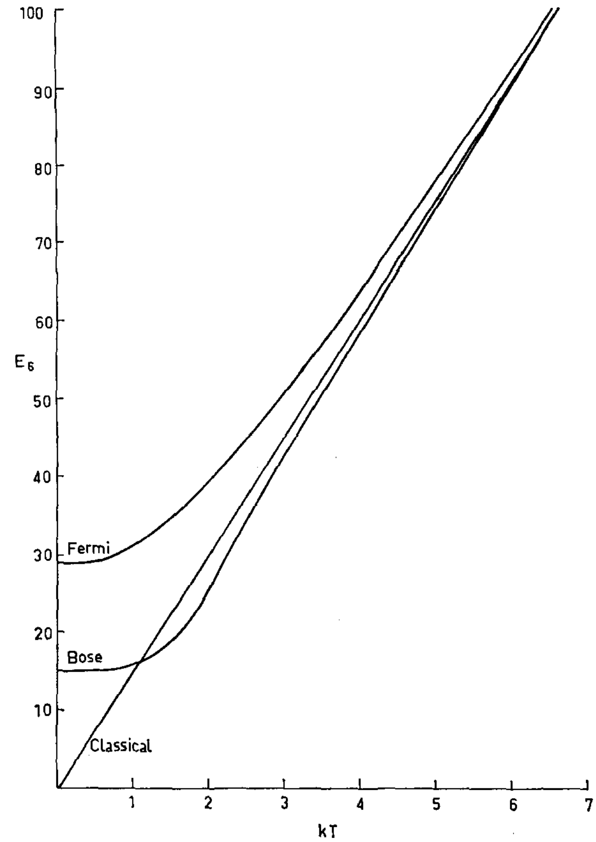

FIG. 4. A comparison between the internal energy (neglecting the center-of-mass contribution) of six bosons or fermions and the corresponding classical expression.

4. TWO-PARTICLE DISTRIBUTION FUNCTIONS

We define the two-particle distribution function as

$$n_2(\mathbf{x}, \mathbf{y}) = \frac{1}{Z_N}\int\cdots\int \rho_{\text{sym}}^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_N;\beta)\delta(\mathbf{X}) \times \sum_{i,j}{}' \delta(\mathbf{x}-\mathbf{x}_i)\delta(\mathbf{y}-\mathbf{x}_j)\,d\mathbf{x}_1\cdots d\mathbf{x}_N. \quad (25)$$

If we replace the δ functions by their Fourier integral representations and use Eq. (11), n_2 can be written

$$n_2(\mathbf{x}, \mathbf{y}) = \frac{(4\pi\beta)^{-\frac{3}{2}}(2\sinh\omega\beta)^3}{Z_N N!} \times \sum_p \epsilon_p \prod_{s=1}^{r}[2\sinh(M_s\omega\beta)]^{-3}\sum_{i,j}{}'(2\pi)^{-6} \times \iint \exp[-\tfrac{1}{4}(K_{ii}k_i^2 + 2K_{ij}\mathbf{k}_i\cdot\mathbf{k}_j + K_{jj}k_j^2) - i\mathbf{k}_i\cdot\mathbf{x} - i\mathbf{k}_j\cdot\mathbf{y}]\,d\mathbf{k}_i\,d\mathbf{k}_j. \quad (26)$$

The sum over permutations in this expression can be reduced, in a manner similar to that used in Sec. 3, by separating the two possibilities: that particles i and j are in two distinct cycles and that i and j are in the same cycle. In the first case, K_{ij} depends only on the size of the cycles containing i and j; however, if i and j are in the same cycle K_{ij} depends on the relative position of i and j in the cycle. Thus Eq. (26) reduces to

$$n_2(\mathbf{x}, \mathbf{y}) = \frac{1}{Z_N}\sum_{M=1}^{N-1}\sum_{L=1}^{N-M} Z_{N-M-L}S_M S_L A_{ML}(\mathbf{x}, \mathbf{y}) + \frac{1}{Z_N}\sum_{M=2}^{N} Z_{N-M}S_M B_M(\mathbf{x}, \mathbf{y}), \quad (27)$$

where S_M is defined by Eq. (19). By picking the appropriate elements from the matrix K [defined in Eq. (13)], we find

$$A_{ML}(\mathbf{x}, \mathbf{y}) = (2\pi)^{-6}\iint d\mathbf{k}_1\,d\mathbf{k}_2 \times \exp\left[-\frac{1}{4\omega}\left(k_1^2\coth(M\omega\beta) + k_2^2\coth(L\omega\beta) - \frac{1}{N}(\mathbf{k}_1+\mathbf{k}_2)^2\coth(\omega\beta)\right) - i\mathbf{k}_1\cdot\mathbf{x} - i\mathbf{k}_2\cdot\mathbf{y}\right] \quad (28)$$

and

$$B_M(\mathbf{x},\mathbf{y}) = \sum_{j=1}^{M-1} (2\pi)^{-6} \iint d\mathbf{k}_1\, d\mathbf{k}_2 \times \exp\Bigg[-\frac{1}{4\omega}\Bigg((k_1^2 + k_2^2)\coth(M\omega\beta) - 2\mathbf{k}_1\cdot\mathbf{k}_2 \frac{\coth(M\omega\beta - 2j\omega\beta)}{\sinh(M\omega\beta)} - \frac{1}{N}(\mathbf{k}_1 + \mathbf{k}_2)^2 \coth(\omega\beta)\Bigg) - i\mathbf{k}_1\cdot\mathbf{x} - i\mathbf{k}_2\cdot\mathbf{y}\Bigg]. \quad (29)$$

It is appropriate to evaluate these expressions in terms of the variables $\mathbf{R} = \frac{1}{2}(\mathbf{x} + \mathbf{y})$ and $\mathbf{r} = \mathbf{x} - \mathbf{y}$. We obtain then

$$A_{ML}(\mathbf{x},\mathbf{y}) = (\omega/\pi)^3 a_{ML}^{-\frac{3}{2}} \times \exp\big(-(\omega/a_{ML})\{[\coth(M\omega\beta) + \coth(L\omega\beta)](R^2 + \tfrac{1}{4}r^2) - (1/N)\coth(\omega\beta) r^2 + [\coth(M\omega\beta) - \coth(L\omega\beta)]\mathbf{R}\cdot\mathbf{r}\}\big), \quad (30)$$

where

$$a_{ML} = \coth(M\omega\beta)\coth(L\omega\beta) - (1/N)\coth(\omega\beta)[\coth(M\omega\beta) + \coth(L\omega\beta)] \quad (31)$$

and

$$B_M(\mathbf{x},\mathbf{y}) = \sum_{j=1}^{M-1} (\omega/\pi)^3 (C_{Mj} S_{Mj})^{-\frac{3}{2}} \times \exp(-\omega R^2/C_{Mj} - \omega r^2/S_{Mj}), \quad (32)$$

where

$$C_{Mj} = \cosh(M\omega\beta - j\omega\beta)\cosh(j\omega\beta)/\sinh(M\omega\beta) - (1/N)\cosh(\omega\beta)$$

and

$$S_{Mj} = 4\sinh(M\omega\beta - j\omega\beta)\sinh(j\omega\beta)/\sinh(M\omega\beta). \quad (33)$$

Inspection of these results indicates that the form of n_2 depends on the position and orientation of the two particles relative to the center-of-mass of the whole system. Typical examples of the shape of the two-particle distribution function are shown in Fig. 5.

A measure of the correlation between two particles is the quantity

$$g_2(\mathbf{x},\mathbf{y}) = n_2(\mathbf{x},\mathbf{y})/N(N-1) - n(\mathbf{x})n(\mathbf{y})/N^2. \quad (34)$$

We would expect that for large $|\mathbf{x} - \mathbf{y}|$ there would be little correlation between the particles, i.e.,

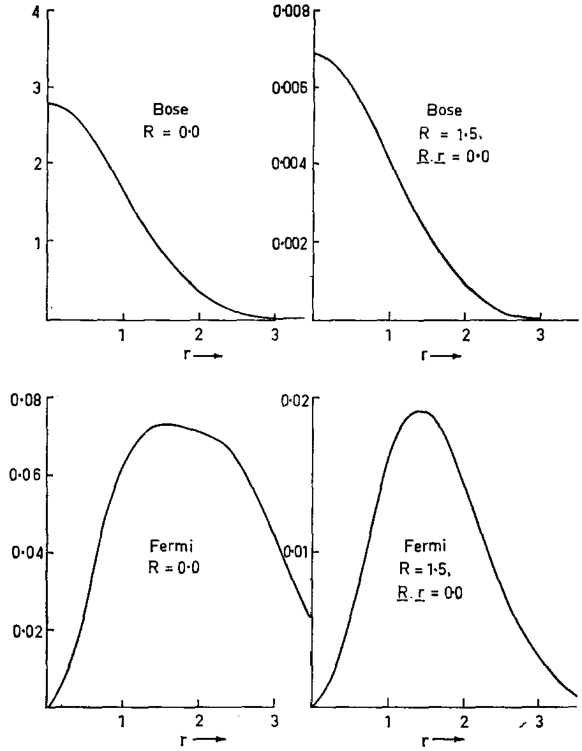

FIG. 5. The two-particle distribution function $n_2(\mathbf{R},\mathbf{r})$ for a system of eight bosons or fermions when the ground state dominates ($\beta = 2.5$) at the center ($R = 0$) and the edge ($R = 1.5$, $\mathbf{R}\cdot\mathbf{r} = 0$) of the system.

$g_2(\mathbf{x},\mathbf{y}) \to 0$; this is verified by explicit calculations. Figure 6 shows the effect of varying β for an eight-fermion system. Note that the range of the correlation is generally less than the diameter of the system and decreases with increasing temperature.

In some circumstances it is useful to know the average pair distribution function defined by

$$n_2(r) = \int n_2(\mathbf{x},\mathbf{y})\, d\mathbf{R}. \quad (35)$$

This quantity coincides with the usual definition of the pair distribution function for a uniform system. Using Eqs. (27) and (30)–(33), we find

$$n_2(r) = \frac{1}{Z_N}\sum_{M=1}^{N-1}\sum_{L=1}^{N-M} Z_{N-M-L} S_M S_L \times \left(\frac{\omega}{\pi[\coth(M\omega\beta) + \coth(L\omega\beta)]}\right)^{\frac{3}{2}} \times \exp\left(\frac{-r^2\omega}{[\coth(M\omega\beta) + \coth(L\omega\beta)]}\right) + \frac{1}{Z_N}\sum_{M=2}^{N} Z_{N-M} S_M \sum_{j=1}^{M-1}\left(\frac{\omega}{\pi S_{Mj}}\right)^{\frac{3}{2}} \exp\left(\frac{-r^2\omega}{S_{Mj}}\right). \quad (36)$$

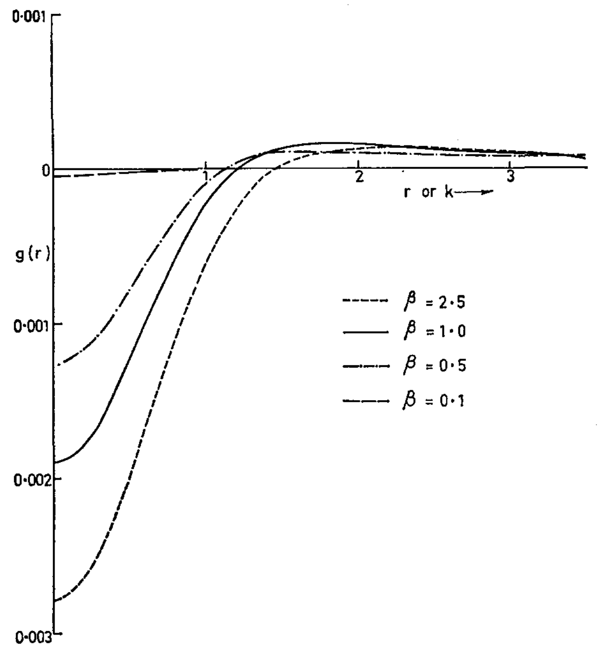

FIG. 6. The two-particle correlation function $g(r)$ for a system of eight fermions at various temperatures. Note the strong negative correlation for small r or k in the ground state.

5. MOMENTUM DISTRIBUTION FUNCTIONS

The momentum distribution functions can be obtained from the momentum space representation of the density matrix $\tilde{\rho}^{(N)}(\mathbf{k}_i \cdots \mathbf{k}_N; \mathbf{k}'_i \cdots \mathbf{k}'_N; \beta)$. This is the double Fourier transform of its representation in configuration space. A direct evaluation of the Fourier transform using the result of Eq. (4) gives

$$\begin{aligned}\tilde{\rho}^{(N)}&(\mathbf{k}_1 \cdots \mathbf{k}_N; \mathbf{k}'_1 \cdots \mathbf{k}'_N; \beta)\\ &= (2\pi)^{-3N} \int \cdots \int \rho^{(N)}(\mathbf{x}_1 \cdots \mathbf{x}'_N; \beta)\\ &\quad \times \exp\left(i \sum_i (\mathbf{k}_i \cdot \mathbf{x}_i - \mathbf{k}'_i \cdot \mathbf{x}'_i)\right) d\mathbf{x}_1 \cdots d\mathbf{x}'_N\\ &= \delta(\mathbf{K} - \mathbf{K}') e^{-\beta K^2} [2\pi\omega \sinh(2\omega\beta)]^{-\frac{3}{2}(N-1)}\\ &\quad \times \exp\left(-\frac{1}{2\omega} \operatorname{csch}(2\omega\beta) \sum_{i=1}^{N} (\mathbf{k}_i - \mathbf{k}'_i)^2\right.\\ &\quad \left. - \frac{1}{2N\omega} \tanh(\omega\beta) \sum_{i<j} (\mathbf{k}_{ij}^2 + \mathbf{k}'^2_{ij})\right), \qquad (37)\end{aligned}$$

where $\mathbf{K} = \sum_i k_i/N$ and $\mathbf{k}_{ij} = \mathbf{k}_i - \mathbf{k}_j$. The resemblance to the form of Eq. (4) is striking. In fact all the results we have derived for the configuration space distribution functions can be used with only minor alterations to obtain the momentum distribution functions.

We define the one-particle momentum distribution function in the zero total momentum frame of reference to be

$$\begin{aligned}\tilde{n}(\mathbf{k}) &= [(4\pi\beta)^{-\frac{3}{2}}/\Omega Z_N]\\ &\quad \times \int \cdots \int \tilde{\rho}^{(N)}_{\text{sym}}(\mathbf{k}_1 \cdots \mathbf{k}_N; \mathbf{k}_1 \cdots \mathbf{k}_N; \beta) \delta(\mathbf{K})\\ &\quad \times \sum_i \delta(\mathbf{k} - \mathbf{k}_i)\, d\mathbf{k}_1 \cdots d\mathbf{k}_N, \qquad (38)\end{aligned}$$

where Z_N is the modified partition function defined by Eq. (6). In terms of $\tilde{\rho}^{(N)}$, Z_N is

$$\begin{aligned}Z_N &= (4\pi\beta)^{-\frac{3}{2}}/\Omega\\ &\quad \times \int \cdots \int \tilde{\rho}^{(N)}_{\text{sym}}(\mathbf{k}_1 \cdots \mathbf{k}_N; \mathbf{k}_1 \cdots \mathbf{k}_N; \beta)\\ &\quad \times \delta(\mathbf{K})\, d\mathbf{k}_1 \cdots d\mathbf{k}_N. \qquad (39)\end{aligned}$$

The volume factor (Ω) arises from the δ function $\delta(\mathbf{K} - \mathbf{K}')$ when $\mathbf{K}$ is set equal to $\mathbf{K}'$. If we then follow through an analysis similar to that of Sec. 3, we find

$$\tilde{n}(\mathbf{k}) = \frac{1}{Z_N} \sum_{M=1}^{N} Z_{N-M} S_M (\pi\kappa_M\omega^2)^{-\frac{3}{2}} \exp\left(\frac{-k^2}{\kappa_M\omega^2}\right). \qquad (40)$$

By comparison with Eq. (18) we see that the shape of the momentum distribution function is exactly that of the configuration space distribution function shown in Figs. 1–3 with the horizontal scale measured in units of (k/ω) and the vertical scale altered by a factor of ω^3.

In a similar manner we can show that the form of the two-particle momentum distribution function is the same as that of the two-particle configuration space distribution function so that Fig. 6 can be interpreted as showing the momentum correlation between two particles. This illustrates in a graphic fashion the phenomena that two fermions have a strong negative correlation when they have similar momenta but are almost uncorrelated when their momenta differ by a large amount. One could speculate that this phenomena would apply to the momentum correlations of particles in a nucleus.

ACKNOWLEDGMENTS

The author is grateful to Professor A. A. Broyles and Professor I. E. McCarthy for useful discussions and advice.

APPENDIX A

Consider the matrix

$$R = NtI^{(N)} - tB^{(N)} + c(A^{(M_1)} \oplus \cdots \oplus A^{(M_r)}), \qquad (A1)$$

where we have let $t = \omega \tanh(\omega\beta)/N$ and $c = \omega \operatorname{csch}(2\omega\beta)/2$. One can diagonalize $A^{(M)}$ by an orthogonal transformation using the matrix $U^{(M)}$

whose elements are

$$U_{jk}^{(M)} = M^{-\frac{1}{2}}[\cos(2\pi jk/M) + \sin(2\pi jk/M)], \quad j, k = 1, \cdots M, \quad (A2)$$

giving the eigenvalues

$$a_j^{(M)} = 2[1 - \cos(2\pi j/M)], \quad j = 1, \cdots M. \quad (A3)$$

This same unitary transformation diagonalizes $B^{(M)}$ giving the eigenvalues

$$b_1^{(M)} = b_2^{(M)} = b_{M-1}^{(M)} = 0; \quad b_M^{(M)} = M. \quad (A4)$$

If we therefore apply a unitary transformation using $U = U^{(M_1)} \oplus \cdots \oplus U^{(M_r)}$ to R, we obtain

$$NtI^{(N)} - t\tilde{B}^{(N)} + c[\tilde{A}^{(M_1)} \oplus \cdots \oplus \tilde{A}^{(M_r)}], \quad (A5)$$

where $\tilde{A}_{jk}^{(M)} = a_j^{(M)}\delta_{jk}$ and $\tilde{B}^{(N)}$ is broken up into blocks of size $M_s \times M_u$, $s, u = 1, \cdots, r$, whose elements are zero except for the lower right-hand corner element in each block which has a value $(M_sM_u)^{\frac{1}{2}}$. Since $a_M^{(M)} = 0$ for all M, the matrix $\tilde{B}^{(N)}$ can now be diagonalized by a transformation which leaves the matrices $\tilde{A}^{(M)}$ unchanged, to give the eigenvalues

$$\tilde{b}_1^{(N)} = \cdots = \tilde{b}_{N-1}^{(N)} = 0, \quad \tilde{b}_N^{(N)} = \sum_{S=1}^{r} M_s = N. \quad (A6)$$

This transformation can be defined by an orthogonal matrix V which has the same general structure as $\tilde{B}^{(N)}$ with the elements

$$V_{us} = (M_{s+1}^{\frac{1}{2}})(M_u^{\frac{1}{2}}) \Big/ \left(\sum_{t=1}^{s+1} M_t\right)^{\frac{1}{2}} \left(\sum_{t=1}^{s} M_t\right)^{\frac{1}{2}}, \quad r > s \geq u,$$

$$V_{s+1\,s} = -\left(\sum_{t=1}^{s} M_t\right)^{\frac{1}{2}} \Big/ \left(\sum_{t=1}^{s+1} M_t\right)^{\frac{1}{2}}, \quad r > s, \quad (A7)$$

$$V_{sr} = M_s^{\frac{1}{2}} \Big/ \left(\sum_{t=1}^{r} M_t\right)^{\frac{1}{2}},$$

$$V_{us} = 0, \quad u > s + 1,$$

at the lower right-hand corner of each $M_s \times M_u$ block, 1 on the remaining diagonal elements, and 0 elsewhere. The matrix R is therefore diagonalized by the product $UV = W$ and has the eigenvalues $\lambda_j = Nt + ca_i^{(M_s)}$, $i = 1, \cdots, M_s$, $s = 1, \cdots, r$, except that $\lambda_N = 0$. An additional result that we require is

$$\prod_{j=1}^{N-1} \lambda_j^{-\frac{1}{2}} = [2\sinh(\omega\beta)]^3[2\sinh(2\omega\beta)/\omega]^{\frac{1}{2}(N-1)} \times \prod_{s=1}^{r} [2\sinh(M_s\omega\beta)]^{-3}, \quad (A8)$$

which has been shown before.[1]

APPENDIX B

The matrix K, defined by Eq. (12), can be calculated in two steps. We use the fact that $W = UV$ and first calculate

$$\tilde{K}_{jl} = \sum_{k=1}^{N-1} V_{jk}V_{lk}\lambda_k^{-1}.$$

This transformation affects only the elements on the lower right-hand corner of each block. Then a canonical transformation of this matrix, using U, gives

$$K = U^+\tilde{K}U = (C^{(M_1)} \oplus C^{(M_2)} \oplus \cdots \oplus C^{(M_r)}) - B^{(N)}/N^2t, \quad (B1)$$

where $B^{(N)}$ is, as before, an $N \times N$ matrix with every element unity and

$$C_{jk}^{(M)} = \frac{1}{M}\sum_{l=1}^{M} \frac{\cos[2\pi(j-k)l/M]}{Nt + 2c[1 - \cos(2\pi l/M)]} = \frac{\sinh(2\omega\beta)}{\omega M}\sum_{l=1}^{M} \frac{\cos[2\pi(j-k)l/M]}{[\cosh(2\omega\beta) - \cos(2\pi l/M)]}. \quad (B2)$$

This sum can be evaluated by using a finite modification of the Poisson sum formula,[2] i.e.,

$$(1/M)\sum_{l=1}^{M} \cos(2\pi\, ln/M)F(2\pi j/M) = \sum_{l=-\infty}^{\infty} a_{|lM+n|}, \quad (B3)$$

where

$$a_n = \frac{1}{2\pi}\int_0^{2\pi} F(\theta)\cos n\theta\, d\theta. \quad (B4)$$

Applying this to Eq. (B2), we find

$$C_{jk}^{(M)} = \frac{1}{\omega}\sum_{l=-\infty}^{\infty} \exp(-|lM + |j-k||\,2\omega\beta) = \frac{\cosh(M\omega\beta - 2\omega\beta\,|j-k|)}{\omega\sinh(M\omega\beta)}, \quad (B5)$$

which is the result quoted in Eq. (14). Note that as $M \to \infty$

$$C_{jk}^{(M)} \to \frac{1}{\omega}\exp(-2\omega\beta\,|j-k|). \quad (B6)$$

* Work supported by the National Science Foundation and the Australian Research Grants Committee.

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[1] R. G. Storer, Phys. Rev. Letters 24, 5 (1970).
[2] P. B. Abraham and G. H. Weiss, J. Math. Phys. 4, 1115 (1963).

New Tool for Scattering Studies*

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(Received 4 January 1971)

In potential scattering, from the transformation kernel, a function $\mathcal{K}(\rho)$ is constructed whose Bessel transforms are the Jost functions. $\mathcal{K}(\rho)$ contains the whole information on the potential $V(\rho)$. There is a one-to-one correspondence between the two functions, and they are related, in both senses of this correspondence, through integral equations. Since the relation between $\mathcal{K}(\rho)$ and the phase shift is very direct, it is a useful tool for all analyses of the relations between the information contained in the dynamics of the problem (viz., the potential) and the measurable information (viz., the phase shifts). This tool will be applied to the inverse problem in forthcoming publications. Besides, the derivation of $\mathcal{K}(\rho)$ makes clear that a similar study can be done in all cases to which the Gel'fand–Levitan scheme applies and therefore in most scattering problems in physics.

1. INTRODUCTION

We study the scattering of a particle obeying the Schrödinger equation with a spherically symmetric potential, at an energy $E = \hbar^2k^2/2m$, m being the reduced mass and k the linear momentum. The direct problem deals with obtaining the scattering amplitude, or, equally, the phase shifts, from the potential, which contains all the dynamical information on the problem. This is done by deriving the wavefunctions and then looking at their asymptotic behavior. In but one partial wave, known as a function of r, the whole dynamical information is contained, and we can straightforwardly derive the potential from it. However, the step of taking the asymptotic behavior corresponds to *an irreversible loss* of information. This makes the inverse problem, viz., the construction of the potentials from the phase shifts, very difficult. In such a problem, one looks for the interaction potential inside a given class of functions. Even in the most restrictive cases, this class is an infinite set, and only an infinite set of phase shifts can contain a significant part of the required information. The trouble is that the set of all the phase shifts at a given energy, or the (continuous) set of the phase shifts at a fixed angular momentum, for all positive energies, do not always contain enough information. On the other hand, the set of all scattering amplitudes for all positive energies can correspond to a local potential if and only if very restrictive conditions are fulfilled, conditions which are broadly unknown. The giving of a set of scattering amplitudes, or a set of phase shifts, has therefore a good chance to lead us to an improperly posed problem, either due to lack of information or due to inconsistency of the information. By looking at the methods currently used for solving the direct and the inverse problem (especially at fixed energy), it has appeared to the author that one of the reasons why the amount of information contained in a set of scattering results is so difficult to analyze is that even the formal way of going from it to the interaction, or conversely, is very devious, and involves in general many intermediate steps.

The aim of this paper is to provide a much more direct formal way of handling these problems. It is nearly hopeless to try to obtain such a method for the largest class of potentials, say, $\bar{\mathcal{T}}$, for which phase shifts are well defined. $\bar{\mathcal{T}}$ not only includes, for instance, the class $\mathcal{V}$ of potentials[1] for which (a being a length)

$$\int_0^a \rho^{1-\epsilon}\,|V(\rho)|\,d\rho + \int_a^\infty |V(\rho)|\,d\rho < \infty, \qquad (1.1)$$

but it also contains the infinitely repulsive potentials whose singularities are very cumbersome. We have limited our study to a class $\mathcal{V}_0$ of potentials which is dense in $\mathcal{V}$ for the norm (1.1) and conveniently chosen. For a scattering problem at a given energy, the key of our method is the existence of a function of r, *independent of l*, which generates all the physical Jost functions through linear (Bessel) transforms and which generates the fundamental transformation kernel through a single integral equation. This function can conversely be obtained from the potential through an integral equation. It should be emphasized that this approach is not confined to the Schrödinger equation and can be introduced with slight modifications in most scattering problems. An analogous method can, moreover, be devised, *mutatis mutandis*, for the scattering problem at fixed angular momentum, but since the information problem there is in much better shape and since other methods there give comparable result, it offers a comparatively smaller interest than the one described in the present paper.

Let us now state the results obtained in this paper, and, for this, let us first introduce some notation.

For the lth partial wave, we write down the Schrödinger equation as

$$[D_0(r) - r^2V(r)]\Phi_l(r) = l(l+1)\Phi_l(r), \quad (1.2)$$

where

$$D_0(r) = r^2\left(\frac{\partial^2}{\partial r^2} + k^2\right). \quad (1.3)$$

The classes of functions of which V can be an element have to be defined. Let j and k be two given numbers; we define $\mathcal{E}_{jk}$ as the (linear) space of all the functions f continuous on $R^+ (= [0, \infty))$, such that, for any of them, two positive numbers ϵ, ϵ' and a nonnegative number C do exist, for which the following inequalities are fulfilled:

$$|r^j f(r)| \leq C(r/a)^\epsilon, \quad |r^k f(r)| \leq C(a/r)^{\epsilon'}. \quad (1.4)$$

We also use the space $\mathcal{E}_{\overline{jk}}$, obtained from $\mathcal{E}_{jk}$ by allowing ϵ and ϵ' to be equal to zero. Let us now define $\mathcal{E}^n_{jk}$ as the set of all the functions having continuous derivatives up to order n on R^+, such that the product by r^n of the nth derivative is an element of $\mathcal{E}_{jk}$. We deal in most cases with $\mathcal{E}^3_{1,3}$, which we simply call $\mathcal{E}$. Clearly $\mathcal{E}^n_{jk}$ is contained in $\mathcal{E}_{jk}$, and $\mathcal{E}_{jk}$ is contained in $\mathcal{E}_{j'k'}$ for $j' \geq j$ and $k' \leq k$. Clearly all these spaces, for $j \leq 2$ and $k \geq 1$, can be normed with (1.1) and are dense in $\mathcal{V}$ for the metric induced by this norm.

For a potential V of class $\mathcal{V}$, let us now introduce the Regge–Newton[1,2] transformation kernel $K(r, r')$, which generates the regular solutions $\Phi_l(r)$ of (1.2) for all l, through the formula

$$\Phi_l(r) = u_l(r) - \int_0^r K(r, \rho)u_l(\rho)\rho^{-2}\, d\rho, \quad (1.5)$$

where

$$u_l(r) = (\tfrac{1}{2}\pi kr)^{\frac{1}{2}} J_{l+\frac{1}{2}}(kr). \quad (1.6)$$

The normalization of $\Phi_l(r)$ is such that it has the behavior of $u_l(r)$ as r goes to zero. According to Loeffel,[1] for any potential in $\mathcal{V}$ and any finite a, $K(r, r')$ does exist and belongs to $L_2(0, a)$.

Throughout this paper, we call any function of r and r' a *negligible function* of r and r', and denote it with the subindex N—for instance, $f_N(r, r')$—if

(a) $f_N(r, r')$ goes to zero for any fixed r' as r goes to ∞,

(b) $\int_0^r |f_N(r, r')|\, r'^{-1}(1 + kr')^{-1}\, dr'$ goes to zero as r goes to ∞.

Now, our first result is the following:

Lemma 1: For any potential V in $\mathcal{E}$, the transformation kernel $K(r, r')$ and its derivative with respect to r can be put into the following form:

$$K(r, r') = \cos(kr)\, k(r') + \sin(kr)\, \bar{k}(r') + P_N(r, r'), \quad (1.7)$$

$$k^{-1}\frac{\partial}{\partial r}K(r, r') = -\sin(kr)\, k(r') + \cos(kr)\, \bar{k}(r') + Q_N(r, r'), \quad (1.8)$$

where P_N and Q_N are negligible functions.

This Lemma is proven in Sec. 5.

Let us now differentiate both sides of (1.5), so as to write their Wronskian successively with $\cos(kr)$ and $\sin(kr)$, and then let us take $r \to \infty$. From (1.7) and (1.8), we get

$$\int_0^\infty \frac{\bar{k}(\rho)}{\rho}\frac{u_l(\rho)}{\rho}\, d\rho = \cos(\tfrac{1}{2}l\pi) - A_l\cos(\tfrac{1}{2}l\pi - \delta_l), \quad (1.9)$$

$$\int_0^\infty \frac{k(\rho)}{\rho}\frac{u_l(\rho)}{\rho}\, d\rho = -\sin(\tfrac{1}{2}l\pi) + A_l\sin(\tfrac{1}{2}l\pi - \delta_l), \quad (1.10)$$

where A_l and δ_l have been defined, as usual, through the asymptotic behavior of $\Phi_l(r)$:

$$\Phi_l(r) = A_l\sin(kr - \tfrac{1}{2}l\pi + \delta_l) + o(1), \quad r \to \infty. \quad (1.11)$$

Introducing now the complex function $\mathcal{K}(\rho) = \rho^{-1}[\bar{k}(\rho) + ik(\rho)]$, we can rewrite (1.9) and (1.10) in the compact form

$$\int_0^\infty \mathcal{K}(\rho)u_l(\rho)\rho^{-1}\, d\rho = \exp(-\tfrac{1}{2}il\pi) - A_l\exp(-\tfrac{1}{2}il\pi + i\delta_l). \quad (1.12)$$

It is clear from (1.12) that knowing $\mathcal{K}(\rho)$ straightforwardly yields the phase shifts and the scattering amplitude. The function $\mathcal{K}(\rho)$ therefore expresses the *whole structure* of the problem so far as we are concerned with *the scattering at energy E*. Its knowledge as a function of E yields the whole structure of the collision problem. For these reasons, and also because the existence of these functions is not confined to quantum mechanics problems, we shall call it the scattering structure function, or, to be brief, the s.s. function, whereas $\rho^{-1}\bar{k}(\rho)$ and $\rho^{-1}k(\rho)$ will be for us the real s.s. functions.

Let us now introduce the notation

$$w = [(r - r')^2 + 4rr'u^2]^{\frac{1}{2}}, \tag{1.13}$$

$$G(r, r', u) = \cos(kw) - \cos[k(r - r')], \tag{1.14}$$

$$K_0^0(r, r') = (2\pi k)^{-1}\int_0^1 G(r, r', u)u^{-2}\,du \int_0^\infty V(s)s\,ds, \tag{1.15}$$

$$K_2(r, r') = K(r, r') - K_0^0(r, r'), \tag{1.16}$$

$$V_0 = \int_0^\infty \rho V(\rho)\,d\rho. \tag{1.17}$$

We prove in Sec. 5 that $K_0^0(r, r')$ can be written as (1.7) and (1.8), and its real s.s. functions are given by

$$\bar{k}_0(r') = (\pi k)^{-1}V_0 \times \left(\sin(kr') - kr'\int_0^\pi \cos(kr'\cos\theta) \times \cos(\tfrac{1}{2}\theta)\,d\theta\right), \tag{1.18}$$

$$k_0(r') = (\pi k)^{-1}V_0 kr'\int_0^\pi \sin(kr'\cos\theta)\cos(\tfrac{1}{2}\theta)\,d\theta. \tag{1.19}$$

The s.s. functions of $K(r, r')$ clearly are the sum of the s.s. functions of $K_0^0(r, r')$ and $K_2(r, r')$; we label the latter with the index 2. Now, our second result, proved in Sec. 5, is the following.

Lemma 2: The s.s. functions $\rho^{-1}k_2(\rho)$ and $\rho^{-1}\bar{k}_2(\rho)$ are bounded functions of $L_2(0, \infty)$, going to zero as ρ^{-1} for $\rho \to \infty$.

This property does not hold for the functions $\rho^{-1}k_0(\rho)$ and $\rho^{-1}\bar{k}_0(\rho)$, which go to zero only as $\rho^{-\frac{1}{2}}$. However, Lemma 2 and Formulas (1.18) and (1.19) give a fairly well-defined mathematical frame, in which the inverse problem at fixed energy can be thoroughly studied as a moment problem. Moreover, the fact that these functions belong to L_2 can be very useful for an approximation theory in the inverse problem at fixed energy. These studies are the subject of two forthcoming papers.[3]

We now have to give a way of constructing the s.s. functions from the potential and a way of constructing the potential from the s.s. functions. The s.s. functions can be readily obtained from the asymptotic behavior of $K(r, r')$, through Eqs. (1.7) and (1.8). On the other hand, $V(r)$ is readily obtained from $K(r, r)$ through the formula

$$V(r) = -2r^{-1}\frac{d}{dr}[r^{-1}K(r, r)]. \tag{1.20}$$

We therefore attain our goal if we give ways of obtaining $K(r, r')$ from the potential and from the s.s. functions. Besides, the transformation kernel readily yields all the wavefunctions, Jost functions, etc., in short, all the information on the problem. The two following lemmas, respectively proved in Secs. 2 and 6, completely fulfill our purpose.

Lemma 3: Given a potential $V(\rho)$ in $\mathcal{V}$, the corresponding transformation kernel $K(r, r')$ is the (unique) solution of the (Volterra-type) integral equation

$$K(r, r') = K_0(r, r') \pm \iint_{D^\pm} N_1(r, r', \rho, \rho') \times \rho^2 V(\rho)K(\rho, \rho')\,d\rho\,d\rho', \tag{1.21}$$

where

$$K_0(r, r') = -\tfrac{1}{2}(rr')^{\frac{1}{2}} \times \int_0^{(rr')^{\frac{1}{2}}} J_0[k(r - r')(1 - \rho^2/rr')^{\frac{1}{2}}]\rho V(\rho)\,d\rho, \tag{1.22}$$

$$N_1(r, r', \rho, \rho') = \tfrac{1}{2}(rr')^{\frac{1}{2}}(\rho\rho')^{-\frac{3}{2}} \times J_0\left(k\left[(rr' - \rho\rho')\left(\frac{r}{r'} + \frac{r'}{r} - \frac{\rho}{\rho'} - \frac{\rho'}{\rho}\right)\right]^{\frac{1}{2}}\right) \tag{1.23}$$

and the $\pm$ signs respectively correspond to the cases $r \geq r'$ and $r \leq r'$. The domains D^+ and D^- are bounded by the straight lines $\rho' = \rho$ and $\rho' = \rho r'/r$ and the hyperbola $\rho\rho' = rr'$ (see Figs. 1 and 2).

(a)

(b)

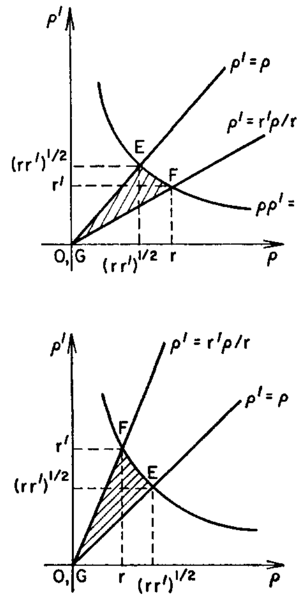

FIG. 1. (a) The integration domain D^+ in the (ρ, ρ') plane. (b) The integration domain D^- in the (ρ, ρ') plane.

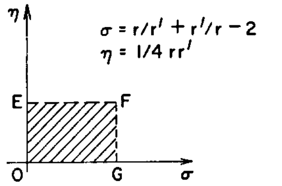

FIG. 2. The integration domains D^+ and D^- in the (σ, η) plane.

Lemma 4: Given the first moment V_0 [$= \int_0^\infty \rho V(\rho)\, d\rho$] of the potential and given two bounded functions of $L_2(0, \infty)$, $\rho^{-1}k_2(\rho)$ and $\rho^{-1}\bar{k}_2(\rho)$, going to zero faster than $\rho^{-\frac{1}{2}-\epsilon}$ as ρ goes to ∞, the transformation kernel $K(r, r')$ can be obtained as the sum of two functions, the first one, $K_0^0(r, r')$, being obtained from V_0 through (1.15) and the second one, $K_2(r, r')$, being obtained as the solution of the integro-differential equation

$$K_2(r, r') = K_2^0(r, r') - 2\iint_G N_1(\rho, \rho'; r, r') \times K(\rho, \rho') \frac{d}{d\rho} [\rho^{-1}K(\rho, \rho)]\rho\, d\rho\, d\rho', \tag{1.24}$$

where we set for convenience

$$K(\rho, \rho') = K_2(\rho, \rho') + K_0^0(\rho, \rho'), \tag{1.25}$$

$$K_2^0(r, r') = (2\pi)^{-\frac{1}{2}}(krr')^{\frac{1}{2}} \times \int_0^\infty \{k_2(\rho) \sin [\varphi(\rho)] - \bar{k}_2(\rho) \cos [\varphi(\rho)]\}\rho^{-\frac{3}{2}}\, d\rho, \tag{1.26}$$

$$\varphi(\rho) = \tfrac{1}{2}k\rho[(rr'/\rho^2) + (r/r') + (r'/r)] + \tfrac{1}{4}\pi. \tag{1.27}$$

For practical purposes, other equations can be obtained for relating the s.s. functions to the potential, using the Gel'fand–Levitan symmetric function as an intermediate step; they will be given in a forthcoming paper.[3] It is clear that Lemmas 1, 2, 3, and 4 enable us to describe the scattering problem completely, at a given energy, by a single function. Since this function can readily generate the scattering amplitude and can be easily related to the potential, it should be a useful tool in potential scattering. Apart from their applications to the inverse problem, which we have already quoted, the s.s. functions can be used for yielding information on the other tools used in scattering problems. As an example, the Jost functions can readily be derived from them. Actually, for any positive value of λ, we can write, instead of (1.5), the formula

$$\Psi_\lambda(r, k) = v_\lambda(r) - \int_0^r K(r, \rho)v_\lambda(\rho)\rho^{-2}\, d\rho, \tag{1.28}$$

where

$$v_\lambda(r) = (\tfrac{1}{2}\pi kr)^{\frac{1}{2}}J_\lambda(kr). \tag{1.29}$$

$K(r, \rho)$ depends also on k, and $\Psi_\lambda(r, k)$ is the regular solution of the Schrödinger equation (1.2) for $l = (\lambda - \frac{1}{2})$. The Jost function is given by[4]

$$f(\lambda, k) = \lim e^{-ikr}[\Psi_\lambda'(r, k) + ik\Psi_\lambda(r, k)] \tag{1.30}$$

and is therefore equal to

$$f(\lambda, k) = k\left(e^{-\frac{1}{2}i(\lambda-\frac{1}{2})\pi} - \int_0^\infty \mathcal{K}(\rho)v_\lambda(\rho)\rho^{-1}\, d\rho\right). \tag{1.31}$$

Integral Representations of the s.s. Functions

The formulas (5.14), (5.15), (5.26), (5.27), (5.29), and (5.30) and (1.18) and (1.19) give integral representations for the s.s. functions, valid for any potential in $\mathcal{E}$. The integral representations (5.29) and (5.30), which correspond to the contribution of $K(r, r') - K_0(r, r')$, are elegant. Unfortunately, their validity seems to require the double differentiability of $V(r)$ and the bounds defined for its derivatives in class $\mathcal{E}$. It is interesting to notice that we can obtain an integral representation of the s.s. function from Eq. (1.21), which is valid for any potential of $\mathcal{E}_{13}$. The derivation is done in Sec. 7. The results are the following:

$$\begin{aligned}\mathcal{K}(r') = {} & -(2\pi k)^{-\frac{1}{2}}r'^{\frac{1}{2}} \\ & \times \Big(\int_0^\infty \exp\{-ik[r' + \tfrac{1}{2}\rho^2(r')^{-1}] \\ & + \tfrac{1}{4}i\pi\}\rho V(\rho)\, d\rho \\ & - \int_0^1 u^{-1}\, du \int_0^\infty \rho V(\rho)k(\rho, \rho u) \\ & \times \exp\{-\tfrac{1}{2}ik[\rho^2u(r')^{-1} + ur' \\ & + r'u^{-1}] + \tfrac{1}{4}i\pi\}\, d\rho\Big),\end{aligned} \tag{1.32}$$

where

$$k(\rho, \rho') = (\rho\rho')^{-\frac{1}{2}}K(\rho, \rho'). \tag{1.33}$$

For proving that (1.32) actually forms the scattering functions of the potential V, we only need in Sec. 7 the assumptions defining the class $\mathcal{E}_{13}$. We are therefore led to the following.

Generalization of the Results to the Class $\mathcal{E}_{13}$

(1') Lemma 1 is valid in $\mathcal{E}_{13}$.

(2') Lemma 2 holds in $\mathcal{E}_{13}$ with a weaker asymptotic behavior of $\mathcal{K}_1(r')$ [see (7.52)].

(3') Lemma 3 is valid, actually, in larger classes then $\mathcal{E}_{13}$.

(4') Lemma 4 has been proved by using bounds derived in $\mathcal{E}$.

However, it is possible to extend it to $\mathcal{E}_{13}$, insofar as the integral equation (1.26) has a solution, since obviously $K_2^0(r, r')$ can be derived from s.s. functions fulfilling condition (2′) above. The conditions of existence and uniqueness of solutions of the nonlinear integral equation (1.26) are not studied in the present paper. However, since the existence proof of solutions of integral equations usually involve bounds on kernels and their integrals only, one may expect that going from $\mathcal{E}$ to $\mathcal{E}_{13}$ does not change these conditions.

Generalization to Other Scattering Problems

The generalization to the potential scattering problem at a fixed value of l, E being the variable parameter, is straightforward. Obviously all the results will have a formal analog in this problem. Generalizations are more generally possible in any case where a transformation kernel can be obtained which generates all the wavefunctions (or their analogs). In other words, the generalization is possible in any case where the Gel'fand–Levitan method applies. This encompasses all the scattering problems involving Sturm–Liouville equations, viz., almost all the linear scattering problems in physics.

2. DERIVATION OF THE TRANSFORMATION KERNEL FROM THE POTENTIAL

Let us be given a potential V in $\mathcal{E}_{21}$. We use this class of potentials rather than $\mathcal{V}$ for avoiding mathematical intricacies. It would be easy to generalize our results. We know[1] that the transformation kernel $K(r, r')$ is a solution of the partial differential equation

$$\left[\rho^2\left(\frac{\partial^2}{\partial\rho^2} + k^2\right) - \rho'^2\left(\frac{\partial^2}{\partial\rho'^2} + k^2\right)\right]K(\rho, \rho') = \rho^2V(\rho)K(\rho, \rho') \quad (2.1)$$

with the boundary conditions

$$[(\rho\rho')^{-\frac{1}{2}}K(\rho, \rho')]_{\rho=0} = [(\rho\rho')^{-\frac{1}{2}}K(\rho, \rho')]_{\rho'=0} = 0, \quad (2.2)$$

$$K(\rho, \rho) = -\tfrac{1}{2}\rho\int_0^\rho \tau V(\tau)\, d\tau. \quad (2.3)$$

Let us now introduce the variables

$$\sigma = (\rho/\rho') + (\rho'/\rho) - 2, \quad \eta = \tfrac{1}{4}\rho\rho' \quad (2.4)$$

and the functions

$$v(\sigma, \eta) = \eta^{-\frac{1}{2}}K(\rho, \rho'), \quad (2.5)$$

$$h(\sigma, \eta) = (\rho^2 - \rho'^2)^{-1}\rho^2V(\rho)v(\sigma, \eta); \quad (2.6)$$

we obtain the normal form of the hyperbolic equation (2.1),

$$\frac{\partial^2}{\partial\sigma\partial\eta} v(\sigma, \eta) + k^2v(\sigma, \eta) = h(\sigma, \eta), \quad (2.7)$$

with the boundary conditions

$$v(\sigma, 0) = 0, \quad (2.8)$$

$$v(0, \eta) = \eta^{-\frac{1}{2}}K(2\eta^{\frac{1}{2}}, 2\eta^{\frac{1}{2}}). \quad (2.9)$$

Let now F be the point whose coordinates are

$$\sigma = s, \quad \eta = y. \quad (2.10)$$

Let E and G be the projections of F on the η axis and on the σ axis, and let D be the square $OEFG$ (Fig. 2). Following Riemann's method,[5] we obtain

$$\begin{aligned} v(s, y) = {} & v(0, y)S(0, y, s, y) \\ & - \int_0^y v(0, \eta)\frac{\partial}{\partial\eta} S(0, \eta, s, y)\, d\eta \\ & + \int_0^s S(\sigma, 0, s, y)\frac{\partial}{\partial\sigma} v(\sigma, 0)\, d\sigma \\ & + \iint_D S(\sigma, \eta, s, y)h(\sigma, \eta)\, d\sigma\, d\eta, \end{aligned} \quad (2.11)$$

where $S(\sigma, \eta, s, y)$ is the Riemann function, defined by the differential system

$$\left(\frac{\partial^2}{\partial\sigma\partial\eta} + k^2\right)S(\sigma, \eta, s, y) = 0,$$

$$\frac{\partial}{\partial\sigma} S(\sigma, y, s, y) = 0, \quad (2.12)$$

$$\frac{\partial}{\partial\eta} S(s, \eta, s, y) = 0, \quad S(s, y, s, y) = 1,$$

and is therefore equal[5] to

$$S(\sigma, \eta, s, y) = J_0(2k[(\sigma - s)(\eta - y)]^{\frac{1}{2}}). \quad (2.13)$$

Let us now introduce the notation

$$x = (r/r') + (r'/r) = s + 2, \quad (2.14)$$

$$y = \tfrac{1}{4}rr', \quad (2.15)$$

$$\bar{K}(x, y) = K(r, r'), \quad (2.16)$$

$$g(x, y) = y^{\frac{1}{2}}h(s, y). \quad (2.17)$$

We can write (2.12) in the form

$$\begin{aligned} \bar{K}(x, y) = {} & \bar{K}(2, y) \\ & - y^{\frac{1}{2}}\int_0^y\left(\frac{\partial}{\partial\eta} S(0, \eta, x - 2, y)\right)\bar{K}(2, \eta)\eta^{-\frac{1}{2}}\, d\eta \\ & + y^{\frac{1}{2}}\int_2^x d\xi \\ & \times \int_0^y S(\xi - 2, \eta, x - 2, y)g(\xi, \eta)\eta^{-\frac{1}{2}}\, d\eta. \end{aligned} \quad (2.18)$$

Now, the continuous mapping $(x, y) \to (r, r')$ is expressed by different formulas, according to the sign of $r - r'$:

for $r \geq r'$

$$\begin{cases} r = y^{\frac{1}{2}}[(x+2)^{\frac{1}{2}} + (x-2)^{\frac{1}{2}}] \\ r' = y^{\frac{1}{2}}[(x+2)^{\frac{1}{2}} - (x-2)^{\frac{1}{2}}] \end{cases}; \quad (2.19)$$

for $r \leq r'$

$$\begin{cases} r = y^{\frac{1}{2}}[(x+2)^{\frac{1}{2}} - (x-2)^{\frac{1}{2}}] \\ r' = y^{\frac{1}{2}}[(x+2)^{\frac{1}{2}} + (x-2)^{\frac{1}{2}}] \end{cases}. \quad (2.20)$$

Let ρ, ρ' be the image of ξ, η in the above mapping. Using it in (2.18) yields the relation

$$\begin{aligned} K(r, r') &= K[(rr')^{\frac{1}{2}}, (rr')^{\frac{1}{2}}] + I(r, r') - \tfrac{1}{2}(rr')^{\frac{1}{2}} \\ &\times \int_0^{\frac{1}{4}rr'} \left\{\frac{\partial}{\partial\eta} J_0\left(2k\left[\left(\frac{r}{r'} + \frac{r'}{r} - 2\right)(\tfrac{1}{4}rr' - \eta)\right]^{\frac{1}{2}}\right)\right\} \\ &\times K(2\eta^{\frac{1}{2}}, 2\eta^{\frac{1}{2}})\eta^{-\frac{1}{2}}\, d\eta. \end{aligned} \quad (2.21)$$

In (2.21), we set, for convenience,

$$\begin{aligned} I(r, r') = \pm(rr')^{\frac{1}{2}} &\times \iint_{D^\pm} J_0\left(k\left[\left(\frac{r}{r'} + \frac{r'}{r} - \frac{\rho}{\rho'} - \frac{\rho'}{\rho}\right)\right.\right. \\ &\times \left.\left.(rr' - \rho\rho')\right]^{\frac{1}{2}}\right)(\rho\rho')^{-\frac{3}{2}} f(\rho, \rho')\, d\rho\, d\rho', \end{aligned} \quad (2.22)$$

where

$$f(\rho, \rho') = \rho^2 V(\rho) K(\rho, \rho'). \quad (2.23)$$

The domains D^+ and D^-, and the signs $+$ and $-$, are to be used, respectively, for $r \geq r'$ and for $r \leq r'$ (Fig. 1). The integral equation (1.21) follows readily from (2.21) by integrating by parts the third term in the right-hand side. It should be noticed that the special properties (2.23) of $f(\rho, \rho')$ have not been used in the derivation. The formula (2.21) actually holds if any integrable function $f(\rho, \rho')$ is the right-hand side of (2.1).

Let us now introduce the functions

$$M(r, r') = r'^2\left(\frac{\partial^2}{\partial r'^2} + k^2\right) K(r, r'), \quad (2.24)$$

$$\begin{aligned} N(r, r') &= r^2\left(\frac{\partial^2}{\partial r^2} + k^2\right) K(r, r') \\ &= M(r, r') + r^2 V(r) K(r, r'). \end{aligned} \quad (2.25)$$

Clearly, $M(r, r')$ is a solution of (2.1). From (2.2) and (2.21), elementary but tedious differentiations enable one to show that if $r^{2-\epsilon}V(r)$ and $r^{3-\epsilon}V'(r)$ remain bounded as $r \to 0$, then $(rr')^{-\frac{1}{2}-\frac{1}{2}\epsilon} M(r, r')$ remains bounded when either of r and r' goes to zero, the other variable keeping constant. $M(r, r')$ therefore fulfills the boundary condition (2.2).

Once again, tedious operations enable us to get $M(r, r)$ from (2.3) and (2.21). The result is

$$M(r, r) = M^+(r, r) + M^-(r, r), \quad (2.26)$$

where

$$M^+(r, r) = -\tfrac{1}{4}k^2 r \int_0^r V(\rho)\rho(r^2 + \rho^2)\, d\rho, \quad (2.27)$$

$$\begin{aligned} M^-(r, r) = \tfrac{1}{8}r \int_0^r \rho^3 V^2(\rho)\, d\rho &+ \tfrac{1}{48}r\left(\int_0^r \rho V(\rho)\, d\rho\right)^3 + \tfrac{1}{8}r \int_0^r \rho V(\rho)\, d\rho \\ &- \tfrac{1}{4}r^3 V(r) - \tfrac{1}{8}r^4 V'(r) \\ &+ \tfrac{1}{8}r^3 V(r) \int_0^r \rho V(\rho)\, d\rho. \end{aligned} \quad (2.28)$$

Setting now

$$\begin{aligned} M_0(r, r') &= M[(rr')^{\frac{1}{2}}, (rr')^{\frac{1}{2}}] \\ &- \tfrac{1}{2}(rr')^{\frac{1}{2}} \int_0^{\frac{1}{4}rr'} M(2\eta^{\frac{1}{2}}, 2\eta^{\frac{1}{2}}) \\ &\times \left\{\frac{\partial}{\partial\eta} J_0\left(2k\left[\left(\frac{r}{r'} + \frac{r'}{r} - 2\right)(\tfrac{1}{4}rr' - \eta)\right]^{\frac{1}{2}}\right)\right\}\eta^{-\frac{1}{2}}\, d\eta, \end{aligned} \quad (2.29)$$

we get, as we did for (2.21),

$$\begin{aligned} M(r, r') &= M_0(r, r') \\ &\pm \iint_{D^\pm} N_1(r, r', \rho, \rho')\rho^2 V(\rho) M(\rho, \rho')\, d\rho\, d\rho'. \end{aligned} \quad (2.30)$$

These results will be of use in Sec. 4 below.

3. PROPERTIES OF $K_0(r, r')$ AND RELATED QUANTITIES

In the following, $V(r)$ belongs to the set $\mathcal{E}$ defined in Sec. 1, and its norm $\|V\|$ is given by (1.1). Some notations are to be introduced for convenience: C is meant as a general nonnegative constant; **V** a general nonnegative constant proportional to $\|V\|$ and therefore going to zero as $\|V\|$ goes to zero; **W** a general nonnegative constant going to zero as $\|V\|$ goes to zero but not necessarily proportional to $\|V\|$; and **V*** and **W*** the products of **V** and **W** by a function of E, finite for $E > 0$, and going to 1 for $E \to \infty$.

Bounds for $K_0(r, r')$

From (1.22), since $V \in \mathcal{E}$, using for J_0 the upper bound 1 yields the absolute upper bounds

$$|K_0(r, r')| < \begin{cases} \mathbf{V}(rr')^{\frac{1}{2}} \\ \mathbf{V}(rr')^{\frac{1}{2}}(rr'/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}} \\ \mathbf{V}(rr')^{\frac{1}{2}}(rr'/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}[1 + (rr'/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}]^{-1}. \end{cases} \quad (3.1)$$

Using for $J_0(z)$ the absolute bound $Cz^{-\frac{1}{2}}$ yields from (1.22) the inequalities

$$|K_0(r, r')| \le \tfrac{1}{2}(rr')^{\frac{1}{2}}\int_0^{(rr')^{\frac{1}{2}}} |V(s)|\, s\left[k\,|r - r'|\left(1 - \frac{s^2}{rr'}\right)^{\frac{1}{2}}\right]^{-\frac{1}{2}} ds \tag{3.2}$$

$$\le C(rr')^{\frac{1}{2}}[k\,|r - r'|]^{-\frac{1}{2}}\left[\int_0^{\frac{1}{2}(rr')^{\frac{1}{2}}} |V(s)|\, ds + V\int_{\frac{1}{2}(rr')^{\frac{1}{2}}}^{(rr')^{\frac{1}{2}}} s^{-1}\left(1 - \frac{s^2}{rr'}\right)^{-\frac{1}{4}} ds\right], \tag{3.3}$$

and therefore

$$|K_0(r, r')| \le \mathbf{V}(rr')^{\frac{1}{2}}[1 + k\,|r - r'|]^{-\frac{1}{2}}. \tag{3.4}$$

Bounds for $M_0(r, r')$

Using (2.27) and (2.28) inside (2.29), we can split $M_0(r, r')$ into two terms, $M_0^+(r, r')$ and $M_0^-(r, r')$. Integrating by parts (2.29) yields

$$M_0^{\pm}(r, r') = \tfrac{1}{2}(rr')^{\frac{1}{2}}\int_0^{(rr')^{\frac{1}{2}}} J_0\left(k\,|r - r'|\left(1 - \frac{s^2}{rr'}\right)^{\frac{1}{2}}\right) \times \frac{d}{ds}[2s^{-1}M^{\pm}(s, s)]\, ds. \tag{3.5}$$

Now, from (2.28), it is clear that $r^{-1}(d/dr)[2r^{-1}M^-(r, r)]$ belongs to $\mathcal{E}$. Since this quantity is used in (3.5) like $V(r)$ in (3.2), we can readily write

$$|M_0^-(r, r')| \le \begin{cases} \mathbf{W}(rr')^{\frac{1}{2}} \\ \mathbf{W}(rr')^{\frac{1}{2}}(rr'/a^2)^{\frac{1}{2}(1+\epsilon)} \\ \mathbf{W}[k\,|r - r'|]^{-\frac{1}{2}}(rr')^{\frac{1}{2}} \end{cases}. \tag{3.6}$$

Integrating by parts twice, we find that the formula for $M_0^+(r, r')$ yields

$$M_0^+(r, r') = -\tfrac{1}{2}k^2(rr')^{\frac{3}{2}}\int_0^{(rr')^{\frac{1}{2}}} J_1\left(k\,|r - r'|\left(1 - \frac{s^2}{rr'}\right)^{\frac{1}{2}}\right) \times [k\,|r - r'|]^{-1}\left(1 - \frac{s^2}{rr'}\right)^{\frac{1}{2}}[3V(s) + sV'(s)]s\, ds. \tag{3.7}$$

From (3.7) we easily derive the inequalities

$$|M_0^+(r, r')| \le \begin{cases} \mathbf{V}k^2(rr')^{\frac{3}{2}} \\ \mathbf{V}k^2(rr')^{\frac{3}{2}}(rr'/a^2)^{\frac{1}{2}(1+\epsilon)} \\ \mathbf{V}k^2(rr')^{\frac{3}{2}}\,|k(r - r')|^{-\frac{3}{2}} \end{cases}. \tag{3.8}$$

Further Properties of $K_0(r, r')$

In (1.22), we can substitute the formula[6]

$$J_0\left[k(r - r')\left(1 - \frac{s^2}{rr'}\right)^{\frac{1}{2}}\right]\Upsilon\left(1 - \frac{s^2}{rr'}\right) = \frac{2}{\pi}\int_0^\infty \{\cos[(k^2(r - r')^2 + z^2)^{\frac{1}{2}}] - \cos[k(r - r')]\}\frac{d}{dz}\left[z^{-1}\cos\left(\frac{sz}{(rr')^{\frac{1}{2}}}\right)\right] dz, \tag{3.9}$$

where $\Upsilon(x)$ is the Heaviside step function. More exactly, we break the right-hand side of (3.9) into two members,

$$\frac{2}{\pi}\int_0^A \{\ \}\, dz + \frac{2}{\pi}\, I(s, r, r', A), \tag{3.10}$$

then substitute (3.10) in (1.22), which yields

$$K_0(r, r') = K_0^A(r, r') + R_0^A(r, r'), \tag{3.11}$$

and show separately that both $|R_0^A(r, r')|$ and the integral $\int_0^\infty |R_0^A(r, r')|^2 r'^{-2}\, dr'$ go to zero when $[1 + k^2(r - r')^2]^{-1}[1 + 2k(rr')^{\frac{1}{2}}]^{-1}A$ goes to infinity. Actually, this can be shown by elementary but tedious operations and majorations, which we do not reproduce here. Clearly, it follows from the result that, as long as we are interested in evaluations of $K_0(r, r')$ or of its square integral, we can use $K_0^A(r, r')$, take advantage of the finiteness of A for proving the validity of changing integrations, and then make A go to infinity. We can therefore forget A, except when justification is required. Once (3.9) has been substituted in (1.22), let us use instead of z the variable t equal to $[2k(rr')^{\frac{1}{2}}]^{-1}z$, and integrate twice by parts with respect to the s variable. We get

$$K_0(r, r') = K_0^0(r, r') + K_3(r, r') + K_4(r, r'), \tag{3.12}$$

where

$$2\pi k K_0^0(r, r') = -\int_0^1 G(r, r', t)t^{-2}\, dt \times \int_0^\infty \left(s\frac{d}{ds}\frac{1}{s}\frac{d}{ds}\right)[s^3V(s)]\, ds, \tag{3.13}$$

$$4\pi k^2 K_3(r, r') = -\int_0^1 G(r, r', t)t^{-2}\, dt \times \int_0^\infty \left(\frac{\sin(2kst)}{t} - 2ks\right)\left(\frac{d}{ds}\frac{1}{s}\frac{d}{ds}[s^3V(s)]\right) ds, \tag{3.14}$$

$$4\pi k^2 K_4(r, r') = -\int_1^\infty G(r, r', t)t^{-2}\, dt \times \int_0^\infty \frac{\sin(2kst)}{t}\left(\frac{d}{ds}\frac{1}{s}\frac{d}{ds}[s^3V(s)]\right) ds. \tag{3.15}$$

The formula (3.14) can also be written in the form (1.15), or, via well-known formulas,[7] as

$$K_0^0(r, r') = -(\pi k)^{-1} V_0 \left(v_0(r) v_0(r') + 2 \sum_{l=1}^{\infty} v_l(r) v_l(r') \right), \tag{3.16}$$

where the v_l have been defined by (1.29). Let us introduce the notation

$$K_0^1(r, r') = K_3(r, r') + K_4(r, r'), \tag{3.17}$$

$$\Phi_3(u) = -\frac{u^{-2}}{4\pi k^2} \int_0^\infty \left(\frac{\sin 2ksu}{u} - 2ks \right) \times \left(\frac{d}{ds} s^{-1} \frac{d}{ds} [s^3 V(s)] \right) ds, \tag{3.18}$$

$$\Phi_4(u) = -\frac{u^{-2}}{4\pi k^2} \int_0^\infty \frac{\sin 2ksu}{u} \left(\frac{d}{ds} s^{-1} \frac{d}{ds} [s^3 V(s)] \right) ds. \tag{3.19}$$

From (3.18), integrating once by parts, we readily derive the inequality

$$|\Phi_3(u)| < C \int_0^\infty \frac{ks}{1 + k^2 s^2 u^2} |s^3 V'(s) + 3s^2 V(s)| \, ds, \tag{3.20}$$

and, from the properties of $\mathcal{E}$, it follows that $|\Phi_3(u)|$ is integrable on $(0, 1)$. From (3.19), integrating once by parts, we readily derive the inequality

$$|\Phi_4(u)| < \tfrac{1}{2} k^{-3} u^{-4} \times \left| \int_0^\infty (1 - \cos 2ksu) \left(\frac{d^2}{ds^2} s^{-1} \frac{d}{ds} s^3 V(s) \right) ds \right|, \tag{3.21}$$

from which the properties of $\mathcal{E}$ enable us to get

$$|\Phi_4(u)| < \mathrm{V} k^{-1} (ka)^{-1-\epsilon} u^{-3-\epsilon}. \tag{3.22}$$

Let us now notice that, replacing, in (1.14), the difference of cosines by a product of sines, we get

$$|G(r, r', u)| < \begin{cases} 2 \\ 2krr' \, |r - r'|^{-1} \, u^2 \end{cases}. \tag{3.23}$$

Using now (3.18)–(3.23) in (3.14) and (3.15), we obtain the following bounds:

$$|K_3(r, r')| < \begin{cases} \mathrm{V}a \\ \mathrm{V}karr' \, |r - r'|^{-1} \end{cases}, \tag{3.24}$$

$$|K_4(r, r')| < \begin{cases} \mathrm{V}k^{-1}(ka)^{-1-\epsilon} \\ \mathrm{V}(ka)^{-1-\epsilon} rr' \, |r - r'|^{-1} \end{cases}. \tag{3.25}$$

$K_0^0(r, r')$ cannot be handled in the same way. Fortunately, it is a series of Bessel functions of a kind we have previously[8] studied, so that we can write down its bounds:

$$|K_0^0(r, r')| < \begin{cases} \mathrm{V}r(1 + kr) \\ \mathrm{V}r'(1 + kr') \end{cases}, \tag{3.26}$$

$$|K_0^0(r, r') - \pi^{-1} V_0 (rr')^{\frac{1}{2}} J_0(k(r - r'))| \le C. \tag{3.27}$$

Bounds for the Derivatives

So as to get bounds for the derivatives of $K_3(r, r')$ and $K_4(r, r')$, we need bounds for, say, $(\partial/\partial r) G(r, r', u)$. We therefore write

$$k^{-1} \frac{\partial}{\partial r} G(r, r', u) = 2 \sin [k(r - r' - w)] \cos [k(r - r' + w)] + \left(1 - \frac{\dot{w}}{2w}\right) \sin kw, \tag{3.28}$$

where

$$\tfrac{1}{2} \dot{w} = r - r' + 2r'u^2. \tag{3.29}$$

Case 1 ($u^2 \le 1$): It is easy to prove that $(\frac{1}{2}\dot{w})^2$ is smaller than w^2, so that $|1 - \dot{w}/2w|$ is smaller than 2. Besides, writing w as $|r - r'| \, [1 + 4rr'u^2/(r - r')^2]^{\frac{1}{2}}$ and using elementary inequalities for $r' \le r$, we get

$$(r - r') \le (r - r') \left(1 + \frac{2rr'u^2}{(r - r')^2} - \frac{2r^2 r'^2 u^4}{(r - r')^4} \right) \le w \le (r - r') \left(1 + \frac{2rr'u^2}{(r - r')^2} \right). \tag{3.30}$$

Since $|1 - \dot{w}/2w|$ is clearly smaller than $|r - r'| \times |\frac{1}{2}\dot{w} - w|$, using (3.30), we can easily show that, for $r' \le \frac{1}{2} r$, $|1 - \dot{w}/2w|$ is smaller than $(4r'/r)u^2$. We summarize this result in the following formula:

$$|(\sin kw)(1 - \dot{w}/2w)| < \begin{cases} 2 \\ 4(r'/r)u^2 & \text{for } r' \le \frac{1}{2} r, \\ Ckr' & \text{for } r' \le \frac{1}{2} r \end{cases} \tag{3.31}$$

where the last inequality has been obtained by using the bound $2kr$ for kw. Besides, the formula (3.30) enables us to get a bound for $|r - r' - w|$, which yields

$$|2 \sin [k(r - r' - w)] \cos [k(r - r' + w)]| \le \begin{cases} 2 \\ Ckr'u^2 & \text{for } r' \le \frac{1}{2} r. \\ Ckr' & \text{for } r' \le \frac{1}{2} r \end{cases} \tag{3.32}$$

From (3.14), (3.20), (3.31), and (3.32), we get

$$\left| \frac{\partial}{\partial r} [K_3(r, r')] \right| < \begin{cases} \mathrm{V}ka \\ \mathrm{V}k^2 r'a & \text{for } r' \le \frac{1}{2} r \end{cases}. \tag{3.33}$$

Case 2 ($u^2 \geq 1$): Again, we have to evaluate (3.27). Clearly, $\dot{w}$ is positive. Therefore, $|1 - \frac{1}{2}\dot{w}/w|$ is smaller than $|1 - (\frac{1}{2}\dot{w}/w)^2|$, so that

$$|1 - \tfrac{1}{2}\dot{w}/w| < C(r'/r)u^2. \tag{3.34}$$

On the other hand, for $r \leq r'$, $2r'u^2$ is a majorant of $|\frac{1}{2}\dot{w}|$ and r' is a minorant of w. We can therefore write

$$|\sin kw|\,|1 - \tfrac{1}{2}\dot{w}/w| < \begin{cases} C(r'/r)u^2 \\ Cu^2 \\ Ckr'u^2 \quad \text{for} \quad r' \leq \frac{1}{2}r \end{cases} \tag{3.35}$$

Besides, the following relations obviously hold for $r' \leq r$:

$$\begin{aligned} |r - r' - w| &= \left|\frac{r^2 - (r' + w)^2}{r + r' + w}\right| \\ &< \left|2r' + \frac{4rr'}{r + r'}(u^2 - 1)\right| \\ &< Cr'u^2. \end{aligned} \tag{3.36}$$

Thus

$$|2 \sin [k(r - r' - w)] \cos [k(r - r' + w)]| < \begin{cases} 2 \\ Ckr'u^2 \quad \text{for} \quad r' \leq r \end{cases}. \tag{3.37}$$

From (3.15), (3.22), (3.35), and (3.36), we get

$$\left|\frac{\partial}{\partial r} K_4(r, r')\right| \leq \begin{cases} \mathbf{V}(ka)^{-1-\epsilon} \\ \mathbf{V}(ka)^{-1-\epsilon}kr' \quad \text{for} \quad r' \leq \frac{1}{2}r \end{cases}. \tag{3.38}$$

Relations (3.24), (3.25) and (3.37), (3.38) can obviously be gathered as follows:

$$|K_0^1(r, r')| \leq \begin{cases} \mathbf{V}^*a \\ \mathbf{V}^*karr'\,|r - r'|^{-1} \end{cases}, \tag{3.39}$$

$$\left|\frac{\partial}{\partial r} K_0^1(r, r')\right| \leq \begin{cases} \mathbf{V}^*ka \\ \mathbf{V}^*k^2r'a \quad \text{for} \quad r' \leq \frac{1}{2}r \end{cases}. \tag{3.40}$$

Owing to the symmetry of $G(r, r', t)$, we have also

$$\left|\frac{\partial}{\partial r'} K_0^1(r, r')\right| \leq \begin{cases} \mathbf{V}^*ka \\ \mathbf{V}^*k^2ra \quad \text{for} \quad r \leq \frac{1}{2}r' \end{cases}. \tag{3.41}$$

4. BOUNDS FOR $K(r, r')$ AND RELATED QUANTITIES

Let us for convenience introduce the notation

$$k(r, r') = (rr')^{-\frac{1}{2}}K(r, r'), \quad k_0(r, r') = (rr')^{-\frac{1}{2}}K_0(r, r'), \tag{4.1}$$

$$\begin{aligned} n(r, r', \rho, \rho') &= \tfrac{1}{2}\rho V(\rho)(\rho')^{-1} \\ &\times J_0\left(k\left[(rr' - \rho\rho')\left(\frac{r}{r'} + \frac{r'}{r} - \frac{\rho}{\rho'} - \frac{\rho'}{\rho}\right)\right]^{\frac{1}{2}}\right) \end{aligned} \tag{4.2}$$

$$\theta = r^{-1}r'. \tag{4.3}$$

Bounds of $|k(r, r')|$ for $r' \leq r$

For $r' \leq r$, (1.21) can be rewritten as

$$\begin{aligned} k(r, r\theta) &= k_0(r, r\theta) \\ &+ \int_\theta^1 du \int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho n(r, r\theta, \rho, \rho u)k(\rho, \rho u)\, d\rho. \end{aligned} \tag{4.4}$$

Let us look for an iteration series:

$$k(r, r\theta) = \sum_{n=0}^{\infty} k_n(r, r\theta), \tag{4.5}$$

$$k_n(r, r\theta) = \int_\theta^1 du \int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho n(r, r\theta, \rho, \rho u)k_{n-1}(\rho, \rho u)\, d\rho. \tag{4.6}$$

For proving the convergence of (4.5) and getting an absolute bound of its sum, we replace the kernel and the free term in (4.4) by absolute majorants and solve the equation thus obtained. Each of the iterated terms of the solution of this "majorant" equation clearly is an absolute bound for the corresponding term in (4.5). Let us first use the absolute majorants

$$|k_0(r, r\theta)| < \mathbf{V}, \tag{4.7}$$

$$|n(r, r\theta, \rho, \rho u)| \leq \tfrac{1}{2}u^{-1}\,|V(\rho)| \tag{4.8}$$

and extend the u integration up to ∞. We thus obtain the majorant equation

$$\bar{k}(r, r\theta) = \mathbf{V} + \tfrac{1}{2}\int_0^r \rho\,|V(\rho)|\, d\rho \int_\theta^{r^2\theta/\rho^2} \bar{k}(\rho, \rho u)u^{-1}\, du, \tag{4.9}$$

whose solution[9] is equal to $\mathbf{V}k(r)$, with $k(r)$ being equal to

$$k(r) = 1 + \int_0^r \rho\,|V(\rho)| \log\left(\frac{r}{\rho}\right)k(\rho)\, d\rho. \tag{4.10}$$

A majorant equation for (4.10) is in turn

$$\begin{aligned} K(r) &= 1 + \int_0^r \rho\,|V(\rho)| \log\left(\frac{a}{\rho}\right)K(\rho)\, d\rho, \quad r \leq a, \\ K(r) &= K(a) + \log\left(\frac{r}{a}\right)\int_0^r \rho\,|V(\rho)|\, K(\rho)\, d\rho, \quad r \geq a, \end{aligned} \tag{4.11}$$

whose solution is

$$K(r) = \exp\left[\int_0^r \rho\,|V(\rho)| \log\left(\frac{a}{\rho}\right) d\rho\right], \quad r \leq a, \tag{4.12}$$

$$= \chi(r) + \left[\log\left(\frac{r}{a}\right)\right]\int_a^r t(\rho) \exp\left(\int_\rho^r w(\tau)\, d\tau\right) d\rho, \quad r \geq a, \tag{4.13}$$

where

$$\chi(r) = K(a) + [\log(r/a)]\int_0^a \rho\,|V(\rho)|\, K(\rho)\, d\rho, \tag{4.14}$$

$$w(r) = r\,|V(r)| \log(r/a), \tag{4.15}$$

$$t(r) = r\,|V(r)|\,\chi(r). \tag{4.16}$$

With the assumptions defining $\mathcal{E}$, $w(r)$ and $t(r)$ belong to $L_1(a, \infty)$, so that

$$|k(r, r\theta)| \le \mathbf{W}[1 + \log(1 + r/a)]. \quad (4.17)$$

Starting now from (3.1) leads us to the majorant equation

$$\bar{k}(r, r\theta) = \mathbf{V}\frac{(r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}{1 + (r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}} + \tfrac{1}{2}\int_0^r \rho\,|V(\rho)|\,d\rho\int_\theta^{r^2\theta/\rho^2}\bar{k}(\rho, \rho u)\frac{du}{u}. \quad (4.18)$$

Trying an iteration series for solving (4.18), let us assume that one of the iterated terms can be bounded as follows:

$$\bar{k}_n(r, r\theta) \le \frac{(r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}{1 + (r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}\bar{k}_n(r). \quad (4.19)$$

Then the following term is bounded by

$$\bar{k}_{n+1}(r, r\theta) \le 2(1 + \epsilon)^{-1}\int_0^r \rho\,|V(\rho)|\,\bar{k}_n(\rho) \times \log\left(\frac{1 + (r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}{1 + (\rho^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}\right)d\rho. \quad (4.20)$$

Using now the following inequality, valid for any nonnegative x, with $0 < s \le 1$,

$$\log[(1 + x)/(1 + sx)] \le [x/(1 + x)]\log(1/s), \quad (4.21)$$

we get

$$\bar{k}_{n+1}(r, r\theta) \le \frac{2(r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}{1 + (r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}} \times \int_0^r \rho\,|V(\rho)|\log(r/\rho)\bar{k}_n(\rho)\,d\rho. \quad (4.22)$$

Now, since (4.19) is valid for $n = 0$ and $k_0(r) = \mathbf{V}$, according to (3.1), it is valid for the $(n + 1)$th-order provided that $\bar{k}_n(r)$ is the nth iterated term of the solution of the equation

$$\bar{k}(r) = \mathbf{V} + 2\int_0^r \rho\,|V(\rho)|\log\left(\frac{r}{\rho}\right)\bar{k}(\rho)\,d\rho. \quad (4.23)$$

Equation (4.23) can be studied like (4.10) and yields

$$|k(r, r\theta| \le \mathbf{W}\frac{(r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}[1 + \log(1 + r/a)]. \quad (4.24)$$

The above bounds do not depend on the energy. Let us now use for n the majorant

$$|n(r, r\theta, \rho, \rho u)| \le Ck^{-\frac{1}{2}}u^{-1}\,|V(\rho)|\,(r^2\theta - \rho^2 u)^{-\frac{1}{2}} \times (\theta^{-1} - u^{-1})^{-\frac{1}{4}}(1 - \theta u)^{-\frac{1}{4}}, \quad (4.25)$$

and let us look for a majorant of $|k(r, r\theta) - k_0(r, r\theta)|$, substituting (4.25) for n and (4.24) for k in (4.4). We obtain the following integral:

$$Ck^{-\frac{1}{2}}\int_\theta^1\left(\frac{u}{\theta} - 1\right)^{-\frac{1}{4}}(1 - \theta u)^{-1}u^{-1}\,du \times \int_0^{(r^2\theta/u)^{\frac{1}{2}}}\rho\,|V(\rho)|\left(\frac{r^2\theta}{u} - \rho^2\right)^{-\frac{1}{2}} \times \frac{(\rho^2u/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (\rho^2u/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}\left[1 + \log\left(1 + \frac{\rho}{a}\right)\right]d\rho. \quad (4.26)$$

Replacing the function of ρ^2u/a^2 by an upper bound and using the Schwarz inequality leads us to the majorant

$$\mathbf{W}(ka)^{-\frac{1}{2}}\int_\theta^1(u/\theta - 1)^{-\frac{1}{4}}(1 - \theta u)^{-1}u^{-1}\,du. \quad (4.27)$$

It is easy to get a constant upper bound for the integral in (4.27), through the intermediate step

$$\int_\theta^1\left(\frac{u}{\theta} - 1\right)^{-\frac{1}{4}}u^{-1}\{1 + [(1 - \theta u)^{-\frac{1}{4}} - 1]\}\,du \le \int_\theta^\infty\left(\frac{u}{\theta} - 1\right)^{-\frac{1}{4}}u^{-1}\,du + \left[\int_\theta^\infty\left(\frac{u}{\theta} - 1\right)^{-\frac{1}{2}}u^{-1}\,du \times \int_0^1 u^{-1}[(1 - u)^{-\frac{1}{4}} - 1]^2\,du\right]^{\frac{1}{2}}. \quad (4.28)$$

We therefore obtain

$$|k(r, r\theta) - k_0(r, r\theta)| < \mathbf{W}(ka)^{-\frac{1}{2}}\frac{(r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}. \quad (4.29)$$

If in (4.26) the ρ integral is split in two parts by the intermediate bound $\frac{1}{2}(r^2\theta/u)^{\frac{1}{2}}$, if $|V(\rho)|$ is bounded by $V\rho^{-1}$ on the lower interval, and if the Schwarz inequality is used for the upper interval, one gets

$$|k(r, r\theta) - k_0(r, r\theta)| \le \mathbf{W}(kr\theta^{\frac{1}{2}})^{-\frac{1}{2}}\frac{(r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}. \quad (4.30)$$

Needless to say, since (4.29) and (4.30) are of the form (4.19), bounds for $|k(r, r\theta) - \sum_0^p k_n(r, r\theta)|$ can be obtained by iteration and are equal to the right-hand side of (4.29) and (4.30), respectively, times a factor $(ka)^{-\frac{1}{2}p}$.

Majorants[10] of $|k(r, r')|$ for $r' \ge r$

(1.21) reduces for $r' \ge r$ to

$$k(r, r\theta) = k_0(r, r\theta) - \int_1^\theta du\int_0^{(r^2\theta/u)^{\frac{1}{2}}}n(r, r\theta, \rho, \rho u)k(\rho, \rho u)\rho\,d\rho. \quad (4.31)$$

The iteration series is now defined by

$$k_{n+1}(r, r\theta) = -\int_1^\theta du \int_0^{(r^2\theta/u)^{\frac{1}{2}}} n(r, r\theta, \rho, \rho u)k_n(\rho, \rho u)\rho\, d\rho \quad (4.32)$$

and

$$|n(r, r\theta, \rho, \rho u)| < Ck^{-\frac{1}{2}}u^{-1}|V(\rho)|(r^2\theta - \rho^2 u)^{-\frac{1}{4}}(\theta - u)^{-\frac{1}{4}}(1 - 1/\theta u)^{-\frac{1}{4}}. \quad (4.33)$$

Assume now that, for a value of n,

$$|k_n(r, r\theta)| \leq A_n B_n(r\theta^{\frac{1}{2}}). \quad (4.34)$$

Inserting (4.34) in (4.32), where each factor should be replaced by its absolute value and $|n|$ by (4.33), we obtain

$$|k_{n+1}(r, r\theta)| \leq \tfrac{1}{2}k^{-\frac{1}{2}}A_n \int_1^\theta u^{-1}(\theta - u)^{-\frac{1}{4}}\left(1 - \frac{1}{\theta u}\right)^{-\frac{1}{4}} du \times \int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho|V(\rho)|(r^2\theta - \rho^2 u)^{-\frac{1}{4}} B_n(\rho u^{\frac{1}{2}})\, d\rho. \quad (4.35)$$

Let β be a positive number. Using twice the Schwarz inequality in the ρ integral yields

$$\left(\int_0^{(r^2\theta/u)^{\frac{1}{2}}} (r^2\theta - \rho^2 u)^{-\frac{1}{2}} d\rho\right)^{\frac{1}{2}} \times \left\{\int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho^5 V^4(\rho)\left[\beta^2 + \log^2\left(\frac{\rho u^{\frac{1}{2}}}{a}\right)\right]\right\}^{\frac{1}{4}} \times \left\{\int_0^{(r^2\theta/u)^{\frac{1}{2}}} B_n^4(\rho u^{\frac{1}{2}})\left[\beta^2 + \log^2\left(\frac{\rho u^{\frac{1}{2}}}{a}\right)\right]^{-1} \rho^{-1}\, d\rho\right\}^{\frac{1}{4}}. \quad (4.36)$$

Owing to the definition of the class, the following numbers are finite:

$$a^2\int_0^\infty \rho^5 V^4(\rho)\, d\rho = 2\beta^{-2}B,$$

$$a^2\int_0^\infty \rho^5 V^4(\rho)\log^2\left(\frac{\rho}{a}\right) d\rho = \tfrac{1}{2}(A - 2B). \quad (4.37)$$

From (4.37) and the inequality

$$[\log(\rho u^{\frac{1}{2}}/a)]^2 \leq 2\log^2(\rho/a) + \tfrac{1}{2}\log^2 u, \quad (4.38)$$

we easily derive

$$|k_{n+1}(r, r\theta)| \leq \mathrm{V}k^{-\frac{1}{2}}A_n \int_1^\theta u^{-1}(\theta - u)^{-\frac{1}{4}}(u - \theta^{-1})^{-\frac{1}{4}} \times (A + B\log^2 u)^{\frac{1}{4}}\, du \times \left(\int_0^{r\theta^{\frac{1}{2}}} B_n^4(x)(\beta^2 + \log^2 x)^{-1}x^{-1}\, dx\right)^{\frac{1}{4}}. \quad (4.39)$$

Replacing now θ^{-1} by 1 and using the Schwarz inequality in the u integral, we obtain

$$|k_{n+1}(r, r\theta)| \leq (ka)^{-\frac{1}{2}}A_n D\left(\int_0^{r\theta^{\frac{1}{2}}} B_n^4(x)(\beta^2 + \log^2 x)^{-1}x^{-1}\, dx\right)^{\frac{1}{4}}, \quad (4.40)$$

where

$$D = \mathrm{V}\left(\int_1^\infty u^{-2}(A + B\log^2 u)^{\frac{1}{2}}\, du\right)^{\frac{1}{2}}. \quad (4.41)$$

Comparing now (4.40) and (4.34), we see that (4.34) is valid for any n if

(1) it is valid for $n = 0$,

(2) $A_n = [(ka)^{-\frac{1}{2}}D]^n$, (4.42)

(3) $B_{n+1}^4(s) = \int_0^s x^{-1}(\beta^2 + \log^2 x)^{-1}B_n^4(x)\, dx.$ (4.43)

$B_n(s)$ is therefore the coefficient of λ^n in the λ powers series expansion of $B(s)$, defined by

$$B(s) = B_0^4(s) + \lambda\int_0^s x^{-1}(\beta^2 + \log^2 x)^{-1}B(x)\, dx. \quad (4.44)$$

Clearly

$$B(s) = B_0^4(s) + \lambda\int_0^s \rho^{-1}(\beta^2 + \log^2\rho)^{-1} \times \exp\left\{\frac{\lambda}{\beta}\left[\tan^{-1}\left(\frac{\log s}{\beta}\right) - \tan^{-1}\left(\frac{\log\rho}{\beta}\right)\right]\right\}B_0^4(\rho)\, d\rho. \quad (4.45)$$

A larger majorant is

$$\bar{B}(s) = B_0^4(s) + \lambda\exp\left(\frac{\pi\lambda}{\beta}\right)\int_0^s B_0^4(\rho)(\beta^2 + \log^2\rho)^{-1}\rho^{-1}\, d\rho. \quad (4.46)$$

Let us now put

$$[A_0(s)]^4 = \int_0^s \rho^{-1}(\beta^2 + \log^2\rho)^{-1}B_0^4(\rho)\, d\rho. \quad (4.47)$$

We obtain

$$B_{n+1}(s) = (n!)^{-\frac{1}{4}}\pi^{\frac{1}{4}n}\beta^{-\frac{1}{4}n}A_0(s). \quad (4.48)$$

From (4.34), (4.42), and (4.48), provided that (4.34) is valid for $k_0(r, r\theta)$, we therefore get

$$|k(r, r\theta) - k_0(r, r\theta)| \leq \mathrm{V}(ka)^{-\frac{1}{2}}A_0(r\theta^{\frac{1}{2}}). \quad (4.49)$$

More generally, if (4.34) holds for $k_{p+1}(r, r\theta)$, it is possible to write

$$\left(k(r, r\theta) - \sum_0^p k_n(r, r\theta)\right) = k_{p+1}(r, r\theta) - \int_1^\theta du\int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho n(r, r\theta, \rho, \rho u) \times \left(k(\rho, \rho u) - \sum_0^p k_n(\rho, \rho u)\right) d\rho \quad (4.50)$$

and study this equation as we did (4.31).

Let us now apply the above results, starting from (3.1), which yield

$$B_0(s) = \mathbf{V}(s/a)^{\epsilon+1}[1 + (s/a)^{\epsilon+1}]^{-1} \tag{4.51}$$

and, with some algebra,

$$A_0(s) = \mathbf{W}(s/a)^{\epsilon+1}[1 + (s/a)^{\epsilon+1}]^{-1}, \tag{4.52}$$

$$|k(r, r\theta)| \leq \mathbf{W}(r\theta^{\frac{1}{2}}/a)^{\epsilon+1}[1 + (r\theta^{\frac{1}{2}}/a)^{\epsilon+1}]^{-1}. \tag{4.53}$$

Bounds for $M(r, r')$

From (3.6) and (3.8), we get for $|M_0(r, r')|$ the upper bound

$$|M_0(r, r')| < \mathbf{W}(1 + k^2rr')(rr')^{\frac{1}{2}} \frac{(rr'/a^2)^{\frac{1}{2}(1+\epsilon)}}{1 + (rr'/a^2)^{\frac{1}{2}(1+\epsilon)}}. \tag{4.54}$$

Since (2.30) is similar to (1.21) and since (4.54) is of the form (4.19) or (4.34), the derivations of (4.29) and (4.49) apply, for $V \in \mathcal{E}$, and yield

$$|M(r, r') - M_0(r, r')| \leq \mathbf{W}(ka)^{-\frac{1}{2}}(1 + k^2rr')(rr')^{\frac{1}{2}} \frac{(rr'/a^2)^{\frac{1}{2}(1+\epsilon)}}{1 + (rr'/a^2)^{\frac{1}{2}(1+\epsilon)}}. \tag{4.55}$$

For getting better bounds, we want to use the trick (4.50). For this, we need to derive $M_1(r, r')$, which is obtained by applying (4.2) to $M_0(r, r')$. We are led to study separately $M_0^+(r, r')$ and $M_0^-(r, r')$. With notations implicitly defined in (4.1), we therefore study $m_1^+(r, r\theta)$ and $m_1^-(r, r\theta)$.

1°$\theta \geq 1$: We have to study the integrals

$$|m_1^+(r, r\theta)| \leq \mathbf{V}k^2\int_1^\theta du\int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho^3\,|V(\rho)|\,[1 + k\rho(u - 1)]^{-\frac{3}{2}}\,d\rho, \tag{4.56}$$

$$|m_1^-(r, r\theta)| \leq \mathbf{V}\int_1^\theta u^{-1}\,du\int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho\,|V(\rho)|\,[k\rho(u - 1)]^{-\frac{1}{2}}\,d\rho, \tag{4.57}$$

where we used (4.8), (3.6), and (3.8). Using now for $[1 + k\rho(u - 1)]^{-\frac{3}{2}}$ the majorant $[k\rho(u - 1)]^{-\frac{3}{2}}$ and using for the upper bound of the ρ integrals, in a first step, the majorant $r^2\theta$ and, in a second step, the majorant $+\infty$, we obtain

$$|m_1^+(r, r\theta)| \leq \mathbf{W}ka\,\frac{(r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}{1 + (r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}, \tag{4.58}$$

$$|m_1^-(r, r\theta)| \leq \mathbf{W}(ka)^{-\frac{1}{2}}\,\frac{(r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}{1 + (r^2\theta/a^2)^{\frac{1}{2}\epsilon+\frac{1}{2}}}. \tag{4.59}$$

From the study done for Eq. (4.31), we easily derive the following inequality, valid for $r' \geq r$:

$$|M(r, r') - M_0(r, r') - M_1(r, r')| \leq \mathbf{W}(rr')^{\frac{1}{2}}(ka)^{\frac{1}{2}} \times [1 + (ka)^{-\frac{3}{2}}]. \tag{4.60}$$

Remark[11]: The inequality (4.58) can be improved for large values of ka, by splitting the u integration interval in (4.56) into two parts, $(1, 1 + \alpha)$ and $(1 + \alpha, \theta)$, with

$$\alpha = \inf\,[(\theta - 1), (ka)^{-1}]. \tag{4.61}$$

In the lower interval, we replace $1 + k\rho(u - 1)$ by 1, in the upper, by $k\rho(u - 1)$. We then obtain, $ka > 1$,

$$|m_1^+(r, r\theta)| < \mathbf{W}(ka)^{\frac{1}{2}}(\theta - 1)^{-\frac{1}{2}}\theta^{\frac{1}{2}}. \tag{4.62}$$

We can gather the results obtained for $\theta \geq 1$ in the following formula:

$$|M(r, r') - M_0(r, r')| < \begin{cases}\mathbf{W}^*(rr')^{\frac{1}{2}}ka \\ \mathbf{W}^*(rr')^{\frac{1}{2}}(ka)^{\frac{1}{2}}[1 + (rr')^{\frac{1}{4}}(r' - r)^{-\frac{1}{2}}]\end{cases}. \tag{4.63}$$

2°$\theta \leq 1$: From (4.25), (3.6), and (3.8), we can write down the following inequalities:

$$|m_1^+(r, r\theta)| \leq \mathbf{V}k^{-\frac{1}{2}}\int_\theta^1 (\theta^{-1} - u^{-1})^{-\frac{1}{2}}(1 - u)^{-\frac{3}{2}}\,du \times \int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho\,|V(\rho)|\,(k\rho)^{\frac{3}{2}}(r^2\theta - \rho^2u)^{-\frac{1}{2}}\,d\rho, \tag{4.64}$$

$$|m_1^-(r, r\theta)| \leq \mathbf{V}k^{-\frac{1}{2}}\int_\theta^1 (\theta^{-1} - u^{-1})^{-\frac{1}{2}}(1 - u)^{-\frac{1}{2}}u^{-1}\,du \times \int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho\,|V(\rho)|\,[r^2\theta - \rho^2u]^{-\frac{1}{2}}\,d\rho. \tag{4.65}$$

Using the Schwarz inequality in (4.65) as we did in (4.26), we readily obtain

$$|m_1^-(r, r\theta)| \leq \mathbf{W}(ka)^{-\frac{1}{2}}\,\frac{(r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}. \tag{4.66}$$

From (4.64) we obtain in the same way

$$\mathbf{V}k^{-\frac{1}{2}}\int_\theta^1 (u/\theta - 1)^{-\frac{1}{2}}(1 - u)^{-\frac{3}{2}}\,du \times \left(\int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho^2V^2(\rho)k^3\rho^3\,d\rho\right)^{\frac{1}{2}} \tag{4.67}$$

and therefore

$$|m_1^+(r, r\theta)| \leq \mathbf{W}ka\,\frac{(r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (r^2\theta/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}. \tag{4.68}$$

The inequality (4.60) is therefore valid for any pair of positive r and r'.

Remark[11]: For improving (4.68) for large values of ka, we can write, instead of (4.64),

$$|m_1^+(r, r\theta)| \le \mathbf{V}k^{-\frac{1}{2}}\int_\theta^1 (\theta^{-1} - u^{-1})^{-\frac{1}{2}}(1-u)^{-\frac{1}{4}}\,du \times \int_0^{(r^2\theta/u)^{\frac{1}{2}}} \rho\,|V(\rho)|\,(r^2\theta - \rho^2 u)^{-\frac{1}{2}} \times k^2\rho^2[1 + k\rho(u-1)]^{-\frac{3}{2}}\,d\rho \quad (4.69)$$

and split the u integration interval by the bound $(1+\theta)/2$. On the lower interval, we can replace $|m_0^+(\rho, \rho u)|$ by $k\rho u(u-1)^{-1}$ and use the Schwarz inequality, which leads to the bound $\mathbf{W}(1-\theta)^{-\frac{1}{2}}\theta^{\frac{1}{2}}(ka)^{\frac{1}{2}}$. On the upper interval, we split the ρ integration interval into two parts, with the boundary $\frac{1}{2}(r^2\theta/u)^{\frac{1}{2}}$, keeping for $m_0^+(r, r\theta)$ the majorant we used in (4.69). On the lower ρ interval, $(r^2\theta - \rho^2 u)^{-\frac{1}{2}}$ remains bounded, proportional to $(r^2\theta)^{-\frac{1}{2}}$. On the upper ρ interval, $\rho^2\,|V(\rho)|$ can be replaced by $\mathbf{V}(\rho/a)^{-\frac{1}{2}}$. In both cases, we again obtain the bound $\mathbf{W}(1-\theta)^{-\frac{1}{2}}\theta^{\frac{1}{2}}(ka)^{\frac{1}{2}}$.

Gathering now the results obtained for $\theta \gtrless 1$, we can write, for any value of r and r',

$$|M(r, r') - M_0(r, r')| \le \begin{cases} \mathbf{W}^*(rr')^{\frac{1}{2}}ka \\ \mathbf{W}^*(rr')^{\frac{1}{2}}(ka)^{\frac{1}{2}}\{1 + (rr')^{\frac{1}{4}}\,|r - r'|^{-\frac{1}{2}}\} \end{cases}, \quad (4.70)$$

$$|M(r, r') - M_0(r, r') - M_1(r, r')| \le \mathbf{W}^*(ka)^{\frac{1}{2}}(rr')^{\frac{1}{2}}, \quad (4.71)$$

and, from (4.29) and (4.49),

$$|K(r, r') - K_0(r, r')| \le \mathbf{W}(ka)^{-\frac{1}{2}}(rr')^{\frac{1}{2}}\frac{(rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}. \quad (4.72)$$

New Bounds of $K(r, r')$

From (2.24), it is easy to derive the formula

$$K(r, r') = \alpha(r)\cos(kr') + \beta(r)\sin(kr') + \int_r^{r'} \frac{\sin k(r'-\rho)}{k}\frac{M(r, \rho)}{\rho^2}\,d\rho. \quad (4.73)$$

$\alpha(r)$ and $\beta(r)$ can be calculated by comparing $K(r, r)$ and $[(\partial/\partial r)K(r, r')]_{r'=r}$ since they can be obtained from (1.21) through elementary and tedious computations, as they are readily obtained from (4.73). The result is

$$K(r, r') = K(r, r)\cos k(r - r') + \eta(r)\sin k(r - r') + \int_r^{r'} \frac{\sin k(r'-\rho)}{k}\frac{M(r, \rho)}{\rho^2}\,d\rho, \quad (4.74)$$

where

$$\eta(r) = \tfrac{1}{4}k^{-1}\{r^2V(r) + k(r, r) + [k(r, r)]^2\}. \quad (4.75)$$

In the same way, from (2.25), we get

$$K(r, r') = K(r', r')\cos k(r' - r) + \zeta(r')\sin k(r' - r) + \int_{r'}^{r} \frac{\sin k(r-\rho)}{k}\frac{N(\rho, r')}{\rho^2}\,d\rho, \quad (4.76)$$

where

$$\zeta(r') = \tfrac{1}{4}k^{-1}\{r'^2V(r') + k(r', r') - [k(r', r')]^2\}. \quad (4.77)$$

Let us now assume for a while that $V(r)$ is replaced in (2.21) by $\lambda V(r)$. Since (2.21) is a Volterra equation, all the iterated series giving either $K(r, r', \lambda)$ or $M(r, r', \lambda)$ or $N(r, r', \lambda)$ are entire functions of λ. They can be twice differentiated with respect to r, or to r'. It follows that the terms in (4.74) and (4.76) which are linear in $V(r)$ are nothing but $K_0(r, r')$. Let us now use, for any quantity, the index L to denote terms which are linear in V. We can write

$$M(r, r') = M_{\mathrm{L}}(r, r') + Q(r, r') \quad (4.78)$$

and, since it follows from (2.25) that the linear part of $N(r, r')$ is the same as for $M(r, r')$,

$$N(r, r') = M_{\mathrm{L}}(r, r') + S(r, r'). \quad (4.79)$$

Bounds for $Q(r, r')$ can be obtained from (3.6) and (4.55); hence

$$|Q(r, r')| \le \mathbf{W}(rr')^{\frac{1}{2}}\frac{(rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}} \times [1 + (ka)^{-\frac{1}{2}}(1 + k^2rr')]. \quad (4.80)$$

One can also use (4.71), (4.58), (4.68), (4.59), (4.66), and (3.6), which yield

$$|Q(r, r')| < \mathbf{W}^*ka(rr')^{\frac{1}{2}}\frac{(rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}. \quad (4.81)$$

From (2.25), (4.81), (3.1), and (4.72) since $|\rho^2V(\rho)|$ is uniformly bounded, we get

$$|S(r, r')| < \mathbf{W}^*ka(rr')^{\frac{1}{2}}\frac{(rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}{1 + (rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}}. \quad (4.82)$$

Separation of the linear and the nonlinear parts in (4.74) and (4.76) yields

$$K(r, r') - K_0(r, r') = \tfrac{1}{4}k^{-1}[k(r, r)]^2\sin[k(r - r')] + k^{-1}\int_r^{r'} \sin k(r'-\rho)Q(r, \rho)\rho^{-2}\,d\rho \quad (4.83)$$

and

$$K(r, r') - K_0(r, r') = -\tfrac{1}{4}k^{-1}[k(r', r')]^2\sin[k(r' - r)] + k^{-1}\int_{r'}^{r} \sin k(r-\rho)S(\rho, r')\rho^{-2}\,d\rho. \quad (4.84)$$

For obtaining upper bounds of $|K(r, r') - K_0(r, r')|$, we use (4.83) for $r' \geq r$ and (4.84) for $r' \leq r$. We replace the sines by their majorant 1, $[k]^2$ by a majorant derived from (1.20) and (4.1), and $|Q(r, \rho)|$ and $|S(\rho, r')|$ by $\mathbf{W}^* ka(rr')^{\frac{1}{2}}$, which follows readily from (4.81) and (4.82). Hence we get, by letting the upper bound of the integral go to ∞,

$$|K(r, r') - K_0(r, r')| \leq a\mathbf{W}^*. \tag{4.85}$$

Replacing the interval (r, r') in (4.83) and (4.84) by $(0, \infty)$ and using (4.81) and (4.82) yields

$$|K(r, r') - K_0(r, r')| \leq \mathbf{W}^* r/(ka), \tag{4.86}$$

$$|K(r, r') - K_0(r, r')| \leq \mathbf{W}^* r'/(ka). \tag{4.87}$$

Bounds for the Derivatives

From (4.83) and (4.84) we readily derive

$$\frac{\partial}{\partial r'}[K(r, r') - K_0(r, r')] = -\tfrac{1}{4}[k(r, r)]^2 \cos[k(r - r')] + \int_r^{r'} \cos k(r' - \rho) Q(r, \rho)\rho^{-2}\, d\rho, \tag{4.88}$$

$$\frac{\partial}{\partial r}[K(r, r') - K_0(r, r')] = \tfrac{1}{4}[k(r', r')]^2 \cos[k(r' - r)] + \int_{r'}^{r} \cos k(r - \rho) S(\rho, r')\rho^{-2}\, d\rho. \tag{4.89}$$

They can be bounded like above. The result is

$$\left.\begin{aligned} &\left|\frac{\partial}{\partial r}[K(r, r') - K_0(r, r')]\right| \\ &\left|\frac{\partial}{\partial r'}[K(r, r') - K_0(r, r')]\right| \end{aligned}\right\} < \mathbf{W}^* ka, \tag{4.90}$$

$$\left|\frac{\partial}{\partial r}[K(r, r') - K_0(r, r')]\right| < \mathbf{W}^* r'/a \quad \text{for} \quad r \geq r', \tag{4.91}$$

$$\left|\frac{\partial}{\partial r'}[K(r, r') - K_0(r, r')]\right| < \mathbf{W}^* r/a \quad \text{for} \quad r' \geq r. \tag{4.92}$$

5. PROOF OF LEMMAS 1 AND 2

We successively prove these lemmas for $K_3(r, r')$, $K_4(r, r')$, $[K(r, r') - K_0(r, r')]$, and $K_0^0(r, r')$.

Proof for $K_3(r, r')$

Since the sine and cosine are uniformly bounded functions, it is sufficient to prove the existence of two functions, $k_3(r')$ and $\bar{k}_3(r')$, and two negligible functions, $R_N^{(3)}(r, r')$ and $\bar{R}_N^{(3)}(r, r')$, such that

$$k_3(r') = \cos(kr) K_3(r, r') - \sin(kr) k^{-1} \frac{\partial}{\partial r} K_3(r, r') + R_N^{(3)}(r, r'), \tag{5.1}$$

$$\bar{k}_3(r') = \sin(kr) K_3(r, r') + \cos(kr) k^{-1} \frac{\partial}{\partial r} K_3(r, r') + \bar{R}_N^{(3)}(r, r'). \tag{5.2}$$

Now, let us introduce the functions

$$R_1^{(3)}(r, r'u) = (1 - \dot{w}/2w) \sin(kw) \cos(kr), \tag{5.3}$$

$$\tfrac{1}{2} R_2^{(3)}(r, r'u) = \sin[\tfrac{1}{2}k(r - r' - w)] \cos[\tfrac{1}{2}k(r + r' - w)] + \sin(kr'u^2) \cos[kr'(1 - u^2)]. \tag{5.4}$$

The two first inequalities in (3.31) obviously hold for $|R_1^{(3)}(r, r')|$. From (3.30), we easily derive the inequalities

$$-\frac{2r'^2u^2}{r - r'} \leq r - r' - w + 2r'u^2 \leq -\frac{2r'^2u^2}{r - r'}\left(1 - \frac{r^2u^2}{(r - r')^2}\right). \tag{5.5}$$

From (5.5) we get, for $r' \leq \frac{1}{2}r$,

$$|r - r' - w + 2r'u^2| \leq C(r'^2/r)u^2 \tag{5.6}$$

and

$$|r + r' - w - 2r'(1 - u^2)| < C(r'^2/r)u^2. \tag{5.7}$$

Referring to (5.4), we see that

$$|R_2^{(3)}(r, r', u)| \leq \begin{cases} C = 4 \\ Ck(r'^2/r)u^2 \quad \text{for} \quad r' \leq \frac{1}{2}r \end{cases}. \tag{5.8}$$

Let us also introduce the functions

$$R_3^{(3)}(r, r', u) = -(1 - \dot{w}/2w) \sin(kr) \sin(kw), \tag{5.9}$$

$$\tfrac{1}{2} R_4^{(3)}(r, r', u) = -\sin[\tfrac{1}{2}k(r + r' - w)] \times \sin[\tfrac{1}{2}k(r - r' - w)] - \sin(kr'u^2) \sin[kr'(1 - u^2)]. \tag{5.10}$$

Therefore, according to (3.31), (5.6), and (5.7),

$$|R_3^{(3)}(r, r', u)| < \begin{cases} C \\ C(r'/r)u^2 \end{cases} \quad \text{for} \quad r' \leq \tfrac{1}{2}r, \tag{5.11}$$

$$|R_4^{(3)}(r, r', u)| < \begin{cases} C \\ Ck(r'^2/r)u^2 \end{cases} \quad \text{for} \quad r' \leq \tfrac{1}{2}r. \tag{5.12}$$

Let us then introduce the notation

$$R_{ij}^{(k)}(r, r', u) = R_i^{(k)}(r, r', u) + R_j^{(k)}(r, r', u) \tag{5.13}$$

and define k_3, $\bar{k}_3$, $R_N^{(3)}$, and $\bar{R}_N^{(3)}$ by the following relations:

$$k_3(r') = 2\int_0^1 \sin(kr'u^2)\sin[kr'(1-u^2)]\Phi_3(u)\,du, \tag{5.14}$$

$$\bar{k}_3(r') = -2\int_0^1 \sin(kr'u^2)\cos[kr'(1-u^2)]\Phi_3(u)\,du, \tag{5.15}$$

$$R_N^{(3)}(r,r') = -\int_0^1 [\sin(kr)R_{2,1}^{(3)}(r,r',u) + \cos(kr)R_{4,3}^{(3)}(r,r',u)]\Phi_3(u)\,du, \tag{5.16}$$

$$\bar{R}_N^{(3)}(r,r') = -\int_0^1 [\cos(kr)R_{2,1}^{(3)}(r,r',u) - \sin(kr)R_{4,3}^{(3)}(r,r',u)]\Phi_3(u)\,du, \tag{5.17}$$

which are consistent with (3.14), (5.1)–(5.10). Since $\Phi_3(u)$, according to (3.20), is integrable on (0, 1), it follows from (3.31), (5.8), (5.11), and (5.12) that

$$|R_N^{(3)}(r,r')| < \begin{cases} C\int_0^1 |\Phi_3(u)|\,du < Ca \\ C\dfrac{r'}{r}(1+kr')\int_0^1 |\Phi_3(u)|\,u^2\,du \quad \text{for} \quad r' \le \tfrac{1}{2}r \end{cases} \tag{5.18}$$

Checking that $R_N^{(3)}(r,r')$ fulfills axioms (a) and (b) of a negligible function is trivial. $R_N^{(3)}(r,r')$ is therefore a negligible function, and similarly $\bar{R}_N^{(3)}(r,r')$. Besides, it readily follows from (5.14) and (5.15) that $r'^{-1}k_3(r')$ and $r'^{-1}\bar{k}_3(r')$ are uniformly bounded functions of r' on $[0,\infty]$, and go to zero like r'^{-1} as r' goes to infinity. They therefore belong to $L_2(0,\infty)$.

Proof for $K_4(r,r')$

The derivation which has been done for $K_3(r,r')$ can be reproduced, except for the following modifications:

(a) $|1 - \frac{1}{2}\dot{w}/w|$ is now bounded by (3.35), so that we get

$$|R_1^{(4)}(r,r',u)| < \begin{cases} Cu^2 \\ C(r'/r)u^2 \end{cases}, \tag{5.19}$$

$$|R_3^{(4)}(r,r',u)| < \begin{cases} Cu^2 \\ C(r'/r)u^2 \end{cases}. \tag{5.20}$$

(b) Let us put

$$R = r + r' - w - 2r'(1-u^2). \tag{5.21}$$

The following relations are easy to prove (for $t' \le r$):

$$R = \left(\frac{4r'^2}{r+r'+w} + 2\frac{w^2-(r+r')^2}{[w+r+r']^2}r'\right)(u^2-1), \tag{5.22}$$

$$\frac{w^2-(r+r')^2}{(w+r+r')^2} = \frac{4rr'(u^2-1)}{(r+r')^2+2(r+r')w+w^2} < \frac{2rr'(u^2-1)}{(r+r')^2+2rr'(u^2-1)}, \tag{5.23}$$

and therefore

$$R < (4r'^2/r)u^2 + 2r'^2u^4/(r+2r'u^2). \tag{5.24}$$

Defining $R_4^{(4)}(r,r',u)$ as the continuation of $R_4^{(3)}(r,r',u)$ for $u^2 \ge 1$, we obtain from (5.24)

$$|R_4^{(4)}(r,r',u)| \le \begin{cases} C = 4 \\ Ck\{(4r'^2/r)u^2 + [2r'^2u^2/(r+2r'u^2)]u^2\} \end{cases}, \quad r' \le r. \tag{5.25}$$

A similar inequality holds for $|R_2^{(4)}(r,r',u)|$. Use of these bounds and of formulas (3.15) and (3.22) leads us to the formulas

$$k_4(r') = 2\int_1^\infty \sin(kr'u^2)\sin[kr'(1-u^2)]\Phi_4(u)\,du, \tag{5.26}$$

$$\bar{k}_4(r') = -2\int_1^\infty \sin(kr'u^2)\cos[kr'(1-u^2)]\Phi_4(u)\,du, \tag{5.27}$$

the inequality

$$|R_N^{(4)}(r,r')| < k^{-1}(ka)^{-1-\epsilon}\begin{cases} C \quad \text{(uniformly)} \\ C(r'/r) + kC(r'^2/r) \\ \quad + kCr'(r'/r)^{\frac{1}{2}\epsilon} \quad \text{for} \quad r' \le r, \end{cases} \tag{5.28}$$

and a similar inequality for $\bar{R}_N^{(4)}(r,r')$. It is a matter of simple algebra to show on (5.28) that $R_N^{(4)}(r,r')$ and $\bar{R}_N^{(4)}(r,r')$ are negligible functions. On the other hand, the majoration of $|\Phi_4(u)|$ by $Cu^{-3-\epsilon}$ in (3.22) enables us to show readily that $|r'^{-1}k_4(r')|$ is uniformly bounded and goes to zero like r'^{-1} as r' goes to infinity and that the same property is true for $\bar{k}_4(r')$.

Proof for $K(r,r') - K_0(r,r')$

We use the label 1 for denoting the quantities related to $K(r,r') - K_0(r,r')$. Referring to (4.84) and (4.89) and comparing with (1.7) and (1.8), we can readily write down

$$k_1(r') = -k^{-1}\left(\tfrac{1}{4}[k(r',r')]^2\sin(kr') + \int_{r'}^\infty \sin(k\rho)S(\rho,r')\rho^{-2}\,d\rho\right), \tag{5.29}$$

$$\bar{k}_1(r') = k^{-1}\left(\tfrac{1}{4}[k(r',r')]^2\cos(kr') + \int_{r'}^\infty \cos(k\rho)S(\rho,r')\rho^{-2}\,d\rho\right), \tag{5.30}$$

$$P_N^{(1)}(r,r') = -k^{-1}\int_r^\infty \sin k(r-\rho)S(\rho,r')\rho^{-2}\,d\rho, \tag{5.31}$$

$$Q_N^{(1)}(r,r') = -k^{-1}\int_r^\infty \cos k(r-\rho)S(\rho,r')\rho^{-2}\,d\rho. \tag{5.32}$$

$P_N^{(1)}(r, r')$ and $Q_N^{(1)}(r, r')$ are obviously negligible if

$$\int_r^\infty |S(\rho, r')|\, \rho^{-2}\, d\rho$$

is negligible. Using for $|S(\rho, r')|$ the bound $C(rr')^{\frac{1}{2}}$, which is readily derived from (4.82), we obtain

$$\int_r^\infty |S(\rho, r')|\, \rho^{-2}\, d\rho < C\left(\frac{r'}{r}\right)^{\frac{1}{2}}, \tag{5.33}$$

and this bound is sufficient for proving the negligibility.

On the other hand, using the bound (4.82) and taking as a new integration variable $x = r'\rho/a^2$, we easily see that

$$\int_0^\infty |S(\rho, r')|\, \rho^{-2}\, d\rho < C\left(\frac{r'}{a}\right). \tag{5.34}$$

Besides, as a special case of (5.33) it is clear that

$$\int_{r'}^\infty |S(\rho, r')|\, \rho^{-2}\, d\rho < C. \tag{5.35}$$

When using these two bounds in (5.29) and (5.30), one sees easily that $r'^{-1}k_1(r')$ and $r'^{-1}\bar{k}_1(r')$ are uniformly bounded functions on $[0, \infty]$, going to zero like r'^{-1} as r' goes to infinity.

Proof for $K_0^0(r, r')$

Again, the argument is similar to the case for $K_3(r, r')$, but we use a different way of bounding the remainders, starting with the following remark: We have essentially to get bounds for $|(1 - \dot{w}/2w) \sin kw|$ and for $k\,|r - r' - w + 2r'u^2|$. Now both these quantities are bounded by $k\,|w - \frac{1}{2}\dot{w}|$, and, by comparing the bound previously derived for $|K_3(r, r')|$, are bounded also by a constant. Now, as we have noticed in Sec. 3, for $u^2 \le 1$ and $r' \le r$, $\frac{1}{2}\dot{w}$ is positive and smaller than w. Therefore, the calculation of the remainders $R_N^{(0)}(r, r')$ and $\bar{R}_N^{(0)}(r, r')$, which is essentially the calculation of

$$\int_0^1 k\,|w - \tfrac{1}{2}\dot{w}|\, u^{-2}\, du, \tag{5.36}$$

reduces to the calculation of

$$k\int_0^\alpha (w - \tfrac{1}{2}\dot{w})u^{-2}\, du + C\int_\alpha^1 u^{-2}\, du, \tag{5.37}$$

where α should be conveniently chosen. The first term in (5.37) can be integrated by parts, and yields

$$-k\alpha^{-1}[w(\alpha) - \tfrac{1}{2}\dot{w}(\alpha)] + 2kr'\int_0^\alpha \left(\frac{r}{w} - 1\right) du. \tag{5.38}$$

We need to know the result only for $r' \le r$. Now, in that case, $(r - w)r^{-1}$ lies between $-r'/w$ and r'/w, so that the second term in (5.38) is absolutely bounded by $2kr'^2\alpha/(r - r')$. The first one is also absolutely bounded by the same quantity. If $kr'^2 < r - r'$, we can take $\alpha = 1$. If not, taking $\alpha = [(r - r')/kr'^2]^{\frac{1}{2}}$ yields

$$|R_N^0(r, r')| < Ck^{-\frac{1}{2}}r'(r - r')^{-\frac{1}{2}}, \tag{5.39}$$

which obviously holds for any $r' \le r$. A similar result is obtained for $|\bar{R}_N^0(r, r')|$. They are therefore negligible functions, and we can write down the s.s. functions

$$k_0(r') = (\pi k)^{-1}V_0\int_0^1 \sin(kr'u^2) \times \sin[kr'(1 - u^2)]u^{-2}\, du, \tag{5.40}$$

$$\bar{k}_0(r') = -(\pi k)^{-1}V_0\int_0^1 \sin(kr'u^2) \times \cos[kr'(1 - u^2)]u^{-2}\, du. \tag{5.41}$$

It is also possible to derive the s.s. functions from the expansion (3.16). One is led in this way to the formulas (1.18) and (1.19), which can easily be proved to be equivalent to (5.40) and (5.41). It is also of interest to obtain the asymptotic behavior of $k_0(r')$ and $\bar{k}_0(r')$. Standard methods, when applied to (5.40) and (5.41), lead us to

$$k_0(r') = -\tfrac{1}{2}V_0(r'/\pi k)^{\frac{1}{2}}[\cos(kr') - \sin(kr')] + (2\pi k)^{-1} \times V_0[\cos(kr') + \sin(kr')/4kr'] + O(1/k^2r'^2), \tag{5.42}$$

$$\bar{k}_0(r') = -\tfrac{1}{2}V_0(r'/\pi k)^{\frac{1}{2}}[\cos(kr') + \sin(kr')] + (2\pi k)^{-1} \times V_0[\sin(kr') + \cos(kr')/4kr'] + O(1/k^2r'^2). \tag{5.43}$$

6. PROOF OF LEMMA 4

Our aim is to obtain $K(\rho, \rho')$ from its values on a straight line $\rho = r$, and ultimately make $r \to \infty$. For convergence reasons, which will clearly appear below, we unfortunately cannot do this for $K(\rho, \rho')$ but rather for $K_2(\rho, \rho')$, which is defined by (1.16). Since it is obvious from (3.16) that $K_0^0(\rho, \rho')$ is a solution of (2.1), with $V(\rho)$ replaced by 0, $K_2(\rho, \rho')$ is a solution of the equation

$$\left[\rho^2\left(\frac{\partial^2}{\partial\rho^2} + k^2\right) - \rho'^2\left(\frac{\partial^2}{\partial\rho'^2} + k^2\right)\right]K_2(\rho, \rho') = \rho^2V(\rho)K(\rho, \rho') \tag{6.1}$$

with the boundary condition

$$[K_2(\rho, \rho')]_{\rho=0} = [K_2(\rho, \rho')]_{\rho'=0} = 0. \tag{6.2}$$

Let Q be the point whose coordinates are

$$Q\begin{cases}\rho = \rho_0\\ \rho' = \rho_0',\end{cases} \tag{6.3}$$

with $\rho_0 \le \rho_0'$, this being the only useful case for our purpose. Clearly, the two characteristics going through Q, namely the straight line $\rho' = \rho\rho_0'/\rho_0$ and the hyperbola $\rho\rho' = \rho_0\rho_0'$, intersect the straight line $\rho = r$ in two points—say D and C—located as shown in Fig. 3. If the right-hand side of (6.1) was a known function, it would therefore be possible[5] to construct the solution of (2.1) and Q from its boundary values on DC, and (2.2) would only give constraints on the choice of that boundary values. So as to obtain a more precise result, let us now use the variables and the functions defined through (2.4), (2.5), and (2.6), and denote by the index 0 the values of these quantities when $\rho = \rho_0$, $\rho' = \rho_0'$. We then obtain Eq. (2.7), and the domain QDC becomes a curvitriangle (Fig. 4), with two orthogonal straight sides QD and QC. The Riemann function is again

$$S(\sigma, \eta; \sigma_0, \eta_0) \equiv S(\sigma, \eta; Q) = J_0(2k[(\sigma - \sigma_0)(\eta - \eta_0)]^{\frac{1}{2}}), \quad (6.4)$$

and we can readily write

$$v(Q) = v(C)S(C; Q) + \iint_G S(\sigma, \eta; Q)\, d\sigma\, d\eta + \int_{CD} S(\sigma, \eta; Q)\left(\frac{\partial}{\partial\sigma} v(\sigma, \eta)\right) d\sigma + v(\sigma, \eta)\left(\frac{\partial}{\partial\eta} S(\sigma, \eta; Q)\right) d\eta, \quad (6.5)$$

where G is the domain QDC. We can now come back to the variables ρ and ρ', through the transformation formulas

$$\rho = \{2\eta[\sigma + 2 + (\sigma^2 + 4\sigma)^{\frac{1}{2}}]\}^{\frac{1}{2}},$$
$$\rho' = \{2\eta[\sigma + 2 - (\sigma^2 + 4\sigma)^{\frac{1}{2}}]\}^{\frac{1}{2}}. \quad (6.6)$$

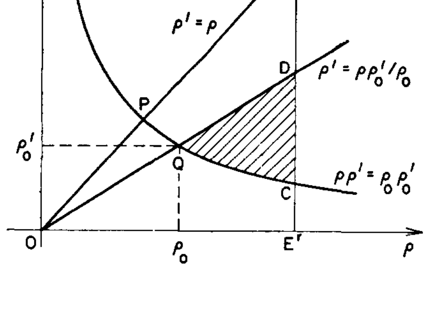

FIG. 3. The integration domain G in the (ρ, ρ') plane.

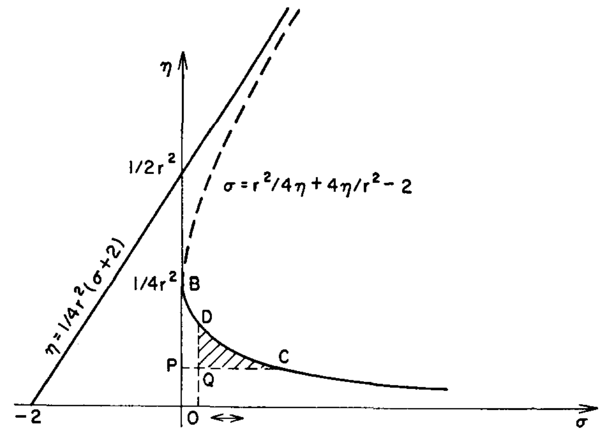

FIG. 4. The integration domain G in the (σ, η) plane.

After one integration by parts, we obtain in this way

$$\begin{aligned} 2(\rho_0\rho_0')^{-\frac{1}{2}}K_2(\rho_0, \rho_0) &= [(r\rho_D')^{-\frac{1}{2}}K_2(r, \rho_D') + (r\rho_C')^{-\frac{1}{2}}K_2(r, \rho_C')] \\ &+ \int_{\rho'_C}^{\rho'_D} r\left\{-S_{r,\rho'}\frac{\partial}{\partial r}[(r\rho')^{-\frac{1}{2}}K_2(r, \rho')] + (r\rho')^{-\frac{1}{2}}K_2(r, \rho')\frac{\partial}{\partial r}S_{r,\rho'}\right\}\frac{d\rho'}{\rho'} \\ &+ \iint_G (\rho\rho')^{-\frac{3}{2}}S_{\rho\rho'}V(\rho)\rho^2K(\rho, \rho')\, d\rho\, d\rho', \end{aligned} \quad (6.7)$$

where

$$\rho_C' = \rho_0\rho_0'/r, \quad \rho_D' = r\rho_0/\rho_0', \quad (6.8)$$

and

$$S_{\rho\rho'} = J_0\left\{k\left[\left(\frac{\rho}{\rho'} + \frac{\rho'}{\rho} - \frac{\rho_0}{\rho_0'} - \frac{\rho_0'}{\rho_0}\right)(\rho\rho' - \rho_0\rho_0')\right]^{\frac{1}{2}}\right\}. \quad (6.9)$$

The brace in the second term of the right-hand side of (6.7) can be rewritten as

$$\tfrac{1}{2}S_{r,\rho'}r^{-\frac{3}{2}}\rho'^{-\frac{1}{2}}K_2(r, \rho') + (r\rho')^{-\frac{1}{2}} \times \left(K_2(r, \rho')\frac{\partial}{\partial r}S_{r,\rho'} - S_{r,\rho'}\frac{\partial}{\partial r}K_2(r, \rho')\right). \quad (6.10)$$

Let us now introduce the following convenient notation:

$$A = \left(\frac{r}{\rho'} + \frac{\rho'}{r} - \frac{\rho_0}{\rho_0'} - \frac{\rho_0'}{\rho_0}\right)(r\rho' - \rho_0\rho_0'), \quad (6.11)$$

$$N = \left(\frac{1}{\rho'} - \frac{\rho'}{r^2}\right)(\rho' r - \rho_0\rho_0') + \rho'\left(\frac{r}{\rho'} + \frac{\rho'}{r} - \frac{\rho_0}{\rho_0'} - \frac{\rho_0'}{\rho_0}\right), \quad (6.12)$$

$$D = A^{\frac{1}{2}}. \quad (6.13)$$

Clearly, S, and its derivative, in (6.10), are equal to

$$S_{r,\rho'} = J_0(kD), \tag{6.14}$$

$$\frac{\partial}{\partial r} S_{r,\rho'} = -\tfrac{1}{2}kND^{-1}J_1(kD). \tag{6.15}$$

Analysis of the behavior of A as r goes to infinity shows that

$$kD = kr - \tfrac{1}{2}k\rho'\left(\frac{\rho_0\rho_0'}{\rho'^2} + \frac{\rho_0}{\rho_0'} + \frac{\rho_0'}{\rho_0}\right) + O\left(\frac{\bar{a} + b\rho'^2}{r^2}\right)\left[1 + O\left(\frac{\rho'}{r}\right)\right], \tag{6.16}$$

where $\bar{a}$ and b are quantities related to ρ_0 and ρ_0', which remain constant as r goes to infinity. Besides

$$\tfrac{1}{2}k(N/D) = k + O((\bar{a} + b\rho'^2)/r^2)[1 + O(\rho'/r)]. \tag{6.17}$$

Formula (6.15) shows that the argument of the Bessel functions in S and $\partial S/\partial r$ go to infinity like kr as r goes to infinity. We are therefore led to use the asymptotic forms of the Bessel functions, which are related to the Bessel functions by the inequalities

$$|J_0(x) - (2/\pi x)^{\frac{1}{2}} \cos (x - \tfrac{1}{4}\pi)| \le C \inf \{x^{-\frac{3}{2}} + x^{-\frac{5}{2}}, 1 + x^{-\frac{1}{2}}\}, \tag{6.18}$$

$$|J_1(x) - (2/\pi x)^{\frac{1}{2}} \sin (x - \tfrac{1}{4}\pi)| \le C \inf \{x^{-\frac{3}{2}} + x^{-\frac{5}{2}}, 1 + x^{-\frac{1}{2}}\}. \tag{6.19}$$

Let us now introduce the functions

$$\varphi = kr - \tfrac{1}{2}k\rho[(\rho_0\rho_0'/\rho'^2) + (\rho_0/\rho_0') + (\rho_0'/\rho_0)] = kr - \bar{\varphi}, \tag{6.20}$$

$$R = C[(\bar{a} + b\rho'^2)/r^2](1 + C\rho'/r). \tag{6.21}$$

As far as S and its derivative are concerned, going to $r = \infty$ in (6.7) leads to replacing kD by φ in the Bessel functions, $\frac{1}{2}(N/D)$ by 1, and the Bessel functions by their asymptotic behaviors (6.18) and (6.19), *and* proving that the over-all remainder goes to zero. For this we use for $|K_2(r, \rho')|$ the bound

$$|K_2(r, \rho')| < Ca[\rho'/(\rho' + a)], \tag{6.22}$$

which follows readily from (3.39) for $r \gg a$, and we use for $|(\partial/\partial r)K_2(r, \rho')|$ the bound

$$\left|\frac{\partial}{\partial r} K_2(r, \rho')\right| < C\frac{\rho'}{\rho' + a}, \tag{6.23}$$

which follows readily from (3.40) for $r \gg a$. Let us then notice that $|x - \varphi|$ is $O(R)$ and therefore $|\cos x - \cos \varphi|$ is $O(R) + O(R^2)$, whereas $|x^{-\frac{1}{2}} - \varphi^{-\frac{1}{2}}|$ is $O(\varphi^{-\frac{3}{2}}R)$ provided that $|R\varphi^{-1}| < 1$, a condition[12] which must be checked when ρ' approaches ρ_C' or ρ_D'. Keeping this caution in mind, we can precisely write that the remainder, when either S or $\partial S/\partial r$ in (6.10) is replaced by its asymptotic form, is given by

$$\mathfrak{R}_\varphi \le C\varphi^{-\frac{1}{2}}(R + R^2 + \varphi^{-1}R) + (1 + \varphi^{-1}R)(\varphi^{-\frac{3}{2}} + \varphi^{-\frac{5}{2}}) \tag{6.24}$$

and, in any case, viz., even if φ is very small,

$$\mathfrak{R}_\varphi \le C(1 + \varphi^{-\frac{1}{2}} + x^{-\frac{1}{2}}), \tag{6.25}$$

where x is the exact value of the argument. When (6.10) is used in (6.7), the contributions to the remainder due to the replacement of S and $\partial S/\partial r$ by their asymptotic form are bounded, for large r, by

$$\mathfrak{R} < C\int_{\rho'_C}^{\rho'_D} r^{\frac{1}{2}}\rho'^{-\frac{1}{2}}\frac{\rho'}{a + \rho'}\mathfrak{R}_\varphi\, d\rho'. \tag{6.26}$$

So as to evaluate (6.26), let us first assume that $\rho_0' \ne \rho_0$ and $\rho_0' \ne 0$. We are led to split the integration path CD as shown in Fig. 5, introducing for convenience the following points: M is the middle of CD, so that its ordinate is approximately $\frac{1}{2}r(\rho_0'/\rho_0)$ for large r. A is the point of ordinate a, which is a fixed length. E and F are the points for which $\varphi = 0$. Their ordinates, α and β, are approximately equal to $\rho_0\rho_0'/r$ and $2(\rho_0/\rho_0' + \rho_0'/\rho_0)^{-1}r$ for large r. Clearly $EF \supset CD$ for large r. Since we assume $\rho_0' \ne \rho_0$, we can always take r large enough so that DF is larger than k^{-1}. This situation is the one taken into account below. Now, for large r, φ can be written as

$$\varphi \sim \tfrac{1}{2}[(\rho_0/\rho_0') + (\rho_0'/\rho_0)](k/\rho')(\rho' - \alpha)(\beta - \rho') = Ck\rho'^{-1}(\rho' - \alpha)(\beta - \rho'). \tag{6.27}$$

According to (6.21)–(6.24), for evaluating $\mathfrak{R}$, we have to calculate

$$I_{p,q} = Ck^{-p}r^{\frac{1}{2}}\int_{\rho'_C}^{\rho'_D}\frac{\rho'}{a + \rho'}\left(\frac{\rho'}{(\rho' - \alpha)(\beta - \rho')}\right)^p \times \left(\frac{\bar{a} + b\rho'^2}{r^2}\right)^q \rho'^{-\frac{1}{2}}\, d\rho', \tag{6.28}$$

for $p = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$ and, for each p, for $q = 0, 1, 2$, except in the case $p = \frac{1}{2}$, where $q = 0$ should be discarded. In (6.28) we have not taken in account the term ρ'/r in (6.21), because it is bounded throughout

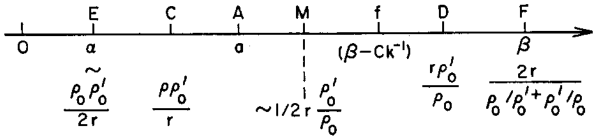

FIG. 5.

the interval. Clearly, if $I_{p,q}$ goes to zero as r goes to infinity for some value of q, the property holds for larger q's. We have therefore to check (6.28) only for $p = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$, $q = 0$, and for $p = \frac{1}{2}$, $q = 1$. On the intervals AM and MD, we replace $\rho'/(a + \rho')$ by 1, and, on the interval CA, we replace it by ρ'/a. We are led in this way to the following integrals.

Interval MD, $p \geq \frac{1}{2}, q = 0$:

$$I < Ck^{-p}r^{-1}\int_M^D (\beta - \rho')^{-p}\, d\rho' < C(kr)^{-1}. \quad (6.29)$$

Interval AM, $p \geq \frac{1}{2}, q \geq 0$:

$$I < Ck^{-p}r^{-p+\frac{1}{2}}\int_A^M \rho'^{-\frac{3}{2}}(\rho^2/r^2)^q\, d\rho'. \quad (6.30)$$

Hence, for $p > \frac{1}{2}$, $q = 0$, we get

$$I < C(kr)^{-p}(r/a)^{\frac{1}{2}} \quad (6.31)$$

and, for $p = \frac{1}{2}$, $q = 1$, we get

$$I < Ck^{-\frac{1}{2}}r^{-2}\int_a^{Cr} \rho'^{\frac{1}{2}}\, d\rho' < C(kr)^{-\frac{1}{2}}. \quad (6.32)$$

Interval CA, $p > \frac{1}{2}, q = 0$:

$$I < Ck^{-p}r^{-p+\frac{1}{2}}a^{-1}\int_{2\alpha}^{a} \rho'^{p-\frac{1}{2}}(\rho' - \alpha)^{-p}\, d\rho' \quad (6.33)$$

and, since $\rho'/(\rho' - \alpha)$ is clearly bounded by 2,

$$I < C(kr)^{-p}(r/a)^{\frac{1}{2}}, \quad (6.34)$$

$p = \frac{1}{2}$, $q = 1$. The same ansatz, combined with the remark that R is there smaller than Ca^2/r^2, yields

$$I < C(ka)^{-\frac{1}{2}}a^2/r^2. \quad (6.35)$$

From (6.29), (6.31), (6.32), (6.34), and (6.35) we see that the remainder go to zero as r goes to infinity. Since the first terms in the right-hand side of (6.7) go to zero as r goes to ∞, K_2 being uniformly bounded by (6.22), we therefore obtain

$$\begin{aligned} 2(\rho_0\rho_0')^{-\frac{1}{2}}K_2(\rho_0, \rho_0') &= -\left(\frac{2k}{\pi}\right)^{\frac{1}{2}} \lim_{r\to\infty}\int_0^{r(\rho_0'/\rho_0)}\Big(K_2(r, \rho')\sin(kr - \bar\varphi - \tfrac{1}{4}\pi) \\ &\quad + k^{-1}\frac{\partial}{\partial r}K_2(r, \rho')\cos(kr - \bar\varphi - \tfrac{1}{4}\pi)\Big)\rho'^{-\frac{3}{2}}\, d\rho' \\ &\quad + \iint_{\bar G} (\rho\rho')^{-\frac{3}{2}}\rho^2 V(\rho)K(\rho, \rho') \\ &\quad \times J_0\left(k\left[\left(\frac{\rho}{\rho'} + \frac{\rho'}{\rho} - \frac{\rho_0}{\rho_0'} - \frac{\rho_0'}{\rho_0}\right)(\rho\rho' - \rho_0\rho_0')\right]^{\frac{1}{2}}\right) \\ &\quad \times d\rho\, d\rho', \end{aligned} \quad (6.36)$$

where $\bar G$ is the domain G for $r = \infty$. Now for being allowed to replace $K_2(r, \rho')$ and $(\partial/\partial r)K^2(r, \rho')$ by their expressions in terms of the s.s. functions, we need only to check that the negligible functions associated with $K_2(r, \rho')$ fulfill also the condition

$$\int_0^r |K_N^{(2)}(r, \rho')|\, \rho'^{-\frac{3}{2}}\, d\rho' \to 0 \quad \text{as} \quad r \to \infty. \quad (6.37)$$

This is easy to check on (5.18), (5.28), and (5.33). It would no longer be true for $|K_0^0(r, r')|$, or our majorants for the remainder either. This is the reason why, unfortunately, we had to use $K_2(r, r')$ instead of $K(r, r')$. The use of the s.s. function yields the equation

$$\begin{aligned} (\rho_0\rho_0')^{-\frac{1}{2}}K_2(\rho_0, \rho_0') &= \left(\frac{k}{2\pi}\right)^{\frac{1}{2}}\int_0^\infty \{[k_2(\rho')\sin[\varphi(\rho')] \\ &\quad - \bar k_2(\rho')\cos[\varphi(\rho')]\}\rho'^{-\frac{3}{2}}\, d\rho' \\ &\quad + \tfrac{1}{2}\iint_{\bar G} (\rho\rho')^{-\frac{3}{2}}\rho^2 V(\rho)K(\rho, \rho') \\ &\quad \times J_0\left[k\left[\left(\frac{\rho}{\rho'} + \frac{\rho'}{\rho} - \frac{\rho_0}{\rho_0'} - \frac{\rho_0'}{\rho_0}\right)(\rho\rho' - \rho_0\rho_0')\right]^{\frac{1}{2}}\right] \\ &\quad \times d\rho\, d\rho', \end{aligned} \quad (6.38)$$

in which $\varphi(\rho')$ is equal to $\bar\varphi + \frac{1}{4}\pi$ and the domain $\bar G$ is the infinite extension of QDC when r goes to $+\infty$.

Remarks: (1) In the case of a finite range potential, equal to zero for $\rho > b$, the integrated term in (6.38) vanishes for ρ_0 larger than b. The part of the wave-functions outside of the range can therefore be readily derived from the s.s. function and, by comparing to what can be directly obtained, gives consistency conditions on s.s. functions for finite-range potentials. A similar study can yield relations between properties of the s.s. functions and asymptotic properties of $V(r)$.

(2) The "boundary condition" (6.2) is obviously fulfilled by any finite solution of (6.38). Existence and uniqueness of solutions of (6.38) are not studied in the present paper.

7. INTEGRAL REPRESENTATION FOR THE s.s. FUNCTIONS

We start from (1.22) and (1.23), which we have to study only in the case $r \geq r'$, according to the definition of the s.s. functions. We successively derive the contributions to the s.s. functions due to $K_0(r, r')$ and to the integrated term. In both cases, we successively derive the corresponding equalities (1.7) and (1.8).

Contribution Due to $K_0(r, r')$

We study (1.22). If r is allowed to go to infinity, a candidate for the asymptotic form of $K_0(r, r')$ is obviously

$$\mathcal{K}_0(r, r') = \frac{-1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}} \times \int_0^\infty \cos\left[k\left(r - r' - \frac{1}{2}\frac{\rho^2}{r'}\right) - \frac{\pi}{4}\right]\rho V(\rho)\, d\rho. \tag{7.1}$$

For proving that (7.1) truly is the nonnegligible part in (1.7), we have to prove that its difference $\mathfrak{R}$ with (1.21) is a negligible function; to get absolute bounds for this difference, we must do the following:

(1) Obviously, we obtain a bound for $\mathfrak{R}$ by just adding up a bound of $|K_0(r, r')|$, as given by (3.4), to a bound coming from (7.1), say $(r'/k)^{\frac{1}{2}}$. We therefore obtain

$$|\mathfrak{R}| < C\{(r'/k)^{\frac{1}{2}} + (rr')^{\frac{1}{2}}[1 + k\,|r - r'|]^{-\frac{1}{2}}\}. \tag{7.2}$$

(2) So as to make the comparisons easier, let us now introduce the functions

$$\mathcal{K}_0^{\mathrm{T}}(r, r') = -\frac{1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}} \times \int_0^{\frac{1}{2}(rr')^{\frac{1}{2}}} \cos\left[k\left(r - r' - \frac{1}{2}\frac{\rho^2}{r'}\right) - \frac{\pi}{4}\right]\rho V(\rho)\, d\rho, \tag{7.3}$$

$$K_0^{\mathrm{T}}(r, r') = -\tfrac{1}{2}(rr')^{\frac{1}{2}} \times \int_0^{\frac{1}{2}(rr')^{\frac{1}{2}}} J_0\left[k(r - r')\left(1 - \frac{\rho^2}{rr'}\right)^{\frac{1}{2}}\right]\rho V(\rho)\, d\rho. \tag{7.4}$$

Since the Bessel function and the cosine function are uniformly bounded functions, it is easy to show that

$$|K_0(r, r') - K_0^{\mathrm{T}}(r, r')| + |\mathcal{K}_0(r, r') - \mathcal{K}_0^{\mathrm{T}}(r, r')| < C\left(1 + \frac{1}{(kr)^{\frac{1}{2}}}\right)\frac{(rr')^{\frac{1}{2}}}{1 + (rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}} \tag{7.5}$$

and is therefore a negligible function. Hence we can limit our study to the comparison of $K_0^{\mathrm{T}}(r, r')$ and $\mathcal{K}_0^{\mathrm{T}}(r, r')$.

(3) Let us put[13]

$$x = k(r - r')[1 - \rho^2/rr']^{\frac{1}{2}}, \tag{7.6}$$

$$\varphi = k(r - r' - \tfrac{1}{2}\rho^2/r'), \tag{7.7}$$

$$R = x - \varphi, \tag{7.8}$$

and let us assume that $r' \leq \frac{1}{4}r$. It follows that x, and φ, remain[12] larger than $\frac{1}{2}kr$ on the integration path and that $|R| \leq \varphi$. Besides, R is given by

$$|R| < Ckr[\rho^2/r^2 + \rho^4/(rr')^2]. \tag{7.9}$$

We also introduce

$$R_1 = |\varphi - kr| = k\,|r' + \tfrac{1}{2}\rho^2/r'|, \tag{7.10}$$

which is also smaller than φ. Now, throughout the transformation of the Bessel function in (7.4) into its asymptotic form, remainders appear at four steps:

(a) $J_0(x) \to x^{-\frac{1}{2}}\cos(x - \pi/4)$. Remainders absolutely bounded by $C(x^{-\frac{3}{2}} + x^{-\frac{5}{2}})$, or $C\varphi^{-\frac{3}{2}}(1 + R/\varphi) + C\varphi^{-\frac{5}{2}}(1 + R/\varphi)$.

(b) $x^{-\frac{1}{2}}\cos(x - \pi/4) \to \varphi^{-\frac{1}{2}}\cos(x - \pi/4)$. Remainders absolutely bounded by $C\varphi^{-\frac{3}{2}}R$.

(c) $\varphi^{-\frac{1}{2}}\cos(x - \pi/4) \to \varphi^{-\frac{1}{2}}\cos(\varphi - \pi/4)$. Remainders absolutely bounded by $C\varphi^{-\frac{1}{2}}R/(1 + R)$.

(d) $\varphi^{-\frac{1}{2}}\cos(\varphi - \pi/4) \to (kr)^{-\frac{1}{2}}\cos(\varphi - \pi/4)$. Remainders absolutely bounded by $(kr)^{-\frac{3}{2}}R_1$.

Gathering these results, and inserting them at their proper place, we see that the remainder $\mathfrak{R}$ of the transformation $K_0^{\mathrm{T}}(r, r') \to \mathcal{K}_0^{\mathrm{T}}(r, r')$ is absolutely bounded by

$$|\mathfrak{R}| \leq C(rr')^{\frac{1}{2}}\int_0^{(rr')^{\frac{1}{2}}} \rho\,|V(\rho)|\, R_{(\varphi)}\, d\rho, \tag{7.11}$$

where

$$R_{(\varphi)} = \varphi^{-\frac{3}{2}} + \varphi^{-\frac{5}{2}} + R(\varphi^{-\frac{5}{2}} + \varphi^{-\frac{7}{2}}) + \varphi^{-\frac{1}{2}}[R/(1 + R)] + (kr)^{-\frac{3}{2}}R_1. \tag{7.12}$$

Clearly, our point is proved if we succeed in showing that the contributions to (7.11) of $\varphi^{-\frac{3}{2}}$, $R\varphi^{-\frac{5}{2}}$, $[R/(1 + R)]\varphi^{-\frac{1}{2}}$, and $(kr)^{-\frac{3}{2}}R_1$ are negligible functions. Now, since φ is larger than Ckr and since $\rho\,|V(\rho)|$ belongs to $L_1(0, \infty)$, the contribution of $\varphi^{-\frac{3}{2}}$ is bounded by

$$Cr'^{\frac{1}{2}}r^{-1}k^{-\frac{3}{2}}. \tag{7.13}$$

The same is true for $R\varphi^{-\frac{5}{2}}$ since R is smaller than kr. So as to get a bound for $\varphi^{-\frac{1}{2}}R/(1 + R)$, we split the integration path in (7.11) into two domains: from 0 to $(rr'/k^2)^{\frac{1}{4}}$, and from $(rr'/k^2)^{\frac{1}{4}}$ to $(rr')^{\frac{1}{2}}$, or to ∞. On the first domain we use $\varphi^{-\frac{1}{2}}R$, on the second one we use $C\varphi^{-\frac{1}{2}}$. We obtain in this way

$$(r'/k)^{\frac{1}{2}}(rr'/k^2)^{-\frac{1}{4}(1+\epsilon)}a^{1+\epsilon}(1 + 1/kr'). \tag{7.14}$$

As for the term $(kr)^{-\frac{3}{2}}$, it yields

$$(r'/k)^{\frac{1}{2}}[(r'/r) + (rr')^{-\frac{1}{2}(1+\epsilon)}a^{1+\epsilon}]. \tag{7.15}$$

(4) Now, by using the bound (7.2) and the bound obtained by adding (7.13), (7.16), and (7.15), it is possible to prove that $\mathfrak{R}$ is a negligible function.

Clearly, the first axiom for a negligible function is fulfilled by $\mathcal{R}$ because if r goes to infinity, r', being fixed, becomes smaller than $\frac{1}{4}r$ and then the bounds (7.13), (7.14), and (7.15) prove that $\mathcal{R}$ goes to zero, at least for $r' \neq 0$, and, according to (7.2), $|\mathcal{R}|$ is zero for $r' = 0$. As for the second axiom, we have to get an appraisal of

$$\int_0^r \mathcal{R}(r, r')r'^{-1}(1 + kr')^{-1}\, dr'. \qquad (7.16)$$

This leads us to evaluate terms which are in any case bounded by (7.2) and which for $r' \leq \frac{1}{4}r$ are bounded by

$$Cr'^{\alpha}r^{-\beta}, \qquad (7.17)$$

where β is strictly positive and $\alpha \leq 1 + \beta - \gamma$, γ being a strictly positive number. The appraisal can be obtained by splitting the path of integration in (7.16) into two parts if $\alpha > 0$, say $\int_0^{\frac{1}{4}r}$ and $\int_{\frac{1}{4}r}^{r}$, and use the bound $Cr'^{\alpha}r^{-\beta}$ on the first part, obtaining a bound in $Cr^{\alpha-\beta-1}$, and the bound $(rr')^{\frac{1}{2}}(r - r')^{-\frac{1}{2}}$ on the second part, obtaining $Cr^{-\frac{1}{2}}$. If $\alpha < 0$, keeping the upper interval, we split the lower one into $\int_0^{\eta}$ and $\int_{\eta}^{\frac{1}{4}r}$, η having to be much smaller than $\frac{1}{4}r$. On the lower interval, we use the bound $Cr'^{-\frac{1}{2}}$, which is readily derived from (7.2) since $r' \ll r$. On the intermediate interval we use $Cr'^{\alpha}r^{-\beta}$, and on the upper we use again $(rr')^{\frac{1}{2}}(r - r')^{-\frac{1}{2}}$. We then see that the bound goes to zero if η is equal to $a(r/a)^{-\beta/(\frac{1}{2}+|\alpha|)}$, like

$$Cr^{-\frac{1}{2}\beta/(\frac{1}{2}+|\alpha|)} + Cr^{-\frac{1}{2}} + Cr^{\alpha-\beta-1}. \qquad (7.18)$$

Since all the terms in $\mathcal{R}$ can be included in this scheme, we have proved that $\mathcal{R}(r, r')$ is a negligible function.

Let us now study $(\partial/\partial r)K_0(r, r')$. Differentiating (1.22) leads us to three terms. The first one, obtained by differentiating $(rr')^{\frac{1}{2}}$, is $\frac{1}{2}r^{-1}K_0(r, r')$. Using the bound (3.4), we readily see that this term is a negligible function. The second one, obtained by differentiating (1.22) with respect to the upper bound of the integral, leads us to a quantity obviously bounded (1 is a majorant of $|J_0|$) by $C(rr')\,|V[(rr')^{\frac{1}{2}}]|\,(r'/r)^{\frac{1}{2}}$, and therefore by $C(r'/r)^{\frac{1}{2}}$, and therefore negligible. The last one is

$$-\tfrac{1}{2}(rr')^{\frac{1}{2}}\int_0^{(rr')^{\frac{1}{2}}} \frac{\partial}{\partial r} J_0\left[k(r - r')\left(1 - \frac{\rho^2}{rr'}\right)^{\frac{1}{2}}\right]\rho V(\rho)\, d\rho. \qquad (7.19)$$

Now

$$\frac{\partial}{\partial r} J_0\left[k(r - r')\left(1 - \frac{\rho^2}{rr'}\right)^{\frac{1}{2}}\right] = -kJ_1\left[k(r - r')\left(1 - \frac{\rho^2}{rr'}\right)^{\frac{1}{2}}\right] \times \frac{1 - \frac{1}{2}\rho^2(r + r')/(r^2r')}{[1 - \rho^2/rr']^{\frac{1}{2}}}. \qquad (7.20)$$

The replacement of the fraction in (7.20) by 1, as r goes to infinity, affords remainders of the order of ρ^2/rr', which are therefore similar to remainders studied above in R_1. As for the Bessel function, it can be studied exactly as we did for J_0. The over-all remainder can therefore be proved to be a negligible function and, apart from this negligible function, (7.19) can be replaced by

$$\frac{1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}}\int_0^{\infty}\sin\left[k\left(r - r' - \frac{1}{2}\frac{\rho^2}{r'}\right) - \frac{\pi}{4}\right]\rho V(\rho)\, d\rho, \qquad (7.21)$$

which is nothing but $(\partial/\partial r)\bar{K}_0(r, r')$. From (7.1) and (7.21), we readily derive the part of the s.s. functions linear in V:

$$k_{\rm L}(r') = -\frac{1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}} \times \int_0^{\infty}\cos\left[k\left(r' + \frac{1}{2}\frac{\rho^2}{r'}\right) + \frac{\pi}{4}\right]\rho V(\rho)\, d\rho, \qquad (7.22)$$

$$\bar{k}_{\rm L}(r') = -\frac{1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}} \times \int_0^{\infty}\sin\left[k\left(r' + \frac{1}{2}\frac{\rho^2}{r'}\right) + \frac{\pi}{4}\right]\rho V(\rho)\, d\rho. \qquad (7.23)$$

Contribution Due to the Integrated Term

Since $r \geq r'$, the integrated term (1.23) can be written

$$I = \tfrac{1}{2}(rr')^{\frac{1}{2}}\int_{r'/r}^{1} du \int_0^{(rr'/u)^{\frac{1}{2}}} \rho V(\rho)k(\rho, \rho u)u^{-1} \times J_0\left[k\left[(rr' - \rho^2 u)\left(\frac{r}{r'} + \frac{r'}{r} - u - \frac{1}{u}\right)\right]^{\frac{1}{2}}\right] d\rho, \qquad (7.24)$$

where the notations have been introduced in Sec. 4. Now, a candidate for its asymptotic form is

$$\bar{I} = (2\pi k)^{-\frac{1}{2}}r'^{\frac{1}{2}}\int_0^1 u^{-1}\, du \times \int_0^{\infty}\rho V(\rho)k(\rho, \rho u)\cos[\varphi' - \tfrac{1}{4}\pi]\, d\rho, \qquad (7.25)$$

where

$$\varphi' = kr[1 - \rho^2 u/(2rr') - \tfrac{1}{2}(u + u^{-1})r'/r]. \qquad (7.26)$$

Let us therefore get bounds for $|I - \bar{I}|$. For this, we use for $k(\rho, \rho u)$ the following bounds, which follow from the combination of (3.1) and (4.29),

$$|k(\rho, \rho u)| < C(\rho u^{\frac{1}{2}})^{\eta}/[a + \rho u^{\frac{1}{2}}]^{\eta}, \qquad (7.27)$$

in which $0 \leq \eta \leq 1 + \epsilon$, and let us assume that $r' \leq \frac{1}{2}r$. A more general bound is obtained later. So as to make the comparison between I and $\bar{I}$ easier, let us introduce the functions

$$I_T = \tfrac{1}{2}(rr')^{\frac{1}{2}} \int_{2r'/r}^{1} u^{-1}\,du \times \int_0^{\frac{1}{2}(rr'/u)^{\frac{1}{2}}} \rho V(\rho) k(\rho, \rho u) J_0[\ ]\,d\rho, \quad (7.28)$$

$$\bar{I}_T = (2\pi k)^{-\frac{1}{2}} r'^{\frac{1}{2}} \int_{2r'/r}^{1} u^{-1}\,du \times \int_0^{\frac{1}{2}(rr'/u)^{\frac{1}{2}}} \rho V(\rho) k(\rho, \rho u) \cos[\ ]\,d\rho. \quad (7.29)$$

Going from I to I_T, and similarly from $\bar{I}$ to $\bar{I}_T$, can be done in two steps:

(1) setting the ρ bound equal to $\frac{1}{2}(rr'/u)^{\frac{1}{2}}$, but leaving the u bound equal to r'/r,

(2) in the result obtained from the first step, shifting the u bound up to $2r'/r$.

It is not difficult to evaluate the differences introduced at the two steps. The result is

$$|I - I_T| + |\bar{I} - \bar{I}_T| < C[1 + (kr)^{-\frac{1}{2}}] \frac{(rr')^{\frac{1}{2}}}{1 + (rr'/a^2)^{\frac{1}{2}+\frac{1}{2}\epsilon}} + \frac{Cr'}{(kr)^{\frac{1}{2}}}. \quad (7.30)$$

Let us now put

$$x' = k\{(rr' - \rho^2 u)[(r/r') + (r'/r) - u - u^{-1}]\}^{\frac{1}{2}}, \quad (7.31)$$

$$R(u) = x' - \varphi', \quad (7.32)$$

and let us assume that $r' \leq \frac{1}{4}r$. It follows[10] that φ' is larger than $\frac{1}{2}kr$ on the domain of integration, whereas x' is smaller than $\frac{3}{2}kr$. $|R(u)|$ is therefore smaller than $|\varphi'|$. We also introduce

$$R_1(u) = |\varphi' - kr| = \tfrac{1}{2}[k\rho^2(u/r') + (u + u^{-1})r'], \quad (7.33)$$

which is also smaller than φ'. Now, throughout the transformation of the Bessel function from I to $\bar{I}$, the same steps are involved which have been studied after Eq. (7.10). We can therefore write readily, for the difference $\mathcal{R}'$ between I_T and $\bar{I}_T$,

$$|\mathcal{R}'| \leq C(rr')^{\frac{1}{2}} \int_{2r'/r}^{1} u^{-1}\,du \times \int_0^{\frac{1}{2}(rr'/u)^{\frac{1}{2}}} \rho\,|V(\rho)|\,|k(\rho, \rho u)|\,R_{\varphi'}\,d\rho, \quad (7.34)$$

where

$$R_{\varphi'} \leq \varphi'^{-\frac{3}{2}} + R(u)\varphi'^{-\frac{5}{2}} + \varphi'^{-\frac{1}{2}}\{R(u)/[1 + R(u)]\} + (kr)^{-\frac{3}{2}} R_1(u). \quad (7.35)$$

Now it is easy to see from (7.31), (7.26), and (7.32) that

$$R(u) < Ckr[\rho^2/r^2 + \rho^4/(r^2 r'^2) + r'^2/r^2 u^2]. \quad (7.36)$$

Bounds for the contributions of the various parts of (7.35) to $\mathcal{R}'$ can be derived as we did above from Eq. (7.13) down. The derivation, which makes use of (7.27), is sometimes tedious, but not difficult. The result for the contributions of $\varphi'^{-\frac{3}{2}}$ and of $\varphi'^{-\frac{5}{2}}R(u)$ is

$$C(rr')^{\frac{1}{2}}(kr)^{-\frac{3}{2}}. \quad (7.37)$$

As for the term $\varphi'^{-\frac{1}{2}}\{R(u)/[1 + R(u)]\}$, where $R(u)$ is given by (7.36), we separately evaluate the contribution which depends on u only and the one which depends on ρ only. The first one can be calculated using (7.27) with $1 > \eta > 0$, and yields

$$Cr'^{\frac{1}{2}+\eta}/r^{\frac{1}{2}+\frac{1}{2}\eta}. \quad (7.38)$$

For the second one, we use the fact that a potential of class $\mathcal{E}$ is as well bounded by $C\rho^{-3+\epsilon'}$, where we can take $\theta \leq \epsilon' \leq 1$. Hence we obtain a bound in

$$C\log(r/r')[(r'/r)^{\frac{1}{2}} + r'^{\frac{1}{2}\epsilon'} r^{-\frac{1}{2}+\frac{1}{2}\epsilon'}]. \quad (7.39)$$

Using (7.27) with $\eta = 0$ for the first term in R_1, with $\eta = 1$ for the second one, we obtain a bound in

$$Cr^{-\epsilon} + Cr'^{\frac{3}{2}} r^{-\frac{1}{2}}. \quad (7.40)$$

All the bounds obtained above are valid only for $r' \leq \frac{1}{4}r$. So as to obtain a bound valid in any other case, we can add an absolute bound for (7.25), which $Cr'^{\frac{1}{2}}$ obviously is (via $\eta = 1$ in 7.27), and a bound for (7.24). For getting an absolute bound for (7.24), we have the choice between the bounds given in Sec. 4 in the case $r \geq r'$. However, let us notice that up to this point, throughout Sec. 7, all the bounds we have used for $k(\rho, \rho u)$ and $K_0(r, r')$ were obtained without making use of the differentials of $V(\rho)$ or the derivation of the bounds for the remainders either. So as to keep a way of proving the validity of our result in a class of potentials larger than $\mathcal{E}$, let us therefore use for $|I|$ the bound (4.30). We get by this way

$$|I| + |\bar{I}| < Cr'^{\frac{1}{2}} + C(rr')^{\frac{1}{4}}. \quad (7.41)$$

Using now (7.41) for $r' \geq \frac{1}{4}r$ and the above bounds for $r' \leq \frac{1}{4}r$, we can easily show on (7.16) that $\mathcal{R}$ is negligible. The only small difficulties come from (7.40), for which we rather split the integration interval in (7.16) into three parts—from 0 to a^3/r^2, which yields, via (7.41), a bound in $Cr^{-\frac{1}{2}}$; from a^3/r^2 to $a^{\frac{3}{2}}/r^{\frac{1}{2}}$, which yields, via (7.40), a bound whose dominant term is $Cr^{-\epsilon}\log|r/a|$; and from $a^{\frac{3}{2}}/r^{\frac{1}{2}}$ to r, which yields, via (7.41), a bound whose dominant term is $Cr^{-\frac{1}{8}}$. All these terms go therefore to zero as r goes to infinity, so that $\mathfrak{R}$ is negligible.

Let us now differentiate I with respect to r, and, for this, let us study (7.24). Differentiating $(rr')^{\frac{1}{2}}$ obviously yields a term bounded by $C(r'/r)^{\frac{1}{2}}$. Differentiating I with respect to the bound r'/r yields $C(r'/r)^{\frac{3}{2}}$ which is also negligible, and so is $C(r'/r)^{\frac{1}{2}} \times \log(r/r')$ which comes from the differentiation of $(rr'/u)^{\frac{1}{2}}$. We are therefore led to a term

$$I_1 = \tfrac{1}{2}(rr')^{\frac{1}{2}}\int_{r'/r}^{1} u^{-1}\,du\int_0^{(rr'/u)^{\frac{1}{2}}} \rho V(\rho)k(\rho,\rho u) \times \frac{\partial}{\partial r} J_0\left[k\left[(rr'-\rho^2 u)\left(\frac{r}{r'}+\frac{r'}{r}-u-u^{-1}\right)\right]^{\frac{1}{2}}\right] \times d\rho. \quad (7.42)$$

A candidate for its asymptotic form is

$$\bar{I}_1 = -(2\pi k)^{-\frac{1}{2}} r'^{\frac{1}{2}} k\int_0^1 u^{-1}\,du \times \int_0^\infty \rho V(\rho)k(\rho,\rho u)\sin(\varphi' - \tfrac{1}{4}\pi)\,d\rho. \quad (7.43)$$

That $|I_1 - \bar{I}_1|$ is a negligible function can be proved by the ways used above. Comparing now (7.25) and (7.43), we readily derive their contributions to the s.s. functions:

$$k_1(r') = (2\pi k)^{-\frac{1}{2}} r'^{\frac{1}{2}}\int_0^1 u^{-1}\,du\int_0^\infty \rho V(\rho)k(\rho,\rho u) \times \cos\left[\tfrac{1}{2}k\left(\frac{\rho^2 u}{r'} + ur' + \frac{r'}{u}\right) + \frac{\pi}{4}\right]d\rho, \quad (7.44)$$

$$\bar{k}_1(r') = (2\pi k)^{-\frac{1}{2}} r'^{\frac{1}{2}}\int_0^1 u^{-1}\,du\int_0^\infty \rho V(\rho)k(\rho,\rho u) \times \sin\left[\tfrac{1}{2}k\left(\frac{\rho^2 u}{r'} + ur' + \frac{r'}{u}\right) + \frac{\pi}{4}\right]d\rho. \quad (7.45)$$

Since, as we have already noticed, all the derivations in this section are valid provided V belongs to $\mathcal{E}_{13}$, it is interesting to see what can be said of the s.s. functions with the only assumptions of $\mathcal{E}_{13}$. This can be done easily. First take (7.22) and write it in the form

$$\begin{aligned} k_L(r') = &-\frac{1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}}\cos(kr' + \tfrac{1}{4}\pi)\int_0^\infty \rho V(\rho)\,d\rho \\ &- \frac{1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}}\cos(kr' + \tfrac{1}{4}\pi) \times \int_0^\infty\left[\cos\left(\frac{\frac{1}{2}k\rho^2}{r'}\right) - 1\right]\rho V(\rho)\,d\rho \\ &- \frac{1}{(2\pi)^{\frac{1}{2}}}\left(\frac{r'}{k}\right)^{\frac{1}{2}}\sin(kr' + \tfrac{1}{4}\pi) \times \int_0^\infty \sin\left(\frac{\frac{1}{2}k\rho^2}{r'}\right)\rho V(\rho)\,d\rho. \end{aligned} \quad (7.46)$$

By using for $|\cos(\frac{1}{2}k\rho^2/r') - 1|$ and $|\sin(\frac{1}{2}k\rho^2/r')|$ the bound $Ck\rho^2/(r' + \rho^2)$ and the properties of $\mathcal{E}_{13}$, it is easy to see that the second and the third term in (7.46) are uniformly bounded by a constant. We notice also that the first term is nothing but the leading term in the asymptotic behavior of $k_0(r')$, as given by (5.42). Therefore, $k_L(r') - k_0(r')$ is uniformly bounded by a constant. Now, let us look for the behavior of $k_L(r')$ as r' goes to zero. $k_L(r')$ can be written as a linear combination of $\int_0^\infty \cos(\frac{1}{2}k\rho^2/r') \times \rho V(\rho)\,d\rho$ and $\int_0^\infty \sin(\frac{1}{2}k\rho^2/r')\rho V(\rho)\,d\rho$ with coefficients behaving at the origin like $r'^{\frac{1}{2}}$. Let us write again one of these terms like

$$\tfrac{1}{2}\int_0^\infty \cos(\tfrac{1}{2}kr'^{-1}x)V(x^2)\,dx. \quad (7.47)$$

For a potential $V(x)$ of class $\mathcal{E}_{13}$, the function $x \to V(x^2)$ belongs to $L_2(0,\infty)$. Therefore, its Fourier transform belongs to $L^2(0,\infty)$, and therefore $r'^{-\frac{3}{2}}k_L(r')$ is square integrable near the origin. Therefore, $r'^{-1}k_L(r')$ remains bounded, and, since this is true for $r'^{-1}k_0(r')$, it is true for $r'^{-1}[k_L(r') - k_0(r')]$.

Let us now study $\mathcal{K}_1(r')$, writing

$$\mathcal{K}_1(r') = (2\pi k r')^{-\frac{1}{2}}[\bar{\mathcal{K}}_1^0(r') + \bar{\mathcal{K}}_1^1(r')], \quad (7.48)$$

where

$$\bar{\mathcal{K}}_1^0(r') = \int_0^1 u^{-1}\exp\left[\tfrac{1}{2}ikr'\left(u + \frac{1}{u}\right)\right]du \times \int_0^\infty \rho V(\rho)k(\rho,\rho u)\,d\rho \quad (7.49)$$

and

$$\bar{\mathcal{K}}_1^1(r') = \int_0^1 u^{-1}\exp\left[\tfrac{1}{2}ikr'\left(u + \frac{1}{u}\right)\right]du \times \int_0^\infty \rho V(\rho)k(\rho,\rho u) \times \left[\exp\left(\tfrac{1}{2}ik\rho^2\frac{u}{r'}\right) - 1\right]d\rho. \quad (7.50)$$

Clearly

$$\bar{\mathcal{K}}_1^0(r') = \int_0^\infty \exp[\tfrac{1}{2}ikr'(1+s)][s^2 + 2s]^{-\frac{1}{2}}\,ds \times \int_0^\infty \rho V(\rho)k[\rho, \rho[1 + s - (s^2+2s)^{\frac{1}{2}}]]\,d\rho. \quad (7.51)$$

Since $|k(\rho,\rho u)|$ can be bounded by $C\rho^\epsilon u^{\frac{1}{2}\epsilon}$, $\bar{\mathcal{K}}_1^0(r')$ is the Fourier transform of a function which belongs to L^p for any p such that $1 \le p < 2$. Hence

$$|\bar{\mathcal{K}}_1^0(r')| \in L_{p'}(0,\infty) \quad (7.52)$$

with

$$2 < p' < \infty. \quad (7.53)$$

As for $|\mathcal{K}_1^1(r')|$, it is clearly bounded by

$$C\int_0^1 u^{-1+\frac{1}{2}\epsilon}\,du\int_0^\infty \rho\,|V(\rho)|\,\rho^\epsilon\,\frac{k\rho^2u}{r'+k\rho^2u}\,d\rho < Cr'^{-\frac{1}{2}}. \tag{7.54}$$

From (7.52) and (7.54), it follows that $r^{\frac{1}{2}}\mathcal{K}_1(r')$ is a function of $L_{p'}(a,\infty)$. On the other hand, the quantity

$$\left|\int_0^1 u^{-1}\rho V(\rho)k(\rho,\rho u)\,d\rho\right|$$

is bounded by $C\rho^{1+\epsilon}\,|V(\rho)|$. We can therefore study the behavior of $\mathcal{K}_1(r')$ near $r'=0$ as we did above for $\mathcal{K}_L(r')$, with the same result: $\mathcal{K}_1(r')$ is bounded for $r'\to 0$. Hence we see that the only modification when we study the problem in $\mathcal{E}_{13}$ instead of $\mathcal{E}$, as regards Lemma 2, concerns the asymptotic behavior of $\mathcal{K}_1(r')$.

ACKNOWLEDGMENTS

The study we have begun to describe in this paper was undertaken, three years ago, in our Département de Physique Mathématique at Montpellier University. Our interest in the use of Riemann's representation arises in large part from an old discussion with J. J. Loeffel. In the last stages of the research, and during the period when the manuscript was being written, we have enjoyed the warm hospitality of the Theoretical Physics Department at Indiana University and useful discussions with Professor R. G. Newton.

APPENDIX

The following trivial inequalities, and similar ones, have been used without quotation: Let x a positive number and y a real number,

$$|(x+y)^{\frac{1}{2}}-x^{\frac{1}{2}}| = |y/[(x+y)^{\frac{1}{2}}+x^{\frac{1}{2}}]| \le |y/x^{\frac{1}{2}}| \quad \text{if} \quad |y|\le|x|, \tag{A1}$$

$$|(x+y)^{-\frac{1}{2}}-x^{-\frac{1}{2}}| = |y/\{x^{\frac{3}{2}}+x^{\frac{1}{2}}(x+y)^{\frac{1}{2}} \times [(x+y)^{\frac{1}{2}}+x^{\frac{1}{2}}]\} \tag{A2}$$

and therefore $\le |y/x^{\frac{3}{2}}|$ if $|y|\le|x|$.

* Supported in part by the U.S. Army Research Office, Durham, North Carolina.

† On leave of absence from Département de Physique Mathématique, Equipe de Recherche Associée au CNRS, Montpellier (France), which is the present address of the author.

[1] J. J. Loeffel, Ann. Inst. Henri Poincaré **8**, 339 (1968).

[2] T. Regge, Nuovo Cimento **14**, 951 (1959); **18**, 947 (1960); R. G. Newton, J. Math. Phys. **3**, 75 (1962).

[3] P. C. Sabatier, unpublished.

[4] V. De Alfaro and T. Regge, *Potential Scattering* (North-Holland, Amsterdam, 1965).

[5] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1966), Vol. II, p. 451.

[6] This formula is readily derived from Formula 1.7(30) of A. Erdélyi *et al.*, *Tables of Integral Transforms* (Bateman Manuscript Project) (McGraw-Hill, New York, 1954).

[7] A. Erdélyi *et al.*, *Higher Transcendental Functions* (Bateman Manuscript Project) (McGraw-Hill, New York, 1956), Formula 7.15(30).

[8] P. C. Sabatier, J. Math. Phys. **7**, 1515 (1966).

[9] It is easy to see on the iterated terms that the solution does not depend on θ.

[10] The majorants for $r'\ge r$ are not directly used in the present paper, but are necessary for getting bounds for the resolvent of the Regge–Newton equation. Those bounds will be derived and used in Ref. 3. The majorants for $K(r,r')$ are much more conveniently studied here.

[11] An improved bound for large energies will be used in the theory of approximation in the inverse scattering problem.

[12] The use of this condition is clearly seen in the Appendix.

[13] The notation, x, φ, and R, in Sec. 7 is independent of that used in Sec. 6.

A Method of Quantization for Relativistic Fields*

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(Received 12 September 1969)

A procedure for quantization is given which does not require the canonical formalism. Only the equation of motion for the field and the resulting conserved current are needed to derive all the necessary commutators or anticommutators, the operators which represent the physical observables, the reduction formulas, and vacuum expectation values for the particle fields. The formalism is sufficiently general so that it holds for fields, or a superposition of fields, of arbitrary mass and spin.

INTRODUCTION

There are two basic ways which are used to quantize fields. One uses a Lagrangian formulation[1] from which the canonical rules can be used to obtain equal time commutators and from which the various invariants which represent the physical observables can be constructed. The commutators are extended to arbitrary times by either using Schwinger's[2] or Peierls'[3] method or a theorem of Takahashi and Umezawa.[4]

The other method[5] utilizes an expansion of the field in terms of plane waves, requiring the Fourier coefficients to be Fock space operators whose commutators are either zero or a delta function. The physical operators are then defined in terms of these Fourier coefficients and the original expansion is inverted to obtain the physical operators as a function of the fields.

The purpose of this paper is to describe still another method which seems to be more general than the other two, in that the commutators of the Fock space operators corresponding to the expansion coefficients for the field do not have to be zero or a delta function. Nevertheless, physical operators, such as the number-of-particles operator, energy, momentum, etc., can be constructed directly from invariant integrals obtained from the equations of motion for the fields. The unequal time commutators are obtained directly from the quantization postulate and are found to preserve microcausality.

It will be seen that this method of quantization is a natural one to use in the Lehmann–Symanzik–Zimmermann (LSZ) formulation (see Refs. 1, 10, and 13) of interacting fields, since everything is derivable from the equations of motion, and the c-number wave packet solutions of the free particle equations no longer need to be restricted to that class of functions which can be orthonormalized. Indeed, the c-number solutions need not even be complete.

It is also possible to reduce the S matrix to vacuum expectation values of field operators which represent particles of arbitrary mass and spin. These expectation values can in turn be expressed as Feynman-type propagators.

In the first section, the creation and annihilation operators are defined in terms of the conserved current and the quantization postulate is given. The second section contains four basic theorems which are necessary for the foundation of the q-number theory. The q-number theory for particles of arbitrary mass and spin is constructed in the third section, and the evaluation of the S matrix in terms of Feynman propagators is given in the final section.

I. BASIC POSTULATES AND DEFINITIONS

In what follows it will be assumed that the fields satisfy a linear differential equation

$$\vec{D}(\partial)\psi(x) = 0, \tag{1}$$

with the adjoint equation

$$\bar{\psi}(x)\overleftarrow{D}(-\partial) = 0, \tag{2}$$

where

$$\bar{\psi}(x) = [\gamma_4\psi(x)]^\dagger,$$
$$-\gamma_4^\dagger D(-\partial) = D^\dagger(\partial)\gamma_4. \tag{3}$$

The arrow indicates the direction of differential operation, and γ_4 is a nonsingular matrix. The explicit form of the differential operator $D(\partial)$ for arbitrary spin can be obtained from either Weinberg[6] or Hammer *et al.*[7] Then γ_4 is the $2(2s+1)$ generalization of the Dirac γ_4 matrix.

If ψ_1 and ψ_2 are any two solutions of Eq. (1), it is further assumed[8] that a conserved current exists with the factors of i chosen so that

$$\frac{\partial}{\partial x_\mu} j_\mu(\bar{\psi}_2(x), \psi_1(x))$$
$$= \bar{\psi}_2(x)\vec{D}(\partial)\psi_1(x) - \bar{\psi}_2(x)\overleftarrow{D}(-\partial)\psi_1(x) = 0, \tag{4}$$

where any 4-vector is defined by

$$A_\mu = (A_i, iA_0).$$

With this definition, j_μ is linear in $\bar{\psi}(x)$ and $\psi(x)$,

$$a j_\mu(\bar{\psi}_2(x), \psi_1(x)) = j_\mu(a\bar{\psi}_2(x), \psi_1(x)) = j_\mu(\bar{\psi}_2(x), a\psi_1(x)), \quad (5)$$

and its Hermitian conjugate is

$$j_i^\dagger(\bar{\psi}_2(x), \psi_1(x)) = j_i(\bar{\psi}_1(x), \psi_2(x)),$$
$$j_0^\dagger(\bar{\psi}_2(x), \psi_1(x)) = j_0(\bar{\psi}_1(x), \psi_2(x)). \quad (6)$$

The definition of the conserved current given in Eq. (4) is chosen because it applies for the free field equations mentioned previously.[6,7] If Eq. (4) is not applicable, but a conserved current does exist, then the proofs given below can serve as an outline for obtaining the altered results.

It is well known that, for fields obeying Eq. (4), the invariant integral

$$I = \int d\mathbf{x}\, j_0(\bar{\psi}_2(x), \psi_1(x)) \quad (7)$$

or its generalization to an arbitrary hypersurface $\sigma_\mu(x)$

$$I = \int d\sigma_\mu(x) j_\mu(\bar{\psi}_2(x), \psi_1(x)) \quad (8)$$

is time-independent, with the Lorentz tensor properties given by $\psi_1(x)$ and $\psi_2(x)$. For example, if $\mathcal{O}_l(\partial)$ is a c-number tensor operator of rank l, and

$$[\mathcal{O}_l(\partial), D(\partial)]_- = 0, \quad (9)$$

then the q-number operator defined by

$$O_l = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), \mathcal{O}_l(\partial)\psi(x)) \quad (10)$$

is independent of time and is a Lorentz tensor of rank l. Consequently, the invariant integral can be used to define the time-independent Fock space operators

$$a_k(\mathbf{p}) = \int d\sigma_\mu(x) j_\mu(\bar{u}_k(\mathbf{p}, x), \psi(x)), \quad (11)$$

where $u_k(\mathbf{p}, x)$ is any c-number solution of

$$\vec{D}(\partial_x) u_k(\mathbf{p}, x) = 0,$$

with discrete eigenvalues k and continuous eigenvalues $\mathbf{p}$. It follows from Eq. (6) that

$$a_k^\dagger(\mathbf{p}) = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), u_k(\mathbf{p}, x)). \quad (12)$$

The basic quantization postulate is

$$[a_k(\mathbf{p}), a_l^\dagger(\mathbf{q})]_\pm = \int d\sigma_\mu(x) j_\mu(\bar{u}_k(\mathbf{p}, x), u_l(\mathbf{q}, x)), \quad (13a)$$

$$[a_k(\mathbf{p}), a_l(\mathbf{q})]_\pm = 0. \quad (13b)$$

It should be noted that the $u_l(\mathbf{p}, x)$ need not be a complete set of orthonormal functions. Thus it may not be possible in general to invert Eq. (11) to obtain $\psi(x)$ as a function of $a_k(\mathbf{p})$. On the other hand, Eqs. (11) and (13) reduce to the usual results if the $u_l(\mathbf{p}, x)$ are a complete set of orthonormal functions.[9]

II. THEOREMS

In this section the commutation rules, which are basic to the construction of a q-number theory for particles of arbitrary mass and spin, are derived for the configuration fields and the operators defined by Eqs. (10), (11), and (12). The rules are presented in the form of four theorems.

Theorem 1: The commutation rules for field operators, which satisfy a differential equation from which a conserved current can be derived, are

$$[\psi(x), \psi(y)]_\pm = 0, \quad (14a)$$

$$[\psi(x), \bar{\psi}(y)]_\pm = G(x-y), \quad (14b)$$

where

$$G(x-y) = G_a(x-y) - G_r(x-y), \quad (15)$$

the advanced and retarded Green's functions, respectively, defined by

$$\vec{D}(\partial_x) G_{a,r}(x-y) = -\delta(x-y), \quad (16a)$$

$$G_{a,r}(x-y) = 0, \quad \text{for} \quad (x_0 - y_0) \gtrless 0. \quad (16b)$$

Proof: The proof exploits the linearity properties of $j_\mu(x)$ given in Eq. (5). For example, from the definition given in Eq. (11),

$$[a_k(\mathbf{p}), a_l(\mathbf{q})]_\pm = \iint d\sigma_\mu(x)\, d\sigma_\nu(y) \times [j_\mu(\bar{u}_k(\mathbf{p},x), \psi(x)), j_\nu(\bar{u}_l(\mathbf{q},y), \psi(y))]_\pm$$
$$= \iint d\sigma_\mu(x)\, d\sigma_\nu(y) \times j_\mu(u_k(\mathbf{p},x), [\psi(x), j_\nu(\bar{u}_l(\mathbf{q},y), \psi(y))]_\pm)$$
$$= \int d\sigma_\mu(x) j_\mu\Big(\bar{u}_k(\mathbf{p}, x), \int d\sigma_\nu(y) \times j_\nu(\bar{u}_l(\mathbf{q}, y), [\psi(x), \psi(y)]_\pm)\Big). \quad (17)$$

However, the left-hand side of this equation must be zero by the quantization postulate of Eq. (13b). Since Eq. (17) must hold for all $\bar{u}_k(\mathbf{p}, x)$ and $\bar{u}_l(\mathbf{q}, y)$ or any variation of them, it follows that

$$[\psi(x), \psi(y)]_\pm = 0.$$

Similarly, by using Eq. (13a),

$$\int d\sigma_\mu(x) j_\mu(\bar{u}_k(\mathbf{p}, x), u_l(\mathbf{q}, x)) = \int d\sigma_\mu(x) j_\mu\Big(\bar{u}_k(\mathbf{p}, x), \int d\sigma_\nu(y) j_\nu([\psi(x), \bar{\psi}(y)]_\pm, u_l(\mathbf{q}, y))\Big), \quad (18)$$

from which it follows that

$$u_l(\mathbf{q}, x) = \int d\sigma(y) j_\mu([\psi(x), \bar{\psi}(y)]_\pm, u_l(\mathbf{q}, y)). \quad (19)$$

It also can be shown (see Appendix) that

$$u_l(\mathbf{q}, x) = \int d\sigma_\mu(y) j_\mu(G(x-y), u_l(\mathbf{q}, y)). \quad (20)$$

Consequently Eqs. (19) and (20) can be combined as

$$\int d\sigma_\mu(y) j_\mu(G(x-y) - [\psi(x), \bar{\psi}(y)]_\pm, u_l(\mathbf{q}, x)) = 0. \quad (21)$$

Since this equation must apply for all $u_l(\mathbf{q}, y)$ or its variations,

$$[\psi(x), \bar{\psi}(y)]_\pm = G(x-y).$$

Theorem 2: The commutation relations between the field operators $\psi(x)$ and the Fock space operators $u_k(\mathbf{p})$ are

$$[\psi(x), a_k^\dagger(\mathbf{p})]_\pm = u_k(\mathbf{p}, x), \quad (22a)$$

$$[\psi(x), a_k(\mathbf{p})]_\pm = 0. \quad (22b)$$

Proof: Equation (22a) follows directly from Eq. (19), which can be expressed as

$$u_k(\mathbf{p}, x) = \left[\psi(x), \int d\sigma_\mu(y) j_\mu(\bar{\psi}(y), u_k(\mathbf{p}, y))\right]_\pm,$$

from the linearity of j_μ. The integral within the commutator brackets can be seen from Eq. (12) to be $a_k^\dagger(\mathbf{p})$. Equation (22b) follows in a similar way from Eq. (14a).

Theorem 3: The commutation relation between a field operator and a q-number operator is

$$[O_l, \psi(x)]_- = -\mathcal{O}_l(\partial_x)\psi(x). \quad (23)$$

Proof: Equation (23) follows from Theorem 1, Eq. (20), and the linearity of j_μ:

$$\begin{aligned}[O_l, \psi(x)]_- &= -\int d\sigma_\mu(y) j_\mu([\psi(x), \bar{\psi}(y)]_\pm, \mathcal{O}_l(\partial_y)\psi(y)) \\ &= -\int d\sigma_\mu(y) j_\mu(G(x-y), \mathcal{O}_l(\partial_y)\psi(y)) \\ &= -\mathcal{O}_l(\partial)\psi(x).\end{aligned}$$

Theorem 4: The commutation relation for q-number operators is

$$[O_l, O_k]_- = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), [\mathcal{O}_l(\partial_x), \mathcal{O}_k(\partial_x)]_-\psi(x)). \quad (24)$$

Proof: Equation (24) also follows from Theorem 1, Eq. (20), and the linearity of j_μ:

$$\begin{aligned}[O_l, O_k]_- &= \int d\sigma_\mu(x) j_\mu\Big(\bar{\psi}(x), \int d\sigma_\nu(y) \\ &\quad \times j_\nu(\mathcal{O}_l(\partial_x)[\psi(x), \bar{\psi}(y)]_\pm, \mathcal{O}_k(\partial_y)\psi(y))\Big) \\ &\quad \mp \int d\sigma_\nu(y) j_\nu\Big(\bar{\psi}(y), \int d\sigma_\mu(x) \\ &\quad \times j_\mu(\mathcal{O}_k(\partial_y)[\bar{\psi}(x), \psi(y)]_\pm, \mathcal{O}_l(\partial_x)\psi(x))\Big) \\ &= \int d\sigma_\mu(x) j_\mu\Big(\bar{\psi}(x), \mathcal{O}_l(\partial_x)\int d\sigma_\nu(y) \\ &\quad \times j_\nu(G(x-y), \mathcal{O}_k(\partial_y)\psi(y))\Big) \\ &\quad - \int d\sigma_\nu(y) j_\nu\Big(\bar{\psi}(y), \mathcal{O}_k(\partial_y)\int d\sigma_\mu(x) \\ &\quad \times j_\mu(G(y-x), \mathcal{O}_l(\partial_x)\psi(x))\Big) \\ &= \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), [\mathcal{O}_l(\partial_x), \mathcal{O}_k(\partial_x)]_-\psi(x)).\end{aligned}$$

III. Q-NUMBER THEORY

Each dynamical system in quantum theory corresponds to a unitary representation of the Poincaré group which is completely specified by a Lie algebra for the infinitesimal generators: P_μ corresponding to four-vector momentum (translations) and $M_{\mu\nu}$ corresponding to four-tensor angular momentum (rotations). It is clear then from Theorems 3 and 4, Eqs. (23) and (24), and from Eq. (10), that the Fock space generators of the Poincaré group, and therefore the physical observables corresponding to linear momentum, energy, etc., are given by

$$P_\mu = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), \mathcal{T}_\mu(x)\psi(x)), \quad (25a)$$

$$M_{\mu\nu} = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), \mathcal{M}_{\mu\nu}(x)\psi(x)), \quad (25b)$$

with the corresponding equations of motion

$$[\psi(x), P_\mu]_- = \mathcal{T}_\mu(x)\psi(x), \quad (26a)$$

$$[\psi(x), M_{\mu\nu}]_- = \mathcal{M}_{\mu\nu}(x)\psi(x), \quad (26b)$$

where $\mathcal{T}_\mu(x)$ and $\mathcal{M}_{\mu\nu}(x)$ are the generators of the Poincaré group in the configuration representation.

In a similar way, Eq. (10) can be used to define any observable which corresponds to a transformation that leaves the equations of motion invariant. If the generators of the transformation form a Lie algebra, then Theorem 4 guarantees that the q-number generators satisfy that algebra. Typical examples might be the $SU(3)$ generators, isospin, and hypercharge.

For those transformations that do not form a group, Eq. (10) of course equally applies. In particular, the number-of-particles operator is

$$N = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), \psi(x)), \tag{27}$$

since, by Eq. (23),

$$[N, \psi(x)]_- = -\psi(x), \tag{28}$$

from which follows

$$[N, \psi^\dagger(x)]_- = \psi^\dagger(x) \tag{29}$$

by Eqs. (6). It also follows from Theorem 2 and Eqs. (11) and (12) that

$$[a_k(\mathbf{p}), N]_- = a_k(\mathbf{p}), \tag{30}$$

$$[a_k^\dagger(\mathbf{p}), N]_- = -a_k^\dagger(\mathbf{p}). \tag{31}$$

It is clear from these last two equations that number of particle states can be constructed from a vacuum in the usual way, even though the operators $a_k(\mathbf{p})$ satisfy Eq. (13) rather than the usual delta-function relationship.

For a relativistic theory, operators are needed to create both particle and antiparticle states. If $u_k(\mathbf{p}, x)$ and $v_k(\mathbf{p}, x)$ are any positive and negative c-number solutions of Eq. (1), it is convenient to redefine Eqs. (11) and (12) to

$$a_k(\mathbf{p}) = \int d\sigma_\mu(x) j_\mu(\bar{u}_k(\mathbf{p}, x), \psi(x)), \tag{32a}$$

$$b_k(\mathbf{p}) = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), v_k(\mathbf{p}, x)) \tag{32b}$$

for the destruction operators of the particle and antiparticle states, respectively. Note that the requirement

$$[a_k(\mathbf{p}), b_l(\mathbf{q})]_\pm = 0$$

implies the orthogonality of $u(p, x)$ and $v(q, x)$, since by Theorem 1

$$[a_k(\mathbf{p}), b_l(\mathbf{q})]_\pm = \int d\sigma_\mu(x) j_\mu(\bar{u}_k(\mathbf{p}, x), v_l(\mathbf{q}, x)).$$

Then, in parallel to Eq. (30),

$$[a_k(\mathbf{p}), N]_- = a_k(\mathbf{p}), \tag{33a}$$

$$[b_k(\mathbf{p}), N]_- = -b_k(\mathbf{p}). \tag{33b}$$

An n-particle and an m-antiparticle state can be constructed from the vacuum state $|0\rangle$ by the operation

$$|\mathbf{p}_1, \cdots, \mathbf{p}_n\rangle = (n!)^{-\frac{1}{2}} a^\dagger(\mathbf{p}_n) \cdots a^\dagger(\mathbf{p}_1) |0\rangle, \tag{34}$$

$$|\mathbf{q}_1, \cdots, \mathbf{q}_n\rangle = (m!)^{-\frac{1}{2}} b^\dagger(\mathbf{q}_n) \cdots b^\dagger(\mathbf{q}_1) |0\rangle, \tag{35}$$

where the discrete indices have been suppressed. As usual, it is postulated that

$$a_k(\mathbf{p}) |0\rangle = 0,$$
$$b_k(\mathbf{q}) |0\rangle = 0.$$

The operator N must now be interpreted as the difference between the number of particles and antiparticles (charge) since by using Eqs. (33) and their Hermitian conjugates,

$$N |\mathbf{p}_1, \cdots, \mathbf{p}_n; \mathbf{q}_1, \cdots, \mathbf{q}_m\rangle = (n - m) |\mathbf{p}_1, \cdots, \mathbf{p}_n; \mathbf{q}_1, \cdots, \mathbf{q}_m\rangle, \tag{36}$$

where now the q-number operators are defined in terms of a normal ordered current

$$O_l = \int d\sigma_\mu(x) :j_\mu(\bar{\psi}(x), \mathcal{O}_l(\partial)\psi(x)):, \tag{37}$$

with

$$:j_\mu(\bar{\psi}, \mathcal{O}_l(\partial)\psi): = \tfrac{1}{2}[j_\mu(\bar{\psi}, \mathcal{O}_l(\partial)\psi) \pm j_\mu(\ , (\mathcal{O}_l(\partial)\psi)\bar{\psi})]. \tag{38}$$

Here the $+/-$ sign is used for bosons/fermions and the second term in the brackets is the same as the first term except that $\bar{\psi}$ and all operations on it are written to the right of ψ.

An equivalent definition for the normal ordered product can be obtained by writing the fields as the sum of positive and negative energy parts

$$\begin{aligned} \psi(x) &= \psi_+(x) + \psi_-(x), \\ \bar{\psi}(x) &= \bar{\psi}_+(x) + \bar{\psi}_-(x), \end{aligned} \tag{39}$$

with

$$\begin{aligned} a_k(\mathbf{p}) &= \int d\sigma_\mu(x) j_\mu(\bar{u}_k(\mathbf{p}, x), \psi_+(x)), \\ b_k^\dagger(\mathbf{p}) &= \int d\sigma_\mu(x) j_\mu(\bar{v}_k(\mathbf{p}, x), \psi_-(x)), \\ a_k^\dagger(\mathbf{p}) &= \int d\sigma_\mu(x) j_\mu(\bar{\psi}_-(x), u_k(\mathbf{p}, x)), \\ b_k(\mathbf{p}) &= \int d\sigma_\mu(x) j_\mu(\bar{\psi}_+(x), v_k(\mathbf{p}, x)), \end{aligned} \tag{40}$$

since u_k and v_k project out the appropriate parts of ψ in Eq. (32). With these definitions

$$\begin{aligned} :j_\mu(\bar{\psi}, \mathcal{O}_l(\partial)\psi): = j_\mu(\bar{\psi}_+, \mathcal{O}_l(\partial)\psi_+) + j_\mu(\bar{\psi}_-, \mathcal{O}_l(\partial)\psi_-) \\ + j_\mu(\bar{\psi}_-, \mathcal{O}_l(\partial)\psi_+) \\ \pm j_\mu(\ , (\mathcal{O}_l(\partial)\psi_-)\bar{\psi}_+). \end{aligned} \tag{41}$$

The connection between Eq. (38) and Eq. (41) is somewhat tedious but straightforward. Because of Eqs. (40), following the proof of Theorem 2,

$$\begin{aligned} [a_k(\mathbf{p}), \psi_+(x)]_\pm &= [a_k(\mathbf{p}), \bar{\psi}_+(x)]_\pm = 0, \\ [a_k(\mathbf{p}), \bar{\psi}_-(x)]_\pm &= \bar{u}_k(\mathbf{p}, x), \\ [b_k^\dagger(\mathbf{p}), \psi_-(x)]_\pm &= [b_k^\dagger(\mathbf{p}), \bar{\psi}_-(x)]_\pm = 0, \\ [b_k(\mathbf{p}), \psi_-(x)]_\pm &= v_k(\mathbf{p}, x). \end{aligned} \tag{42}$$

These equations along with Eq. (40), in parallel to the proofs of Theorem 1, imply

$$[\psi_+(x), \bar{\psi}_-(y)]_\pm = G_+(x-y),$$
$$[\psi_-(x), \bar{\psi}_+(y)]_\pm = G_-(x-y), \tag{43}$$

with all other commutators equal to zero, where $G_+(x)$ and $G_-(x)$ are the positive and negative frequency parts of $G(x)$,

$$G(x) = G_+(x) + G_-(x),$$
$$D(\partial)G_\pm(x) = 0. \tag{44}$$

The equivalence of the two forms for the normal ordered product is then established by observing that the divergence of the right-hand sides of Eqs. (38) and (41) are equal. Therefore they differ by at most a c-number which may be taken equal to zero.

The q-number operators O_l, when operating on an n-particle state, give

$$O_l\,|\mathbf{p}_1, \cdots, \mathbf{p}_n\rangle = (n!)^{-\frac{1}{2}}[O_l, a^\dagger(\mathbf{p}_n)\cdots a^\dagger(\mathbf{p}_1)]_-\,|0\rangle. \tag{45}$$

However, from Eq. (37) and Theorem 2,

$$[O_l, a^\dagger(\mathbf{p})] = \int d\sigma_\mu(x) j_\mu(\bar{\psi}(x), \mathcal{O}_l(\partial)u(\mathbf{p}, x))$$
$$= \mathcal{O}_l(\mathbf{p})a^\dagger(\mathbf{p}), \tag{46}$$

where $\mathcal{O}_l(\mathbf{p})$ is the eigenvalue

$$\mathcal{O}_l(\partial)u(\mathbf{p}, x) = \mathcal{O}_l(\mathbf{p})u(\mathbf{p}, x). \tag{47}$$

Therefore Eq. (45) becomes

$$O_l\,|\mathbf{p}_1, \cdots, \mathbf{p}_n\rangle = \sum_{i=1}^{n}\mathcal{O}_l(p_i)\,|\mathbf{p}_1, \cdots, \mathbf{p}_n\rangle, \tag{48}$$

as expected.

It is also possible to define the charge conjugation operation as

$$Ca_k(\mathbf{p})C^{-1} = b_k(\mathbf{p}),$$
$$C\psi(x)C^{-1} = \mathcal{C}\psi^\dagger \equiv \psi^c, \tag{49}$$

where

$$v_k(\mathbf{p}, x) = \mathcal{C}u_k^*(\mathbf{p}, x),$$
$$u_k(\mathbf{p}, x) = \mathcal{C}v_k^*(\mathbf{p}, x), \tag{50}$$

and $\dagger$ means Hermitian-conjugate the Fock space part of ψ and complex-conjugate the c-number part. Equations (49) can then be used in conjunction with Eqs. (32) to show

$$j_\mu(\bar{u}_k(\mathbf{p}, x), \psi^c(x)) = j_\mu(\bar{\psi}(x), v_k(\mathbf{p}, x)). \tag{51}$$

This in turn requires that

$$\mathcal{C}D^*(\partial)\mathcal{C}^{-1} = -D(\partial),$$
$$\mathcal{C}^\dagger\gamma_4\mathcal{C}^{-1} = -\gamma_4^*. \tag{52}$$

These last equations are in agreement with the standard treatment.[5]

IV. REDUCTION FORMULAS AND VACUUM EXPECTATION VALUES

The definitions of the Fock space operators given in Eqs. (32) provide a natural starting point for developing reduction formulas for field operators satisfying the inhomogeneous equation

$$\vec{D}(\partial)\psi(x) = J(x). \tag{53}$$

Corresponding to free field operators $\psi_{\text{in}}(x)$, $\psi_{\text{out}}(x)$ satisfying Eq. (11), the Fock space operators a_{in}, a_{out} are defined by

$$a_{\substack{\text{in}\\\text{out}}}(\mathbf{p}) = \int d\sigma_\mu(x) j_\mu(\bar{u}(\mathbf{p}, x), \psi_{\substack{\text{in}\\\text{out}}}(x)); \tag{54}$$

corresponding to operators $\psi(x)$ satisfying Eq. (53), the operator $a(\mathbf{p}, \sigma)$ is

$$a(\mathbf{p}, \sigma) = \int d\sigma_\mu(x) j_\mu(\bar{u}(\mathbf{p}, x), \psi(x)), \tag{55}$$

where $u(\mathbf{p}, x)$ is any wave packet c-number solution to Eq. (1). The operators $a_{\text{in}}(\mathbf{p})$, $a_{\text{out}}(\mathbf{p})$, and $a(\mathbf{p}, \sigma)$ are then related by the weak limit condition[10]

$$a_{\substack{\text{in}\\\text{out}}}(\mathbf{p}) = \lim_{\sigma\to\mp\infty} a(\mathbf{p}, \sigma). \tag{56}$$

Consider the scattering matrix element for an initial configuration

$$|\mathbf{p}, \alpha\rangle_{\text{in}} = a_{\text{in}}^\dagger(\mathbf{p})\,|\alpha\rangle_{\text{in}}, \tag{57}$$

and a final configuration

$$|\mathbf{q}, \beta\rangle_{\text{out}} = a_{\text{out}}^\dagger(\mathbf{q})\,|\beta\rangle, \tag{58}$$

with

$$a_{\text{in}}(\mathbf{p})\,|\alpha\rangle_{\text{in}} = a_{\text{out}}(\mathbf{p})\,|\beta\rangle_{\text{out}} = 0, \tag{59}$$

and the S matrix defined by

$$S(\mathbf{q}, \beta \mid \mathbf{p}, \alpha) = {}_{\text{out}}\langle \mathbf{q}, \beta \mid \mathbf{p}, \alpha\rangle_{\text{in}}. \tag{60}$$

Using the standard techniques for deriving reduction formulas,[11] it is found that

$$S(\mathbf{q}, \beta \mid \mathbf{p}, \alpha) = {}_{\text{out}}\langle\beta \mid a_{\text{in}}(\mathbf{q}) \mid \mathbf{p}, \alpha\rangle_{\text{in}}$$
$$+ \int dx\; {}_{\text{out}}\langle\beta|\,\frac{\partial}{\partial x_0}\,j_0(\bar{u}(\mathbf{q}, x), \psi(x))\,|\mathbf{p}, \alpha\rangle_{\text{in}}. \tag{61}$$

Since the divergence of the current $j_\mu(\bar{u}(\mathbf{q}, x), \psi(x))$ is just

$$\frac{\partial}{\partial x_\mu}\,j_\mu(\bar{u}(\mathbf{q}, x), \psi(x)) = \bar{u}(\mathbf{q}, x)J(x) = \bar{u}(\mathbf{q}, x)\vec{D}(\partial)\psi(x), \tag{62}$$

Eq. (61) can be rewritten

$$S(\mathbf{q}, \beta \mid \mathbf{p}, \alpha) = {}_{\text{out}}\langle\beta|\,[a_{\text{in}}(\mathbf{q}), a_{\text{in}}^\dagger(\mathbf{p})]_\pm\,|\alpha\rangle_{\text{in}}$$
$$+ \int dx\; \bar{u}(\mathbf{q}, x)\vec{D}(\partial_x)\;{}_{\text{out}}\langle\beta|\,\psi(x)\,|\mathbf{p}, x\rangle_{\text{in}}. \tag{63}$$

Continuing with the standard procedure we find that

$$S(\mathbf{q},\beta\mid\mathbf{p},\alpha)={}_{\text{out}}\langle\beta|\,[a_{\text{in}}(\mathbf{q}),a_{\text{in}}^{\dagger}(\mathbf{p})]_{\pm}\,|\alpha\rangle_{\text{in}}-\iint dx\,dy\bar{u}(\mathbf{q},x)\vec{D}(\partial_x)\,{}_{\text{out}}\langle\beta|\,\frac{\partial}{\partial y_0}\times j_0(T[\psi(x)\bar{\psi}(y)],u(\mathbf{p},y))\,|\alpha\rangle_{\text{in}},\quad(64)$$

where T indicates the time ordered product. However, it is clear from the form of j_μ that

$$\frac{\partial}{\partial y_\mu}j_\mu(T[\psi(x)\bar{\psi}(y)],u(\mathbf{p},y))=-T[\psi(x)\bar{\psi}(y)]\overleftarrow{D}(-\partial_y)u(\mathbf{p},y).\quad(65)$$

Thus it is found that the reduction formula for fields satisfying Eq. (53) is

$$S(\mathbf{q},\beta\mid\mathbf{p},\alpha)={}_{\text{out}}\langle\beta|\,[a_{\text{in}}(\mathbf{q}),a_{\text{in}}^{\dagger}(\mathbf{p})]_{\pm}\,|\alpha\rangle_{\text{in}}+\iint dx\,dy\bar{u}(\mathbf{q},x)\vec{D}(\partial_x)\times{}_{\text{out}}\langle\beta|\,T[\psi(x)\bar{\psi}(y)]\,|\alpha\rangle_{\text{in}}\,\overleftarrow{D}(-\partial_y)u(\mathbf{p},y).\quad(66)$$

Evidently this procedure can be continued until the vacuum expectation is reached. For example,

$$\begin{aligned}&{}_{\text{out}}\langle q_1\cdots q_n\mid p_1\cdots p_m\rangle_{\text{in}}\\&=\int dx_1\cdots\int dx_n\int dy_1\cdots\int dy_m\bar{u}(\mathbf{q}\ ,x_1)\cdots\bar{u}(\mathbf{q}_n,x_n)\\&\quad\times\vec{D}(\partial_{x_1})\cdots\vec{D}(\partial_{x_n})\\&\quad\times\langle 0|\,T\psi(x_1)\cdots\psi(x_n)\bar{\psi}(y_1)\cdots\bar{\psi}(y_m)\,|0\rangle\\&\quad\times\overleftarrow{D}(-\partial_{y_1})\cdots\overleftarrow{D}(-\partial_{y_m})u(p_1,y_1)\cdots u(p_m,y_m),\end{aligned}\quad(67)$$

where forwardlike scattering terms have been neglected.

The vacuum expectation value for the time ordered product follows just as for Klein-Gordon or Dirac theory. By definition

$$\langle 0|\,T[\psi(x)\bar{\psi}(y)]\,|0\rangle=\theta(x-y)\,\langle 0|\,\psi(x)\bar{\psi}(y)\,|0\rangle\mp\theta(y-x)\,\langle 0|\,\bar{\psi}(y)\psi(x)\,|0\rangle.\quad(68)$$

However, from Eqs. (40) and (43),

$$\langle 0|\,\psi(x)\bar{\psi}(y)\,|0\rangle=\langle 0|\,[\psi_+(x),\bar{\psi}_-(y)]_{\pm}\,|0\rangle=G_+(x-y),\quad(69)$$

$$\langle 0|\,\bar{\psi}(y)\psi(x)\,|0\rangle=\langle 0|\,[\bar{\psi}_+(y),\psi_-(x)]_{\pm}\,|0\rangle=G_-(x-y).\quad(70)$$

Consequently Eq. (68) becomes

$$\langle 0|\,T[\psi(x)\bar{\psi}(y)]\,|0\rangle=\theta(x-y)G_+(x-y)-\theta(y-x)G_-(x-y)\quad(71)$$

in analogy to the Feynman propagator for the spin-0 and -½ cases.

This result may be extended to the time ordered product of any number of field operators by Wick's theorem[12] or by using a functional differentiation technique.[13] Feynman rules can therefore be constructed for any field that has a conserved current of the type discussed here. Weinberg[6] has already treated the subject of high spin propagators in detail.

V. DISCUSSION

A quantization procedure has been presented which does not depend on the canonical formalism and which is more general in that the Fock space operators create and annihilate particles that have internal degrees of freedom or whose wavefunctions are arbitrary wave packets. Since the spinors $u(\mathbf{p},x)$ can always be expressed in terms of their plane wave counter parts through the use of form factors, form factors enter into a scattering calculation based on the formalism of the preceding section in a very natural way.

The formalism also applies for a superposition of fields. For example, consider the field operator ψ,

$$(\gamma p-im_1)(\gamma p-im_2)\psi=0.\quad(72)$$

It is apparent that ψ is any linear combination of fields φ_1 and φ_2:

$$\begin{aligned}(\gamma p-im_1)\varphi_1&=0,\\(\gamma p-im_2)\varphi_2&=0.\end{aligned}\quad(73)$$

The invariant integral associated with Eq. (72) is

$$I=\frac{m_1+m_2}{m_1-m_2}\int d\mathbf{x}\times\left\{\bar{\varphi}_2(x)\gamma_4\varphi_1(x)+\frac{i}{m_1+m_2}\left[\bar{\varphi}_2(x)\frac{\overleftrightarrow{\partial}}{\partial t}\varphi_1(x)\right]\right\},\quad(74)$$

where

$$\bar{\varphi}_2(x)\frac{\overleftrightarrow{\partial}}{\partial t}\varphi_1(x)=\left(\frac{\partial}{\partial t}\varphi_2(x)\right)\varphi_1(x)-\bar{\varphi}_2(x)\frac{\partial}{\partial t}\varphi_1(x).$$

Consequently, annihilation operators can be defined according to Eqs. (11),

$$a(p)=\frac{m_1+m_2}{m_1-m_2}\int d\mathbf{x}\times\left\{\bar{u}(p,x)\gamma_4\psi(x)+\frac{i}{m_1+m_2}\left[\bar{u}(p,x)\frac{\overleftrightarrow{\partial}}{\partial t}\psi(x)\right]\right\},\quad(75)$$

where $u(p,x)$ is a c-number solution of Eq. (72) and consequently any linear combinations of c-number solutions of Eq. (73). The same process can be repeated for Eq. (73):

$$a_1(p) = \int d\mathbf{x}\bar{u}_1(p, x)\gamma_4\varphi_1(x),$$
$$a_2(p) = \int d\mathbf{x}\bar{u}_2(p, x)\gamma_4\varphi_2(x). \qquad (76)$$

It is then a straightforward calculation to show that if

$$\psi = A_1\varphi_1 + A_2\varphi_2,$$
$$u = B_1u_1 + B_2u_2,$$

then

$$a(p) = A_2B_2^*a_2(p) - A_1B_1^*a_1(p). \qquad (77)$$

Thus Eqs. (75) and (76) are equivalent.

ACKNOWLEDGMENTS

The authors wish to acknowledge the many helpful discussions with their colleagues Dr. David S. Moroi of Kent State University and Dr. Derek Pursey of Iowa State University.

APPENDIX

Given that $\psi(x)$ satisfies an equation

$$\vec{D}(\partial)\psi(x) = 0, \qquad (\text{A1})$$

from which a conserved current can be derived, and given an invariant Green's function $G(x)$ where

$$G(x) = G_a(x) - G_r(x), \qquad (\text{A2})$$
$$\vec{D}(\partial_x)G_{a,r}(x - y) = -\delta(x - y), \qquad (\text{A3})$$
$$G_{a,r}(x) = 0 \quad \text{for} \quad x_0 \gtrless 0, \qquad (\text{A4})$$

then $\psi(x)$ can be expressed as

$$\psi(x) = \int d\sigma_\mu(y)j_\mu(G(x - y), \psi(y)). \qquad (\text{A5})$$

Proof: It is convenient to rewrite Eqs. (A1) and (A3) as

$$\vec{D}(\partial)\psi(y) = 0, \qquad (\text{A6})$$
$$G_{a,r}(x - y)\overleftarrow{D}(-\partial_y) = -\delta(x - y), \qquad (\text{A7})$$

where Eq. (A7) follows from Eq. (A3) by the fact that the right-hand side of Eq. (A3) is diagonal. It is readily seen that

$$\frac{\partial}{\partial y_\mu}j_\mu(G_{a,r}(x - y), \psi(y)) = \delta(x - y)\psi(y) \quad (\text{A8})$$

from the form of j_μ. Integrating Eq. (A8) from $y_0 < x_0$ to $y_0 > x_0$ and over all space yields

$$\int d\mathbf{y}j_0(G_{a,r}(x - y), \psi(y))\Big|_{y_0<x_0}^{y_0>x_0} = \psi(x). \qquad (\text{A9})$$

Then from Eq. (A4),

$$\int_{y_0>x_0} d\mathbf{y}j_0(G_a(x - y), \psi(y)) = \psi(x), \qquad (\text{A10a})$$
$$\int_{y_0<x_0} d\mathbf{y}j_0(G_r(x - y), \psi(y)) = -\psi(x). \quad (\text{A10b})$$

Using the definition of $G(x)$, Eqs. (A10) can be combined to give

$$\int d\mathbf{y}j_0(G(x - y), \psi(y)) = \psi(x) \qquad (\text{A11})$$

for all x_0 and y_0. By generalizing $d\mathbf{x}$ to an arbitrary hypersurface, Eq. (A11) can be written

$$\int d\sigma_\mu(y)j_\mu(G(x - y), \psi(y)) = \psi(x). \qquad (\text{A12})$$

* Work performed in the Ames Laboratory of the U.S. Atomic Energy Commission, contribution No. 2629.

[1] See, e.g., S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row Peterson, Elmsford, N.Y., 1961).

[2] J. Schwinger, Phys. Rev. **74**, 1439 (1948).

[3] R. E. Peierls, Proc. Roy. Soc. (London) **A214**, 143 (1952).

[4] Y. Takahashi and H. Umezawa, Progr. Theoret. Phys. (Kyoto) **9**, 14 (1953).

[5] T. J. Nelson and R. H. Good, Jr., Rev. Mod. Phys. **40**, 508 (1968).

[6] S. Weinberg, Phys. Rev. **133**, B1318 (1964).

[7] C. L. Hammer, S. C. McDonald, and D. L. Pursey, Phys. Rev. **171**, 1349 (1968).

[8] See Y. Takahashi, *An Introduction to Field Quantization* (Pergamon, London, 1969), Chap. IV. He also defines a conserved current which is subsequently used to define invariant integrals representing the physical observables.

[9] If the u_k are a complete set of orthonormal functions, then

$$\psi(x) = \sum_k \int d\mathbf{p}a_k(\mathbf{p})u_k(\mathbf{p}, x).$$

Substitution for $a_k(\mathbf{p})$ from Eq. (11) gives rise to the completeness relationship

$$\sum_k \int d\mathbf{p}u_k(p, x)\bar{u}_k(p, y) = G(x - y).$$

The proof parallels the proof leading to Eq. (21).

[10] H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo Cimento **11**, 342 (1954).

[11] See Ref. 1, pp. 692–94.

[12] See Ref. 1, p. 435.

[13] See, e.g., S. Gasiorowicz, *Elementary Physics* (Wiley, New York, 1966), p. 121.

Nonlinear Spinor Equation and Asymmetric Connection in General Relativity

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(Received 17 August 1970)

In order to take full account of spin in general relativity, it is necessary to consider space-time as a metric space *with* torsion, as was shown elsewhere. We treat a Dirac particle in such a space. The generalized Dirac equation turns out to be of a Heisenberg-Pauli type. The nonlinear terms induced by torsion express a universal spin-spin interaction of range zero.

1. INTRODUCTION

The realization that momentum and spin angular momentum are, in a certain sense, quantities of the same kind suggests a generalization of the general theory of relativity which encompasses spin angular momentum.[1-4] Momentum is a dynamic quantity which corresponds to translation, whereas spin angular momentum corresponds to rotation. If one further observes that in differential geometry the metric tensor field is related in a definite way to translations and the torsion tensor field to rotations, one is led to consider a geometry with curvature *and torsion* (Riemann-Cartan geometry) in place of the Riemannian geometry.[5,6]

The physical model now proposed is as follows: The matter-free space-time continuum has neither curvature nor torsion and therefore possesses Minkowskian structure. (This is merely a model. Strictly speaking, according to general relativity, space-time does not exist in the absence of matter.) Imagine that in this space-time continuum matter with momentum and spin angular momentum is introduced and distributed continuously. Owing to the influence of matter, curvature and torsion are produced. The curvature can be derived from metric and torsion in a well-known way. Hence, there should exist functional relationships between momentum and spin angular momentum on one side and metric and torsion on the other side. These relationships are the field equations (generalized Einstein field equations); the momentum and the spin angular momentum densities appear as the sources of the metric and torsion fields.

The solutions of these equations are of the following type: Given the densities of momentum and spin angular momentum, the metric and torsion fields are to be found. These solutions obviously touch only a part of the physical problem. Therefore, one should also be able to calculate the momentum and the spin angular momentum densities from the physical conditions. These conditions could perhaps be given in terms of the (classical) wave amplitude of matter on a spacelike hypersurface. What one still needs in the theory are the matter equations. (These are of course not entirely independent of the field equations.)

The field equations as well as the matter equations will be derived from a variational principle. In order to obtain the conventional form of general relativity in the case of vanishing spin, one introduces a Lagrangian density which is the sum of the field Lagrangian and the matter Lagrangian. The field Lagrangian density is determined by metric and torsion; the usual arguments of simplicity lead to the curvature density. The material Lagrangian density can be obtained from that of special relativity by minimal coupling to metric and torsion, i.e., the partial derivatives are replaced by the derivatives which are covariant with respect to the curved and contorted Riemann-Cartan space-time.

In this paper, we treat a classical *Dirac field* in the way discussed above; hence the matter field will be represented by a four-component spinor.

Note added in proof: The whole theory for arbitary matter fields is represented in an article by one of the authors (F. W. Hehl, "Spin und Torsion in der Allgemeinen Relativitätstheorie Oder die Riemann-Cartansche Geometrie der Welt," Habilitation thesis TU Clausthal, 1970). An English version has been submitted for publication to Fortsch Physik.

In accord with these preliminary remarks, we set up the theory in the following way.

In Sec. 2 we summarize all the geometrical apparatus necessary for our theory. In Sec. 3 we introduce in a well-known manner orthonormal tetrads as anholonomic coordinates in the space-time under consideration. This allows us to define the covariant differentiation of a spinor in a straightforward way.

In Sec. 4 we introduce the action function of a Dirac particle interacting with a gravitational field. We explicitly compute the additional terms characteristic for our non-Riemannian geometry. Through a variational procedure we deduce the field equations in Sec. 5 and the matter equations which constitute the generalized Dirac equation in Sec. 6. Eliminating the contortion in the Dirac equation, we arrive at a nonlinear spinor equation of the Heisenberg–Pauli type, thereby generalizing somewhat similar results obtained first by Rodichev.[7]

After the general theory, in Sec. 7 we work out and stress the difference between conventional general relativity and our non-Riemannian theory. The torsion terms in the action function and therefore the nonlinear term in the spinor equation are recognized as corresponding to a universal spin–spin contact interaction. We propose to regard this universal spin–spin interaction as a classical model of weak interaction.

2. RIEMANN–CARTAN GEOMETRY

As was shown elsewhere,[3,4] it is reasonable to assume for the affine connection of space–time the expression

$$\Gamma^k_{ij} = \{{}_i{}^k{}_j\} + S_{ij}{}^k - S_j{}^k{}_i + S^k{}_{ij}. \tag{2.1}$$

In our notation we essentially follow the book of Schouten.[8] The physical conventions are taken from Landau-Lifshitz.[9] In (2.1), $\{{}_i{}^k{}_j\}$ is Christoffel's symbol of the second kind belonging to the metric g_{ij}. Cartan's torsion tensor is defined according to

$$S_{ij}{}^k = \tfrac{1}{2}(\Gamma^k_{ij} - \Gamma^k_{ji}) \equiv \Gamma^k_{[ij]}. \tag{2.2}$$

Latin indices run from 0 to 3. With the contortion tensor

$$K_{ij}{}^k = -S_{ij}{}^k + S_j{}^k{}_i - S^k{}_{ij}, \tag{2.3}$$

(2.1) can be written as

$$\Gamma^k_{ij} = \{{}_i{}^k{}_j\} - K_{ij}{}^k. \tag{2.4}$$

We remark that (2.1) and therefore (2.4) are equivalent to the relation

$$\nabla_i g_{jk} = 0. \tag{2.5}$$

The manifold equipped with a connection of the form (2.1) will be called a U_4 ("Riemann–Cartan space"). It is the most general metric space with a linear affine connection. For vanishing torsion we arrive at a Riemannian space V_4.

The Riemann–Christoffel curvature tensor is defined in the usual way as

$$R_{ijk}{}^l = 2\partial_{[i}\Gamma^l_{j]k} + 2\Gamma^l{}_{[i|m|}\Gamma^m_{j]k}. \tag{2.6}$$

The first two identities of the curvature tensor are valid in each affine space:

$$\tfrac{1}{2}(R_{ijk}{}^l + R_{jik}{}^l) \equiv R_{(ij)k}{}^l = 0, \tag{2.7}$$

$$R_{[ijk]}{}^l = 2\nabla_{[i}S_{jk]}{}^l - 4S_{[ij}{}^m S_{k]m}{}^l. \tag{2.8}$$

The third identity for a U_4 reads

$$R_{ij(kl)} = 0. \tag{2.9}$$

For these and other formulas the book of Schouten[8] should be referred to. Bianchi's identity is given by

$$\nabla_{[i}R_{jk]l}{}^m = 2S_{[ij}{}^n R_{k]nl}{}^m. \tag{2.10}$$

We define the Ricci tensor $R_{ij} = R_{kij}{}^k$ and the Einstein tensor as

$$G_{ij} = R_{ij} - \tfrac{1}{2}g_{ij}R_k{}^k. \tag{2.11}$$

For a V_4 (2.8) with (2.9) *inter alia* tells us that the antisymmetric part of the Einstein tensor vanishes; but not so for a U_4. We contract (2.8) and get

$$\tfrac{3}{2}R_{[kij]}{}^k = \overset{*}{\nabla}_k T_{ij}{}^k, \tag{2.12}$$

where we have introduced a modified torsion tensor

$$T_{ij}{}^k = S_{ij}{}^k + \delta^k_i S_{jl}{}^l - \delta^k_j S_{il}{}^l \tag{2.13}$$

and used the notation

$$\overset{*}{\nabla}_i = \nabla_i + 2S_{ik}{}^k. \tag{2.14}$$

(2.12) together with (2.9) and (2.11) yields

$$\overset{*}{\nabla}_k T_{ij}{}^k - G_{[ij]} = 0. \tag{2.15}$$

As we have shown,[4] (2.15) is the geometrical image of the angular momentum conservation theorem.

Bianchi's identity can also be written in a contracted form. Using (2.10), (2.11), and (2.13) we get

$$\overset{*}{\nabla}_j G_i{}^j + 2S_{ji}{}^k G_k{}^j = T_{jk}{}^l R_{il}{}^{jk}. \tag{2.16}$$

Of course this relation corresponds to energy–momentum conservation; therefore the right-hand side will represent a certain volume force density apart from a dimensional factor.

3. TETRADS AS ANHOLONOMIC COORDINATES

Equation (2.1) determines the geometry of space–time. There is nothing in our formalism like an independent tetrad connection or similar entities often described in the literature. Thus there is no place for the so-called Palatini formalism in our theory. We prefer the method worked out for instance in Ref. 7. The independent geometrical quantities describing the U_4 are metric and torsion (or contortion). One is then able to introduce anholonomic coordinates. Let us choose at each point a tetrad $e_\alpha{}^i$. $\alpha = 1, 2, 3, 4$, numbers the four different and linearly independent vectors. Because we treat a metric space, it is convenient to use (pseudo-)orthonormal tetrads. This yields the relations ($e^\beta{}_j$ is the reciprocal of $e_\alpha{}^i$):

$$e_\alpha{}^i e^\alpha{}_j = \delta^i_j, \quad e_\alpha{}^i e^\beta{}_i = \delta^\beta_\alpha, \tag{3.1}$$

$$e_\alpha{}^i = g_{\alpha\beta} g^{ij} e^\beta{}_j, \quad g_{\alpha\beta} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 \end{pmatrix}. \tag{3.2}$$

The object of anholonomity

$$\Omega^\gamma_{\alpha\beta} = e_\alpha{}^i e_\beta{}^j \partial_{[i} e^\gamma{}_{j]}, \quad \Omega_{\alpha\beta\gamma} = g_{\gamma\delta} \Omega^\delta_{\alpha\beta} \tag{3.3}$$

depends on the coordinates we chose.

The reason for introducing orthonormal tetrads is the following. As is well known, tensors are connected with the group of general coordinate transformations. Accordingly, there exists no necessity for introducing anholonomic coordinates for computations with tensors in the U_4. Spinors, however, are connected with the Lorentz group. We are compelled therefore to define at each point of the U_4 a tangent Minkowski space R_4 via the tetrads $e_\alpha{}^i$. This procedure cannot be circumvented in principle because of the very nature of spinors mentioned above. The details of this discussion will be worked out in a forthcoming publication.

The covariant derivative in anholonomic coordinates reads

$$\nabla_\alpha \psi = \partial_\alpha \psi + \Gamma^\gamma_{\alpha\beta} f_\gamma{}^\beta \psi. \tag{3.4}$$

Because of (3.1) and (3.2) the operator $f_\gamma{}^\beta$ describes the behavior of ψ under an infinitesimal Lorentz transformation δx^γ:

$$\delta\psi = \partial_\beta(\delta x^\gamma) f_\gamma{}^\beta \psi. \tag{3.5}$$

If we remember (3.1) and (3.2), the connection (2.1) expressed in anholonomic coordinates is given by

$$\Gamma_{\alpha\beta\gamma} = g_{\gamma\delta}\Gamma^\delta_{\alpha\beta} = -\Omega_{\alpha\beta\gamma} + \Omega_{\beta\gamma\alpha} - \Omega_{\gamma\alpha\beta} - K_{\alpha\beta\gamma}. \tag{3.6}$$

This yields the formulas

$$\Gamma_{\alpha(\beta\gamma)} = 0, \tag{3.7}$$

$$\Gamma_{[\alpha\beta\gamma]} = -\Omega_{[\alpha\beta\gamma]} - K_{[\alpha\beta\gamma]} \tag{3.8}$$

$$g^{\beta\gamma}\Gamma_{\beta\gamma\alpha} = -2\Omega^\beta_{\alpha\beta} + K_{\beta\alpha}{}^\beta. \tag{3.9}$$

Let us define for later use the scalar density

$$e = (-\det g_{ij})^{\frac{1}{2}} = \det(e^\alpha{}_i). \tag{3.10}$$

The definition of the determinant together with (3.1) leads to

$$(\partial_\alpha e)/e = e_\beta{}^k \partial_\alpha e^\beta{}_k. \tag{3.11}$$

Later we will also be concerned with the ordinary divergence of tetrads. With (3.1), (3.3), and (3.11) we arrive at

$$\partial_k e_\alpha{}^k = 2\Omega^\beta_{\alpha\beta} - e_\beta{}^k \partial_\alpha e^\beta{}_k = 2\Omega^\beta_{\alpha\beta} - (\partial_\alpha e)/e. \tag{3.12}$$

Let us now turn to 4-spinors, because we want to treat a Dirac particle in a U_4. From Corson,[10] for instance, we get

$$f_{\alpha\beta} = \tfrac{1}{4}\gamma_{[\alpha}\gamma_{\beta]} \tag{3.13}$$

with the well-known Dirac matrices. Covariant differentiation of a 4-spinor is hence given by

$$\nabla_\alpha \psi = \partial_\alpha \psi - \tfrac{1}{4}\Gamma_{\alpha\beta\gamma}\gamma^\beta\gamma^\gamma\psi. \tag{3.14}$$

The derivative of the Dirac adjoint $\psi^+ = \psi^*\gamma_4$ can be calculated easily:

$$\nabla_\alpha \psi^+ = \partial_\alpha \psi^+ - \tfrac{1}{4}\Gamma_{\alpha\beta\gamma}\psi^+\gamma^\gamma\gamma^\beta. \tag{3.15}$$

For later purpose we also introduce a covariant derivative with respect to a V_4:

$$\overset{\{\}}{\nabla}_\alpha \psi = \partial_\alpha\psi + \tfrac{1}{4}(\Omega_{\alpha\beta\gamma} - \Omega_{\beta\gamma\alpha} + \Omega_{\gamma\alpha\beta})\gamma^\beta\gamma^\gamma\psi. \tag{3.16}$$

4. ACTION FUNCTION OF A DIRAC PARTICLE INTERACTING WITH A GRAVITATIONAL FIELD

For the special relativistic Lagrangian density of a Dirac particle we use the usual expression in a R_4, given, for example, in Ref. 10. Instead of taking the partial derivatives, we substitute the covariant ones of (3.14) and (3.15) in the sense of minimal coupling to metric and torsion. This results in ($2\pi\hbar$ = Planck's constant, c = velocity of light, $\hbar m/c$ = mass of the electron)

$$\mathfrak{L} = -e(i\hbar c/2)[(\nabla_\alpha\psi^+)\gamma^\alpha\psi - \psi^+\gamma^\alpha\nabla_\alpha\psi + 2im\psi^+\psi]. \tag{4.1}$$

Hence, we assume that Pauli-type terms do not enter (4.1). Substituting (3.14) and (3.15) in (4.1) and noting (3.16), we have

$$\mathfrak{L} = -e(i\hbar c/2)[(\overset{\{\}}{\nabla}_\alpha\psi^+)\gamma^\alpha\psi - \psi^+\gamma^\alpha\overset{\{\}}{\nabla}_\alpha\psi + 2im\psi^+\psi] + e(i\hbar c/4)K_{\alpha\beta\gamma}\psi^+\gamma^{[\alpha|}\gamma^\beta\gamma^{|\gamma]}\psi. \tag{4.2}$$

The first term on the right-hand side is identically the same as one would get in a V_4 or already in a R_4 in curvilinear coordinates. The second term can be simplified using the formula

$$\gamma^\alpha\gamma^\beta\gamma^\gamma = \gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]} + g^{\alpha\beta}\gamma^\gamma + g^{\beta\gamma}\gamma^\alpha - g^{\gamma\alpha}\gamma^\beta \tag{4.3}$$

or more specifically

$$\gamma^{[\alpha|}\gamma^\beta\gamma^{|\gamma]} = \gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]}, \tag{4.4}$$

which follows from the anticommutation relations for the γ's. Thus, we have for (4.2)

$$\mathfrak{L} = \mathfrak{L}(\{\}) - e(i\hbar c/4)\psi^+\gamma^{[\gamma}\gamma^\beta\gamma^{\alpha]}\psi K_{\alpha\beta\gamma}. \quad (4.5)$$

A similar consideration leads to the equivalent expression

$$\mathfrak{L} = \mathfrak{L}(\partial_\alpha) + e(i\hbar c/4)\psi^+\gamma^{[\gamma}\gamma^\beta\gamma^{\alpha]}\psi\Gamma_{\alpha\beta\gamma}, \quad (4.6)$$

where $\mathfrak{L}(\partial_\alpha)$ is the Lagrangian (4.1), but with the difference that partial derivatives replace the covariant ones.

According to the general theory treated in Refs. 3 and 4, spin angular momentum $\tau_{ij}{}^k$ is coupled to the contortion of the U_4:

$$e\tau_k{}^{ji} = \delta\mathfrak{L}/\delta K_{ij}{}^k. \quad (4.7)$$

(4.5) and (4.7) yield

$$\tau^{\alpha\beta\gamma} = e^\alpha{}_i e^\beta{}_j e^\gamma{}_k \tau^{ijk} = \tau^{[\alpha\beta\gamma]} = -\frac{i\hbar c}{4}\psi^+\gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]}\psi. \quad (4.8)$$

This is the well-known canonical spin angular momentum as required by the theory of Refs. 1, 2, and 4. It is totally antisymmetric and hence has only four independent components. Thus (4.5) and (4.6) can be written in the form

$$\mathfrak{L} = \mathfrak{L}(\{\}) + e\tau^{\gamma\beta\alpha}K_{\alpha\beta\gamma} = \mathfrak{L}(\partial_\alpha) - e\tau^{\gamma\beta\alpha}\Gamma_{\alpha\beta\gamma}. \quad (4.9)$$

(In spite of some other remarks in the literature, a material Lagrangian density generally contains a third term depending on the contortion. A formula of the type (4.9) is valid only if the spin is independent of contortion, as in Dirac's case. This remark is not crucial, however, because the mentioned third term represents only a correction.)

Let the field Lagrangian be given by

$$\mathfrak{R} = eR_k{}^k. \quad (4.10)$$

This is the only scalar density which can be derived from the curvature tensor by contraction. Additional torsion-dependent terms[4] destroy the simplicity of the theory. Thus (4.10) is suggested by analogy with conventional relativity. A straightforward but lengthy calculation reveals that (4.10) can be separated into a Riemannian and a torsion part:

$$\mathfrak{R} = \mathfrak{R}(\{\}) + \partial_i(2eK_k{}^{ik}) - eT_k{}^{ji}K_{ij}{}^k. \quad (4.11)$$

Since in what follows we do not vary on the boundary of the integration volume of the action function, we can forget the divergence in (4.11). The last term of (4.11) can be written in anholonomic coordinates as well.

Correspondingly the total action function is given by

$$W = \frac{1}{c}\int d\Omega\left[\mathfrak{L}(\{\}) + e\tau^{\gamma\beta\alpha}K_{\alpha\beta\gamma} + \frac{1}{2k}\mathfrak{R}(\{\}) - \frac{e}{2k}T^{\gamma\beta\alpha}K_{\alpha\beta\gamma}\right], \quad (4.12)$$

where $kc^4/8\pi$ is Newton's gravitational constant. Observe that we get two different additional terms characteristic for a U_4: a term coupling spin and contortion and a term quadratic in the contortion. (Using a tetrad formalism and quantizing a Dirac particle interacting with a gravitational field, Kibble[11] and Kannenberg and Arnowitt[12] subtracted out such terms, because they wanted to have the Riemannian result. The same is true for Lemmer,[13] who quantized a general matter field under the same conditions.)

Rodichev[7] was the first who stated an action function similar to (4.12). He treated the case of $\mathfrak{R}(\{\}) = 0$, which leads to a sort of a teleparallelism, and required the torsion to be totally antisymmetric *a priori*, which is not necessary in our theory. See also Braunss[14] for an interpretation of Rodichev's results. For vanishing spin the theory presented here simplifies to ordinary general relativity; furthermore the constant in front of the last term of (4.12) is specified. For related papers with action functions resembling (4.12), in which torsion is considered more as a secondary concept, see Peres,[15] Lenoir,[16] and Wainwright.[17,18]

5. FIELD EQUATIONS

We must now vary (4.12) with respect to $e^\alpha{}_i$ and $K_{ij}{}^k$ and equate the variations to zero as required by Hamilton's principle. This yields

$$\frac{\delta\mathfrak{L}}{\delta e^\alpha{}_i}e^\beta{}_i \stackrel{\text{def}}{=} e\sigma_\alpha{}^\beta = -\frac{1}{2k}\frac{\delta\mathfrak{R}}{\delta e^\alpha{}_i}e^\beta{}_i, \quad (5.1)$$

$$\frac{\delta\mathfrak{L}}{\delta K_{ij}{}^k} \stackrel{\text{def}}{=} e\tau_k{}^{ji} = -\frac{1}{2k}\frac{\delta\mathfrak{R}}{\delta K_{ij}{}^k}. \quad (5.2)$$

Here the left-hand side of (5.1) is by definition the metric energy–momentum density $e\sigma_\alpha{}^\beta$ and the left-hand side of (5.2) the spin angular momentum density according to (4.7).

Notice that $\mathfrak{R}$ depends on $e^\alpha{}_i$ only via g_{kl}. Thus we can use the variational method worked out in detail in Ref. 4. If we define the canonical energy–momentum tensor according to

$$\Sigma_{\alpha\beta} \stackrel{\text{def}}{=} \sigma_{\alpha\beta} + \overset{*}{\nabla}_\gamma(\tau_{\alpha\beta}{}^\gamma - \tau_\beta{}^\gamma{}_\alpha + \tau^\gamma{}_{\alpha\beta}) \quad (5.3)$$

(see Ref. 4), the above-mentioned procedure applied to (5.1) leads to the equations

$$G_{\alpha\beta} = k\Sigma_{\alpha\beta}. \quad (A)$$

Using (4.12) and (5.2) we immediately have

$$T_{\alpha\beta\gamma} = k\tau_{\alpha\beta\gamma}. \tag{5.4}$$

(A) and (5.4) are the field equations which are generally valid in this form.

Using now (4.8) we see that in the Dirac case discussed here the contortion tensor is totally antisymmetric and the second set of field equations can be specialized to

$$\begin{aligned} T^{\alpha\beta\gamma} &= T^{[\alpha\beta\gamma]} = S^{[\alpha\beta\gamma]} = -K^{[\alpha\beta\gamma]} = k\tau^{\alpha\beta\gamma} \\ &= -(il^2/4)\psi^+\gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]}\psi. \end{aligned} \tag{B}$$

Here we have introduced $l^2 = \hbar ck$ or $l \approx 10^{-32}$ cm.

This results in a very special U_4: Only four independent components of $K_{\alpha\beta\gamma}$ are "excited" by a Dirac particle, and this indicates the relatively simple nature of such a particle. It is of course possible to introduce the axial vector corresponding to $\tau_{\alpha\beta\gamma}$ making explicit the independence of only four components. We use the well-known relation (see Ref. 9, for instance)

$$i\gamma_5\gamma^\alpha = \frac{1}{3!}\epsilon^{\alpha\beta\gamma\delta}\gamma_\beta\gamma_\gamma\gamma_\delta. \tag{5.5}$$

[$\epsilon^{\alpha\beta\gamma\delta} = \pm 1/e$ if α, β, δ is an even (odd) permutation of 1, 2, 3, 4; otherwise 0.] Inverting (5.5) and substituting it in (B) yields

$$K_{\alpha\beta\gamma} = -k\tau_{\alpha\beta\gamma} = \tfrac{1}{4}l^2\epsilon_{\alpha\beta\gamma\delta}\psi^+\gamma_5\gamma^\delta\psi. \tag{5.6}$$

Squaring (5.5), we get for later use

$$\gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]}\gamma_\alpha\gamma_\beta\gamma_\gamma = -6(\gamma_5\gamma^\alpha)(\gamma_5\gamma_\alpha). \tag{5.7}$$

6. GENERALIZED DIRAC EQUATION

We vary (4.12) with respect to ψ and ψ^+, and then the action principle yields the Euler–Lagrange equations

$$\frac{\partial\mathfrak{L}}{\partial\psi^{(+)}} - \partial_k\left(e_\alpha{}^k\frac{\partial\mathfrak{L}}{\partial(\partial_\alpha\psi^{(+)})}\right) = 0. \tag{6.1}$$

In view of (3.12) we get

$$\frac{\partial\mathfrak{L}}{\partial\psi^{(+)}} - \left(\partial_\alpha + 2\Omega^\beta_{\alpha\beta} - \frac{(\partial_\alpha e)}{e}\right)\frac{\partial\mathfrak{L}}{\partial\partial_\alpha\psi^{(+)}} = 0. \tag{6.2}$$

For convenience we now use the Lagrangian in the form (4.6). Computing the necessary partial derivatives, we obtain from (6.2)

$$[\gamma^\alpha\partial_\alpha - \tfrac{1}{4}\Gamma_{\alpha\beta\gamma}\gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]} + \Omega^\beta_{\alpha\beta}\gamma^\alpha]\psi = im\gamma. \tag{6.3}$$

The partial derivative can be transformed into a derivative with respect to a V_4 or a U_4. Substituting (3.14) in (6.3) we have

$$[\gamma^\alpha\nabla_\alpha + \tfrac{1}{4}\Gamma_{\alpha\beta\gamma}(\gamma^\alpha\gamma^\beta\gamma^\gamma - \gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]}) + \Omega^\beta_{\alpha\beta}\gamma^\alpha]\psi = im\psi. \tag{6.4}$$

With (4.3), (3.7), and (3.9) one is led to

$$\gamma^\alpha[\nabla_\alpha + \tfrac{1}{2}K_{\beta\alpha}{}^\beta]\psi = im\psi \tag{6.5}$$

and with (3.14), (3.6), (3.16), and (4.3) to

$$[\gamma^\alpha\overset{\{\}}{\nabla}_\alpha + \tfrac{1}{4}K_{\alpha\beta\gamma}\gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]}]\psi = im\psi. \tag{C}$$

The comparison of this equation with the result in a V_4 is especially instructive.

With the help of (B) it is possible to eliminate the contortion everywhere. Substituting (B) in (C), we immediately have

$$[\gamma^\alpha\overset{\{\}}{\nabla}_\alpha + (il^2/16)(\psi^+\gamma^{[\alpha}\gamma^\beta\gamma^{\gamma]}\psi)\gamma_\alpha\gamma_\beta\gamma_\gamma]\psi = im\psi \tag{6.6}$$

or together with (5.7)

$$[\gamma^\alpha\overset{\{\}}{\nabla}_\alpha - \tfrac{3}{8}il^2(\psi^+\gamma_5\gamma^\alpha\psi)\gamma_5\gamma_\alpha]\psi = im\psi. \tag{C$'$}$$

This is a classical spinor equation of the Heisenberg–Pauli type and because of (6.5) it can be equivalently written as

$$\gamma^\alpha\nabla_\alpha\psi = im\psi. \tag{6.7}$$

It should be noted that we arrive at this simple equation only in view of (B).

In addition to the above-mentioned authors of Refs. 7 and 14–18, Gürsey[19] and Finkelstein[20] discussed nonlinear spinor equations, more or less resembling (C′), in space–times with torsion. They both worked with a connection allowing teleparallelism, and Finkelstein even used a space with constant torsion.

7. UNIVERSAL SPIN–SPIN INTERACTION OF RANGE ZERO

Let us now reflect on the difference between the theory presented here and usual general relativity. With the help of the field equations (B) we can collect the contortion terms in the Lagrangian scalar of (4.12) in one term

$$\tfrac{1}{2}\tau^{\gamma\beta\alpha}K_{\alpha\beta\gamma} = \tfrac{1}{2}\tau^{[\gamma\beta\alpha]}K_{\alpha\beta\gamma} = \tfrac{1}{2}k\tau^{[\alpha\beta\gamma]}\tau_{[\alpha\beta\gamma]}. \tag{7.1}$$

We recognize the interaction term (7.1), characteristic for a U_4, as a universal spin–spin contact interaction. That is to say there is nothing like a "spin field" which is emitted and which is the carrier of a new interaction; there is rather a very weak classical interaction as soon as any spinning matter is overlapping. This leads also to a certain self-interaction of spinning matter automatically introducing nonlinearities as in (C′). This interaction is very weak, as can be seen from the smallness of 1 in (C′). Hence this theory describes in a unified manner two universal interactions: the far reaching gravitational interaction and a weak spin–spin interaction of vanishing range. It is very tempting to regard such a theory as a *classical model* unifying gravitational and *weak interaction.*

For a Dirac particle according to (5.6) the canonical spin can be represented by an axial vector. A spin–spin interaction thus leads in this special case to an axial vector interaction and (7.1) can be rewritten, using (B) and (5.7), in the form

$$\tfrac{1}{2}\tau^{\gamma\beta\alpha}K_{\alpha\beta\gamma} = \frac{3l^4}{16k}(\psi^+\gamma_5\gamma_\alpha\psi)(\psi^+\gamma_5\gamma^\alpha\psi). \quad (7.2)$$

(7.2) naturally corresponds to the nonlinear term entering the spinor equation (C′). It is easy to obtain a V–A interaction instead of (7.2) by modifying the matter Lagrangian in a suitable way.

Apart from all speculations, we have formally arrived at the result that the second term of (C′) can be derived from the first term just by using the connection (2.1) of a U_4 instead of the Christoffel symbol of a V_4. This leads to a deeper understanding of such nonlinear spinor equations and their connection with geometry of space–time.

ACKNOWLEDGMENTS

We especially thank Professor E. Kröner for many discussions and for suggestions improving our paper. One author (F. H.) gratefully acknowledges support from the Deutsche Forschungsgemeinschaft.

[1] D. W. Sciama, in *Recent Developments in General Relativity* (Pergamon, New York, 1962), p. 415.
[2] T. W. B. Kibble, J. Math. Phys. **2**, 212 (1961).
[3] F. Hehl and E. Kröner, Z. Physik **187**, 478 (1965).
[4] F. Hehl, Abhandl. Braunschweiger Wiss. Ges. **18**, 98 (1966).
[5] E. Cartan, Compt. Rend. Acad. Sci. (Paris) **174**, 593 (1922).
[6] E. Cartan, Ann. Ecole Norm. Sup. **40**, 325 (1923); **41**, 1 (1924); **42**, 17 (1925).
[7] V. I. Rodichev, Zh. Eksp. Teor. Fiz **40**, 1469 (1961) [Sov. Phys. JETP **13**, 1029 (1961)].
[8] J. A. Schouten, *Ricci-Calculus* (Springer-Verlag, Berlin, 1954), 2nd ed.
[9] L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields* (Pergamon, New York, 1962), 2nd ed.
[10] E. M. Corson, *Introduction to Tensors, Spinors, and Relativistic Wave Equations* (Blackie, London, 1953).
[11] T. W. B. Kibble, J. Math. Phys. **4**, 1433 (1963).
[12] L. Kannenberg and R. Arnowitt, Ann. Phys. (N.Y.) **45**, 416 (1967).
[13] G. Lemmer, Nuovo Cimento **37**, 1647 (1965).
[14] G. Braunss, Z. Naturforsch. **19a**, 825 (1964).
[15] A. Peres, Nuovo Cimento Suppl. **24**, 389 (1962).
[16] M. Lenoir, Compt. Rend. Acad. Sci. (Paris) **259**, 3701 (1964).
[17] J. Wainwright, in *Colloquium on the Calculus of Variations* (University of South Africa, Pretoria, 1966), p. 98.
[18] J. Wainwright, Tensor **19**, 217, 266 (1968).
[19] F. Gürsey, Nuovo Cimento **5**, 154 (1957).
[20] R. Finkelstein, J. Math. Phys. **1**, 440 (1960).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Phase-Plane Analysis of Nonlinear, Second-Order, Ordinary Differential Equations*

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(Received 12 October 1970)

Group invariance is used to analyze the solutions of several well-known differential equations.

INTRODUCTION

Nonlinear mechanics is the name generally given to the study of nonlinear, second-order, ordinary differential equations. The independent variable is usually interpreted as time. The principal tool in nonlinear mechanics is the phase plane, the plane in which the dependent variable and its first derivative are the coordinates. The phase plane is particularly useful for studying autonomous differential equations, i.e., those equations in which the independent variable does not appear. For them, the paths in the phase plane traced out by the solutions are independent of time and can be obtained from the solution of a first-order differential equation. In the event that the first-order equation cannot be solved in terms of elementary functions, which is frequently the case, its direction field can be sketched in the phase plane and the qualitative nature of the paths determined. From these paths, certain properties of the solutions of the original equation can be inferred: whether they are oscillatory or monotone, whether they are stable or unstable, whether they have any asymptotic limits, whether they have roots or singularities.

When the differential equation is not autonomous, the paths in the phase plane are no longer time-independent nor are they determined by a first-order differential equation. The phase plane loses much of its usefulness. However, if the differential equation is interactions: the far reaching gravitational interaction and a weak spin–spin interaction of vanishing range. It is very tempting to regard such a theory as a *classical model* unifying gravitational and *weak interaction.*

For a Dirac particle according to (5.6) the canonical spin can be represented by an axial vector. A spin–spin interaction thus leads in this special case to an axial vector interaction and (7.1) can be rewritten, using (B) and (5.7), in the form

$$\tfrac{1}{2}\tau^{\gamma\beta\alpha}K_{\alpha\beta\gamma} = \frac{3l^4}{16k}(\psi^+\gamma_5\gamma_\alpha\psi)(\psi^+\gamma_5\gamma^\alpha\psi). \qquad (7.2)$$

(7.2) naturally corresponds to the nonlinear term entering the spinor equation (C′). It is easy to obtain a V–A interaction instead of (7.2) by modifying the matter Lagrangian in a suitable way.

Apart from all speculations, we have formally arrived at the result that the second term of (C′) can be derived from the first term just by using the connection (2.1) of a U_4 instead of the Christoffel symbol of a V_4. This leads to a deeper understanding of such nonlinear spinor equations and their connection with geometry of space–time.

ACKNOWLEDGMENTS

We especially thank Professor E. Kröner for many discussions and for suggestions improving our paper. One author (F. H.) gratefully acknowledges support from the Deutsche Forschungsgemeinschaft.

[1] D. W. Sciama, in *Recent Developments in General Relativity* (Pergamon, New York, 1962), p. 415.
[2] T. W. B. Kibble, J. Math. Phys. **2**, 212 (1961).
[3] F. Hehl and E. Kröner, Z. Physik **187**, 478 (1965).
[4] F. Hehl, Abhandl. Braunschweiger Wiss. Ges. **18**, 98 (1966).
[5] E. Cartan, Compt. Rend. Acad. Sci. (Paris) **174**, 593 (1922).
[6] E. Cartan, Ann. Ecole Norm. Sup. **40**, 325 (1923); **41**, 1 (1924); **42**, 17 (1925).
[7] V. I. Rodichev, Zh. Eksp. Teor. Fiz **40**, 1469 (1961) [Sov. Phys. JETP **13**, 1029 (1961)].
[8] J. A. Schouten, *Ricci-Calculus* (Springer-Verlag, Berlin, 1954), 2nd ed.
[9] L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields* (Pergamon, New York, 1962), 2nd ed.
[10] E. M. Corson, *Introduction to Tensors, Spinors, and Relativistic Wave Equations* (Blackie, London, 1953).
[11] T. W. B. Kibble, J. Math. Phys. **4**, 1433 (1963).
[12] L. Kannenberg and R. Arnowitt, Ann. Phys. (N.Y.) **45**, 416 (1967).
[13] G. Lemmer, Nuovo Cimento **37**, 1647 (1965).
[14] G. Braunss, Z. Naturforsch. **19a**, 825 (1964).
[15] A. Peres, Nuovo Cimento Suppl. **24**, 389 (1962).
[16] M. Lenoir, Compt. Rend. Acad. Sci. (Paris) **259**, 3701 (1964).
[17] J. Wainwright, in *Colloquium on the Calculus of Variations* (University of South Africa, Pretoria, 1966), p. 98.
[18] J. Wainwright, Tensor **19**, 217, 266 (1968).
[19] F. Gürsey, Nuovo Cimento **5**, 154 (1957).
[20] R. Finkelstein, J. Math. Phys. **1**, 440 (1960).

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INTRODUCTION

Nonlinear mechanics is the name generally given to the study of nonlinear, second-order, ordinary differential equations. The independent variable is usually interpreted as time. The principal tool in nonlinear mechanics is the phase plane, the plane in which the dependent variable and its first derivative are the coordinates. The phase plane is particularly useful for studying autonomous differential equations, i.e., those equations in which the independent variable does not appear. For them, the paths in the phase plane traced out by the solutions are independent of time and can be obtained from the solution of a first-order differential equation. In the event that the first-order equation cannot be solved in terms of elementary functions, which is frequently the case, its direction field can be sketched in the phase plane and the qualitative nature of the paths determined. From these paths, certain properties of the solutions of the original equation can be inferred: whether they are oscillatory or monotone, whether they are stable or unstable, whether they have any asymptotic limits, whether they have roots or singularities.

When the differential equation is not autonomous, the paths in the phase plane are no longer time-independent nor are they determined by a first-order differential equation. The phase plane loses much of its usefulness. However, if the differential equation is invariant to a one-parameter group of transformations of the variables, an analysis very similar to phase-plane analysis is possible. In fact, when the group of transformations is the group of translations of the independent variable, the analysis is identical with phase-plane analysis.

The new analysis is based on a theorem of Lie,[1] namely, if an invariant u and a first differential invariant v of the group are substituted in the original (invariant) second-order equation, the resulting equation in u and v is of first order. (An invariant u of the group is a function of x, the independent variable, and y, the dependent variable, which is invariant to the transformations of the group. A first differential invariant v is an invariant function of x, y, and $\dot{y} \equiv dy/dx$.) We now study the paths in the (u, v) plane (henceforth called the Lie plane), which is the analog of the phase plane of an autonomous differential equation.

The remainder of this paper will be devoted to the analysis of several well-known equations to show how the method works. The equations are the Bessel (zero-order), Emden–Fowler, Poisson–Boltzmann, and Fermi–Thomas equations. Bessel's equation, while linear, is included by way of introduction because the properties of its solutions are well known.

BESSEL'S EQUATION

Bessel's equation of order zero is

$$x^2\ddot{y} + x\dot{y} + x^2 y = 0. \tag{1}$$

(The dot denotes differentiation with respect to the independent variable.) Equation (1), like all linear equations, is invariant to the group of transformations

$$y' = \lambda y, \tag{2a}$$

$$x' = x, \tag{2b}$$

$0 < \lambda < \infty$. $u = x$ and $v = \dot{y}/y$ are an invariant and a first differential invariant, respectively. (There is a systematic method of calculating these invariants, but we shall be content to display them without proof. For the uncomplicated groups treated in this paper, the invariants u and v are evident on inspection.) Now

$$du = dx, \tag{3a}$$

$$dv = \frac{\ddot{y}}{y}\,dx - \frac{\dot{y}^2}{y^2}\,dx, \tag{3b}$$

so that

$$p \equiv \frac{dv}{du} = \frac{\ddot{y}}{y} - \frac{\dot{y}^2}{y^2} = -\frac{v}{u} - 1 - v^2. \tag{3c}$$

In obtaining the last equality, we give $\ddot{y}$ its value from Eq. (1).

Figure 1 shows the direction field of Eq. (3c) in the Lie plane. Shown also in Fig. 1 are the $p = 0$ and $|p| = \infty$ isoclines. The origin 0 ($u = 0$, $v = 0$) is a critical point, and it is clear from the figure that it is a saddle point. Two separatrices intersect at 0, dividing the Lie plane into four distinct parts. One of the separatrices is the $|p| = \infty$ isocline, that is, the v axis. The other we find by noting that, in the neighborhood of 0, the separatrix obeys the equation $dv/du = v/u$. We see then from (3c) that $(dv/du)_0 = -\frac{1}{2}$. Having found the slope of the separatrix at the origin, we can calculate it by integrating (3c) away from the origin in both directions. The separatrices are shown in Fig. 1.

The integral curves of (3c) have many branches, and away from the origin are reminiscent of the curves $v = -\tan u$. On each branch, save the two that are asymptotic to the v axis, v goes from $+\infty$ to $-\infty$ as u increases. When $|v|$ is sufficiently large, $dv/du \approx -v^2$. Thus $1/v = u - a$, where a is a constant of integration. Since $v = \dot{y}/y$ and $u = x$, this last equation is the same as $\dot{y}/y = 1/(x - a)$. Integrating again we find $y = b(x - a)$, where b is another constant of integration. Thus each singularity of an integral curve in the Lie plane, with the possible exception of that at $u = 0$, marks a root of the one-parameter family of solutions corresponding to the integral curve. Thus Bessel's equation of zero order only has oscillatory solutions.

The singularity at $u = 0$ requires more analysis since the term v/u cannot necessarily be neglected when compared with the term v^2. The 1 on the right-hand side of Eq. (3c) can be dropped since $p = \pm\infty$

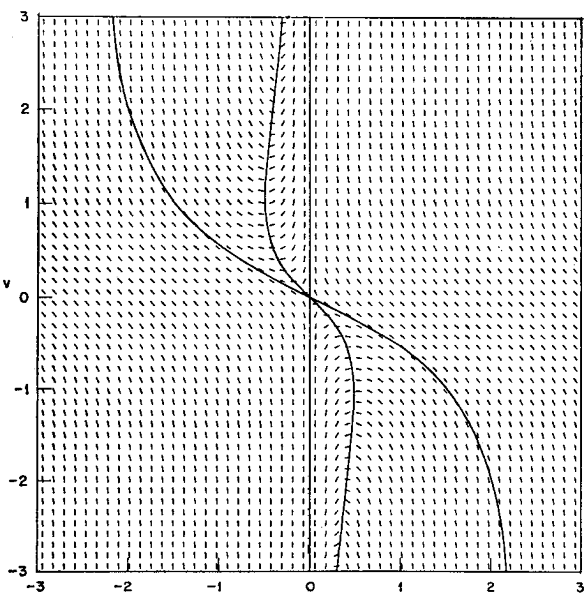

FIG. 1. The direction field in the Lie plane for Bessel's equation of order zero.

on $u = 0$. Then (3c) can be integrated: Near $u = 0$, $v = [u \ln (u/a)]^{-1}$, where a is a constant of integration. This last equation can be integrated again and gives $y = b \ln (x/a)$, where b is a second constant of integration. Thus the families of solutions corresponding to integral curves of (3c) that are singular at the origin themselves have logarithmic singularities at their origins.

There is a one-parameter family of solutions whose integral curve in the Lie plane is nonsingular at the origin, namely, that corresponding to the separatrix. Since $(dv/du)_0 = -\frac{1}{2}$ for this separatrix, this family has the form $y = ae^{-x^2/4} = a(1 - x^2/4 + \cdots)$ near the origin. The curves of this family are all multiples of the Bessel function of order zero $J_0(x)$.

When $u \gg 1$, we can easily find the form of the solutions of (1), for $v \approx -\tan (u - a) - 1/2u$ and $y = bx^{-\frac{1}{2}} \cos (x - a)$, where a and b are constants of integration. This is the asymptotic form of all the solutions of Bessel's equation of zero order.

POISSON-BOLTZMANN EQUATION

The one-dimensional Poisson–Boltzmann equation is

$$\ddot{y} + (\nu/x)\dot{y} = e^y, \tag{4}$$

where $\nu = 0, 1$, or 2 according to whether we work in plane, cylindrical, or spherical geometry, respectively. Equation (4) is invariant to the one-parameter group of transformations

$$x' = \lambda x, \tag{5a}$$

$$y' = y - 2 \ln \lambda. \tag{5b}$$

An invariant and a first differential invariant of this group are

$$u = x^2 e^y, \tag{6a}$$

$$v = x\dot{y}. \tag{6b}$$

According to Lie's theorem, u and v should be connected by a first-order differential equation. A short calculation shows it to be

$$\frac{dv}{du} = \frac{u + (1 - \nu)v}{u(v + 2)}. \tag{7}$$

When $\nu = 1$, (7) can easily be integrated. The resulting relation between u and v can be integrated again, and leads in a straightforward way to the solution of Walker and Lemke.[2] When $\nu = 0$, Eq. (7) is not easily integrated, but then (4) simplifies and can easily be integrated directly. When $\nu = 2$, neither Eq. (7) nor Eq. (4) can be easily integrated.

When $\nu = 1$, the integral curves of (7) in the Lie plane are the parabolas

$$(v + 2)^2 = 2(u - a), \tag{8}$$

where a is a parameter. These parabolas all have the line $v = -2$ as their common axis and the points $(a, -2)$ as their vertices. In terms of the variables x and y, (8) becomes

$$[(2x^2e^y - 2a)^{\frac{1}{2}} - 2]\, dx - x\, dy = 0. \tag{9}$$

Another theorem of Lie's[3] tells us that $[x(2x^2e^y - 2a)^{\frac{1}{2}}]^{-1}$ is an integrating factor for (9). When $a > 0$, integration of (9) gives

$$(2/a)^{\frac{1}{2}} \operatorname{arccot} (x^2e^y/a - 1)^{\frac{1}{2}} + \ln (x/b) = 0, \tag{10}$$

where b is another parameter. Using (10), we can easily show that

$$y = 2 \ln |\csc [(2/a)^{-\frac{1}{2}} \ln (x/b)]| - 2 \ln x + \ln a, \tag{11a}$$

$$u = a \csc^2 [(2/a)^{-\frac{1}{2}} \ln (x/b)], \tag{11b}$$

$$v = -(2a)^{\frac{1}{2}} \cot [(2/a)^{-\frac{1}{2}} \ln (x/b)] - 2. \tag{11c}$$

From (11a) we see that y has a logarithmic singularity whenever $(2/a)^{-\frac{1}{2}} \ln (x/b)$ is an even multiple of $\pi/2$. When $(2/a)^{-\frac{1}{2}} \ln (x/b)$ is an odd multiple of $\pi/2$, $y = \ln a - 2 \ln x$. A sketch of y as a function of x is shown in Fig. 2. In cylindrical geometry we are only interested in $x \geq 0$.

When $(2/a)^{-\frac{1}{2}} \ln (x/b)$ is just slightly less than some even multiple of $\pi/2$, both u and v are large and positive. When $(2/a)^{-\frac{1}{2}} \ln (x/b)$ is just slightly greater than some even multiple of $\pi/2$, u is large and positive,

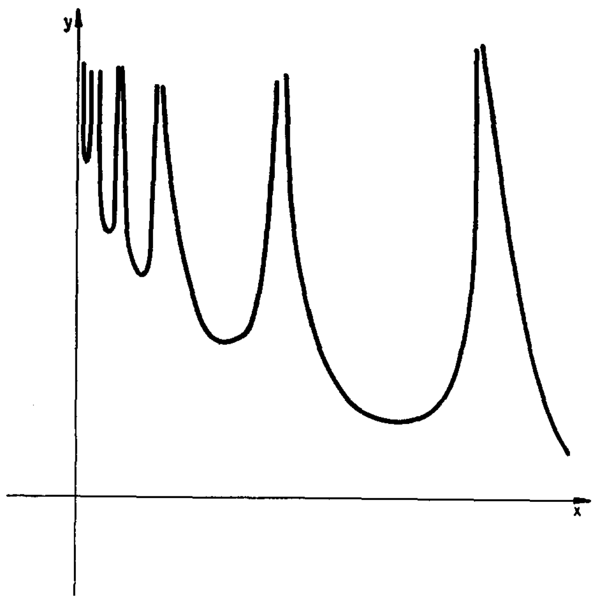

FIG. 2. A sketch of y vs x for the Poisson–Boltzmann equation in cylindrical geometry when $a > 0$.

while v is large and negative. When $(2/a)^{-\frac{1}{2}} \ln (x/b)$ is an odd multiple of $\pi/2$, $u = a$, and $v = -2$. Thus as we pass from one singularity to the next on a curve of y vs x, we traverse the *entire* integral curve in the Lie plane in the direction shown in Fig. 3.

When $a < 0$, (10) becomes

$$\frac{(x^2e^y/|a| + 1)^{\frac{1}{2}} + 1}{(x^2e^y/|a| + 1)^{\frac{1}{2}} - 1} = \left(\frac{x}{b}\right)^{-(2|a|)^{\frac{1}{2}}}, \tag{12}$$

from which it follows that

$$y = \ln \left[\left(\frac{(x/b)^{(2|a|)^{\frac{1}{2}}} + 1}{(x/b)^{(2|a|)^{\frac{1}{2}}} - 1}\right)^2 - 1\right] - 2 \ln x + \ln |a|, \tag{13a}$$

$$u = |a| \left[\left(\frac{(x/b)^{(2|a|)^{\frac{1}{2}}} + 1}{(x/b)^{(2|a|)^{\frac{1}{2}}} - 1}\right)^2 - 1\right], \tag{13b}$$

$$v = -(2\,|a|)^{\frac{1}{2}} \frac{(x/b)^{(2|a|)^{\frac{1}{2}}} + 1}{(x/b)^{(2|a|)^{\frac{1}{2}}} - 1} - 2. \tag{13c}$$

The only singularities which y has now are at $x = 0$, $x = b$, and $x = \infty$, except when $|a| = 2$, when there is no singularity at $x = 0$. When $0 < |a| < 2$, $\dot{y} < 0$ near $x = 0$. When $|a| = 2$, $\dot{y} = 0$ at $x = 0$. When $|a| > 2$, $\dot{y} > 0$ near $x = 0$. The behavior of y is shown in Fig. 4.

When $x = 0$, $v = (2\,|a|)^{\frac{1}{2}} - 2$ and $u = 0$. When $x = \infty$, $v = -(2\,|a|)^{\frac{1}{2}} - 2$ and $u = 0$. When $x = b$, both u and $v = \infty$. When x/b is slightly less than 1, v is positive; when x/b is slightly greater than 1, v is negative. Thus as x increases from zero to infinity, the integral curves in the Lie plane are traversed in the direction shown in Fig. 5. (Only the right-hand half-plane is of interest since $u = x^2e^v > 0$.)

From this analysis, we see, for example, that only the integral curve corresponding to $a = -2$ in the

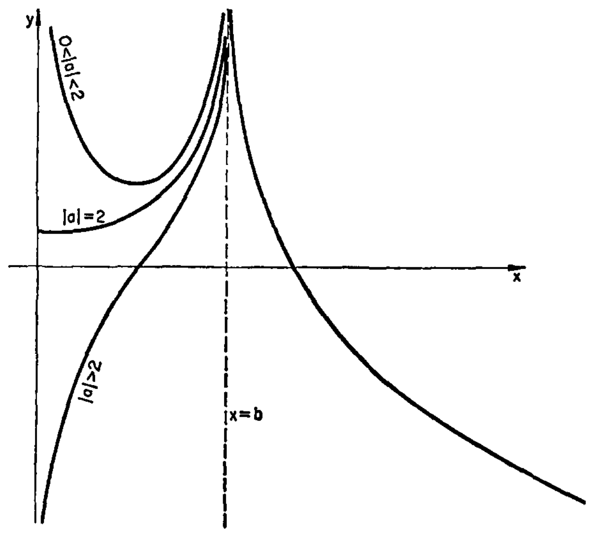

FIG. 4. A sketch of y vs x for the Poisson–Boltzmann equation in cylindrical geometry when $a < 0$.

Lie plane leads to solutions that are nonsingular at the origin. The solutions all form a one-parameter family, but transform into one another under the transformations of the group (5). In this sense, there is but one solution nonsingular at the origin. According to (13a), it can be written $y = \ln [8b^2/(x^2 - b^2)^2]$.

Figure 6 shows the direction field of (7) when $\nu = 2$. Again only the first and fourth quadrant are of interest. The lines $u = 0$ and $v = -2$ are the $|p| = \infty$ isoclines; the line $v = u$ is the $p = 0$ isocline. The origin is a saddle point. The separatrices are the lines $u = 0$ and a curve, shown in Fig. 6, which crosses the origin with a slope of $\frac{1}{3}$.

We pursue our analysis by studying the singularities

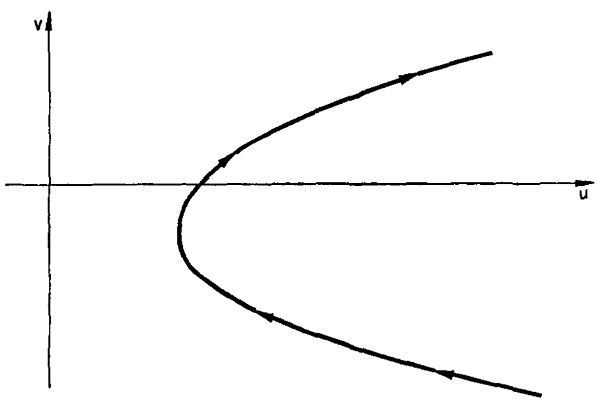

FIG. 3. The direction in which the integral curves are traversed—Poisson–Boltzmann equation in cylindrical geometry, $a > 0$.

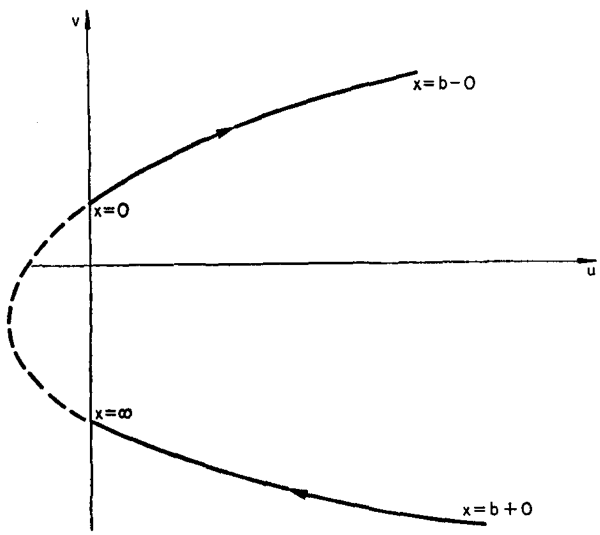

FIG. 5. The direction in which the integral curves are traversed—Poisson–Boltzmann equation in cylindrical geometry, $a < 0$.

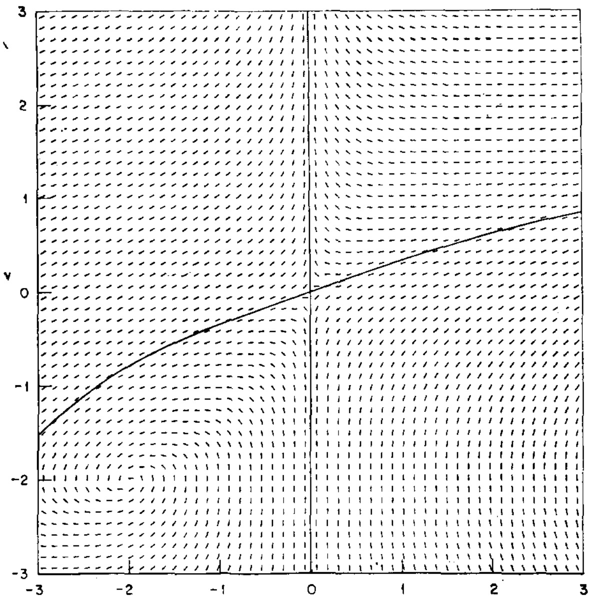

FIG. 6. The direction field in the Lie plane for the Poisson–Boltzmann equation in spherical geometry.

of the solutions in the (x, y) plane. First off, we ask whether a finite point $(0 \leq |v| < \infty, 0 < u < \infty)$ of the Lie plane can correspond to a singularity in the (x, y) plane. In the neighborhood of any point in the (u, v) plane, $\dot{y}^2 = (v^2/u)e^y$. Near a singularity of y, v^2/u may be considered constant. The solution to this differential equation is then

$$y = -\ln [b - (v^2/4u)^{\frac{1}{2}}x]^2. \tag{14a}$$

Furthermore,

$$v = \frac{(v^2/u)^{\frac{1}{2}}x}{b - (v^2/4u)^{\frac{1}{2}}x} \tag{14b}$$

and

$$u = \frac{x^2}{[b - (v^2/4u)^{\frac{1}{2}}x]^2}. \tag{14c}$$

For y to be singular, $b - (v^2/4u)^{\frac{1}{2}}x$ must vanish, and then u and v are infinite, contrary to hypothesis. The only possible exception occurs when $b = 0$, in which case $v = -2$, u can have any nonzero positive value, and $y = \ln u/x^2$. Substitution into (4) shows that u must equal -2 if (4) is to be satisfied by $y = \ln u/x^2$ near $x = 0$. Thus y can have no singularity corresponding to a finite point in the (u, v) plane. All singularities in the (x, y) plane correspond to points at infinity in the Lie plane.

When u and v are both $\gg 1$, $|dv/du| \sim |1/v - 1/u| \ll 1$. Hence, eventually, u far outweighs v. Then $dv/du \simeq 1/v$ so that $v^2 \simeq 2u + a$, where a is a constant of integration. No matter what value a has, when v and u are large enough, both will be $\gg a$. Then $v^2 \sim 2u$, which can be written $\dot{y}^2 = 2e^y$ in terms of x and y. The solution of this differential equation is $y = \ln [2/(x - b)^2]$, where b is a constant of integration, corresponding to a logarithmic singularity. Moreover, $v = x\dot{y} = -2x/(x - b)$, so that when $x = b - 0$, $v = +\infty$ and, when $x = b + 0$, $v = -\infty$. Thus when we traverse the integral curves lying below the separatrix in the direction shown in Fig. 3, we advance from one singularity to the next in the (x, y) plane. Furthermore, b must be positive for y to be singular; it cannot equal zero, since then $|v|$ would not be $\gg 1$ near $x = b$.

Let us now consider the behavior of the solutions determined by the behavior of the integral curves in the Lie plane near the positive part of the v axis. When $v \gg 1$, $dv/du = -1/u$ so that $v + \ln u = a$. When v is large enough, the constant a may be neglected, and $v + \ln u = 0$. The latter can be written $d(xy) + 2 \ln x\, dx = 0$, so that $xy + 2x \ln x - 2x = b'$. If we calculate v from this last equation, we find $v = -b'/x - 2$. Since v must be large and positive, $0 < x \ll 1$ and $b' < 0$ (remember $x > 0$ in spherical geometry). Thus $y \sim -|b'|/x$ near $x = 0$.

Now we are in a position to consider the kind of solutions (4) can have when $\nu = 2$. Either the solutions are singular or nonsingular at $x = 0$. If they are nonsingular, $\dot{y}$ and y are finite at $x = 0$, and $u = v = 0$ there. The only integral curve traversing the origin is the separatrix, so these solutions start off with $u = 3v$, i.e., with $\dot{y}e^{-y} = x/3$. This equation integrates to give $y = \ln [6/(b - x^2)]$, $b \neq 0$, in the neighborhood of $x = 0$. Advancing along the separatrix leads to a singularity as u and v approach ∞ [arc (a), Fig. 7]. If the solutions are singular at the origin, their behavior there corresponds to the positive v axis, i.e., $a - 1/x$

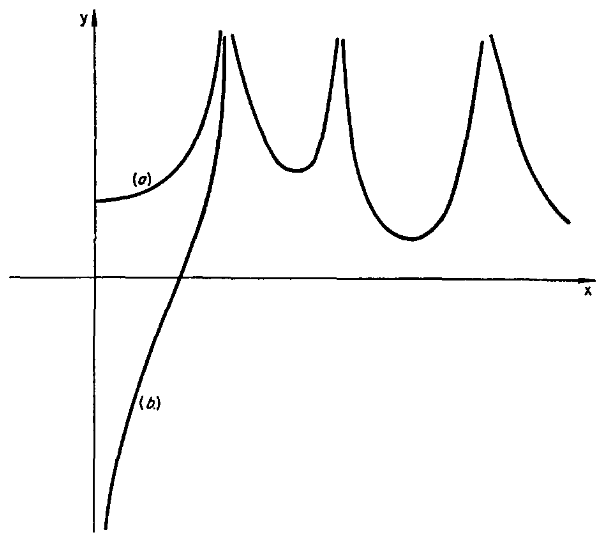

FIG. 7. A sketch of y vs x for the Poisson–Boltzmann equation in spherical geometry.

singularity [arc (b), Fig. 7]. In each case, a singularity is reached. From the first singularity on, the solution corresponds to traversals of integral curves in the Lie plane below the separatrix, these being the only ones both of whose extremes can correspond to points on the finite x axis. The behavior of the possible solutions is shown in Fig. 7.

EMDEN-FOWLER EQUATION

The Emden–Fowler equation has the form

$$\ddot{y} + (2/x)\dot{y} + y^n = 0, \quad x \geq 0, \tag{15}$$

where $n \geq 0$. Equation (15) is invariant under the group of transformations

$$x' = \lambda x, \tag{16a}$$

$$y' = \lambda^{2/(1-n)}y, \tag{16b}$$

except when $n = 1$. An invariant u and a first differential invariant v of this group are

$$u = x^{-2/(1-n)}y, \tag{17a}$$

$$v = x^{(n+1)/(n-1)}\dot{y}. \tag{17b}$$

In terms of these invariants, (15) becomes

$$\frac{dv}{du} = \frac{(1-n)u^n + (3-n)v}{2u - (1-n)v}. \tag{18}$$

We begin by considering the case $n = 5$. Equations (17) and (18) then become

$$u = x^{\frac{1}{2}}y, \tag{19a}$$

$$v = x^{\frac{3}{2}}\dot{y}, \tag{19b}$$

$$\frac{dv}{du} = -\frac{2u^5 + v}{u + 2v}. \tag{19c}$$

The direction field of (19c) in the Lie plane is shown in Fig. 8. There are three critical points: $(\sqrt{2}/2, -\sqrt{2}/4)$, $(-\sqrt{2}/2, \sqrt{2}/4)$, and $(0, 0)$. The first two critical points are vortex points, the origin is a saddle point. Two separatrices cross the origin; in the neighborhood of the origin they are the curves $v = -u$ and $v = -\frac{1}{3}u^5$. The two separatrices join smoothly to form a figure eight. Integral curves inside the loops of the figure eight are closed curves surrounding the vortex points; integral curves outside the figure eight are closed curves surrounding the entire figure eight.

Our analysis is aided in this case by the fact that (19c) can be integrated to give

$$3uv + 3v^2 + u^6 = b, \tag{20}$$

where b is a constant.

In terms of x and y, (20) becomes

$$3x^2y\dot{y} + 3x^3\dot{y}^2 + x^3y^6 = b. \tag{21}$$

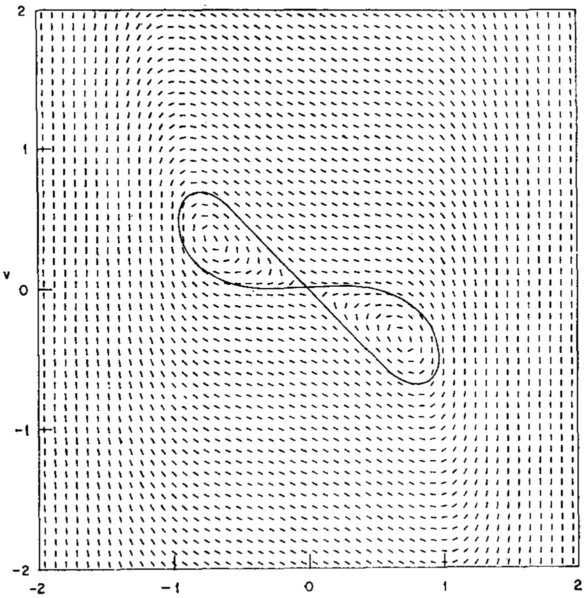

FIG. 8. The direction field in the Lie plane for the Emden–Fowler equation, $n = 5$.

Equation (21) is also invariant to the group (16b). Another theorem of Lie's shows that the substitution $w = y^2x$ will lead to a differential equation for w in which the variables are separable. After some computation we find

$$\frac{dx}{x} = (\sqrt{3}/2)\, dw(w^2(\tfrac{3}{4} - w^2) + bw)^{-\frac{1}{2}}. \tag{22}$$

$b = 0$ for the separatrices since they pass through the point $u = v = 0$. For $b = 0$, (22) can be integrated using the trigonometric substitution $w = (\sqrt{3}/2)\sin\theta$. Again after some calculation we at last find

$$y = [3a/(x^2 + 3a^2)]^{\frac{1}{2}} \tag{23}$$

as the family of solutions all of which correspond to the separatrix in the Lie plane. These solutions are already known.[4]

Having the explicit solution (23) enables us to find directly how a point in the Lie plane traces out the separatrix as x increases from zero to infinity. From (23) we find

$$u = [3ax/(x^2 + 3a^2)]^{\frac{1}{2}}, \tag{24a}$$

$$v = -(3a)^{\frac{1}{2}}x^{\frac{3}{2}}/(x^2 + 3a^2)^{\frac{3}{2}}. \tag{24b}$$

When x is small ($\ll a$), $u \sim (x/a)^{\frac{1}{2}}$ and

$$v \sim -\tfrac{1}{3}(x/a)^{\frac{5}{2}} = -\tfrac{1}{3}u^5.$$

Hence, as x advances away from the origin, the point in the Lie plane moves away from the origin in the Lie plane along the branch of the separatrix that has zero slope at the origin (see Fig. 8). When x is large ($\gg a$), $u \sim (3a/x)^{\frac{1}{2}}$ and $v \sim -(3a/x)^{\frac{1}{2}} = -u$. Thus as x approaches ∞, the point in the Lie plane returns to the origin in the Lie plane along the separatrix that has a slope of -1 at the origin. *One circuit in the Lie plane* corresponds to passage of x from 0 to ∞. The two halves of the figure eight correspond to families of solutions which are negatives of each other, i.e., to opposite choices of the sign of the square root in (23).

Equation (22) can be integrated in terms of elliptic integrals, but this is a laborious task. To determine the qualitative behavior of the solutions, we return to (21). When $x \to 0$, at least one of the terms on the left-hand side must remain finite. [None can become infinite since (21) is the same as (20), and u and v are bounded on any integral curve.] No matter which one we choose, we see that $y \sim x^{-\frac{1}{2}}$ as $x \to 0$. If this is so, $v \sim -\frac{1}{2}u$ when $x \to 0$. The same argument also holds as $x \to \infty$. Then half a circuit of each integral curve from one intersection with the line $v = -\frac{1}{2}u$ to the other corresponds to passage of x from zero to infinity. The two halves of the same integral curve in the Lie plane correspond to families of solutions which are negatives of each other. Thus the solutions of (15) corresponding to $b \neq 0$ all vary as $x^{-\frac{1}{2}}$ near $x = 0$ and $x = \infty$. Then $u = y\sqrt{x} =$ const in these extremes, and its value can be found from the equation $u^6 - \frac{3}{4}u^2 = b$, which results from substituting $v = -\frac{1}{2}u$ in (20).

b is greater than zero for the integral curves in the Lie plane outside the figure eight, and b is less than zero for those inside the loops of the figure eight. $v = 0$ at one point on each half of the curves for which $b > 0$. Since this occurs at a finite value of x, $\dot{y} = 0$ *once* on each curve for which $b > 0$. $v \neq 0$ on the integral curves in the Lie plane for which $b < 0$, and y has no extremum at all on these curves. Thus the solutions of (15) for $n = 5$ look like those sketched in Fig. 9. Each vortex point corresponds to an entire solution. These two solutions are $y = \pm\sqrt{2}/2\sqrt{x}$. For these solutions $b = -\frac{1}{4}$.

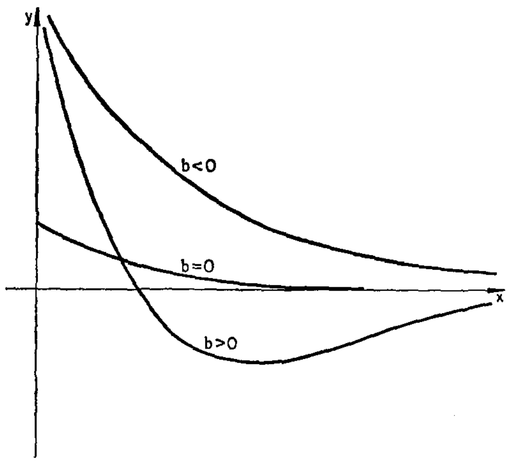

FIG. 9. A sketch of y vs x for the Emden–Fowler equation, $n = 5$.

EMDEN–FOWLER EQUATION: $n = 3$

A different type of behavior is exhibited by the Emden–Fowler equation when $n = 3$. Then,

$$u = xy, \tag{25a}$$

$$v = x^2\dot{y}, \tag{25b}$$

$$\frac{dv}{du} = -\frac{u^3}{u+v}. \tag{25c}$$

The only critical point is the origin; it is a node. (See Fig. 10.) All of the integral curves approach the line $v = -u$ as they approach the origin except that for which $dv/du = 0$ at the origin.

Let us now ask whether any finite point of the Lie plane ($0 < |u| < \infty, 0 < |v| < \infty$) can correspond to a singularity in the (x, y) plane. Near such a singularity, $\dot{y}/y^2 = v/u^2$; the right-hand side of this equation may be treated as a constant. Then $y = [a - (v/u^2)x]^{-1}$, where a is a constant of integration. Then $u = x[a - (v/u^2)x]^{-1}$ and $v = (v/u^2)x^2[a - (v/u^2)x]^{-2}$. If u and v are finite in the neighborhood of the singularity, a must equal zero. But then $u = -u^2/v$ and $v = u^2/v$. The only solution of these equations is $v = -u$. Thus, if there are singularities corresponding to finite points in the Lie plane, the latter must be on the line $v = -u$. The corresponding solutions are $y = u/x$ in the neighborhood of the singularity, which occurs at

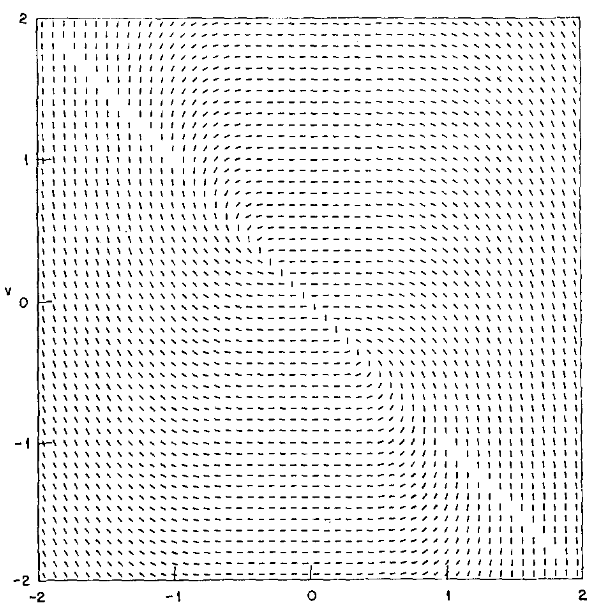

FIG. 10. The direction field in the Lie plane for the Emden–Fowler equation, $n = 3$.

$x = 0$ in the (x, y) plane. However, substitution into (15) shows that $y = u/x$ cannot satisfy (15) even to leading order near $x = 0$. Hence, finite points of the Lie plane correspond to ordinary points in the (x, y) plane.

Let us now consider the behavior of the solutions when the point in the Lie plane approaches the origin. In general, as the integral curves in the Lie plane approach the origin they draw ever closer to the line $v = -u$, but there is one exception—the integral curve that approaches the line $v = 0$ as it crosses the origin. The integral curves which approach the line $v = -u$ have equations near the origin of the form $v + u = f(u, u_0)$. Here u_0 is the abscissa at which the curve first cuts the line $v = -u$ as we proceed away from the origin, and $f(u, u_0)$ is a function with the following properties. It has the same sign as u for u between zero and u_0, and it vanishes more rapidly than u as $u \to 0$. Thus, in the neighborhood of the origin $v = u = 0$,

$$x\frac{du}{dx} = x\frac{d}{dx}(xy) = x^2\dot{y} + xy = u + v = f(u, u_0) \tag{26a}$$

or

$$\ln\left(\frac{x}{a}\right) = -\int_u^{u_0}\frac{du}{f(u, u_0)}, \tag{26b}$$

where a is a constant of integration. As $u \to 0$, the right-hand side of (26b) approaches $-\infty$, so that $x \to 0$. Furthermore, since $f(u, u_0)$ approaches zero faster than u does, x must approach zero faster than u does. But then (25a) shows that $y \to \pm\infty$ as $x \to 0$, the sign depending on the sign of u.

The integral curve which approaches the origin with zero slope has the equation $v = -\frac{1}{3}u^3 + \cdots$ in the neighborhood of the origin. This integrates to give $y = [3/(x^2 + a)]^{\frac{1}{2}}$, where $a > 0$ is a constant of integration. For this solution, $u = x[3/(x^2 + a)]^{\frac{1}{2}}$, $v = -x^3\sqrt{3}(x^2 + a)^{-\frac{3}{2}}$. u and v can only vanish if $x \to 0$. Hence, this integral curve leads to a solution that is nonsingular at the origin; the others treated above lead to solutions singular at the origin.

As we advance away from the origin in the Lie plane, the integral curves spiral outwards around the origin. Each time they cross the line $u = 0$, $y = 0$; each time they cross the line $v = 0$, $\dot{y} = 0$. Clearly, then, the solution oscillates as x increases. The oscillations are bounded. This is easier to prove starting from (15) than by using the Lie plane. If we multiply (15) by $\dot{y}\,dx = dy$ and integrate, we get $\frac{1}{2}(\dot{y})^2 + \int_a^x (2/x)(\dot{y})^2 \times dx + \frac{1}{4}y^4 = \text{const}$, where $x = a$ is some point at which y is nonsingular. When $x > a$, all the terms in the sum are positive, and therefore they must be bounded. Then y and $\dot{y}$ are both bounded for $x > a$.

The solutions of (15) for $n = 3$ are thus all oscillatory and bounded at ∞. They have no singularities when $x > 0$. At $x = 0$ they are singular, except for a one-parameter family of solutions that are regular everywhere.

FERMI–THOMAS EQUATION

The Fermi–Thomas equation has the form

$$\ddot{y} = x^{-\frac{1}{2}}y^{\frac{3}{2}} \tag{27}$$

and is invariant to the group of transformations

$$y' = \lambda^{-3}y, \tag{28a}$$

$$x' = \lambda x, \tag{28b}$$

whose invariant u and first differential invariant v are

$$u = x^3y, \tag{29a}$$

$$v = x^4\dot{y}. \tag{29b}$$

In terms of u and v, (27) becomes

$$\frac{dv}{du} = \frac{u^{\frac{3}{2}} + 4v}{v + 3u}. \tag{30}$$

The critical points of (30) are (0, 0) and (144, −432). The direction field in the Lie plane is shown in Fig. 11. The abscissas in Fig. 11 have been reduced by a factor of 64, the ordinates by a factor of 200. Only the right half-plane is considered since u cannot be less than zero. The origin is a nodal point; the point P: (144, −432) is a saddle point. The separatrices cross the

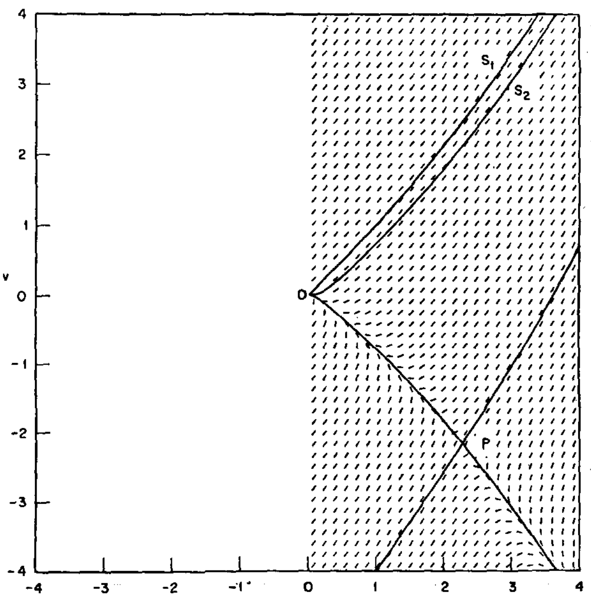

FIG. 11. The direction field in the Lie plane for the Fermi–Thomas equation.

saddle point with slopes of $\frac{1}{2}(1 \pm \sqrt{73})$. One of them, the one with the negative slope, also passes through the origin.

Let us now study the asymptotic behavior of the separatrices. On any integral curve in the Lie plane on which $|u|$ and $|v| \to \infty$, five possibilities are open:

$$|v| \ll |u|, \quad \text{i.e.,} \quad \lim_{|u|\to\infty} |v/u| = 0,$$

$$|v| \sim |u|, \quad \text{i.e.,} \quad \lim_{|u|\to\infty} |v/u| = \text{const},$$

$$|v| \gg |u|, \quad \text{i.e.,} \quad \lim_{|u|\to\infty} |v/u| = \infty.$$

The latter case comprises three subcases, $|v| \ll |u|^{\frac{3}{2}}$, $|v| \sim |u|^{\frac{3}{2}}$, or $|v| \gg |u|^{\frac{3}{2}}$.

Case 1: $|v| \ll |u|$. Then $dv/du \sim \frac{1}{3}u^{\frac{1}{2}}$, $v \sim \frac{2}{9}u^{\frac{3}{2}}$ so that $|v|$ is not $\ll |u|$, a contradiction.

Case 2: $|v| \sim |u|$. $dv/du \sim \text{const} \times u^{\frac{1}{2}}$, $v \sim \text{const} \times u^{\frac{3}{2}}$, which is a contradiction.

Case 3: $|u|^{\frac{3}{2}} \gg |v| \gg |u|$. $dv/du \sim u^{\frac{3}{2}}/v$, $v \sim (2/\sqrt{5})u^{\frac{5}{4}}$. This last equation can be integrated again to give

$$y = [(2/3\sqrt{5})x^{\frac{3}{4}} - a]^{-4}, \tag{31a}$$

$$u = x^3[(2/3\sqrt{5})x^{\frac{3}{4}} - a]^{-4}, \tag{31b}$$

$$v = -(2/\sqrt{5})x^{\frac{15}{4}}[(2/3\sqrt{5})x^{\frac{3}{4}} - a]^{-5}, \tag{31c}$$

where a is a constant of integration. $|u|$ and $|v|$ can only approach ∞ if $(2/3\sqrt{5})x^{\frac{3}{4}} \to a$. If the approach to a is from below, $u \to +\infty$ and $v \to +\infty$; if the approach is from above, $u \to +\infty$ and $v \to -\infty$.

Case 4: $|v| \sim |u|^{\frac{3}{2}}$. $dv/du \sim \text{const}$, so that $|v| \sim |u|$, again a contradiction.

Case 5: $|v| \gg |u|^{\frac{3}{2}}$. The proof is the same as in Case 4.

Next let us locate the singularities, if any, in the finite portion of the Lie plane. In the neighborhood of a singularity, we have $\dot{y}^3/y^4 = v^3/u^4$, where the right-hand side can be considered as constant. Integration gives $y = 27[a - (v/u^{\frac{4}{3}})x]^{-3}$, $u = 27x^3[a - (v/u^{\frac{4}{3}})x]^{-3}$, $v = 81x^4(v/u^{\frac{4}{3}})[a - (v/u^{\frac{4}{3}})x]^{-4}$. At a singularity, u and v would thus become infinite, contrary to hypothesis, unless the constant $a = 0$. If $a = 0$, $u = -27u^4/v^3$, and $v = 81u^4/v^3$, so that $v = -3u$ and $y = u/x^3$. Thus the only possible singularity in the finite part of the Lie plane corresponds to an x^{-3} singularity in the (x, y) plane at $x = 0$. If we substitute $y = u/x^3$ into (27), we find that it will only satisfy (27) if $u = 144$; but then it satisfies (27) for all x. Hence only the special solution $y = 144/x^3$ can have a singularity in the finite part of the Lie plane; the singularity occurs at the point P.

Next let us study the behavior of the solutions corresponding to integral curves near the origin. Again we analyze (30) by cases. As $|u|$ and $|v|$ approach zero, five possibilities exist.

Case 1: $|v| \ll |u|^{\frac{3}{2}}$. $dv/du = \frac{1}{3}u^{\frac{1}{2}}$, $v = \frac{2}{9}u^{\frac{3}{2}}$, which is a contradiction.

Case 2: $|v| \sim |u|^{\frac{3}{2}}$. Set $v = \lambda u^{\frac{3}{2}}$. $dv/du = \frac{1}{3}(1 + 4\lambda)u^{\frac{1}{2}}$ or $v = \frac{2}{9}(1 + 4\lambda)u^{\frac{3}{2}}$. Therefore, $\lambda = 2$ and $v = 2u^{\frac{3}{2}}$.

Case 3: $|u| \gg |v| \gg |u|^{\frac{3}{2}}$. $dv/du = 4v/3u$. $v = au^{\frac{4}{3}}$, $a = \text{const}$.

Case 4: $|v| \sim |u|$. Set $v = \lambda u$. $\lambda = 4\lambda/(\lambda + 3)$ or $\lambda = 1$. Therefore, $v = u$.

Case 5: $|v| \gg |u|$. $dv/du = 4$, $v = 4u$, which is a contradiction.

The separatrix OP has a negative slope; for small u it therefore has the form $v = au^{\frac{4}{3}}$. The value of a has been determined by Fermi as -1.58 and by Baker as -1.588588.[5] Any attempt to determine a by integrating from the origin outwards is plagued by two difficulties: First, it must be a trial and error method; second, it will be unstable against small errors, e.g., roundoff and truncation errors. In contrast, a can be determined by a *single* inward integration from the saddle point, which is, moreover, stable. The starting values are $(+144, -432)$ and the starting slope (necessary at the critical point) is $\frac{1}{2}(1 - \sqrt{73})$. In fact, if we only want the value of a and not the equation of the separatrix, it is enough to start at any convenient point in the Lie plane and integrate inwards to the origin.

The solutions in the (x, y) plane corresponding to $v = au^{\frac{4}{3}}$ are $y = (b - \frac{1}{3}ax)^{-3}$, $u = x^3(b - \frac{1}{3}ax)^{-3}$, $v = ax^4(b - \frac{1}{3}ax)^{-4}$. If u and v are both to vanish, x must $\to 0$ and b cannot equal zero. Thus, in the neighborhood of the origin, the solutions corresponding to the separatrix OP behave like $y = (b - \frac{1}{3}ax)^{-3}$.

How do these solutions behave as we move along the separatrix OP towards the saddle point? In the vicinity of the saddle point, $u = 144 + u'$, $v = -432 + v'$, $v' = mu'$, $m = \frac{1}{2}(1 - \sqrt{73})$. Then $v - mu = -432 + v' - 144m - mu' = -(432 + 144m)$. In terms of x and y this becomes $x^4\dot{y} - mx^3y = -(432 + 144m)$. This last equation is linear, and, to solve it, we set $y = 144x^{-3} + w$. Then $x^4\dot{w} - mx^3w = 0$ so that $w = cx^m$, $c = \text{const}$. Hence $y = 144x^{-3} + cx^m$, $u = 144 + cx^{3+m}$, $v = -432 + mcx^{m+3}$. As we approach the saddle point then, x^{3+m} must approach zero and, since $3 + m < 0$, x must clearly $\to \infty$. Thus the arc of the separatrix between the origin and the saddle point corresponds to a one-parameter family of solutions having the behavior $y = (b - \frac{1}{3}ax)^{-3}$ at the origin and $y = 144/x^3$ for large x. All the members of this family transform into one another under the group (28). The member for which $b = 1$ is the solution originally obtained by Fermi and by Bush and Caldwell.[6]

The same analysis holds when we approach the saddle point along the other separatrix, except that now $m + 3 > 0$. Clearly, then, $x = 0$ at the saddle point for curves corresponding to this separatrix. These curves all behave like $144x^{-3}$ at the origin.

So far we have only considered Case 3 of the three noncontradictory possibilities for the behavior of u and v as both approach zero. Case 4 implies the existence of an integral curve S_1 entering the origin with $v = u$. Near $u = 0$, this integral curve has the series expansion $v = u + \frac{1}{3}u^{\frac{3}{2}} - \frac{1}{30}u^2 + \frac{1}{180}u^{\frac{5}{2}} + \cdots$. Along this curve, $y = bx$, to lowest order, where b is a constant of integration. All of these solutions form a one-parameter family, transformable into one another according to (28). The one for which $b = 1$ has the following power series expansion around $x = 0$:

$$y = x + \tfrac{1}{6}x^3 + \tfrac{1}{80}x^5 + \tfrac{1}{1440}x^7 + \cdots. \quad (32)$$

Eventually this solution becomes singular (since the integral curve starting with $v = u$ at the origin lies above the separatrix with positive slope).

Case 2 implies an integral curve S_2 which enters the origin with $v = 2u^{\frac{3}{2}}$. S_2, which has the series expansion $2u^{\frac{3}{2}} - 3u^2 + 6u^{\frac{5}{2}} + 66u^3 + \cdots$, corresponds to a family of solutions behaving like $y = (b - \frac{2}{3}x^{\frac{3}{2}})^{-2}$, $b \neq 0$, near $x = 0$. The member of the family for which $b = 1$ has the following expansion around $x = 0$:

$$y = 1 + \tfrac{4}{3}x^{\frac{3}{2}} + \tfrac{1}{3}x^3 + \tfrac{2}{27}x^{\frac{9}{2}} + \tfrac{4}{405}x^6 + \cdots. \quad (33)$$

Next, what happens when we approach the line $u = 0$ away from the origin? $dv/du = 4$ when $|u| \ll |v|$. Then $v - v_0 = 4u$. In terms of x and y, $x^4\dot{y} = 4x^3y + v_0$. We can solve this as we did above: $y = -\frac{1}{7}v_0x^{-3} + Ax^4$, $A = \text{const.}$ $u = -\frac{1}{7}v_0 + Ax^7$ and $v = \frac{3}{7}v_0 + 4Ax^7$. For u to vanish, x must equal $x_0 = (v_0/7A)^{\frac{1}{7}}$. Then $v = v_0$ as it should, and $y(x_0) = 0$. Thus the line $u = 0$ corresponds to a root of the solution. It is an upcrossing for positive v_0 and a downcrossing for negative v_0. In either case, the solution cannot be advanced analytically, since u can never be negative. One may skip from a point on the negative v axis to a point on the positive v axis, and the solution has a discontinuity in slope at $y = 0$.

We break off the analysis of the Fermi–Thomas equation here even though some interesting questions still remain unanswered, e.g., how do the integral curves between S_1 and S_2 approach the origin? A wide variety of solutions is possible, but only those corresponding to the segment OP of the separatrix are known to be of physical significance.

DISCUSSION

The equations discussed here are all invariant under extremely simple groups, and the group invariance is evident on inspection. Many interesting differential equations are invariant under somewhat more complicated groups, but the group invariance is hard to recognize. Lie[7] has shown how to calculate the most general differential equation of given order invariant under a specified group. Tables have been prepared of these differential equations for various groups.[8] A given differential equation can be compared with the entries in the tables and, if it is found to have one of the forms entered in the table, a group under which it is invariant can be identified. In this way, the differential equation $x^3\ddot{y} = f(x\dot{y} - y)$, which is a generalization of Eq. (6.93) in Kamke's compilation,[9] is found to be invariant to the group of transformations $x' = x(1 + x\lambda)^{-1}$, $y' = y(1 + x\lambda)^{-1}$ (group X in Table II of Ref. 1). In spite of these tables, however, one often encounters equations for which no group invariance is obvious; in fact, it has been shown that there are second-order differential equations that are not invariant under any group.[10] The application of Lie's method thus depends to some extent on fortunate circumstances, but, as the examples given in this paper have shown, such circumstances are not rare.

* Research sponsored by the U.S. Atomic Energy Commission under contract with the Union Carbide Corporation.

[1] A. Cohen, *An Introduction to the Lie Theory of One-Parameter Groups with Applications to the Solution of Differential Equations* (Stechert, New York, 1931), Sec. 27, pp. 86–89.
[2] G. W. Walker, Proc. Roy. Soc. (London) **A41**, 410 (1915); H. Lemke, J. Math., No. 2, **142**, 118 (1913).
[3] Reference 1, Sec. 12, pp. 37, 38.
[4] H. T. Davis, *Introduction to Nonlinear Differential and Integral Equations* (U.S. Govt. Printing Office, Washington, D.C., 1960), p. 373.
[5] Reference 4, p. 406.
[6] Reference 4, p. 407.
[7] Reference 1, Chap. IV, pp. 82–103.
[8] Reference 1, Tables I and II.
[9] E. Kamke, *Differentialgleichungen—Lösungsmethoden und Lösungen* (Edwards Brothers, Ann Arbor, Michigan, 1945), Vol. I.
[10] Reference 1, Note IV, pp. 206–08.

Electromagnetic Sources in a Moving Conducting Medium

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(Received 26 June 1970)

The problem of an arbitrary source distribution in a uniformly moving, homogeneous, isotropic, nondispersive, conducting medium is solved. The technique used is to solve the problem in the rest system of the medium and then write the result in an appropriate four-dimensional, covariant form which is valid in any inertial system.

I. INTRODUCTION

Recently Besieris and Compton[1] solved the problem of electromagnetic radiation by an arbitrary source in a uniformly moving, homogeneous, isotropic, nondispersive, conducting medium by making use of a relation between the fundamental solution of a radiation problem and that of a corresponding Cauchy initial value problem. An alternative method was provided by Chen and Yen,[2] who applied judiciously chosen affine transformations to the pertinent differential equation.

It is the purpose of this paper to solve the same problem but in a different way. The most essential feature of the technique used in the present paper is that the problem is handled in the rest system K' of the medium "as long as possible," because the pertinent differential equations are much simpler in K'. In fact the whole problem is solved in K' by making use of the known fundamental solution of the Klein–Gordon differential equation; the result is then transformed to an arbitrary inertial system K by means of an appropriate tensor formulation.

We use Cartesian tensor notation as in Ref. 3. By a tensor we understand a tensor defined on the Lorentz transformation group. Latin subscripts run from 1 to 4, Greek subscripts run from 1 to 3. The coordinate $x_4 \equiv ict$, where t is the time and c the speed of light in vacuum; therefore, the metric tensor in 4-space is equal to the Kronecker symbol δ_{ij} (when Cartesian spatial coordinates are used) and we do not distinguish between contravariant and covariant tensors. Repeated subscripts obey the summation convention, and commas in subscripts denote partial differentiation with respect to coordinates (or covariant differentiation since the metric tensor is independent of the coordinates).

II. THE POTENTIAL TENSOR (4-VECTOR)

In any inertial system Maxwell's equations are

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_f + \mathbf{J},$$

$$\nabla \cdot \mathbf{D} = \rho_f + \rho,$$

$$\nabla \cdot \mathbf{B} = 0, \tag{1}$$

where **E**, **H**, **D**, **B** are familiar symbols for the field quantities, $\mathbf{J}_f$, ρ_f denote the free current and charge densities, and **J**, ρ the externally applied current and charge densities.

In the rest system K' of the medium, the following constitutive relations are assumed to be valid:

$$\mathbf{D}' = \epsilon \mathbf{E}',\quad \mathbf{B}' = \mu \mathbf{H}',\quad \mathbf{J}_f' = \sigma \mathbf{E}', \tag{2}$$

where ϵ, μ, σ are the dielectric constant, the permeability and the conductivity, respectively.

It is well known[4] that vector and scalar potentials $\mathbf{A}'$, Φ' can be introduced in K', satisfying the equations

$$\nabla^2 \mathbf{A}' - \mu\epsilon \frac{\partial^2 \mathbf{A}'}{\partial t'^2} - \sigma\mu \frac{\partial \mathbf{A}'}{\partial t'} = -\mu \mathbf{J}',$$
$$\nabla^2 \Phi' - \mu\epsilon \frac{\partial^2 \Phi'}{\partial t'^2} - \sigma\mu \frac{\partial \Phi'}{\partial t'} = -\frac{1}{\epsilon}\rho', \tag{3}$$

where we have assumed that $\rho_f' = 0$ because of the brevity of usual relaxation times.

$\mathbf{A}'$ and Φ' are connected by the gauge condition

$$\nabla \cdot \mathbf{A}' + \mu\epsilon \frac{\partial \Phi'}{\partial t'} + \sigma\mu\Phi' = 0. \tag{4}$$

The translation of (3) into tensor language is given in Ref. 5 for the case $\sigma = 0$. It is not difficult to show that if $\sigma \neq 0$, a single term has to be added so that the tensor wave equation for the potential tensor A_i (consult Ref. 6) which is valid in any inertial system K may be written as

$$A_{i,nn} - \kappa A_{i,rs} U_r U_s - \sigma\mu A_{i,r} U_r = -S_i, \tag{5}$$

where $\kappa \equiv (n^2 - 1)/c^2$, $n \equiv c/c'$, $c' \equiv (\mu\epsilon)^{-\frac{1}{2}}$, $S_i \equiv \mu(J_i + \kappa/n^2 J_r U_r U_i)$, U_r is the velocity 4-vector, and finally J_i is the current density 4-vector (consult Ref. 6) of the external source.

The tensor equation for the gauge condition turns out to be

$$A_{r,r} - \kappa A_{r,s}U_rU_s - \sigma\mu A_rU_r = 0. \qquad (6)$$

III. INTEGRATION OF THE TENSOR EQUATION FOR DAMPED WAVES

The first-order term in (5) may be eliminated. Let k_i denote a constant 4-vector (i.e., independent of the space–time coordinates x_r). Also, tensor functions B_i and T_i are defined by

$$B_i \equiv A_i e^{-k_r x_r}, \quad T_i \equiv S_i e^{-k_r x_r}. \qquad (7)$$

From (5) and (7) we derive

$$B_{i,nn} - \kappa B_{i,rs}U_rU_s + l^2 B_i = -T_i, \qquad (8)$$

where

$$l \equiv [k_rk_r - \kappa(k_rU_r)^2 - \sigma\mu k_rU_r]^{\frac{1}{2}} \qquad (9)$$

and k_r is subjected to the condition

$$2k_i - (2\kappa k_rU_r + \sigma\mu)U_i = 0. \qquad (10)$$

Since $U_i' = (0, 0, 0, ic)$, (10) is satisfied in K' if we define

$$k_i' \equiv \left(0, 0, 0, i\frac{\sigma\mu c}{2n^2}\right). \qquad (11)$$

Because (10) is a tensor equation, it holds in any system of inertia K since it holds in K'. [In K we can get k_r from (11) by means of the tensor transformation law.]

l is defined by (9) and transforms like an invariant under a Lorentz transformation. It is easily shown (in K') that

$$l = \tfrac{1}{2}\sigma(\mu/\epsilon)^{\frac{1}{2}}. \qquad (12)$$

In K' (8) reduces to

$$\left(\nabla'^2 + n^2\frac{\partial^2}{\partial x_4'^2} + l^2\right)B_i' = -T_i'. \qquad (8')$$

In preparation for the integration of this equation, consider

$$\left(\nabla'^2 - (in)^2\frac{\partial^2}{\partial x_4'^2} - (il)^2\right)G' = -4\pi\delta(u_r'), \qquad (13)$$

where $u_r' \equiv x_r' - z_r'$; z_r' are parameters and $\delta(u_r') \equiv \delta(u_1')\delta(u_2')\delta(u_3')\delta^\star(u_4')$. $\delta^\star(u_4')$ is a delta-function with purely imaginary argument, i.e., $\int_{-i\infty}^{i\infty} f(z)\delta^\star(z)\,dz = f(0)$ for a great class of functions f.

Equation (13) is the Klein–Gordon equation for the time-dependent Green's function G'. The solution of (13) for the whole space is given in Ref. 7 for real constants (in) and (il). It is readily seen that the solution also holds when (in) and (il) are purely imaginary; therefore

$$G'(x_r', z_r') = \begin{cases} \dfrac{\delta^\star(u_4' - inr')}{r'} - i\dfrac{l}{n}\dfrac{J_1(lR')}{R'}1_+^\star(u_4' - inr'), & \dfrac{u_4'}{i} > 0 \\ 0, & \dfrac{u_4'}{i} < 0 \end{cases}, \qquad (14)$$

where

$$R' \equiv [r'^2 + (u_4'/n)^2]^{\frac{1}{2}}, \quad r' \equiv (u_\nu'u_\nu')^{\frac{1}{2}}. \qquad (15)$$

J_1 is the Bessel function of first kind and first order, and $1_+^\star$ denotes the unit step function with purely imaginary argument, i.e.,

$$1_+^\star(x) = \begin{cases} 1, & x/i \geq 0 \\ 0, & x/i < 0 \end{cases}.$$

By means of G' we are able to write down an integral representation for the potentials A_i' connected with B_i' by (7):

$$A_i'(x_r') = \frac{1}{4\pi}\iiint_{-\infty}^{\infty}\int_{-i\infty}^{i\infty} e^{k_r'u_r'}G'(x_r', z_r') \times S_i'(z_r')\,du_1'\,du_2'\,du_3'\,du_4'. \qquad (16)$$

IV. TRANSFORMATION TO AN ARBITRARY INERTIAL SYSTEM

Let a_{ji} be the transformation matrix for a proper Lorentz transformation, i.e., $x_r = a_{rs}x_s'$. Multiplying (16) by a_{ji}, we see that the left side is equal to $A_j(x_r)$ because A_j is a tensor. a_{ji} may be taken under the integral and, since S_i is a tensor, $a_{ji}S_i'(z_r') = S_j(z_r)$ if the Lorentz transformation is also applied to the integration variables, i.e., if $z_r = a_{rs}z_s'$ which implies $u_r = a_{rs}u_s'$. Furthermore, k_r is a tensor so that $e^{k_r'u_r'} = e^{k_ru_r}$.

Next we investigate how the Green's function G' is transformed. Without loss of generality, we choose a_{rs} so that $x_1 = x_1'$, $x_2 = x_2'$, $x_3 = \gamma(x_3' + i\beta x_4')$, $x_4 = \gamma(x_4' - i\beta x_3')$, where $\gamma \equiv (1 - \beta^2)^{-\frac{1}{2}}$, $\beta \equiv v/c$, and v is the velocity of K relative to K'.

Consider a three-dimensional hypersurface in Minkowski space, which in K' is given by $R'^2 = 0$, $u_4'/i > 0$ (Fig. 1) (cf. Ref. 3). In order to express the surface independently of the inertial system, we define

$$R \equiv \left[u_ru_r + \kappa\left(\frac{u_rU_r}{n}\right)^2\right]^{\frac{1}{2}}. \qquad (17)$$

Obviously R is an invariant function of u_r, and it is easily seen that $R = R'$ in K'. Therefore, the

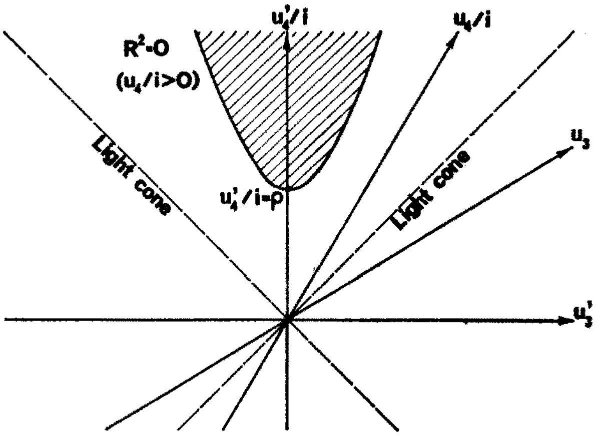

FIG. 1. Location of zeros of the function R^2 in Minkowski 4-space for $u_4/i > 0$.

hypersurface is also given by $R^2 = 0$, $u_4/i > 0$ because it is located entirely in that part of Minkowski space where the condition $u_4/i = (x_4 - z_4)/i > 0$ is valid in any inertial system K.

u_4 is purely imaginary so R^2 may be negative, which is the case inside the hatched domain in Fig. 1. The roots of $R^2 = 0$ are given by (cf. Ref. 3)

$$\frac{u_4}{i} = \tau_\pm \equiv \frac{n\beta}{1-(n\beta)^2}\left[\left(n - \frac{1}{n}\right)u_3 \pm \left(\frac{1}{\beta} - \beta\right)(u_3^2 + a\rho^2)^{\frac{1}{2}}\right], \quad (18)$$

where $a \equiv [1 - (n\beta)^2]/(1 - \beta^2)$, $\rho \equiv (u_1^2 + u_2^2)^{\frac{1}{2}}$.

It is seen that $n\beta < 1$ implies $\tau_+ > 0$, $\tau_- < 0$. In the domain $u_4/i > 0$ the equation $R^2 = 0$ defines a one to one correspondence between u_3 and u_4 (for given ρ). This is not the case for $n\beta > 1$ (Čerenkov region) because $\tau_\mp > 0$ for $u_4/i < -\rho\,|a|^{\frac{1}{2}}$, and both roots are complex or do not belong to the domain $u_4/i > 0$ for $u_4/i > -\rho\,|a|^{\frac{1}{2}}$.

From the preceding remarks we conclude that the step function in (14) may be written in covariant form as $1_+(-R^2)$, $u_4/i > 0$.

As to the δ function in (14), we have

$$\frac{\delta^\star(u_4' - inr')}{-(dR^2/du_4')_{u_4'=inr'}} = \frac{\delta^\star(u_4' - inr')}{i(2/n)r'} = \delta(-R^2), \quad u_4/i > 0. \quad (19)$$

Finally we observe that the limits of integration in (16) remain unchanged because a Lorentz transformation is a one-to-one mapping of the Minkowski space on itself.

We are now able to write down the covariant forms of (14) and (16) valid in an arbitrary inertial system:

$$A_i(x_r) = \frac{1}{4\pi}\iiint_{-\infty}^{\infty}\int_{-i\infty}^{i\infty} e^{k_r u_r} G(x_r, z_r) \times S_i(z_r)\, du_1\, du_2\, du_3\, du_4, \quad (20)$$

$$G(x_r, z_r) = \begin{cases} i\dfrac{2}{n}\,\delta(-R^2) - i\dfrac{l}{n}\dfrac{J_1(lR)}{R}\,1_+(-R^2), & \dfrac{u_4}{i} > 0 \\ 0, & \dfrac{u_4}{i} < 0 \end{cases} \quad (21)$$

When $n\beta < 1$,

$$i\frac{2}{n}\,\delta(-R^2) = i\frac{2}{n}\frac{\delta^\star(u_4 - i\tau_+)}{-(dR^2/du_4)_{u_4=i\tau_+}} = \frac{\delta^\star(u_4 - i\tau_+)}{(u_3^2 + a\rho^2)^{\frac{1}{2}}}, \quad u_4/i > 0. \quad (22)$$

When $n\beta > 1$, both roots $\tau_\pm$ play a part as pointed out before. In this case it turns out that

$$i\frac{2}{n}\,\delta(-R^2) = \frac{\delta^\star(u_4 - i\tau_+) + \delta^\star(u_4 - i\tau_-)}{(u_3^2 + a\rho^2)^{\frac{1}{2}}}, \quad u_4/i > 0. \quad (22')$$

If the medium is nonconductive, i.e., $\sigma = 0$, then $k_r u_r = 0$ and $l = 0$ [cf. (11) and (12)], furthermore, the second term in (21) evidently vanishes. This problem has been investigated previously by Compton,[8] Lee and Papas,[9] Tai,[10,11] and the author.[3] As pointed out by Tai,[11] the first term in (21) is equivalent to the corresponding expression found by Compton.[8]

As to the general case ($\sigma \neq 0$), the result given by Besieris and Compton[1,12] is in error[13] due to miscalculation, and there is a formal error in Ref. 2,[14] so the author hopes deeply that he is right in asserting that the results in Refs. 1 and 2 can be brought into agreement with the results given here.

[1] I. M. Besieris and R. T. Compton, Jr., J. Math. Phys. **8**, 2445 (1967).

[2] K. C. Chen and J. L. Yen, J. Math. Phys. **9**, 2081 (1968).

[3] G. Johannsen, J. Math. Phys. **11**, 3251 (1970).

[4] D. S. Jones, *The Theory of Electromagnetism*, Vol. 47 (Pergamon, New York, 1964).

[5] J. M. Jauch and K. M. Watson, Phys. Rev. **74**, 950 (1948).

[6] C. Møller, *The Theory of Relativity* (Oxford U.P., London, 1952).

[7] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, Vol. I (McGraw-Hill, New York, 1953), pp. 854–857.

[8] R. T. Compton, Jr., J. Math. Phys. **7**, 2145 (1966).

[9] K. S. H. Lee and C. H. Papas, J. Math. Phys. **5**, 1688 (1964).

[10] C. T. Tai, IEEE Trans. Antennas Propagation **AP-13**, 322 (1965).

[11] C. T. Tai, J. Math. Phys. **8**, 646 (1967).

[12] I. M. Besieris, J. Math. Phys. **8**, 409 (1967).

[13] As pointed out in Ref. 2, there is an algebraic error in Eq. (18a), Ref. 1 (v should be replaced by γv); furthermore, the factor before the second term of (59), Ref. 12, is not correct, which in turn influences the results in Ref. 1.

[14] In Eq. (21) etc., Ref. 2, the argument of the Bessel function is in error.

Equivalence of Different Representations of the Generalized Bose Operator

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(Received 12 November 1970)

The infinite series representation of the generalized Bose operator given by Brandt and Greenberg is shown to be equal to an operator introduced by Demkov.

Generalized Bose operators b which reduce by two the number of quanta of a Bose operator a have recently been studied by Brandt and Greenberg.[1] The representations obtained for these operators are normal ordered infinite-degree power series of a, namely

$$b = \sum_{j=0}^{\infty} \alpha_j (a^\dagger)^j a^{j+2}, \tag{1}$$

where

$$\alpha_j = \frac{1}{2j!} \sum_{r=0}^{j} \binom{j}{r} (-1)^{j-r} \left(\frac{2r + 3 + (-1)^r}{(r+2)(r+1)}\right)^{\frac{1}{2}} \exp(i\theta_r), \tag{2}$$

the θ_r being arbitrary real numbers.

Demkov,[2] studying the symmetry group of the two-dimensional anisotropic oscillator, introduced the operator

$$\begin{aligned} B &= B_+\Lambda_+ + B_-\Lambda_-, \\ B_+ &= 2^{-\frac{1}{2}} a(a^\dagger a)^{-\frac{1}{2}} a, \quad B_- = 2^{-\frac{1}{2}} a(aa^\dagger)^{-\frac{1}{2}} a, \\ \Lambda_+ &= \cos^2(\pi a^\dagger a/2), \quad \Lambda_- = \sin^2(\pi a^\dagger a/2). \end{aligned} \tag{3}$$

This operator will now be shown, in a representation-independent manner, to be equal to the generalized Bose operator b, provided that the choice $\theta_r = 0$, $r = 0, \cdots, \infty$, is made and thus constitutes a compact and convenient representation of it.

Lemma:

$$a\Lambda_\pm = \Lambda_\mp a. \tag{4}$$

Proof: Using the normal ordered expansion formula[3]

$$f(a^\dagger a) = \sum_{r=0}^{\infty} \sum_{s=0}^{r} \frac{(-1)^{r-s} f(s)}{s!\,(r-s)!} (a^\dagger)^r a^r \tag{5}$$

and the fact that $[a, (a^\dagger)^r] = r(a^\dagger)^{r-1}$, we get

$$\begin{aligned} a\Lambda_+ &= a\cos^2(\tfrac{1}{2}\pi a^\dagger a) \\ &= \sum_{r=0}^{\infty} \sum_{s=0}^{r} \frac{(-1)^{r-s}\cos^2(\frac{1}{2}\pi s)}{s!\,(r-s)!} [(a^\dagger)^r a^{r+1} + r(a^\dagger)^{r-1} a^r]. \end{aligned}$$

Separating the two terms, changing the summation index in the second to $r' = r - 1$, and noting that, by continuing the first for $s > r$, vanishing terms are added [as then $1/(r-s)! = 0$], we get

$$\begin{aligned} a\Lambda_+ &= \sum_{r=0}^{\infty} \sum_{s=0}^{r+1} \frac{(-1)^{r-s}}{s!\,(r-s)!} \left(1 - \frac{(r+1)}{(r+1-s)}\right) \\ &\quad \times \cos^2(\tfrac{1}{2}\pi s)(a^\dagger)^r a^{r+1} \\ &= \sum_{r=0}^{\infty} \sum_{s=0}^{r+1} \frac{(-1)^{r+1-s}}{(s-1)!\,(r+1-s)!} \cos^2(\tfrac{1}{2}\pi s)(a^\dagger)^r a^{r+1}. \end{aligned}$$

Noting that the term $s = 0$ vanishes and changing to $s' = s - 1$, we get

$$\begin{aligned} a\Lambda_+ &= \sum_{r=0}^{\infty} \sum_{s=0}^{r} \frac{(-1)^{r-s}}{s!\,(r-s)!} \sin^2(\tfrac{1}{2}\pi s)(a^\dagger)^r a^{r+1} \\ &= \sin^2(\tfrac{1}{2}\pi a^\dagger a) a \equiv \Lambda_- a, \end{aligned}$$

Eq. (5) having been used in the last step. The identity $a\Lambda_- = \Lambda_+ a$ follows analogously. One might suspect that the proper form of the operator B should be

$$B = \Lambda_+ B_+ \Lambda_+ + \Lambda_- B_- \Lambda_-, \tag{6}$$

but, by a straightforward use of the lemma and the relations $[\Lambda_\pm, (a^\dagger a)^{-\frac{1}{2}}] = 0$ and $\Lambda_\pm^2 = \Lambda_\pm$, one easily shows that the expression given in Eq. (6) is equal to that given in Eq. (3).

Using the lemma, we note that

$$B = 2^{-\frac{1}{2}} a[(a^\dagger a)^{-\frac{1}{2}}\Lambda_- + (aa^\dagger)^{-\frac{1}{2}}\Lambda_+]a. \tag{7}$$

If we introduce the expansion (5), it follows that

$$\begin{aligned} B &= 2^{-\frac{1}{2}} a \sum_{r=0}^{\infty} \sum_{s=0}^{r} \frac{(-1)^{r-s}}{s!\,(r-s)!} \\ &\quad \times \left(\frac{\sin^2(\frac{1}{2}\pi s)}{s^{\frac{1}{2}}} + \frac{\cos^2(\frac{1}{2}\pi s)}{(s+1)^{\frac{1}{2}}}\right)(a^\dagger)^r a^{r+1}. \end{aligned}$$

By a sequence of operations analogous to that used in the proof of the lemma, we obtain

$$\begin{aligned} B = \sum_{r=0}^{\infty} \frac{1}{2r!} \sum_{s=0}^{r} (-1)^{r-s} \binom{r}{s} \Bigg[2^{\frac{1}{2}} \Bigg(& \frac{\cos^2(\frac{1}{2}\pi s)}{(s+1)^{\frac{1}{2}}} \\ & + \frac{\sin^2(\frac{1}{2}\pi s)}{(s+2)^{\frac{1}{2}}} \Bigg) \Bigg] (a^\dagger)^r a^{r+2}. \end{aligned} \tag{8}$$

Using the fact that for integral s

$$\cos^2(\pi s/2) = [1 + (-1)^s]/2,$$

we get

$$[\cos^2(\tfrac{1}{2}\pi s)/(s+1)^{\frac{1}{2}} + \sin^2(\tfrac{1}{2}\pi s)/(s+2)^{\frac{1}{2}}]^2$$
$$= \tfrac{1}{2}\{[2s + 3 + (-1)^s]/(s+1)(s+2)]\}. \quad (9)$$

From Eqs. (1), (2), (8), and (9) we finally get, for $\theta_r = 0$, $r = 0, \cdots, \infty$, $B = b$.

[1] R. A. Brandt and O. W. Greenberg, J. Math. Phys. **10**, 1168 (1969).
[2] Yu. N. Demkov, Zh. Eksp. Teor. Fiz. **44**, 2007 (1963) [Sov. Phys. JETP **17**, 1349 (1963)].
[3] R. M. Wilcox, J. Math. Phys. **8**, 962 (1967).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Micromagnetism and Superconductivity*

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(Received 6 October 1970)

The balance laws of microelectromagnetic theory developed by Eringen and Kafadar [J. Math. Phys. **11**, 1984 (1970)] are shown to contain, as special cases, the classical theories of micromagnetism and Londons' equation of superconductivity. Various generalizations are indicated.

1. INTRODUCTION

Recently[1] we gave a relativistic theory of microelectromagnetism which is intended for the prediction of physical phenomena involving ferromagnetism, micromagnetism, electrets, microwave propagations, and other related microelectromechanical effects. A hierarchy of balance laws was derived for all order moments of electromagnetic fields. The field equations for the zeroth-order moments are Maxwell's equations of the classical electromagnetic theory, and those for the first-order moments are entirely new and possess extra internal degrees of freedom for the description of a large class of microelectromagnetic phenomena not describable by Maxwell's equations.

The main purpose of the present paper is twofold: (i) to derive the basic balance laws of ferromagnetism as a special case of the theory and (ii) to show that Londons' equation of superconductivity is contained in our theory. Various rational extensions of both theories are suggested.

The literature is extensive on both ferromagnetism and superconductivity. Since the introduction of molecular fields by Weiss in 1907, ferromagnetism has been developed in various directions. Both quantum mechanical approaches (Heisenberg,[2] Dirac,[3] and Bloch[4]) and phenomenological work (Landau and Lifshitz,[5] Brown,[6,7] Tiersten,[8] Amari,[9] and Alblas[10]) exist. A number of books and reviews on the subject have also been published (Kittel,[11] Kittel and Galt,[12] and Brown[7]). The basic micromagnetic balance law in most of these works is argued on the basis of its origin through electronic spin. The discussion of magnetic domains, the instability of domain walls, and the micromagnetic resonance phenomena requires knowledge of this law. In phenomenological approaches to the subject, this law is often derived by a variational principle for the static case; afterwards, suitable dynamical terms are added[5–7,10,11] or certain inertia terms or a kinetic energy are postulated.[8,10] A rational and unified approach should provide not only a deeper understanding but also extensions of the existing theories in various fruitful directions.

In Sec. 3 we arrive at the balance law of spin moment of momentum by specializing the general theory given in Ref. 1 and by providing physical interpretations to new magnetic field tensors. Complete balance laws and jump conditions are obtained. Various dynamical generalizations of the theory are indicated.

In Sec. 4 another special case of the basic equations of the microelectromagnetic theory of Ref. 1 is considered. This leads to Londons' equations of superconductivity[13,14] and its generalizations.

Proper reference to works in both fields is beyond the scope of this paper.

We believe it is interesting and important to find that on a microcontinuum basis such seemingly diverse fields as ferromagnetism and superconductivity have the same unified foundations. In addition, various dynamical generalizations and new physical interpretations suggest new directions for research in these fields.

Using the fact that for integral s

$$\cos^2(\pi s/2) = [1 + (-1)^s]/2,$$

we get

$$[\cos^2(\tfrac{1}{2}\pi s)/(s+1)^{\frac{1}{2}} + \sin^2(\tfrac{1}{2}\pi s)/(s+2)^{\frac{1}{2}}]^2 = \tfrac{1}{2}\{[2s + 3 + (-1)^s]/(s+1)(s+2)]\}. \quad (9)$$

From Eqs. (1), (2), (8), and (9) we finally get, for $\theta_r = 0$, $r = 0, \cdots, \infty$, $B = b$.

[1] R. A. Brandt and O. W. Greenberg, J. Math. Phys. **10**, 1168 (1969).
[2] Yu. N. Demkov, Zh. Eksp. Teor. Fiz. **44**, 2007 (1963) [Sov. Phys. JETP **17**, 1349 (1963)].
[3] R. M. Wilcox, J. Math. Phys. **8**, 962 (1967).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

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We believe it is interesting and important to find that on a microcontinuum basis such seemingly diverse fields as ferromagnetism and superconductivity have the same unified foundations. In addition, various dynamical generalizations and new physical interpretations suggest new directions for research in these fields.

2. MICROMAGNETIC BALANCE LAWS

Balance laws (5.11) and (5.13) and jump conditions (5.12) and (5.14) of microelectromagnetic theory given in Ref. 1 may be simplified a great deal in the case of negligible electric fields. Here we are interested in micromagnetism. For this case we set

$$\mathbf{D} = \mathfrak{D} = \mathbf{P} = \mathbf{E} = \mathcal{E} = \boldsymbol{\pi} = \mathbf{0}, \quad q = \sigma = 0,$$
$$E_{kl} = H_{kl} = 0, \quad E_{k4} = H_{k4} = D_{k4} = B_{k4} = 0. \quad (2.1)$$

With this, the balance laws reduce to

$$D^{lk}{}_{;l} = 0, \quad (2.2a)$$
$$\epsilon^{klm} H_{m;l} = (4\pi/c) J^k, \quad (2.2b)$$
$$\epsilon^{kmn} H_n{}^l{}_{;m} - \frac{1}{c}\frac{\partial D^{kl}}{\partial t} + \epsilon^{klm}(H_m - \mathcal{H}_m + 4\pi M_m) = 0, \quad (2.2c)$$
$$B^k{}_{;k} = 0, \quad (2.2d)$$
$$B_k = \mathcal{B}_k, \quad (2.2e)$$
$$B^{lk}{}_{;l} = 0, \quad (2.2f)$$
$$\epsilon^{klm}(\mathcal{H}_m - 4\pi M_m)_{;l} = (4\pi/c) J^k, \quad \text{in} \quad \mathcal{V} - \Gamma, \quad (2.2g)$$

valid in the region $\mathcal{V}$ excluding the discontinuity surface Γ. For the corresponding jump conditions from (5.12) and (5.14) of Ref. 1 we have

$$[D^{lk}] n_l = 0, \quad (2.3a)$$
$$\epsilon^{klm} n_l [H_m] = (4\pi/c) K^k, \quad (2.3b)$$
$$\epsilon^{kmn} n_m [H_n{}^l] + \nu_{(\mathbf{n})} c^{-1} [D^{kl}] = -4\pi \epsilon^{klm} \mu n_m, \quad (2.3c)$$
$$[B^k] n_k = 0, \quad (2.3d)$$
$$[B^{kl}] n_k = 0, \quad (2.3e)$$
$$\epsilon^{klm} n_l [\mathcal{H}_m] = 4\pi (x^k{}_{,a} \epsilon^{ab} \mu_{,b} + \epsilon^{klm} n_l [M_m]) + (4\pi/c) K^k, \quad (2.3f)$$

valid on the discontinuity surface Γ, which may be moving with a normal velocity $\nu_{(\mathbf{n})}$ in the direction of its positive unit normal $\mathbf{n}$. Various tensorial quantities appearing in these equations are:

D^{lk} = electric displacement tensor, H_k = magnetic field vector, $H_k{}^l$ = magnetic field tensor, $\mathcal{H}_k$ = local mean magnetic field, M_k = magnetization vector, $B_k = H_k + 4\pi M_k$ = magnetic flux vector, B^{lk} = magnetic flux tensor, μ = surface magnetization, c = speed of light in vacuum, J^k = the current vector, K^k = the surface current vector.

Throughout this paper we employ the summation convention over the repeated indices, and use the semicolon to indicate covariant partial differentiation with metric tensor g_{kl} and the comma to indicate partial differentiation with respect to the curvilinear coordinates x^k, e.g.,

$$B^k{}_{;l} \equiv B^k{}_{,l} + \left\{{k \atop lm}\right\} B^m, \quad B^k{}_{,l} \equiv \frac{\partial B^k}{\partial x^l}.$$

Also, ϵ^{klm}, $k, l, m = 1, 2, 3$ and ϵ^{ab}, $a, b = 1, 2$, are, respectively, three- and two-dimensional alternating tensors, and indices a, b following a comma indicate the surface gradient on the discontinuity surface Γ given by its Gaussian form $x^k = x^k(u^a)$. Quantities enclosed in boldface brackets are the jumps of these quantities at Γ.

Note that the above set of equations contain the field equations of the classical theory of magnetism, namely,

$$\nabla \times \mathbf{H} = (4\pi/c)\mathbf{J}, \quad \nabla \cdot \mathbf{B} = 0 \quad \text{in} \quad \mathcal{V} - \Gamma, \quad (2.4)$$
$$\mathbf{n} \times [\mathbf{H}] = (4\pi/c)\mathbf{K}, \quad [\mathbf{B}] \cdot \mathbf{n} = 0 \quad \text{on} \quad \Gamma. \quad (2.5)$$

The remaining equations are new.

The field equations (2.2a) and (2.2f) are the generalizations of Gauss' law to the *first moments* of dielectric displacement and magnetic induction in the absence of charges. Equation (2.2c) extends Ampère's law to the *first moment of the magnetic field*, and the last equation of (2.2) is the extension of Ampère's law to the surface average of magnetic field. In the present theory, the magnetic field $\mathbf{H}$ (which is the local line average of the microscopic field) is distinguished from the local surface average $\mathcal{H}$ of the magnetic field. The second-order tensor H^{lk} is the average of the first moment of the local magnetic field and D^{lk} is that of the local dielectric displacement. These equations arise from the consideration of macroscopic electromagnetic fields as *distributions* over macroelements of the body (cf. Ref. 1). We note that these new equations are not the result of multipole expansions. In fact, as we shall see, (2.2c) are the field equations for the micromagnetic fields and spin inertia whose special forms are discussed by Landau and Lifshitz,[5] Brown,[6] and others.

Any second-order tensor may be expressed as

$$D^{kl} = D^{(kl)} + D^{[kl]}, \quad (2.6)$$

where

$$D^{(kl)} \equiv \tfrac{1}{2}(D^{kl} + D^{lk}), \quad D^{[kl]} \equiv \tfrac{1}{2}(D^{kl} - D^{lk})$$

are, respectively, symmetric and antisymmetric parts of D^{kl}. Upon substituting (2.6) into (2.2a) and (2.2c), we get

$$D^{(lk)}{}_{;l} + D^{[lk]}{}_{;l} = 0, \quad (2.7a)$$
$$\epsilon^{mn(k} H_n{}^{l)}{}_{;m} - \frac{1}{c}\frac{\partial D^{(kl)}}{\partial t} = 0, \quad (2.7b)$$
$$\epsilon^{mn[k} H_n{}^{l]}{}_{;m} - \frac{1}{c}\frac{\partial D^{[kl]}}{\partial t} + \epsilon^{klm}(H_m - \mathcal{H}_m + 4\pi M_m) = 0. \quad (2.7c)$$

We now define

$$d_r \equiv \tfrac{1}{2}\epsilon_{klr}D^{[kl]}, \tag{2.8a}$$

$$T^l{}_r \equiv \tfrac{1}{2}(H_r{}^l - H_k{}^k\delta^l{}_r), \tag{2.8b}$$

which possess the inverses

$$D^{[kl]} = \epsilon^{klr}d_r, \tag{2.9a}$$

$$H_r{}^l = 2T^l{}_r - T^k{}_k\delta^l{}_r. \tag{2.9b}$$

Upon introducing these into (2.7), we obtain

$$D^{(lk)}{}_{;l} - \epsilon^{klr}d_{r;l} = 0, \tag{2.10a}$$

$$2\epsilon^{mn(k}T^{l)}{}_{n;m} - \frac{1}{c}\frac{\partial D^{(kl)}}{\partial t} = 0, \tag{2.10b}$$

$$\frac{1}{c}\frac{\partial d_r}{\partial t} = T^l{}_{r;l} + H_r - \mathcal{H}_r + 4\pi M_r. \tag{2.10c}$$

The jump conditions corresponding to these follow from (2.3a) and (2.3c):

$$[D^{(lk)}]n_l + \epsilon^{klr}n_l[d_r] = 0, \tag{2.11a}$$

$$2\epsilon^{mn(k}n_m[T^{l)}{}_n] + \nu_{(\mathbf{n})}c^{-1}[D^{(kl)}] = 0, \tag{2.11b}$$

$$[T^l{}_r]n_l + \nu_{(\mathbf{n})}c^{-1}[d_r] = -4\pi\mu n_r. \tag{2.11c}$$

If d_r is determined by solving (2.10c) under the jump conditions (2.11c), then $D^{(kl)}$ would be determined by the two first sets of (2.10) under the jump conditions (2.11a), (2.11b). Finally, the last two equations of (2.2) and the corresponding jump conditions are necessary in the determination of $\mathcal{H}_m$ and $H_l{}^n$ (equivalently $T^n{}_l$). To this end, however, one alternately needs a set of constitutive equations, which has been ignored so far.

3. BALANCE OF SPIN MOMENT OF MOMENTUM

In the literature there exists a dynamical law for the spin moment of momentum. This law is usually written down on some quantum mechanical arguments (cf. Refs. 2–4) or in analogy with the moment of momentum of an electron.[5–7] A model based on two superposed continua, one mechanical and one spin, was also proposed.[8] All these theories contain certain analogies and rationale. We believe, however, that micromagnetic phenomena is an integral part of microelectromagnetism. Naturally, this important connection could not have been established on any rational basis before a unified theory was available. Here we establish this connection by showing that the dynamical law of spin moment of momentum is a special case of the present theory.

Multiplication of (2.10c) by $\epsilon^{kmr}M_m$ gives

$$\frac{1}{c}\epsilon^{kmr}M_m\frac{\partial d_r}{\partial t} = \epsilon^{kmr}M_m(T^l{}_{r;l} + H_r - \mathcal{H}_r). \tag{3.1}$$

This equation may be made identical to those postulated by Landau and Lifshitz,[6] Brown,[7] Herring,[11] and Tiersten[8] by setting

$$\frac{1}{c}\epsilon^{kmr}M_m\frac{\partial d_r}{\partial t} = \frac{1}{\gamma_0}\frac{\partial M^k}{\partial t}, \tag{3.2}$$

with gyromagnetic ratio $\gamma_0 = ge/2mc$, ($g \simeq 2$), where e/m is the ratio of charge of an electron to its mass.

We now investigate the nature of (3.2). In vector notation

$$\frac{\partial \mathbf{M}}{\partial t} = \frac{\gamma_0}{c}\mathbf{M} \times \frac{\partial \mathbf{d}}{\partial t}. \tag{3.3}$$

From this it follows that

$$\mathbf{M}\cdot\frac{\partial \mathbf{M}}{\partial t} = 0 \quad \text{or} \quad |\mathbf{M}| = M(\mathbf{x}). \tag{3.4}$$

Thus the magnetization must have a magnitude independent of time. This is the assumption used by most previous writers for the saturation of magnetization. In fact most authors take $M = \text{const}$.

An examination of (3.3) indicates that $\partial\mathbf{M}/\partial t$ is perpendicular to the plane of $\mathbf{M}$ and $\mathbf{d}$; thus, if $\mathbf{M}$ is proportional to the mechanical moment of momentum, then

$$\mathbf{\Omega} \equiv \frac{\gamma_0}{c}\frac{\partial \mathbf{d}}{\partial t} \tag{3.5}$$

is the angular velocity with which $\mathbf{M}$ rotates at $\mathbf{x}$. This interpretation may be arrived at also by considering the definition of D^{kl} as given in our work,[1] namely,

$$D^{kl} \equiv \langle D'^k\xi'^l\rangle, \tag{3.6}$$

where an angular bracket indicates the average over a macroelement and $\boldsymbol{\xi}'$ may be taken as the directed segment from a point to the position of the electric displacement vector $\mathbf{D}'$. According to (2.8a), then,

$$\mathbf{d} = \tfrac{1}{2}\langle\mathbf{D}' \times \boldsymbol{\xi}'\rangle. \tag{3.7}$$

With (2.1), we assumed $\mathbf{D} = \langle\mathbf{D}'\rangle = \mathbf{0}$. Now suppose that $\mathbf{D}'$ is independent of time and that the microelements are rigid. If the operator $\partial/\partial t$ is commutative with the angular bracket, then

$$2\frac{\partial \mathbf{d}}{\partial t} = \langle\mathbf{D}' \times \dot{\boldsymbol{\xi}}'\rangle = \langle\mathbf{D}' \times (\boldsymbol{\omega}' \times \boldsymbol{\xi}')\rangle$$
$$= \langle\mathbf{D}'\cdot\boldsymbol{\xi}'\boldsymbol{\omega} - \mathbf{D}'\cdot\boldsymbol{\omega}\boldsymbol{\xi}'\rangle,$$

where $\boldsymbol{\omega}$ is the constant spin angular velocity (the gyration vector) of any point $\boldsymbol{\xi}'$ in macroelement. Thus we may take $\boldsymbol{\omega}$ outside of the angular bracket. Hence

$$2\frac{\partial d_r}{\partial t} = (D^n{}_n\delta^s{}_r - D^s{}_r)\omega_s, \tag{3.8}$$

where we used the definition (3.6). Consequently

$$\Omega_r = \frac{\gamma_0}{2c}(D^n{}_n\delta^s{}_r - D^s{}_r)\omega_s. \quad (3.9)$$

This provides the relation of the gyration vector $\boldsymbol{\omega}$ to angular velocity $\boldsymbol{\Omega}$. It is clear that D^{kl} must have the same dimension as γ_0/c. From (2.2c) we have

$$\dim D^{kl} = ct \dim H^k.$$

Upon using this in (3.5), we see that

$$\gamma_0 \sim \frac{\dim \boldsymbol{\Omega}}{\dim \mathbf{H}} = \frac{e}{mc},$$

which is well known from the theory of electrons (cf. Landau and Lifshitz,[15] p. 121).

Upon introducing (2.9a) for the $D_{[sr]}$, (3.9) may be written as

$$\Omega_r = \frac{\gamma_0}{2c}(D^n{}_n g_{sr} - D_{(sr)})\omega^s - \frac{\gamma_0}{2c}\epsilon_{srn}d^n\omega^s, \quad (3.10)$$

which serves to determine $\boldsymbol{\omega}$ when $\boldsymbol{\Omega}$ (equivalently $\mathbf{d}$) is known.

In the special case when $D_{(sr)} = 0$, (3.10) reduces to

$$\boldsymbol{\Omega} = \frac{\gamma_0}{2c}\boldsymbol{\omega} \times \mathbf{d}. \quad (3.11)$$

In this case $\mathbf{d}$ is to be determined from

$$\frac{\partial \mathbf{d}}{\partial t} = \tfrac{1}{2}\boldsymbol{\omega} \times \mathbf{d}, \quad (3.12)$$

which indicates that $\mathbf{d}$ has a magnitude independent of time and rotates with the angular velocity $\boldsymbol{\omega}$.

Under the above special conditions, (3.1) takes the form

$$\frac{1}{\gamma_0}\frac{\partial M^k}{\partial t} = \epsilon^{kmr}M_m(T^l{}_{r;l} + H_r - \mathcal{H}_r), \quad (3.13)$$

which, as stated, has the form encountered in the literature. Of course, the tensor $T^l{}_r$ and the field $\mathcal{H}_r$ in literature are replaced, respectively, by forms that are derivable from a potential, the free energy. From Brown[16] and Tiersten,[8] for example, we have the identifications[17]

$$\mathcal{H}_r = \frac{\partial F}{\partial M^r}, \quad T^k{}_r = \frac{\partial F}{\partial M^r{}_{,K}}x^k{}_{,K}, \quad (3.14)$$

where $F = F(M^r, M^r{}_{,K}, x^k{}_{,K})$ is the free energy. To obtain such equivalence, one needs the mechanical balance laws (mass, momenta, energy) and a constitutive theory.

The present theory is broader in its scope and coverage. It is a dynamical theory, and the inertia terms are not brought in as a modification to a static theory. Additional developments on thermodynamics and constitutive theory are required for a proper development of a constitutive theory leading to (3.14) and its generalizations. This development is beyond the scope of this paper.

Finally, we consider the jump conditions (2.11c) relevant to spin moment of momentum. By taking the product of this with $\epsilon^{kmr}M_m$, we write

$$\epsilon^{kmr}M_m[(T^l{}_r + 4\pi\mu\delta^l{}_r)n_l + \nu_{(n)}c^{-1}d_r] = 0. \quad (3.15)$$

Aside from the terms containing $\nu_{(n)}$, which drop out for the stationary discontinuity surfaces, this equation is similar to those obtained by others in an entirely different fashion.

We emphasize the fact that, in the present theory, we have six extra degrees of freedom $D^{(kl)}$ which affect the magnetization. These degrees of freedom arise from the nonrigid character of the position vectors of the polarization vectors associated with different points in a macroelement. For magnetism, (2.7a), (2.7b) and the corresponding jump conditions (2.11a), (2.11b) may be used to determine $D^{(kl)}$. In the general theory of microelectromagnetism, the situation is much more complicated, and separate constitutive equations for D^{kl} are needed involving the electric field tensors as well.

4. SUPERCONDUCTIVITY

Here we shall show that the micromagnetic balance laws (2.2), in a special case, reduce to the field equations of superconductivity derived by F. and H. London in 1935.[13] Thus the present theory encompasses the diamagnetism.

We can always take

$$H_{rl} = 2\lambda^2\mathcal{H}_{r;l} + \bar{\mathcal{H}}_{rl}, \quad (4.1)$$

where λ is a scalar and $\bar{\mathcal{H}}_{rl}$ is a tensor field.[18] Introducing the *magnetic stress tensor* $\bar{T}^l{}_r$ in the same way as in (2.8b), we have

$$H_{rl} = 2\lambda^2\mathcal{H}_{r;l} + 2\bar{T}_{lr} - \bar{T}^k{}_k g_{rl}, \quad (4.2)$$

where

$$\bar{T}^l_r \equiv \tfrac{1}{2}(\bar{\mathcal{H}}_r{}^l - \bar{\mathcal{H}}_k{}^k\delta^l{}_r). \quad (4.3)$$

Substituting (4.2) into (2.7) and using (2.2g), we get

$$D^{(kl)}{}_{;k} - \epsilon^{klr}d_{r;l} = 0, \quad (4.4)$$

$$\frac{8\pi\lambda^2}{c}j^{(k;l)} + 2\epsilon^{mn(k}\bar{T}^{l)}{}_{n;m} - \frac{1}{c}\frac{\partial D^{(kl)}}{\partial t} = 0, \quad (4.5)$$

$$\lambda^2(\nabla \times \nabla \times \mathcal{H})_k + \mathcal{H}_k - B_k - \bar{T}^l_{k;l} + \frac{1}{c}\frac{\partial d_k}{\partial t} = 0, \quad (4.6)$$

where *super current* field $\mathbf{j}$ is defined by

$$\mathbf{j} = \mathbf{J} + c\nabla \times \mathbf{M}. \tag{4.7}$$

In a special case when the magnetic stress tensor is negligibly small, i.e., $\bar{\mathbf{T}} = \mathbf{0}$, Eqs. (4.4) and (4.5) serve to determine $D^{(kl)}$. However, compatible with this limit we can also take $D^{(kl)} = 0$ and disregard Eq. (4.5). This simply means that the gradient of current field is small. In this case the above system reduces to

$$\nabla \times \mathbf{d} = \mathbf{0}, \tag{4.8}$$

$$\lambda^2 \nabla \times \nabla \times \boldsymbol{\mathcal{H}} + \boldsymbol{\mathcal{H}} = \mathbf{B} - \frac{1}{c}\frac{\partial \mathbf{d}}{\partial t}. \tag{4.9}$$

The remaining equations of the system (2.2) are

$$\nabla \times \mathbf{H} = (4\pi/c)\mathbf{J}, \quad \nabla \cdot \mathbf{B} = 0,$$
$$\nabla \times \boldsymbol{\mathcal{H}} = (4\pi/c)\mathbf{j}. \tag{4.10}$$

These equations take the form of Londons' equations of superconductivity if one further neglects the magnetic inertia term $\partial \mathbf{d}/\partial t$, by taking $\mathbf{d} = \mathbf{0}$. Thus

$$\lambda^2 \nabla \times \nabla \times \boldsymbol{\mathcal{H}} + \boldsymbol{\mathcal{H}} = \mathbf{B}, \tag{4.11}$$

$$\nabla \times \boldsymbol{\mathcal{H}} = (4\pi/c)\mathbf{j}, \quad \nabla \cdot \boldsymbol{\mathcal{H}} = 0, \tag{4.12}$$

$$\nabla \times \mathbf{H} = (4\pi/c)\mathbf{J}, \quad \nabla \cdot \mathbf{B} = 0, \tag{4.13}$$

of which $(4.12)_2$ follows from (4.11) by taking the divergence of both sides and using the second of Eqs. (4.13). Equations (4.13) are Maxwell's equations of magnetism.

Equations (4.11) differ from those of the Londons by the presence of $\mathbf{B}$, instead of $\mathbf{0}$. However, it is well known that (cf. de Gennes,[14] p. 58) in the core of supermagnets Londons' equation must be modified by a flux term. This term is usually introduced heuristically by some arguments based on experimental observations. The present theory gives rise to this effect in a rational manner. Moreover, dynamical generalization of the superconductivity is suggested by the set of equations (4.8)–(4.10) in which a magnetic inertia term $\partial \mathbf{d}/\partial t$ appears. Still further generalization, (4.4)–(4.6), contains micromagnetic effects not usually included in a discussion of diamagnetism. The physical phenomena contained in these equations present interesting challenges for future workers.

The jump conditions corresponding to (4.4)–(4.6) follow from (2.3) by using (4.2). Below we give the boundary conditions corresponding to (4.8)–(4.10), valid on Γ:

$$\mathbf{n} \times [\mathbf{d}] = \mathbf{0}, \tag{4.14a}$$

$$\lambda^2[\boldsymbol{\mathcal{H}}_{,l}]n^l + \lambda^2 c^{-1}\left[\frac{\partial}{\partial t}\nabla \cdot \mathbf{d}\right]\mathbf{n} + \nu_{(\mathbf{n})}c^{-1}[\mathbf{d}] = -4\pi\mu\mathbf{n}, \tag{4.14b}$$

$$\lambda^2[\mathcal{H}^k{}_{;l}]n_k = -2\pi[M^k{}_l]n_k, \tag{4.14c}$$

$$\epsilon^{klm}n_l[\mathcal{H}_m] = 4\pi(x^k{}_{,a}\epsilon^{ab}\mu_{,b} + \epsilon^{klm}n_l[M_m]) + (4\pi/c)K^k, \tag{4.14d}$$

$$\mathbf{n} \times [\mathbf{H}] = (4\pi/c)\mathbf{K}, \tag{4.14e}$$

$$[\mathbf{B}] \cdot \mathbf{n} = 0, \tag{4.14f}$$

where (4.14b) follows from (2.3c) by multiplying it by ϵ_{klr} and using (2.8a), (4.9), and (4.2) with $\bar{T}_{lr} = 0$. The jump condition (4.14c) is the result of substituting

$$B_{kl} = H_{kl} + 4\pi M_{kl} = 2\lambda^2\mathcal{H}_{k,l} + 4\pi M_{kl}, \tag{4.15}$$

since $\bar{H}_{kl} = 0$. From the third of Eqs. (4.10), it follows that

$$\mathcal{H}_{k;l} = \mathcal{H}_{l;k} + (4\pi/c)\epsilon_{lkr}j^r.$$

Upon substituting this into (4.14c) and combining with (4.14b), we obtain

$$(c/2)[M^{kl}]n_k\mathbf{g}_l = c\mu\mathbf{n} + \lambda^2[\mathbf{j}] \times \mathbf{n} + (\nu_{(\mathbf{n})}/4\pi)[\mathbf{d}] + \frac{\lambda^2}{4\pi}\left[\frac{\partial}{\partial t}\nabla \cdot \mathbf{d}\right]\mathbf{n}, \quad \text{on } \Gamma, \tag{4.16}$$

which may be used in place of (4.14c). The scalar and vector products of (4.16) with $\mathbf{n}$ gives

$$\frac{c}{2}[M^{kl}]n_k n_l = c\mu + \frac{\nu_{(\mathbf{n})}}{4\pi}[\mathbf{d}] \cdot \mathbf{n} + \frac{\lambda^2}{4\pi}\left[\frac{\partial}{\partial t}\nabla \cdot \mathbf{d}\right],$$

$$\frac{c}{2}[M^{kl}]n_k\mathbf{n} \times \mathbf{g}_l = \lambda^2[\mathbf{j}_{(t)}] - \frac{\nu_{(\mathbf{n})}}{4\pi}[\mathbf{d}] \times \mathbf{n}, \tag{4.17}$$

on Γ, where

$$[\mathbf{j}_{(t)}] \equiv [\mathbf{j}] - [\mathbf{j}] \cdot \mathbf{n}\mathbf{n} \tag{4.18}$$

is the jump of the super current tangential to the surface Γ. Equations (4.17) express, respectively, the balance of the normal and tangential components of the magnetization tensor on the surface Γ with the surface magnetization μ and the magnetization due to super currents and displacements of the surface dipoles.

The magnetization tensor M^{kl} can be eliminated from (4.16) and (4.17) by observing that from (4.9) we have

$$\mathcal{H}^k{}_{;k} + \frac{1}{c}\frac{\partial}{\partial t}(d^k{}_{;k}) = 0, \tag{4.19a}$$

$$\mathcal{H}^k{}_{;kl} + \frac{1}{c}\frac{\partial}{\partial t}d^k{}_{;kl} = 0, \tag{4.19b}$$

with the corresponding jump condition for the latter

$$[\mathcal{H}^k{}_{;l}]n_k + \frac{1}{c}[d^k{}_{;l}]n_k = 0,$$

on Γ, which is equivalent to (4.14c). From this and

(4.14c), by comparison, we have the identification

$$2\pi[M^k{}_l]n_k = \frac{\lambda^2}{c}[d^k{}_{;l}]n_k.$$

Using this, we can eliminate $M^k{}_l$ from (4.16) and (4.17). Thus in place of the jump condition (4.16) we may use

$$\lambda^2[\mathbf{j}] \times \mathbf{n} + c\mu\mathbf{n} + \frac{v_{(n)}}{4\pi}[\mathbf{d}] + \frac{\lambda^2}{4\pi}\left[\frac{\partial}{\partial t}\nabla\cdot\mathbf{d}\right]\mathbf{n} - \frac{\lambda^2}{4\pi}\left[\frac{\partial}{\partial t}\mathbf{d}_{,l}\right]\cdot\mathbf{n}\mathbf{g}^l = 0. \quad (4.20)$$

The jump conditions corresponding to (4.11)–(4.13) follow from (4.14) and (4.20) by taking $\mathbf{d} = \mathbf{0}$. In this case (4.20) gives $\mu = 0$. Thus, for $\lambda \neq 0$,

$$[\mathcal{H}_{,l}]n^l = \mathbf{0}, \quad (4.21a)$$

$$[\mathbf{j}] \times \mathbf{n} = \mathbf{0}, \quad (4.21b)$$

$$\mathbf{n} \times [\mathcal{H}] = (4\pi/c)\mathbf{k}, \quad (4.21c)$$

$$\mathbf{n} \times [\mathbf{H}] = (4\pi/c)\mathbf{K}, \quad (4.21d)$$

$$[\mathbf{B}]\cdot\mathbf{n} = 0, \quad \text{on } \Gamma, \quad (4.21e)$$

where

$$\mathbf{k} \equiv \mathbf{K} + c\mathbf{n} \times \mathbf{M}, \quad \text{on } \Gamma, \quad (4.22)$$

is the surface super current vector. In this case, clearly

$$\mathbf{k}\cdot\mathbf{n} = 0, \quad \mathbf{K}\cdot\mathbf{n} = 0,$$

which express the fact that in the absence of external currents fed into the system, the normal components of surface current vanish (cf. Ref. 14, p. 19). In the present case, probably the jump condition (4.21b) should be replaced by

$$[\mathcal{H}]\cdot\mathbf{n} = 0, \quad (4.23)$$

which is a condition associated with (4.19a).

* This work was supported by the National Science Foundation.

[1] A. C. Eringen and C. B. Kafadar, J. Math. Phys. **11**, 1984 (1970).
[2] W. Heisenberg, Z. Angew. Phys. **49**, 619 (1928); **69**, 287 (1931).
[3] P. A. M. Dirac, Proc. Roy. Soc. (London) **123**, 714 (1928).
[4] F. Bloch, Z. Angew. Phys. **61**, 206 (1930); **74**, 295 (1932).
[5] L. Landau and E. M. Lifshitz, Phys. Z. (USSR) **8**, 153 (1935).
[6] W. F. Brown, Phys. Rev. **105**, 139 (1941).
[7] W. F. Brown, *Magnetostatic Principles in Ferromagnetism* (North-Holland, Amsterdam, 1962).
[8] H. F. Tiersten, J. Math. Phys. **5**, 1298 (1964); **6**, 779 (1965).
[9] S. I. Amari, *RAAG Memoirs*, edited by K. Kondo (Tokyo, 1962), Vol. 3.
[10] J. B. Alblas, *Mechanics of Generalized Continua*, edited by E. Kröner (Springer-Verlag, Berlin, 1968).
[11] C. Kittel, Rev. Mod. Phys. **21**, 541 (1949).
[12] C. Kittel and J. K. Galt, Solid State Phys. **3**, 437 (1956).
[13] H. London and F. London, *Superfluids* (Dover, New York, 1961), 2nd ed., Vol. I.
[14] P. G. de Gennes, *Superconductivity* (Benjamin, New York, 1966).
[15] L. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, New York, 1965).
[16] W. Brown, *Magnetoelastic Interactions* (Springer-Verlag, Berlin, 1966).
[17] In the literature the magnetization per unit mass $\mu^k = M^k/\rho$ is used. However, by use of the equation of mass conservation, one can show that these forms are equivalent.
[18] In superconductivity $\lambda = (mc^2/4\pi n_s e^2)^{\frac{1}{2}}$, where m and e are respectively the mass and charge of the electron and where n_s is the number of superconducting electrons per unit volume.

Vacuum Expectation Values as Indicatrices of Maximal Regularity*

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(Received 7 July 1970)

Matrix elements and propagators of renormalizable field theories are defined in terms of indicatrices of maximal regularity. The relation of the indicatrix approach with analytic regularization and with the subtraction formalism is established. It is shown that the indicatrix formalism gives rise to well-defined propagators and that the self-energy of a particle vanishes on the mass shell so that no mass renormalization is necessary. The renormalization constant Z_3 equals one without the theory becoming a free one. This implies that, within the frame of the indicatrix approach, convergence of the theory is assured and renormalization actually is superfluous.

INTRODUCTION

In this paper we develop a general theory of propagators and matrix elements of renormalizable field theories in terms of indicatrices of maximal regularity. We also show how this formalism renders the mass renormalization of the theory equal to zero and yields for the renormalization constant Z_3 the value $Z_3 = 1$, without the theory becoming a free one. The results are valid also for unrenormalizable interactions.

By an indicatrix of maximal regularity we understand an analytic function of the 4-momentum squared, whose discontinuity across the real axis equals the given spectral function and whose high energy growth is as small as possible (see Secs. 2 and 3). The connection of the indicatrix approach with analytic regularization (cf. also Refs. 1, 2, and 3) and with the subtraction formalism (Ref. 4) is established (see Sec. 4). The indeterminacy of the indicatrix in coordinate space is given by a generalized function concentrated at the origin of the light cone and does not influence observable quantities (see Sec. 5). The indicatrix formalism gives rise to a well-defined propagator and in turn to a well-defined expression for the self-energy of the particle. This self-energy vanishes on the mass shell. Therefore, mass renormalization turns out to be zero (see Sec. 6). On the mass shell the propagator behaves as the free one with residue -1, i.e., $Z_3 = 1$ (see Sec. 6). This implies that, within the frame of the indicatrix approach, convergence of the theory is assured and renormalization actually is superfluous. The results are illustrated by an example in quantum electrodynamics in Sec. 7.

1. NOTATIONS AND DEFINITIONS

We use the notations and definitions of Ref. 1: The Feynman, anti-Feynman, retarded, and advanced propagators Δ'_F, $\Delta'_{\bar F}$, Δ'_R, Δ'_A, which are the vacuum expectation values of time-ordered, anti-time-ordered, retarded, and advanced products of a scalar field operator Φ are called "inhomogeneous" propagators and denoted by Δ'_I. The vacuum expectation value of the field commutator, Δ', and its positive and negative frequency parts Δ'_+ and Δ'_- are called "homogeneous" propagators and denoted by Δ'_H. In the case of a superrenormalizable theory, where by definition all renormalization constants are finite, the Lehmann representation[5]

$$\Delta'_I(x) = \int d\varkappa^2 \rho(\varkappa^2)\Delta_I(x, \varkappa^2) \tag{1.1}$$

$$\Delta'_H(x) = \int d\varkappa^2 \rho(\varkappa^2)\Delta_H(x, \varkappa^2) \tag{1.2}$$

makes sense. In (1.1) and (1.2), $\Delta_{I,H}(x, \varkappa^2)$ are the propagators corresponding to free particles with mass $\varkappa$ satisfying the homogeneous and inhomogeneous Klein–Gordon equation

$$(\Box + \varkappa^2)\Delta_I(x, \varkappa^2) = \delta(x), \tag{1.3}$$

$$(\Box + \varkappa^2)\Delta_H(x, \varkappa^2) = 0. \tag{1.4}$$

We assume that the usual spectrum conditions hold for the spectral function ρ:

$$\rho = 0 \quad \text{for} \quad \varkappa^2 < 0, \tag{1.5}$$

$$\rho \geq 0 \quad \text{otherwise.} \tag{1.6}$$

In momentum space (1.1) reads

$$\Delta'_I(p) = \int d\varkappa^2 \frac{\rho(\varkappa^2)}{-p^2 + \varkappa^2}, \tag{1.7}$$

where

$$\Delta'_I(p) = \mathcal{F}\Delta'_I(x) \tag{1.8}$$

is the Fourier transform of $\Delta'_I(x)$. If in (1.7) we assume p^2 to be a complex variable, then all the inhomogeneous propagators can be obtained from (1.7) by letting p^2 approach the real axis in an appropriate way. For example, we have

$$\Delta'_F(p) = \int d\varkappa^2 \frac{\rho(\varkappa^2)}{-p^2 + \varkappa^2 - i0} = \Delta'_I(p^2 + i0). \tag{1.9}$$

Therefore Δ_{I}' from (1.7), with p^2 being considered as a complex variable, represents all the propagators Δ_{F}', $\Delta_{\bar{\mathrm{F}}}'$, etc., and is simply called the inhomogeneous propagator.

In order to give a precise meaning to the notion of superrenormalizable, renormalizable, and unrenormalizable spectral functions, we define the order N of a spectral function ρ, characterizing its behavior for $\varkappa^2 \to \infty$ as follows.

Definition 1: N is the order of the spectral function ρ if and only if (a) N integer or $+\infty$, (b) the integral

$$\int^{\infty} d\varkappa^2 \rho(\varkappa^2)/(\varkappa^2)^{n+1} \tag{1.10}$$

is divergent at infinity for any integer $n < N$, and (c) there exists an $\epsilon > 0$ such that

$$\rho(\varkappa^2) = O[(\varkappa^2)^{N-\epsilon}], \quad \varkappa^2 \to \infty. \tag{1.11}$$

It follows that we have $N = \infty$ if (1.10) diverges for any integer n. Furthermore we have

$$\int^{\infty} d\varkappa^2 \rho(\varkappa^2)/(\varkappa^2)^{n+1} \begin{cases} < \infty & \text{for} \quad n \geq N \\ = \infty & \text{for} \quad n < N \end{cases}. \tag{1.12}$$

Definition 2: A spectral function is of superrenormalizable, renormalizable, or unrenormalizable type if and only if $N < 0$, $0 \leq N < \infty$, $N = \infty$.

We use the following abbreviations: SR for "superrenormalizable," R for "renormalizable," NR for "unrenormalizable," mr for "maximal regularity." "*" means complex conjugation, $\mathcal{F}$ ($\mathcal{F}^{-1}$) denotes (inverse) Fourier transformation. T_D is the support of a distribution D.

2. THE INDICATRIX OF A DISTRIBUTION

We introduce the notion of the indicatrix of a distribution as follows:

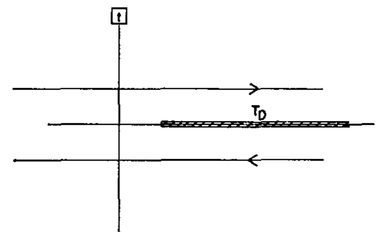
Definition 3: Let $D(r)$ be a distribution on a space of test functions ϕ, r being a one-dimensional variable, and let D be concentrated on some part T_D of the real r axis. Then $I(t)$, $t = r + is$, is called an indicatrix of D if and only if

$$\begin{aligned} D(r) &= (1/2\pi i)[I(r + i0) - I(r - i0)] \\ &= (1/2\pi i) \operatorname{disc.} I(r), \end{aligned} \tag{2.1}$$

i.e.,

$$D(r)\langle\phi(r)\rangle = \frac{1}{2\pi i}\int_{\mathrm{C}} dt I(t)\phi(t) \tag{2.2}$$

for all $\phi(t)$ which are analytic functions of t in some



region containing T_D such that

$$D(r)\langle\phi(r)\rangle = D(r)\langle\phi(t)_{s=0}\rangle \tag{2.3}$$

exists. C is any contour equivalent to the contour of Fig. 1, i.e., any contour which runs clockwise around the support T_D of D and lies inside the domain of analyticity of ϕ.

From this definition it follows that $I(t)$ is analytic in t for all t outside the support T_D of D. D is uniquely determined by I, whereas I is determined by D only up to an entire function $u(t)$.[6]

It is easily seen that the general form of I is given by

$$\begin{aligned} I(t) &= W(t)\int dr \frac{D(r)}{W(r)(-t + r)} + u(t) \\ &= W(t)D(r)\left\langle\frac{1}{W(r)(-t + r)}\right\rangle + u(t), \end{aligned} \tag{2.4}$$

where W is any entire function of t for which the integral in (2.4) exists, u being an arbitrary entire function. If D exists for all bounded test functions ϕ, then we can choose

$$W = 1 \tag{2.5}$$

in (1.4) and obtain

$$I(t) = \int dr \frac{D(r)}{(-t + r)} + u(t). \tag{2.6}$$

If in this case we require that $I(t)$ behaves as regularly as possible (i.e., grows as slowly as possible) for $t \to \infty$, we have to choose $u = 0$ in (2.6) since the first term on the rhs of (2.6) behaves as const/t for $t \to \infty$.

Definition 4: Let $D(r)$ be a distribution which exists for all bounded test functions $\phi(r)$. Then we call $\Delta_{\mathrm{I}}'(t)$ the indicatrix of maximal regularity (mr) of D if and only if (a) $\Delta_{\mathrm{I}}'(t)$ is an indicatrix of D and (b) $\Delta_{\mathrm{I}}'(t)$ behaves as regularly as possible for $t \to \infty$, namely

$$\Delta_{\mathrm{I}}'(t) = O(1/t) \tag{2.7}$$

for $t \to \infty$ in such a way that

$$d(t, T_D) \geq \vartheta\, |t|, \tag{2.8}$$

where $d(t, T_D)$ is the shortest distance between t and T_D:

$$d(t, T_D) = \min \{|t - r|, r \in T_D\}, \qquad (2.9)$$

and $\vartheta > 0$ may be arbitrarily small.

Of course, Definition 4 is a rather complicated formulation of the simple fact that Δ_I' is given by

$$\Delta_I'(t) = \int dr \frac{D(r)}{-t + r} = D(r)\left\langle \frac{1}{-t + r} \right\rangle. \qquad (2.10)$$

This, however, is no longer true if we are concerned with distributions D which grow like some power of r at infinity and therefore do not exist for all bounded test functions ϕ. In this case (2.10) does not make sense. Definition 4, however, can be extended also to this case and also to the case where D grows faster than any power of r,[2] as will be shown in the following sections and in a sequel to this paper.[7]

From Definition 4 or Formula (2.10) the following theorem emerges.

Theorem 1: In an SR theory the propagator $\Delta_I'(p)$ from (1.7) is the indicatrix of mr of the spectral function ρ and may also be defined by this property. Furthermore, it is real analytic, i.e.,

$$\Delta_I'(p^{2*}) = [\Delta_I'(p^2)]^*. \qquad (2.11)$$

Similarly as for Ref. 1 we have considered here p^2 as a one-dimensional variable. This procedure is justified by using Gårding's mapping of invariant four-dimensional distributions onto the space of distributions of one variable.[8]

In Sec. 3 of Ref. 1 we have shown how to reduce the case of spinor fields to the scalar case. Therefore, with slight modifications, the results of the following sections apply also to the case of propagators corresponding to spin or vector particles.

3. RENORMALIZABLE SPECTRAL FUNCTIONS AND THEIR INDICATRICES

In the following we confine ourselves to spectral functions of finite order

$$N < \infty. \qquad (3.1)$$

In case of an SR theory, we have seen in Sec. 2 that the inhomogeneous propagator Δ_I' could be defined as the indicatrix of mr of ρ. It seems reasonable, therefore, to use this definition also in the case of R theories. First we show how to calculate any indicatrix of a spectral function of finite order N. Immediate consequences of (2.4) are the following theorems.

Theorem 2: The general form of the indicatrix I of ρ (cf. Definition 1) is given by

$$I(p^2) = W(p^2)\int d\varkappa^2 \frac{\rho(\varkappa^2)}{W(\varkappa^2)(-p^2 + \varkappa^2)} + u(p^2), \qquad (3.2)$$

where W is an arbitrary entire function of its argument without zeros inside the support T_ρ of ρ, such that the integral in (3.2) exists, i.e., W has to satisfy the condition

$$|W(\varkappa^2)| \geq \text{const}\,(\varkappa^2)^N, \quad \varkappa^2 \to \infty, \qquad (3.3)$$

and $u(p^2)$ is an arbitrary entire function.

Theorem 3: The general form of the real analytic indicatrix I_r of ρ is given by the real analytic part of (3.2)

$$I_r(p^2) = \text{Re}\left(W(p^2)\int d\varkappa^2 \frac{\rho(\varkappa^2)}{W(\varkappa^2)(-p^2 + \varkappa^2)}\right) + \text{Re}\, u(p^2), \qquad (3.4)$$

where, for arbitrary F, Re (F) is defined by

$$\text{Re}\, F(p^2) = \tfrac{1}{2}[F(p^2) + F^*(p^2)] = \tfrac{1}{2}\{F(p^2) + [F(p^{2*})]^*\}. \qquad (3.5)$$

Equation (3.4) can also be written in the form

$$I_r(p^2) = W_r(p^2)\int d\varkappa^2 \frac{\rho(\varkappa^2)}{W_r(\varkappa^2)(-p^2 + \varkappa^2)} + u_r(p^2), \qquad (3.6)$$

where W_r is an arbitrary entire real analytic function without zeros inside the support T_ρ of ρ, such that the integral in (3.6) exists and $u_r(p^2)$ is an arbitrary real analytic entire function.

Proof: Formula (3.6) is obtained by noting that

$$W_r(p^2)\int d\varkappa^2 \frac{\rho(\varkappa^2)}{W_r(\varkappa^2)(-p^2 + \varkappa^2)} \qquad (3.7)$$

is real analytic and that the general form of any real analytic indicatrix differs from (3.7) by an entire real analytic function u_r. The rest of the theorem is trivial. QED

In order to introduce the concept of "maximal regularity" (mr) also for R spectral functions, we note that the least possible growth of $I(p^2)$ at infinity is $O(|p^2|^{N-\epsilon})$ with some $\epsilon > 0$. Therefore, we use the following definition.

Definition 5: Let ρ be of order N. Then Δ_I' is called an indicatrix of mr if and only if (a) Δ_I' is an indicatrix of ρ and (b) there exists an $\epsilon > 0$ such that

$$\Delta_I'(p^2) = O(|p^2|^{N-\epsilon}) \qquad (3.8)$$

for $p^2 \to \infty$ in such a way that

$$\arg(p^2) \geq \vartheta \tag{3.9}$$

for arbitrary $\vartheta > 0$. Note that (3.9) is equivalent to (2.8), since T_ρ is part of the positive real x^2 axis.

Theorem 4: The general form of the indicatrix of mr of ρ is

$$\Delta_I'(p) = w(p^2)\int dx^2 \frac{\rho(x^2)}{w(x^2)(-p^2+x^2)} + u(p^2), \tag{3.10}$$

where w is a polynomial of degree N, its zeros being localized outside the support T_ρ of ρ, and u is an arbitrary polynomial of degree $\leq N-1$. If, in addition, real analyticity of Δ_I' is required, one has to take the real analytic part of (3.10), or choose w and u as real analytic functions, as in (3.6).

Proof: We note first that the integral in (3.10) exists since

$$w(x^2) \sim \text{const}\,(x^2)^N, \quad x^2 \to \infty, \quad \text{const} \neq 0. \tag{3.11}$$

Comparing (3.10) and (3.2), we see that (3.10) yields an indicatrix of ρ. Furthermore, according to (1.11), we have

$$\int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2+x^2)} = O(|p^2|^{-\epsilon}) \tag{3.12}$$

for $p^2 \to \infty$ as in (3.9) with some $\epsilon > 0$. Therefore,

$$w(p^2)\int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2+x^2)} = O(|p^2|^{N-\epsilon}) \tag{3.13}$$

is an indicatrix of mr. Because of (3.8) the general form of Δ_I' differs from (3.13) by a polynomial $u(p^2)$ of degree $\leq N-1$. QED

A further remark should be added: It is often convenient to admit also for functions W, w with zeros inside the support T_ρ of ρ, at $x^2 = M_j^2$, say,

$$W(p^2) = W(p^2, M_j^2) = \prod_j (p^2 - M_j^2)^{\alpha_j}\overline{W}(p^2),$$
$$\overline{W}(p^2) \neq 0 \quad \text{for} \quad p^2 \in T_\rho. \tag{3.14}$$

Then an indicatrix of ρ is, e.g., given by

$$I_\epsilon(p^2) = \tfrac{1}{2}\Big(W(p^2, M_j^2 + i\epsilon_j) \times \int dx^2 \frac{\rho(x^2)}{W(x^2, M_j^2 + i\epsilon_j)(-p^2+x^2)} + W(p^2, M_j^2 - i\epsilon_j) \times \int dx^2 \frac{\rho(x^2)}{W(x^2, M_j^2 - i\epsilon_j)(-p^2+x^2)}\Big), \tag{3.15}$$

since the zeros $M_j^2 \pm i\epsilon_j$ of $W(p^2, M_j^2 \pm i\epsilon_j)$ are outside T_ρ. One can easily prove that

$$\lim_{\epsilon_j \to 0} I_\epsilon \tag{3.16}$$

is also an indicatrix of ρ, if the limit exists uniformly in every compact region of the p^2 plane minus T_ρ. [A sufficient condition is that $\rho(x^2)$, considered as an ordinary function, possesses derivatives up to order $\alpha_j - 1$ at $x^2 = M_j^2$ and that $(d/dx^2)^{\alpha_j}\rho(x^2)$ is integrable at $x^2 = M_j^2$.] Though W is analytic, (3.16) is not necessarily equal to

$$W(p^2, M_j^2)\,\mathrm{Pf}\int dx^2 \frac{\rho(x^2)}{W(x^2, M_j^2)(-p^2+x^2)}, \tag{3.17}$$

Pf $\cdots$ being defined as

$$\tfrac{1}{2}\lim_{\epsilon_j \to 0}\left(\int dx^2 \frac{\rho(x^2)}{W(x^2, M_j^2 + i\epsilon_j)(-p^2+x^2)} + \int dx^2 \frac{\rho(x^2)}{W(x^2, M_j^2 - i\epsilon_j)(-p^2+x^2)}\right); \tag{3.18}$$

for we have

$$\text{disc.}\ W(p^2, M_j^2)\,\mathrm{Pf}\int dx^2 \frac{\rho(x^2)}{W(x^2, M_j^2)(-p^2+x^2)} = \begin{cases} 2\pi i\rho(p^2), & p^2 \neq M_j^2 \\ 0, & p^2 = M_j^2. \end{cases} \tag{3.19}$$

If, therefore, ρ contains a δ function concentrated at $x^2 = M_j^2$ [higher derivatives of $\delta(x^2 - M_j^2)$ are excluded because of the positive definiteness of the spectral function ρ], then (3.17) does not yield an indicatrix of ρ and we have to use (3.15) or (3.16); if, however, ρ is an ordinary function at $x^2 = M_j^2$, then the rhs of (3.19), considered as a distribution, is equivalent to $2\pi i\rho$, and we can use (3.17).

4. RELATION TO SUBTRACTION PROCEDURE AND RESIDUE PRESCRIPTIONS

It is well known that, in case of spectral functions of order $N > 0$, one possibility of giving a meaning to the divergent rhs of (1.7) is the subtraction procedure (cf. also Ref. 4): One subtracts and adds from the integrand

$$\frac{1}{-p^2+x^2} \tag{4.1}$$

in (1.7) N terms of its Taylor series at $x^2 = \infty$, or, equivalently, at $p^2 = M^2$, M^2 being an arbitrary complex number localized outside the support T_ρ of ρ:

$$\frac{1}{-p^2+x^2} = \frac{1}{-p^2+x^2} - \sum_0^{N-1}\frac{(p^2-M^2)^\mu}{(x^2-M^2)^{\mu+1}} + \sum_0^{N-1}\frac{(p^2-M^2)^\mu}{(x^2-M^2)^{\mu+1}}. \tag{4.2}$$

Then one splits the integral in (1.7) into a convergent and a divergent part:

$$\int dx^2 \frac{\rho(x^2)}{-p^2+x^2} = \int dx^2 \rho(x^2)\left(\frac{1}{-p^2+x^2} - \sum_0^{N-1} \frac{(p^2-M^2)^\mu}{(x^2-M^2)^{\mu+1}}\right) + \sum_0^{N-1} C_\mu (p^2-M^2)^\mu, \tag{4.3}$$

where the divergent constants C_μ are given by

$$C_\mu = \int dx^2 \frac{\rho(x^2)}{(x^2-M^2)^{\mu+1}} = \infty. \tag{4.4}$$

Finally one replaces the divergent constants C_μ by arbitrary finite ones,

$$C_\mu = \infty \to C_\mu < \infty, \tag{4.5}$$

and arrives at

$$\Delta_{\mathrm{I}}'(p)|_{\mathrm{subtr}} = \int dx^2 \rho(x^2) \times \left(\frac{1}{-p^2+x^2} - \sum_0^{N-1} \frac{(p^2-M^2)^\mu}{(x^2-M^2)^{\mu+1}}\right) + \tilde{u}(p^2), \tag{4.6}$$

where $\tilde{u}$ is an arbitrary polynomial of degree $\leq N-1$. Now we prove the following theorem.

Theorem 5: The subtraction procedure (4.3) to (4.6) is equivalent to the definition of Δ_{I}' as an indicatrix of ρ of mr. Therefore, if w and u are the same functions as in Theorem 4 and if $\Delta_{\mathrm{I}}'|_{\mathrm{subtr}}$ is given by (4.6), then

$$\Delta_{\mathrm{I}}'(p)|_{\mathrm{subtr}} = w(p^2)\int dx^2 \frac{\rho(x^2)}{w(x^2)(-p^2+x^2)} + u(p^2) \tag{4.7}$$

if u or $\tilde{u}$ are chosen appropriately.

Proof: We use the fact that

$$\frac{1}{-p^2+x^2} - \sum_0^{N-1} \frac{(p^2-M^2)^\mu}{(x^2-M^2)^{\mu+1}} = w_0(p^2)\frac{1}{w_0(x^2)(-p^2+x^2)}, \tag{4.8}$$

where

$$w_0(p^2) = (p^2-M^2)^N \tag{4.9}$$

is a polynomial of degree N. Therefore, the first term on the rhs of (4.6) is an indicatrix of mr. It differs from the rhs of (4.7) at most by a polynomial of degree $N-1$. The rest of the theorem is trivial. QED

A remark should be added: If ρ is of order N, $\Delta_{\mathrm{I}}'(p^2)$ is determined up to a polynomial of degree $\leq N-1$. Therefore, we can, e.g., require

$$\left(\frac{d}{dp^2}\right)^\mu \Delta_{\mathrm{I}}'(p)|_{p^2=M^2} = 0, \quad \mu = 0, \cdots, N-1. \tag{4.10}$$

This requirement determines Δ_{I}' uniquely:

$$\Delta_{\mathrm{I}}'(p) = (p^2-M^2)^N \int dx^2 \frac{\rho(x^2)}{(x^2-M^2)^N(-p^2+x^2)}. \tag{4.11}$$

Because of (4.8), (4.11) is equal to

$$\int dx^2 \rho(x^2)\left[\frac{1}{-p^2+x^2} - \sum_0^{N-1} \frac{(p^2-M^2)^\mu}{\mu!} \times \left(\frac{d}{dp^2}\right)^\mu \frac{1}{(-p^2+x^2)|_{p^2=M^2}}\right]. \tag{4.12}$$

A more general result follows from the next theorem.

Theorem 6: The requirement

$$\left(\frac{d}{dp^2}\right)^\mu \Delta_{\mathrm{I}}'(p)_{p^2=M_j^2} = C_{j\mu}, \quad \mu = 0, 1, \cdots, \alpha_j - 1, \quad \alpha_j \geq 0, \quad \sum_j \alpha_j = N, \tag{4.13}$$

determines Δ_{I}' uniquely and we obtain

$$\Delta_{\mathrm{I}}'(p) = w_1(p^2)\int dx^2 \frac{\rho(x^2)}{w_1(x^2)(-p^2+x^2)} + u_1(p^2), \tag{4.14}$$

where

$$w_1(p^2) = \prod_j (p^2 - M_j^2)^{\alpha_j} \tag{4.15}$$

and $u_1(p^2)$ is the interpolating polynomial of degree $\leq N-1$ satisfying (4.13) with Δ_{I}' replaced by u_1. The proof is trivial. QED

In Ref. 1 we have seen that for a large class of spectral functions ρ of R type the corresponding propagator Δ_{I}' could be defined by

$$\Delta_{\mathrm{I}}'(p) = \operatorname*{Res}_{z=0} \frac{a^{2z}}{z}\int dx^2 \frac{\rho(x^2)}{(-p^2+x^2)^{1-z}}. \tag{4.16}$$

[For the definition of the residue prescription in (4.16) see Ref. 1.] We now prove the following theorem.

Theorem 7: If the residue prescription (4.16) exists, it yields an indicatrix of ρ.

Proof: Since the residue prescription is a linear operation and since

$$\text{disc.}\,[1/(-p^2+x^2)^{1-z}] = 2i(p^2-x^2)^{-1+z}\theta(p^2-x^2)\sin \pi z, \tag{4.17}$$

we obtain

$$\text{disc.}\ \operatorname*{Res}_{z=0} \frac{a^{2z}}{z}\int dx^2 \frac{\rho(x^2)}{(-p^2+x^2)^{1-z}}$$
$$= 2\pi i \operatorname{Res} \frac{\sin \pi z}{\pi z}\int dx^2 \frac{\rho(x^2)\theta(p^2-x^2)}{(p^2-x^2)^{1-z}}$$
$$= 2\pi i \int dx^2 \rho(x^2)\delta(p^2-x^2) = 2\pi i \rho(p^2), \quad (4.18)$$

for we have

$$\operatorname*{Res}_{z=0} \frac{\theta(p^2-x^2)}{(p^2-x^2)^{1-z}} = z(p^2-x^2)^{-1+z}\theta(p^2-x^2)|_{z\to 0}$$
$$= \delta(p^2-x^2). \quad (4.19)$$

QED

In a similar manner one can treat the residue prescription

$$\operatorname{Res} \frac{1}{z}\int dx^2 \frac{\rho(x^2)[a^2(x^2-M^2)]^z}{-p^2+x^2} \quad (4.20)$$

(cf. Ref. 1). We have

$$\text{disc.}\ \operatorname*{Res}_{z=0} \frac{1}{z}\int dx^2 \frac{\rho(x^2)[a^2(x^2-M^2)]^z}{-p^2+x^2}$$
$$= 2\pi i \operatorname*{Res}_{z=0} \frac{1}{z}\int dx^2 \rho(x^2)[a^2(x^2-M^2)]^z \delta(p^2-x^2)$$
$$= \begin{cases} 2\pi i \rho(p^2), & p^2 \neq M^2 \\ 0, & p^2 = M^2 \end{cases}. \quad (4.21)$$

Therefore, if M^2 is outside the support T_ρ of ρ, or, if M^2 is inside T_ρ and ρ is equal to an integrable function at $p^2 = M^2$, (4.20) gives a correct indicatrix of ρ, whereas if ρ contains a term const $\delta(p^2 - M^2)$, one has to apply (4.20) only to the function $\rho -$ const $\times\ \delta(p^2 - M^2)$ in order to get a correct indicatrix.

In case of the spectral function

$$\rho(x^2) = \rho^{(\lambda)}(x^2, m^2) = \frac{(x^2-m^2)^{\lambda-1}\theta(x^2-m^2)}{(\lambda-1)!}, \quad (4.22)$$

considered in Ref. 1, and the corresponding propagator

$$\Delta_{\mathrm{I}}'(p) = \Delta_{\mathrm{I}}^{(\lambda)}(p, m^2), \quad (4.23)$$

the connection between the residue prescription (4.20) (and therefore between the residue prescriptions of Ref. 1) and the definition of Δ_{I}' as indicatrix of mr of ρ is established by the next theorem.

Theorem 8: Formula (3.10) with

$$w(p^2) = \begin{cases} (p^2-m^2)^{[\lambda]}, & \lambda \neq 1, 2, \cdots, \\ (p^2-m^2)^{k-1}[1 + a^2(p^2-m^2)], & \\ & \lambda = k, k = 1, 2, \cdots \end{cases} \quad (4.24)$$

—i.e., a polynomial of degree $[\lambda]$—and

$$u(p^2) = 0 \quad (4.25)$$

yields exactly

$$\Delta_{\mathrm{I}}'(p) = \Delta_{\mathrm{I}}^{(\lambda)}(p, m^2) = \operatorname*{Res}_{z=0} \frac{a^{2z}}{z}\int dx^2 \frac{\rho(x^2)}{(-p^2+x^2)^{1-z}}, \quad (4.26)$$

i.e., (4.20) with $\rho = \rho^{(\lambda)}$, $m^2 = M^2$. By comparison with Theorem 6, it follows that $\Delta_{\mathrm{I}}^{(\lambda)}$ from (4.26) may be defined by the requirement to be the indicatrix of $\rho^{(\lambda)}$ of mr with

$$\left(\frac{d}{dp^2}\right)^{\mu} \Delta_{\mathrm{I}}^{(\lambda)}(p, m^2)_{p^2=m^2} = 0, \quad \mu = 0, \cdots, [\lambda]-1,$$
$$\text{for} \quad \lambda \neq 1, 2, \cdots, \quad (4.27)$$

and

$$\left(\frac{d}{dp^2}\right)^{\mu} \Delta_{\mathrm{I}}^{(\lambda)}(p, m^2)_{p^2=m^2} = 0, \quad \mu = 0, \cdots, k-2,$$
$$\Delta_{\mathrm{I}}^{(\lambda)}(p^2 = m^2 - 1/a^2) = 0 \quad \text{for} \quad \lambda = k, k = 1, 2, \cdots. \quad (4.28)$$

Proof: From Ref. 1 we know that $\Delta_{\mathrm{I}}^{(\lambda)}$ from (4.26) is explicitly given by

$$\Delta_{\mathrm{I}}^{(\lambda)}(p, m^2)$$
$$= \begin{cases} (\lambda)!\,(-p^2+m^2)^{\lambda-1}, & \lambda \neq 1, 2, \cdots, \\ [(-1)^k/(k-1)!](-p^2+m^2)^{k-1} & \\ \quad \times \log[a^2(-p^2+m^2)], & \lambda = k, k = 1, 2, \cdots. \end{cases} \quad (4.29)$$

We see that (4.29) is of mr and satisfies (4.27), (4.28). The rest follows from Theorem 6. QED

5. THE ARBITRARINESS OF INHOMOGENEOUS PROPAGATORS AND MATRIX ELEMENTS

Up to now we have only considered renormalizable theories with spectral functions of finite order N. Since the results of the following two sections are valid for all causal theories—R and NR ones—we first want to summarize the basic results for the inhomogeneous propagators corresponding to NR spectral functions with infinite order $N = \infty$, which are discussed in the sequel of this paper[7] (cf. also Refs. 2, 6, 9): (a) The vacuum expectation value Δ' of the field commutator satisfies causality, i.e., vanishes for spacelike distances $x^2 < 0$ if and only if the spectral function ρ satisfies the high energy bound

$$\rho(x^2)e^{-\epsilon x} \to 0, \quad x^2 \to \infty, \; \epsilon > \text{arbitrary small.} \qquad (5.1)$$

(b) Also in NR causal theories the definition of the inhomogeneous propagator Δ_I' as indicatrix of mr of the spectral function ρ makes sense. Δ_I' can always be written in the form

$$\Delta_I'(p) = W(p^2)\int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2+x^2)} + u(p^2), \qquad (5.2)$$

where W is an entire function which has no zeros for $\arg(p^2)$ sufficiently small, and satisfies

$$\frac{W(x^2)}{\rho(x^2)} = O(|p^2|^{-\epsilon}), \qquad (5.3)$$

with an $\epsilon > 0$ which may be arbitrary small. u is an arbitrary entire function satisfying

$$u(p^2) = O(W(p^2)\,|p^2|^{-\epsilon'}), \qquad (5.4)$$

with an appropriate $\epsilon' > 0$. (c) The inhomogeneous propagator satisfies a similar high energy bound as the spectral function ρ, viz.,

$$\Delta_I'(p)e^{-\epsilon(|p^2|)^{\frac{1}{2}}} \to 0, \quad p^2 \to \infty, \quad \epsilon > 0 \text{ arbitrary small.} \qquad (5.5)$$

(d) In momentum space Δ_I' is determined up to an entire function

$$u(p^2) = \sum_0^\infty C_\mu (p^2)^\mu \qquad (5.6)$$

satisfying the high energy bound

$$u(p^2)e^{-\epsilon(|p^2|)^{\frac{1}{2}}} \to 0, \quad p^2 \to \infty, \quad \epsilon > 0 \text{ arbitrary small.} \qquad (5.7)$$

In x space, therefore, u is determined up to a (Lorentz invariant) distribution

$$u(x) = \mathcal{F}^{-1}u(p^2) = \sum_0^\infty C_\mu(-\Box)^\mu \delta(x) \qquad (5.8)$$

concentrated on the origin of the light cone $x = 0$.

Via the results of Secs. 3 and 4 of this paper, it is easily seen that the statements (b)–(d) are valid also for spectral functions of R type and therefore for all ρ's corresponding to a causal commutator. In the following we discuss this general case, including R and NR spectral functions.

We may summarize our results as follows: Our definitions of the inhomogeneous propagators are free of divergencies. What we have to pay for this advantage is that all our definitions give rise to some arbitrariness in Δ_I' in the following sense: If N is the order of the spectral function ρ, then Δ_I' is defined up to a polynomial of degree $\leq N-1$. For $N = \infty$ the "polynomial of degree $\leq N-1$" is to be interpreted as an entire function satisfying (5.7). It is not at all clear how this arbitrariness—we have N arbitrary constants—should be removed by physical arguments. On the contrary, it seems rather probable that it does not influence the physical content of the corresponding matrix element: The only physical quantity connected with the two-point function is the transition probability of an incoming one-particle state $|1, p\rangle$ with momentum p to a state $|p'\rangle$ with momentum p', namely

$$|\langle p'|\,\mathcal{U}(t,-\infty)\,|1,p\rangle|^2 \sim |\langle 0|\,\Phi(0)\,|p\rangle|^2\,\delta(\mathbf{p}-\mathbf{p}') \sim \rho(p^2)\delta(\mathbf{p}-\mathbf{p}'). \qquad (5.9)$$

Because of

$$\rho(p^2) = (1/2\pi i)\,\text{disc.}\,\Delta_I'(p), \qquad (5.10)$$

this transition probability is independent of the arbitrariness of Δ_I', since the discontinuity of an entire function vanishes.

Similar arguments show that also in case of higher-order matrix elements the arbitrariness of these does not affect the physical results of the theory: Generalizing our formulas to inhomogeneous (i.e., time ordered, retarded, or advanced) n-point functions, we may expect that they are determined up to an entire function

$$u(p_1, \cdots p_n) \qquad (5.11)$$

satisfying the high energy bound (5.6) with respect to every variable p_k. Observable quantities can be calculated from the scattering amplitudes describing 1 incoming and $n-1$ outgoing particles of mass m_k, $k = 1, \cdots n$. These amplitudes are proportional to

$$\int dx_1 \cdots dx_n e^{-i\Sigma_1^n p_k x_k} \prod_{k=1}^n D_k \times \langle 0|\, I\Phi_1(x_1)\cdots\Phi_n(x_n)\,|0\rangle. \qquad (5.12)$$

Here the $\Phi_k(x_k)$ are the field operators corresponding to the various incoming and outgoing particles (spin, isospin indices, etc., have been suppressed) and $I\Phi_1 \cdots \Phi_n$ means an inhomogeneous, i.e., time-ordered ($I = T$), retarded ($I = R$), or advanced product of the Φ_k. The D_k are covariant differential operators (acting on the kth space–time variable x_k) whose homogeneous solutions are the wavefunctions describing the correspondent free particles. For example, if Φ_k is the field operator corresponding to an incoming scalar or spin-$\frac{1}{2}$ particle of mass m_k, then

D_k is the usual Klein–Gordon or Dirac differential operator

$$(\Box_{x_k} + m_k^2) \quad [\text{resp. } (i\gamma\partial_{x_k} - m_k)]. \tag{5.13}$$

The arbitrariness of the inhomogeneous n-point functions—which in x space is given by

$$u(i\partial_{x_1}, \cdots i\partial_{x_n})\delta(x_1, \cdots x_n) \tag{5.14}$$

and represents a functional concentrated at the point $x_1 = x_2 = \cdots = x_n$ of coinciding arguments $x_1, x_2, \cdots x_n$—gives rise to an indeterminacy of the scattering amplitude proportional to

$$\prod_{k=1}^{n} \tilde{D}_k(p_k)u(p_1, \cdots, p_n). \tag{5.15}$$

$\tilde{D}_k$ is obtained from D_k by replacing $i\partial_{x_k}$ by p_k. The essential point is now the following: The scattering amplitude has a physical meaning only on shell, i.e., for $p_k^2 = m_k^2$. Since by definition all the $\tilde{D}_k$ vanish on the mass shell, we obtain the result that the physical quantities are unique despite the arbitrariness of the time ordered functions.

6. RENORMALIZATION AND SELF ENERGY PROBLEMS

Let us adopt the point of view of Ref. 10, i.e., we start from the field equations in the integrated form

$$\Phi_k(x) = \Phi_{k_{\text{in}}}(x) + \int dx' D_k^{(-1)}(x - x')\mathfrak{J}_k(x'). \tag{6.1}$$

The Φ_k are field operators corresponding to the different interacting particles k, $k = 1, 2, \cdots n$; the $\Phi_{k,\text{in}}$ are the usual in operators and the D_k^{-1} are essentially the causal Green's functions of the differential operators D_k in (5.12), i.e.,

$$D_k D_k^{-1}(x) = \delta(x),$$
$$D_k^{-1}(x) = 0 \quad \text{for} \quad x^0 < 0, \tag{6.2}$$

e.g.,

$$D_k^{-1}(x) = \lim_{\epsilon \to 0} \frac{1}{(2\pi)^4} \int dp \frac{e^{-ipx}}{-(p + i\epsilon\eta)^2 + m_k^2},$$
$$\eta^2 = 1, \eta^0 > 0, \tag{6.3}$$

if the kth particle is a scalar particle of mass m_k. Making an iteration procedure for the spectral function $\rho = \rho_k$, we arrive at

$$\rho(\varkappa^2) = \delta(\varkappa^2 - m^2) + \sigma(\varkappa^2). \tag{6.4}$$

(We have suppressed the index k.) Clearly the zeroth approximation must be the free-particle spectral function $\delta(\varkappa^2 - m^2)$; σ involves higher order corrections. Using our definition for the corresponding inhomogeneous propagator, we obtain, e.g., assuming for simplicity a real scalar field,

$$\begin{aligned}\Delta_{\text{I}}'(p) &= \Delta_{\text{I}}(p, m^2) + \Delta_{\text{I}}^{\text{corr}}(p) \\ &= 1/(-p^2 + m^2) \\ &\quad + W(p^2)\int d\varkappa^2 \frac{\sigma(\varkappa^2)}{W(\varkappa^2)(-p^2 + \varkappa^2)} + u(p^2).\end{aligned} \tag{6.5}$$

Here W and u are polynomials of degree N and $\leq N - 1$ [resp. entire functions satisfying (5.3), and (5.7) in the case $N = \infty$] if ρ (and therefore σ) is of order N. In general σ will be a continuous function at $p^2 = m^2$. For instance it will be zero if $m^2 > 0$ is the smallest mass of all interacting particles. This follows from energy momentum conservation if one remembers[5]

$$\theta(p^0)\rho(p^2) = \sum_{\alpha} \langle 0| \Phi(0) |p\alpha\rangle\langle p\alpha| \Phi(0) |0\rangle, \tag{6.6}$$

$$\theta(p^0)\sigma(p^2) = \sum_{\substack{\alpha \\ |p\alpha\rangle \neq |1,p\rangle}} \langle 0| \Phi(0) |p\alpha\rangle\langle p\alpha| \Phi(0) |0\rangle, \tag{6.7}$$

where the set of states $|p, \alpha\rangle$ is a complete set of in-states normalized to $\delta(p - p')\delta_{\alpha\alpha'}$ and $|1, p\rangle$ is the one-particle in state corresponding to the field Φ. In what follows it will be sufficient, however, to assume that σ behaves in such a way for $p^2 \to m^2$ that for some $\gamma > 0$

$$\int_{|\varkappa^2 - m^2| < \gamma} d\varkappa^2 \frac{\sigma(\varkappa^2)}{-p^2 + \varkappa^2} = O\left(\frac{1}{-p^2 + m^2}\right). \tag{6.8}$$

This is satisfied, e.g., if

$$\sigma(\varkappa^2) = O(1/|\varkappa^2 - m^2|^{1-\epsilon}), \quad \varkappa^2 \to m^2, \quad \epsilon > 0. \tag{6.9}$$

Condition (6.8) means essentially that the Φ particle is not a bound state of other particles taking part in the interaction (which guarantees that σ does not have a δ singularity at $p^2 = m^2$) and furthermore that there is no too strong UR interaction, i.e., an interaction with mass-zero particles giving rise to the existence of "too many" states $|p, \alpha\rangle$ with total mass p^2 arbitrary close to m^2 (this guarantees that the contribution to the whole spectral function of the stable one-particle state dominates the contribution of the nearby states $|p, \alpha\rangle$, $p^2 \approx m^2$. We obtain the following theorem.

Theorem 9: If (6.8) or (6.9) is satisfied, then

$$\Delta_{\text{I}}'(p) = 1/(-p^2 + m^2) + O[1/(-p^2 + m^2)]. \tag{6.10}$$

Proof: We have

$$\Delta_{\mathrm{I}}^{\mathrm{corr}}(p) = \int_{|x^2-m^2|<\gamma} dx^2 \frac{\sigma(x^2)}{-p^2+x^2} + \int_{|x^2-m^2|<\gamma} dx^2 \frac{\sigma(x^2)}{W(x^2)} \frac{W(p^2)-W(x^2)}{-p^2+x^2} + W(p^2)\int_{|x^2-m^2|\geq\gamma} dx^2 \frac{\sigma(x^2)}{W(x^2)(-p^2+x^2)} + u(p^2). \quad (6.11)$$

The last three terms are easily seen to be bounded for $p^2 \to m^2$. Using (6.8), we obtain

$$\Delta_{\mathrm{I}}^{\mathrm{corr}}(p) = O[1/(-p^2+m^2)]. \quad (6.12)$$

QED

This means that Δ_{I}' has a pole at $p^2 = m^2$ with residue -1, and therefore may be looked upon as what one usually calls the renormalized propagator for the physical (and not the bare) particle without handling with divergent constants Z_3^{-1}, which would be divergent in the usual point of view. Furthermore, we obtain a new and unobjectionable possibility to define the self-energy Π. Usually Π is defined by a sum over all irreducible Feynman diagrams corresponding to one-particle propagation with the external lines amputated, and satisfies formally[11,4]

$$\Delta_{\mathrm{I}}'(p) = \Delta_{\mathrm{I}}(p, m^2) - \Delta_{\mathrm{I}}(p, m^2)\Pi(p)\Delta_{\mathrm{I}}'(p) \quad (6.13)$$

or

$$\Pi(p) = \Delta_{\mathrm{I}}'^{-1}(p) - \Delta_{\mathrm{I}}^{-1}(p, m^2), \quad (6.14)$$

i.e.,

$$\Delta_{\mathrm{I}}'(p) = 1/[-p^2+m^2+\Pi(p)]. \quad (6.15)$$

Usually some or all of these diagrams are divergent. In order to get rid of these difficulties, one puts[12]

$$\Delta_{\mathrm{I}}'(p) = [-p^2 + m_{\mathrm{Ph}}^2 + \Pi(p) - \Pi(p)_{p^2=m_{\mathrm{Ph}}^2}]^{-1}, \quad (6.16)$$

$$m_{\mathrm{Ph}}^2 = m^2 + \delta m^2, \quad (6.17)$$

$$\delta m^2 = \Pi(p)_{p^2=m_{\mathrm{Ph}}^2}, \quad (6.18)$$

and chooses $m^2 = \infty$ such that

$$m_{\mathrm{Ph}}^2 = m^2 + \Pi(p)_{p^2=m_{\mathrm{Ph}}^2} < \infty, \quad (6.19)$$

and interprets the quantity (6.16) which behaves for $p^2 \to m_{\mathrm{Ph}}^2$ as

$$\Delta_{\mathrm{I}}'(p) \sim Z_3/(-p^2 + m_{\mathrm{Ph}}^2), \quad (6.20)$$

with

$$Z_3^{-1} = 1 - \frac{\partial}{\partial p^2}\Pi(p)|_{p^2=m_{\mathrm{Ph}}^2} \quad (6.21)$$

as the propagator for the "physical particle" with the renormalized mass $m_{\mathrm{Ph}}^2 = m^2 + \delta m^2$, the difference of which to the "bare particle" is due to interaction.

Clearly this procedure is a rather dubious mathematical trick and—even worse—it does not work in general: If, e.g., some or all of the formal integrals corresponding to the irreducible self-energy diagrams diverge in such a way that formal differentiation with respect to the external variable p^2 yields a divergent result too, the quantity (6.21) is meaningless, or, introducing a cutoff Λ depends in such a way on Λ that it is by no means possible to define new propagators and field operators for which the divergencies cancel for $\Lambda \to \infty$ (e.g., in NR theories). If instead we use our method, the way out is clear: We simply have to define Π by one of the relations (6.13)–(6.15). This is possible since Δ_{I}' is already a well-defined quantity.

In Theorem 9 we saw that Δ_{I} and Δ_{I}' have a pole at the same value $p^2 = m^2$ if (6.8) holds. We may suppose, therefore, that no mass renormalization is necessary at all. This result holds even independently of the requirement (6.8) according to the next theorem.

Theorem 10: If Δ_{I}' is defined by (6.5), then no mass renormalization is necessary.

Proof: We have to show that

$$\delta(m^2) = \Pi\,(p^2 = m^2) = 0, \quad (6.22)$$

where the self-energy Π is defined by (6.13) or (6.18). Since

$$\Delta_{\mathrm{I}}^{-1}(p, m^2) = 0 \quad \text{for} \quad p^2 = m^2, \quad (6.23)$$

the condition (6.22) is equivalent to

$$\Delta_{\mathrm{I}}' \to \infty \quad \text{for} \quad p^2 \to m^2. \quad (6.24)$$

Equation (6.24) follows from the fact that σ is nonnegative and that

$$\Delta_{\mathrm{I}}'(p) = \frac{1}{-p^2+m^2} + \int_{|x^2-m^2|<\gamma} dx^2 \frac{\sigma(x^2)}{(-p^2+x^2)} + O(1), \quad p^2 \to m^2. \quad (6.25)$$

QED

7. THE PHOTON PROPAGATOR IN QUANTUM ELECTRODYNAMICS

Let us illustrate the results of the last sections in a simple example in quantum electrodynamics. Here the field equations read

$$A_\mu(x) = A_{\mu_{\mathrm{in}}}(x) + \int dx' D_R^{-1}(x-x')j_\mu(x'), \quad (7.1)$$

where D_R^{-1} is the retarded Green's function of the mass zero Klein–Gordon operator and

$$j_\mu(x) = -(e/2)[\tilde{\psi}(x)\gamma_\mu, \psi(x)]_- \qquad (7.2)$$

is the current operator. It is worth mentioning that the simple form (7.2) of j_μ, obtained by proper antisymmetrization of the fermion fields, is sufficient to yield convergent results. It is unnecessary to consider the current as a weak limit of products of fermion fields, as has been done by various authors.[13,14]

We wish to calculate the photon Feynman propagator

$$\begin{aligned}\Delta_F'^{\mu\nu}(x) &= -i\langle 0|\, TA^\mu(y)A^\nu(y')\,|0\rangle \\ &= \Delta_F'^{\mu\nu(0)}(x) + \Delta_F'^{\mu\nu(1)}(x) + O(e^4), \qquad (7.3)\end{aligned}$$

$x = y - y'$, up to order e^2. In the transverse gauge [which is consistent with (7.1)] we have

$$\Delta_F'^{\mu\nu}(p) = \left(g^{\mu\nu} - \frac{p^\mu p^\nu}{p^2}\right)\Delta_F'(p), \qquad (7.4)$$

$$\Delta_F'(p) = \Delta_F^{(0)}(p) + \Delta_F^{(1)}(p) + O(e^4) = \tfrac{1}{3}\Delta_F'^{\mu}{}_{\mu}(p). \qquad (7.5)$$

The formal Lehmann representation reads

$$\Delta_F'(p) = \int d\varkappa^2 \rho(\varkappa^2)\Delta_F(p, \varkappa^2), \qquad (7.6)$$

where ρ is defined by

$$\begin{aligned}&\theta(\eta p)\rho(p^2) \\ &\quad = -\tfrac{1}{3}(2\pi)^3 \sum_\alpha \langle 0|\, A^\mu(0)\,|p, \alpha\rangle\langle p, \alpha|\, A_\mu(0)\,|0\rangle, \\ &\qquad\qquad \eta^2 = 1, \quad \eta^0 > 0. \qquad (7.7)\end{aligned}$$

The direct but quite complicated calculation method for ρ starts from (7.7) and the perturbation expansion of (7.1) and (7.2), i.e.,

$$A_\mu(x) = A_{\mu_{\rm in}}(x) + \int dx' D_R^{-1}(x - x')j_{\mu_{\rm in}}(x') + O(e^2), \qquad (7.8)$$

$$j_{\mu_{\rm in}}(x) = -(e/2)[\tilde{\psi}_{\rm in}(x)\gamma_\mu, \psi_{\rm in}(x)]_-. \qquad (7.9)$$

A much more elegant procedure uses a Wightman function approach (cf. also Ref. 15, where this approach has been discussed in a general form). Let

$$-i\Delta_+'^{\mu\nu}(x) = \langle 0|\, A^\mu(y)A^\nu(y')\,|0\rangle. \qquad (7.10)$$

Then we have in momentum space that[16]

$$\Delta_+'^{\mu\nu}(p) = (g^{\mu\nu} - p^\mu p^\nu/p^2)\Delta_+'(p), \qquad (7.11)$$

$$\Delta_+'(p) = \tfrac{1}{3}\Delta_+'^{\mu}{}_{\mu}(p) = 2\pi i\theta(\eta p)\rho(p^2). \qquad (7.12)$$

Therefore,

$$\begin{aligned}\theta(\eta p)\rho(p^2) &= (1/6\pi i)\Delta_+'^{\mu}{}_{\mu}(p) \\ &= -(6\pi)^{-1}(2\pi)^{-4}\int dk\,\langle 0|\, A^\mu(p)A_\mu(-k)\,|0\rangle. \qquad (7.13)\end{aligned}$$

Inserting the Fourier transformed form of (7.8) into (7.13) and taking into account that the matrix element $\langle 0|\, A_{\mu_{\rm in}} j^\mu_{\rm in}\,|0\rangle$ vanishes, we obtain[16]

$$\begin{aligned}&\theta(\eta p)\rho(p^2) \\ &\quad = -(6\pi)^{-1}(2\pi)^{-4}\Big(\int dk\,\langle 0|\, A^\mu_{\rm in}(p)A_{\mu_{\rm in}}(-k)\,|0\rangle \\ &\qquad + \int dk\, D_R^{-1}(p)\,\langle 0|\, j^\mu_{\rm in}(p)j_{\mu_{\rm in}}(-k)\,|0\rangle\, D_R^{-1}(-k) \\ &\qquad + O(e^4)\Big) \\ &\quad = \theta(\eta p)[\rho^{(0)}(p^2) + \rho^{(1)}(p^2) + O(e^4)]. \qquad (7.14)\end{aligned}$$

Clearly the first term on the rhs of (7.14) turns out to be the free one-photon spectral function

$$\rho^{(0)}(p^2) = \delta(p^2). \qquad (7.15)$$

Using (7.9) and applying Wick's rules to the matrix element in the second integral of (7.14), one finds after some calculation that

$$\begin{aligned}\rho^{(1)}(p^2) &= e^2(6\pi)^{-1}(2\pi)^{-4}D_R^{-1}(p)(p^2 + 2\mu^2) \\ &\quad \times (1 - 4\mu^2/p^2)^{\frac{1}{2}}\theta(1 - 4\mu^2/p^2)D_R^{-1}(-p), \qquad (7.16)\end{aligned}$$

where μ is the electron mass. Thus

$$\begin{aligned}\rho(\varkappa^2) &= \delta(\varkappa^2) + e^2(12\pi^2\varkappa^2)^{-1}(1 + 2\mu^2/\varkappa^2) \\ &\quad \times (1 - 4\mu^2/\varkappa^2)^{\frac{1}{2}}\theta(1 - 4\mu^2/\varkappa^2) + O(e^4). \qquad (7.17)\end{aligned}$$

Since $\rho^{(1)}$ has the order $N = 0$, we obtain, according to (6.5), that

$$\begin{aligned}\Delta_I^{(1)}(p) &= \int d\varkappa^2 \frac{\rho^{(1)}(\varkappa^2)}{-p^2 + \varkappa^2} \\ &= e^2(12\pi^2p^2)^{-1}\{\tfrac{5}{3} + 4\mu^2/p^2 - (2 + 4\mu^2/p^2) \\ &\quad \times (4\mu^2/p^2 - 1)^{\frac{1}{2}} \tan^{-1}[(4\mu^2/p^2 - 1)^{-\frac{1}{2}}]\}. \qquad (7.18)\end{aligned}$$

Therefore,

$$\begin{aligned}\Delta'_I(p) &= \Delta_I^{(0)}(p) + \Delta_I^{(1)}(p) + O(e^4) \\ &= -1/p^2 + e^2(12\pi^2p^2)^{-1} \\ &\quad \times \{\tfrac{5}{3} + 4\mu^2/p^2 - (2 + 4\mu^2/p^2)(4\mu^2/p^2 - 1)^{\frac{1}{2}} \\ &\quad \times \tan^{-1}[(4\mu^2/p^2 - 1)^{-\frac{1}{2}}]\} + O(e^4). \qquad (7.19)\end{aligned}$$

$\Delta_F'(p)$ can then easily be obtained by letting p^2 approach the real axis from above.

We see that—contrary to the conventional treatment[11]—our approach gives a unique finite result for the photon propagator in momentum space up to first order; no arbitrary or infinite constants are present. For the low energy behavior of $\Delta_I'(p)$ we have

$$\Delta_I^{(0)}(p) + \Delta_I^{(1)}(p) = -1/p^2 + e^2(60\pi^2\mu^2)^{-1} + O(p^2), \qquad p^2 \to 0, \quad (7.20)$$

and we see that Δ_I' has a pole at the value of the "bare" photon mass $m^2 = 0$ with residue -1 in accordance with Theorem 9. The high energy behavior of Δ_I' is given by

$$\Delta_I^{(0)}(p) + \Delta_I^{(1)}(p) = -1/p^2 - e^2(12\pi^2 p^2)^{-1} \times [\log(4 - p^2/\mu^2) - \tfrac{5}{3}] + O(\log p^2/(p^2)^2), \quad p^2 \to \infty. \tag{7.21}$$

The first order contribution to the photon self energy

$$\Pi(p) = \Pi^{(1)}(p) + O(e^4) \tag{7.22}$$

can easily be computed according to (6.13): We obtain

$$\Pi^{(1)}(p) = (-p^2)^2 \Delta_I^{(1)}(p) = e^2(12\pi^2)^{-1} p^2 \{\tfrac{5}{3} + 4\mu^2/p^2 - (2 + 4\mu^2/p^2) \times (4\mu^2/p^2 - 1)^{\frac{1}{2}} \tan^{-1}[(4\mu^2/p^2 - 1)^{-\frac{1}{2}}]\}. \tag{7.23}$$

The first-order contribution to the vacuum polarization tensor $\Pi_{\mu\nu}(p)$ can easily be obtained from (7.23) by multiplication with the factor $(g_{\mu\nu} - p_\mu p_\nu/p^2)$.

In accordance with Theorem 10 we have

$$\Pi^{(1)}(p^2 = 0) = 0, \tag{7.24}$$

and we see that no photon mass renormalization is necessary. Note that this result does not depend upon any gauge invariance arguments.

The conventional calculation method of the first-order photon self-energy (Ref. 12; cf. also Ref. 14), working from the very beginning with time-ordered functions, yields instead of the convergent expression (7.23) the divergent result

$$\tilde{\Pi}^{(1)}(p) = e^2(12\pi^2)^{-1} p^2 \lim_{\Lambda\to\infty} \log(\Lambda/\mu^2) + \Pi^{(1)}(p). \tag{7.25}$$

We see that with our treatment of the problem the first-order corrections turn out to be small (and not divergent) quantities thus satisfying the most immediate requirement of any concept of perturbation theory. In addition, the difficulties in obtaining a finite, divergence-free, polarization tensor, discussed, e.g., in Ref. 14, are not all present in our approach, at least in the approximation considered.

8. CONCLUSIONS

We have seen that the indicatrix approach to renormalizable and unrenormalizable interacting quantized fields yields a vanishing mass renormalization and $Z_3 = 1$, without the theory reducing to a free one. This means that, in a field theory, renormalization is actually superfluous if the theory is properly formulated in terms of generalized functions. In a sequel to this paper we extend the formalism to equal time commutator problems.

ACKNOWLEDGMENTS

The author expresses his sincere thanks to Professor W. Güttinger, Dr. F. Constantinescu, and Dr. R. Blomer for helpful discussions and to Professor D. J. Prowse and Professor W. T. Grandy for the hospitality of the Physics Department, University of Wyoming. He is indebted to the Deutsche Forschungsgemeinschaft for supporting part of this work.

* Work supported in part by the Deutsche Forschungsgemeinschaft.

[1] E. Pfaffelhuber, "Propagators in Terms of Generalized Functions," University of Wyoming Preprint (1970).
[2] E. Pfaffelhuber, thesis, University of Munich (1966); W. Güttinger and E. Pfaffelhuber, Nuovo Cimento **52A**, 389 (1967); SIAM J. Appl. Math. **15**, 1030 (1967); E. Pfaffelhuber and R. Blomer, Ann. Phys. **45**, 404 (1967).
[3] P. Breitenlohner and H. Mitter, Nucl. Phys. **B7**, 443 (1968); E. R. Speer, J. Math. Phys. **9**, 1404 (1968).
[4] F. J. Dyson, Phys. Rev. **75**, 486, 1736 (1949), A. Salam, *ibid.* **82**, 217 (1951); **84**, 426 (1951).
[5] G. Källen, Helv. Phys. Acta **25**, 417 (1952); H. Lehmann, Nuovo Cimento **11**, 342 (1954); O. Steinmann, J. Math. Phys. **4**, 583 (1963).
[6] W. Güttinger, Fortschr. Phys. **14**, 483 (1966).
[7] E. Pfaffelhuber, J. Math. Phys. **12**, 319 (1970).
[8] L. Gårding and J. L. Lions, Nuovo Cimento Suppl. **14**, 9 (1959).
[9] K. Bardakci and B. Schroer, J. Math. Phys. **7**, 10, 16 (1966).
[10] H. Lehmann, K. Symanzik, and W. Zimmermann, Nuovo Cimento **1**, 205 (1955).
[11] S. Schweber, *Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1962).
[12] W. Güttinger, Nuovo Cimento **36**, 968 (1965).
[13] K. Wilson, "On Products of Quantum Field Operators at Short Distances," unpublished Cornell Report; R. A. Brandt, Phys. Rev. **180**, 1490 (1969); Ann. Phys. **44**, 221 (1967).
[14] R. A. Brandt, Ann. Phys. **52**, 122 (1969).
[15] E. Pfaffelhuber, Z. Physik **229**, 264 (1969).
[16] We wish to point out that the first-order correction

$$-i\Delta_+^{\mu\nu(1)}(p) = (2\pi)^{-4} \int dk\, D_R^{-1}(p) \langle 0| j_{\rm in}^{\mu}(p) j_{\rm in}^{\nu}(-k) |0\rangle D_R^{-1}(-k)$$

to the Whiteman function $-i\Delta_+'^{\mu\nu}$ is really (and not only formally) divergence free, i.e., $p_\mu \Delta_+^{\mu\nu(1)}(p) = 0$. Therefore, it is sufficient to calculate only the trace $-i\Delta_{+\mu}^{\mu(1)}(p) = 6\pi\theta(\eta p)\rho^{(1)}(p^2)$ and to use (7.14).

Propagators of Unrenormalizable Fields*

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(Received 7 July 1971)

A general definition of propagators of causal unrenormalizable fields corresponding to rapidly increasing spectral functions is given in terms of indicatrices. The order of growth of the propagators is determined in terms of that of the spectral functions. The high energy bound is rigorously proved and the indeterminacy of the propagators is shown to be concentrated at the origin of the light cone. Theorems are proved concerning the approximation of unrenormalizable propagators by renormalizable ones.

INTRODUCTION

Unrenormalizable interactions are characterized by rapidly increasing spectral functions and discontinuities.[1-3] It is well known that the conventional regularization procedures [analytic regularization[4-7] subtraction,[8] and propagator product definition[4,9]] cannot be applied to these theories.[1,2] In this paper it is shown that a general theory of unrenormalizable theories can be developed in terms of indicatrices of maximal regularity.[10] After having set up the general definition of the indicatrix (Sec. 2), we discuss its general properties and determine the order of growth of the momentum space propagators in terms of that of the spectral function (Sec. 3). The high energy bound is rigorously proved, and the indeterminacy of the propagators in coordinate space is shown to be concentrated at the origin of the light cone (Sec. 3). In Sec. 4 we prove some theorems concerning the approximation of unrenormalizable spectral functions by renormalizable ones. The theorems also extend to certain matrix elements. They give criteria under which unrenormalizable interactions can be dealt with by perturbation approximation.

1. GENERAL PROPERTIES OF UNRENORMALIZABLE SPECTRAL FUNCTIONS IN A CAUSAL THEORY

Let us first introduce the notion of unrenormalizability and of causality.

Definition 1: A spectral function ρ is of unrenormalizable (NR) type if and only if

$$\int^{\infty} dx^2 \rho(x^2)/(x^2)^{n+1} \qquad (1.1)$$

is divergent at infinity for any integer n. Since by definition the order N of a spectral function ρ is essentially the smallest integer n for which (1.1) is convergent, we may also say that spectral functions of unrenormalizable type are characterized by the property that their order N is infinite (cf. Ref. 10).

We see that spectral functions of NR type grow faster than any power of x^2, e.g.,

$$\rho(x^2) \sim \exp(\beta(x^2)^\alpha), \quad x^2 \to \infty, \quad \alpha > 0, \quad \beta > 0. \qquad (1.2)$$

Definition 2: The vacuum expectation value

$$\Delta'(y - y') = -i \langle 0| [\Phi(y), \Phi(y')]_- |0\rangle \qquad (1.3)$$

of the commutator of the field operator Φ is called causal if and only if it vanishes for spacelike distances:

$$\Delta'(x) = 0 \quad \text{for} \quad x^2 < 0. \qquad (1.4)$$

Causality imposes a severe restriction on the growth of the spectral function: ρ must satisfy the condition

$$\rho(x^2)e^{-\epsilon x} \to 0, \quad x^2 \to \infty, \quad \epsilon > 0 \text{ arbitrary small} \qquad (1.5)$$

in order that (1.4) holds.[2,3,11,12] Therefore in (1.2) we must have $\alpha < \frac{1}{2}$ or $\alpha = \frac{1}{2}$, $\beta = 0$ if ρ corresponds to a causal commutator. More generally, if we define the order of growth σ and the type of growth τ of the spectral function by

$$\sigma = \inf\{\sigma' : \rho(x^2) = O(\exp(x^2)^{\sigma'})\}, \quad 0 \le \sigma \le \infty, \qquad (1.6)$$

$$\tau = \inf\{\tau' : \rho(x^2) = O(\exp\tau'(x^2)^{\sigma})\}, \quad 0 \le \tau \le \infty, \qquad (1.7)$$

then we see from (1.5) that in case of a causal commutator σ cannot exceed $\frac{1}{2}$ and, if it equals $\frac{1}{2}$, then the type τ must be zero:

$$\sigma \le \tfrac{1}{2}; \quad \text{if} \quad \sigma = \tfrac{1}{2}, \quad \text{then} \quad \tau = 0. \qquad (1.8)$$

Such functions are called of growth $(\frac{1}{2}, 0)$.[13] In the following, we shall assume that (1.5) and (1.8) hold.

2. THE INHOMOGENEOUS PROPAGATORS IN UNRENORMALIZABLE THEORIES

The Feynman, anti-Feynman, retarded, and advanced propagators Δ'_F, $\Delta'_{\bar F}$, Δ'_R, Δ'_A, which are the vacuum expectation values of time-ordered, anti-time-ordered, retarded, and advanced products of the scalar field operator Φ, are called the "inhomogeneous propagators" and denoted by Δ_I'. The "homogeneous propagators" Δ_H' are Δ' and its positive and negative frequency parts Δ_+' and Δ_-'. Formally we have the Lehmann representation for Δ_I':

$$\Delta_I'(x) = \int d\varkappa^2 \rho(\varkappa^2)\Delta_I(x,\varkappa^2), \tag{2.1}$$

where $\Delta_I(x, \varkappa^2)$ are the propagators corresponding to free particles of mass $\varkappa$. In momentum space, (2.1) is

$$\Delta_I'(p) = \int d\varkappa^2 \frac{\rho(\varkappa^2)}{-p^2 + \varkappa^2}. \tag{2.2}$$

In (2.2) we may consider p^2 as a complex variable and calculate all inhomogeneous propagators by letting p^2 approach the real axis in an appropriate way.[10] Δ_I' from (2.1) and (2.2) is therefore simply called the inhomogeneous propagator. Another representation for the inhomogeneous propagators is given by the following products of singular distributions[2]:

$$\begin{aligned} \Delta_F'(x) &= -\theta(x\eta)\Delta_+'(x) + \theta(-x\eta)\Delta_-'(x), \\ \Delta_{\bar F}'(x) &= -\theta(x\eta)\Delta_-'(x) + \theta(-x\eta)\Delta_+'(x), \\ \Delta_R'(x) &= -\theta(x\eta)\Delta'(x), \\ \Delta_A'(x) &= \theta(-x\eta)\Delta'(x). \end{aligned} \tag{2.3}$$

η is a unit vector of the forward light cone L^+ ($\eta^2 = 1$, $\eta^0 > 0$) characterizing the time direction in the frame of reference. A third representation is given in Ref. 4: If $\rho(l^2)$ is the one-dimensional inverse Fourier transformation of $\rho(p^2)$, i.e., formally

$$\rho(l^2) = \mathcal{F}^{-1}\rho(p^2) = \frac{1}{2\pi}\int dp^2 e^{-il^2p^2}\rho(p^2) \tag{2.4}$$

(l^2 conjugate to p^2), then we have

$$\Delta_F'(p) = \mathcal{F}\Delta_F'(l^2) = \int dl^2 e^{ip^2l^2}\Delta_F'(l^2) \tag{2.5}$$

with

$$\Delta_F'(l^2) = 2\pi i \rho(l^2)\cdot\theta(l^2). \tag{2.6}$$

All these representations for Δ_I' are meaningful in the case of superrenormalizable theories where the spectral function is integrable:

$$\int d\varkappa^2 \rho(\varkappa^2) < \infty. \tag{2.7}$$

In the case of renormalizable (R) theories where ρ possesses a finite order N with $0 \leq N < \infty$, we have developed in Ref. 4 some procedures based on the theory of generalized functions which give a meaning to these representations also in the R case. These procedures, however, do not work if ρ is of NR type, i.e., $N = \infty$. Let us consider, e.g., the subtraction procedure in momentum space. According to Ref. 4, we have to subtract from the integrand $1/(-p^2 + \varkappa^2)$ in (2.2) a sufficiently large part of the Taylor expansion of the integrand at $p^2 = M^2$, M^2 being an arbitrary complex number, such that the modified integrand in (2.2) yields a convergent integral. In the case $N = \infty$, however, sufficiently large means infinite and, therefore, we would arrive at a modified integrand of the form

$$\frac{1}{-p^2+\varkappa^2} - \sum_0^\infty \frac{(p^2-M^2)^\mu}{\mu!}\left(\frac{d}{dp^2}\right)^\mu \left(\frac{1}{-p^2+\varkappa^2}\right)_{p^2=M^2} = \frac{1}{-p^2+\varkappa^2} - \sum_0^\infty \frac{(p^2-M^2)^\mu}{(\varkappa^2-M^2)^{\mu+1}}, \tag{2.8}$$

which is zero for $|p^2 - M^2| < |\varkappa^2 - M^2|$ and divergent for $|p^2 - M^2| > |\varkappa^2 - M^2|$ and therefore would lead to a meaningless result when inserted in (2.2) instead of $1/(-p^2 + \varkappa^2)$. Also the residue prescription of Ref. 4 does not work: We have shown in Ref. 4 that for a large class of spectral functions of R type, Δ_I' can be defined by

$$\operatorname*{Res}_{z=0} \frac{\alpha^{2z}}{z}\int d\varkappa^2 \frac{\rho(\varkappa^2)}{(-p^2+\varkappa^2)^{1-z}} \quad \text{or} \quad \operatorname*{Res}_{z=0}\frac{1}{z}\int d\varkappa^2 \frac{\rho(\varkappa^2)[\alpha^2(\varkappa^2-M^2)]^z}{-p^2+\varkappa^2}, \tag{2.9}$$

where the residue prescription (2.9) is to be interpreted in such a way that one first has to choose z in (2.9) sufficiently large negative so that the integrals in (2.9) exist and then continue the resulting functions of z analytically to a region containing the origin $z = 0$ and finally take the residue according to (2.9). Because of Definition 1, however, we cannot find a z for which the integral in (2.9) converges if ρ is of NR type, and therefore this procedure fails too.

The same arguments apply to the representations (2.3), (2.6): Since the order N of ρ is infinite, Δ_+', Δ_-', Δ', and $\rho(l^2)$ have essential singularities at $(x\eta) = 0$ (resp. $l^2 = 0$) and cannot be regularized by multiplication with appropriate smoothing factors $(x\eta)^n$ [resp. $(l^2)^n$]. Therefore the products (2.3) and (2.6) cannot be defined as in Ref. 4.

In Ref. 10 we have given another possibility of defining the inhomogeneous propagator Δ_I', namely as the indicatrix of maximal regularity (mr) of the spectral function ρ. Furthermore we have shown in Ref. 10 that this possibility is equivalent to the various procedures developed in Ref. 4 for defining Δ_I' in the case of spectral functions of R type. This definition works also in the case of NR spectral functions, as we shall see in the following paragraphs. First we have to introduce some mathematical notations.

Definition 3: Let $\rho(x^2)$ be a spectral function. The support of ρ is called T_ρ. Let $W(x^2)$ be an arbitrary entire function. The set of zeros of W is called Z_W

$$Z_W = \{x_1^2, x_2^2, \cdots\} = \{x^2: W(x^2) = 0\}. \quad (2.10)$$

Definition 4: Let ρ be a spectral function with support T_ρ. Then $I(p^2)$ is called an indicatrix of ρ if and only if

$$2\pi i\rho(x^2) = I(x^2 + i0) - I(x^2 - i0) = \text{disc. } I(x^2), \quad (2.11)$$

i.e., if and only if

$$\rho(x^2)\langle\phi(x^2)\rangle = \int dx^2 \rho(x^2)\phi(x^2) = \frac{1}{2\pi i}\int_C dp^2 I(p^2)\phi(p^2) \quad (2.12)$$

for all $\phi(p^2)$ which are analytic functions of p^2 in some region containing T_ρ such that

$$\rho(x^2)\langle\phi(x^2)\rangle \quad (2.13)$$

exists. C is any contour equivalent to the contour of Fig. 1, i.e., any contour which runs clockwise around the support T_ρ of ρ and lies inside the domain of analyticity of ϕ.

It follows that $I(p^2)$ is analytic in p^2 for all p^2 outside T_ρ. ρ is uniquely determined by I, whereas I is determined by ρ only up to an entire function $u(p^2)$ (cf. also Ref. 10). The general form of the indicatrix I of ρ is given by

$$I(p^2) = W(p^2)\int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2 + x^2)} + u(p^2), \quad (2.14)$$

where W is an entire function of p^2 for which the integral in (2.14) exists, u being an arbitrary entire function.

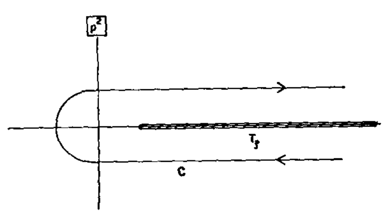

FIG. 1. Integration contour C.

Definition 5: Let ρ be a spectral function. The set $\mathcal{M}_\rho$ is defined as follows: It consists of all entire functions $W(p^2)$ with the properties (a) $W(p^2) \neq 0$ for $\arg(p^2)$ sufficiently small (therefore also for $p^2 \in T_\rho$) and (b) there exists an $\epsilon > 0$ such that

$$\rho(x^2) = O(W(x^2)(x^2)^{-\epsilon}), \quad x^2 \to \infty. \quad (2.15)$$

The existence of such functions W follows immediately from (1.5), (1.8), e.g., $W(p^2) = \exp(\alpha p^2)$, $\alpha > 0$. Now we are able to define the indicatrix of maximal regularity (mr) of a spectral function. Loosely speaking the indicatrix of mr is an indicatrix which behaves as regularly as possible (i.e., grows as slowly as possible) for $p^2 \to \infty$.

Definition 6: $\Delta_I'(p^2)$ is an indicatrix of mr of the spectral function ρ if and only if (a) Δ_I' is an indicatrix of ρ and (b) if $W \in \mathcal{M}_\rho$, then there exists an $\epsilon > 0$ with the property

$$\Delta_I'(p) = O(W(p^2)\,|p^2|^{-\epsilon}) \quad (2.16)$$

for $p^2 \to \infty$ such that

$$d(p^2, T_\rho + Z_W) \geq \vartheta\,|p^2|, \quad (2.17)$$

where $\vartheta > 0$ is arbitrary small and $d(p^2, T_\rho + Z_W)$ is the shortest distance between p^2 and the points $x \in T_\rho + Z_W$ (cf. Definition 3).

It is easily seen that this definition is equivalent to the definition of the indicatrix of (mr) of spectral functions of renormalizable type (i.e., of finite order N) given in Ref. 10. Note that up to now we have not assumed that ρ be of NR type; it may be as well of R or superrenormalizable type. The following theorem gives an explicit representation of the indicatrix of mr.

Theorem 1: Δ_I' is an indicatrix of mr of ρ if and only if, for every $W \in \mathcal{M}_\rho$, Δ_I' can be written in the form

$$\Delta_I'(p) = W(p^2)\int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2 + x^2)} + u(p^2). \quad (2.18)$$

Here u is an entire function satisfying

$$u(p^2) = O(W(p^2)\,|p^2|^{-\epsilon}) \quad (2.19)$$

with an appropriate $\epsilon > 0$, if $p^2 \to \infty$ as in (2.17).

Proof: Suppose (2.18), (2.19) are valid. From (2.18), it follows that Δ_I' is an indicatrix of ρ, and, from (2.16), (2.19) we conclude that there exists an $\epsilon > 0$ such that

$$\frac{\Delta_I'(p)}{W(p^2)} = \int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2 + x^2)} + \frac{u(p^2)}{W(p^2)} = O(|p^2|^{-\epsilon}) \quad (2.20)$$

if $p^2 \to \infty$ as in (2.17). Therefore Δ_I' is an indicatrix of mr. On the other hand, if Δ_I' is an indicatrix of mr of ρ and $W \in \mathcal{M}_\rho$ then we obtain, using Cauchy's formula

$$\frac{\Delta_I'(p^2)}{W(p^2)} = \frac{1}{2\pi i}\int_{C_\Lambda} dx^2 \frac{\Delta_I'(x^2)}{W(x^2)(-p^2+x^2)} \tag{2.21}$$

if p^2 lies in some arbitrary compact domain D of the complex p^2 plane minus $(T_\rho + Z_W)$. C_Λ is given in Fig. 2.

It consists of the large circle $|x^2| = \Lambda$, the contour parallel to T_ρ and small circles running around the zeros x_i^2 of W with $|x_i^2| < \Lambda$. Since Δ_I' is an indicatrix of ρ, we have,

$$\text{disc.}\, \Delta_I'(x^2) = 2\pi i \rho(x^2). \tag{2.22}$$

If $\Lambda_v \to \infty$ for $v \to \infty$, it follows that

$$\begin{aligned}\frac{\Delta_I'(p)}{W(p^2)} &= \frac{1}{2\pi i}\lim_{v\to\infty}\int_{C_{\Lambda_v}} dx' \frac{\Delta_I'(x^2)}{W(x^2)(-p^2+x^2)} \\ &= \lim_{v\to\infty}\left(\int_0^{\Lambda_v} dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2+x^2)}\right. \\ &\quad + \oint_{|x^2|=\Lambda_v} dx^2 \frac{\Delta_I'(x^2)}{W(x^2)(-p^2+x^2)} \\ &\quad \left. - \sum_{|x_i^2|<\Lambda_v} \operatorname*{Res}_{\{x^2=x_i^2\}} \frac{\Delta_I'(x^2)}{W(x^2)(-p^2+x^2)}\right).\end{aligned} \tag{2.23}$$

Because of (2.16) the first term tends towards

$$\int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2+x^2)} \tag{2.24}$$

and the second one vanishes because of (2.16) and (2.17) if we choose the sequence $\Lambda_v \to \infty$ in such a way that the circles $|x^2| = \Lambda_v$ do not contain a $x^2 \in Z_W$. Both limits are uniform with respect to p^2, $p^2 \in D$. Therefore also the third term must converge uniformly in the domain D and is therefore analytic in p^2 for $p^2 \in D$. We obtain

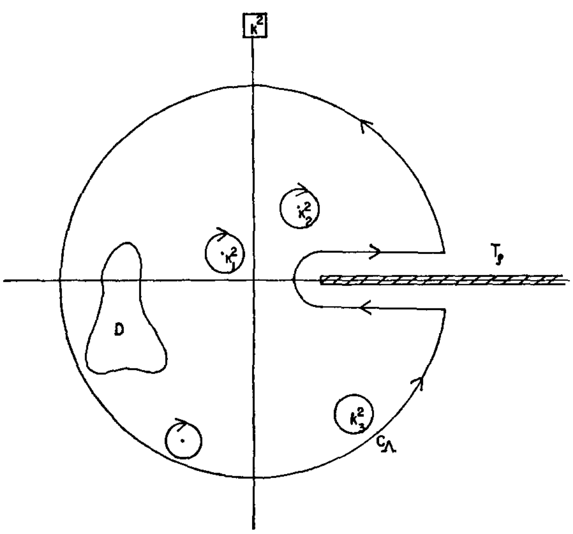

FIG. 2. Integration contour C_Λ.

$$\frac{\Delta_I'(p)}{W(p^2)} = \int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2+x^2)} + \frac{u(p^2)}{W(p^2)}, \tag{2.25}$$

$$u(p^2) = -W(p^2)\sum_i \operatorname*{Res}_{x^2=x_i^2} \frac{\Delta_I'(x^2)}{W(x^2)(-p^2+x^2)}. \tag{2.26}$$

From (2.26) it follows that $u(p^2)$ is regular also for $p^2 \in T_\rho$. Furthermore it is analytic if p^2 coincides with one of the zeros x_i^2 of W, for if x_i^2 is zero of W

$$W(x^2) = (x^2 - x_i^2)^{\alpha_i}\overline{W}(x^2), \quad \overline{W}(x_i^2) \neq 0, \tag{2.27}$$

then

$$-\operatorname*{Res}_{x^2=x_i^2} \frac{\Delta_I'(x^2)}{W(x^2)(-p^2+x^2)}, \tag{2.28}$$

as a function of p^2, is given by

$$\frac{1}{(\alpha_i - 1)!}\left(\frac{d}{dx^2}\right)^{\alpha_i - 1} \frac{\Delta_I'(x^2)}{(p^2 - x^2)\overline{W}(x^2)}\bigg|_{x^2=x_i^2}, \tag{2.29}$$

which is of the form

$$\sum_{\mu=1}^{\alpha_i} \frac{r_\mu}{(p^2 - x_i^2)^\mu}. \tag{2.30}$$

Therefore, according to (2.26), u is regular at $p^2 = x_i^2$ since

$$-\lim_{p^2\to x_i^2} W(p^2) \operatorname*{Res}_{x^2=x_i^2} \frac{\Delta_I'(x^2)}{W(x^2)(-p^2+x^2)} = r_{\alpha_i}\overline{W}(x_i^2) \tag{2.31}$$

exists. We conclude that u is an entire function since the domain D was arbitrary. If $p^2 \to \infty$ as in (2.17), the lhs and also the first term on the rhs of (2.25) are bounded by const $|p^2|^{-\epsilon}$ with some appropriate $\epsilon > 0$. Therefore u satisfies (2.19). If we multiply (2.25) with $W(p^2)$, the resulting formula (2.18) holds also for $p^2 \in Z_W$, for Δ_I' is an indicatrix of ρ which is analytic for all values $p^2 \notin T_\rho$. This completes the proof.

QED

Again we did not make any assumptions about the type of the spectral function ρ. Suppose now that ρ is of superrenormalizable type, satisfying (2.7); then $\mathcal{M}_\rho$ contains the function $W = 1$, and we obtain in this case from (2.18)

$$\Delta_I'(p) = \int dx^2 \frac{\rho(x^2)}{-p^2+x^2} \tag{2.32}$$

since $u = 0$ because of (2.19). We conclude that in this case (2.18) is identical with the Lehmann representation (2.2), and we see that the inhomogeneous propagator is identical with the indicatrix of mr of the spectral function. It is reasonable to take this as a definition of the inhomogeneous propagator if ρ is of R (cf. Ref. 4) or NR type, which we shall do in the following sections.

Since in a causal theory $\rho(x^2)$ is at most of order of growth $\frac{1}{2}$, we may assume without restriction that W is of order < 1 and therefore may be written in the form

$$W(p^2) = (p^2)^k \prod_{i>1} \left(1 - \frac{p^2}{x_i^2}\right), \tag{2.33}$$

where $x_1^2 = 0$ (if $k > 0$) and x_i^2, $i > 1$, are the zeros of W. Then we see from (2.18) that the choice of u is equivalent to fixing the values of

$$\left(\frac{d}{dp^2}\right)^{\mu} \Delta_{\rm I}'(p^2)_{p^2=x_i^2}, \quad \mu = 0, 1, \cdots, \alpha_i - 1 \tag{2.34}$$

if α_i is the multiplicity of the root x_i^2 of W. It is clear therefore that the usual subtraction method, i.e., the choice of a sufficiently large number of derivatives of $\Delta_{\rm I}'$ at the same point $p^2 = M^2$ cannot work for NR theories; for "sufficiently large" means infinite in this case, and choosing all the values $(d/dp^2)^{\mu}\Delta_{\rm I}'(p^2)_{p^2=M^2}$ would already determine the whole function (if any) which might have nothing to do with the propagator $\Delta_{\rm I}'$, since these values were arbitrary. Similarly we see that any method based on the choice of the values (2.34) does not work if all x_i^2 lie in some compact domain of the p^2 plane. Equation (2.18), however, works since the zeros x_i^2 of W have an accumulation point at infinity according to the theory of entire functions.

3. PROPERTIES OF THE INDICATRIX $\Delta_{\rm I}'$ OF MAXIMAL REGULARITY

In Sec. 1 we saw that causality imposes the restriction (1.5) on ρ which, combined with Theorem 1 yields a universal bound for the high energy behavior of the indicatrix of mr of ρ according to the following theorem.

Theorem 2: We have for all $\epsilon > 0$

$$\Delta_{\rm F}'(p)e^{-\epsilon|p^2|^{\frac{1}{2}}} \to 0 \tag{3.1}$$

if $p^2 \to \infty$ as in (2.17). $\Delta_{\rm I}'$ is defined up to an entire function u with

$$u(p^2)e^{-\epsilon|p^2|^{\frac{1}{2}}} \to 0, \quad \epsilon > 0 \text{ arbitrary.} \tag{3.2}$$

Proof: Choose an entire function $W \in \mathcal{M}_\rho$ of growth $(\frac{1}{2}, \epsilon/2)$, i.e., a function

$$W(p^2) = \sum_{v\geq 0} |a_v| (p^2)^v \tag{3.3}$$

with

$$\limsup_{v\to\infty} \frac{v \log v}{\log 1/|a_v|} = \frac{1}{2},$$

$$\frac{2}{e} \limsup_{v\to\infty} v\, |a_v|^{1/2v} = \frac{\epsilon}{2}, \tag{3.4}$$

e.g.,

$$\cosh\,[(\epsilon/2)(p^2)^{\frac{1}{2}}] \quad \text{or} \quad (p^2)^{-\frac{1}{2}} \sinh\,[(\epsilon/2)(p^2)^{\frac{1}{2}}]. \tag{3.5}$$

Because of (2.16) we have

$$\frac{\Delta_{\rm I}'(p)}{W(p^2)} \to 0, \quad p^2 \to \infty. \tag{3.6}$$

Therefore

$$\Delta_{\rm I}'(p)e^{-\epsilon|p^2|^{\frac{1}{2}}} = \frac{\Delta_{\rm I}'(p)}{W(p^2)} W(p^2)e^{-\epsilon|p^2|^{\frac{1}{2}}} \to 0 \tag{3.7}$$

since

$$W(p^2) = O[\exp{(\epsilon/2 + \epsilon')|p^2|^{\frac{1}{2}}}] \quad \text{for all} \quad \epsilon' > 0. \tag{3.8}$$

(3.2) follows immediately from (3.7) and (2.19). QED

Theorem 3 then follows.

Theorem 3: In a causal theory the inhomogeneous propagator $\Delta_{\rm I}'(x)$ is determined up to a distribution concentrated on the origin $x = 0$ of the light cone.

Proof: It is well known[14] that (3.2) is necessary and sufficient for the fact that the inverse Fourier transform

$$\sum_0^{\infty} C_\mu(-\Box)^\mu \delta(x) \tag{3.9}$$

of

$$u(p^2) = \sum_0^{\infty} C_\mu (p^2)^\mu \tag{3.10}$$

from (3.2) can be extended to all test functions $\varphi(x)$ which are analytic at $x = 0$. Therefore the support of (3.9) is the point $x = 0$. QED

Theorem 2 yields, of course, only an upper bound for the growth of $\Delta_{\rm I}'$, which can often be improved if we know the high energy behavior of ρ.

Theorem 4: If the order of growth of ρ is σ and its type is τ, i.e.,

$$\rho(x^2) = O[\exp{(x^2)^{\sigma+\epsilon}}], \quad x^2 \to \infty, \quad \epsilon > 0 \text{ arbitrary,}$$

$$\rho(x^2) = O[\exp{(\tau + \epsilon)(x^2)^{\sigma}}], \quad x^2 \to \infty, \quad \epsilon > 0 \text{ arbitrary,} \tag{3.11}$$

then

$$\Delta_I'(p)\exp[-|p^2|^{\frac{1}{2}(\sigma+\epsilon)}]\to 0,\quad p^2\to\infty,\quad \epsilon>0 \text{ arbitrary},$$

$$\Delta_I'(p)\exp[-(\tau+\epsilon)|p^2|^{\sigma/2}]\to 0,\quad p^2\to\infty,\quad \epsilon>0 \text{ arbitrary}. \tag{3.12}$$

Therefore Δ_I' is defined up to an entire function $u(p^2)$ satisfying (3.12) with Δ_I' replaced by u. The proof goes as in Theorem 2. QED

4. UNRENORMALIZABLE SPECTRAL FUNCTIONS AS A LIMITING CASE OF RENORMALIZABLE ONES

It is often desirable to represent ρ as

$$\rho=\lim_{\alpha\to\alpha_0}\rho_\alpha, \tag{4.1}$$

where the ρ_α can be treated more easily. In perturbation theory, e.g., we have in case of a NR spectral function

$$\rho=\lim_{n\to\infty}\rho_n,\quad \rho_n=\sum_{i=0}^{n}\rho^{(i)}, \tag{4.2}$$

and each $\rho^{(i)}$ and therefore each ρ_n is of R type. To establish the relation of the propagators Δ_{I_α}' and Δ_I' corresponding to the ρ_α and to the exact spectral function ρ, respectively, we first have to give a precise meaning to (4.1): We shall assume in Theorems 5–8 that

$$\lim_{\alpha\to\alpha_0}\int dx^2\rho_\alpha(x^2)\phi(x^2)=\int dx^2\rho(x^2)\phi(x^2) \tag{4.3}$$

for all ϕ for which the rhs of (4.3) exists. [A sufficient condition for (4.3) is that the ρ_α, considered as ordinary functions, converge uniformly towards ρ in every finite interval of the x^2 axis.] Now we prove the following theorem.

Theorem 5: Let $I_\alpha(p^2)$ be an indicatrix of ρ_α. Assume that

$$I=\lim_{\alpha\to\alpha_0}I_\alpha \tag{4.4}$$

exists uniformly in every compact domain D of the complex p^2 plane. Then I is an indicatrix of ρ.

Proof: Suppose that

$$\rho\langle\phi\rangle=\int dx^2\rho(x^2)\phi(x^2) \tag{4.5}$$

exists and that ϕ is analytic for $x^2\in T_\rho$. Then also

$$\int dx^2\rho_\alpha(x^2)\phi(x^2) \tag{4.6}$$

exists for α sufficiently close to α_0, according to (4.3). We have

$$\int_C dp^2 I_\alpha(p^2)\phi(p^2)=2\pi i\int dx^2\rho_\alpha(x^2)\phi(x^2), \tag{4.7}$$

using the definition of I_α. Because of the uniform convergence of (4.4), we obtain

$$\lim_{\alpha\to\alpha_0}\int dp^2 I_\alpha(p^2)\phi(p^2)=\int dp^2 I(p^2)\phi(p^2). \tag{4.8}$$

Therefore, taking the limit $\alpha\to\alpha_0$ in (4.7), we arrive at

$$\frac{1}{2\pi i}\int_C dp^2 I(p^2)\phi(p^2)=\int dx^2\rho(x^2)\phi(x^2). \tag{4.9}$$

QED

Theorem 6: Let I be an indicatrix of ρ. Then there exists a sequence of indicatrices I_α of ρ_α with

$$I_\alpha\to I,\quad \alpha\to\alpha_0, \tag{4.10}$$

uniformly in every compact domain D of the p^2 plane minus T_ρ.

Proof: I can be written in the form

$$I(p^2)=W(p^2)\int dx^2\frac{\rho(x^2)}{W(x^2)(-p^2+x^2)}+u(p^2). \tag{4.11}$$

Define

$$I_\alpha(p^2)=W(p^2)\int dx^2\frac{\rho_\alpha(x^2)}{W(x^2)(-p^2+x^2)}+u(p^2). \tag{4.12}$$

Then I_α is an indicatrix of ρ_α and (4.10) holds, the limit being uniform with respect to p^2, $p^2\in D$, since both I_α and I are analytic for $p^2\in D$. QED

An immediate consequence is the following theorem.

Theorem 7: Let I_α and I be indicatrices of ρ_α and ρ respectively. Then there exist entire functions u_α such that

$$I_\alpha+u_\alpha\to I,\quad \alpha\to\alpha_0, \tag{4.13}$$

uniform in every compact domain D of the complex p^2 plane minus T_ρ.

Proof: I_α differs from the special indicatrix (4.12) at most by an entire function $-u_\alpha$. QED

An important case is the one in which each ρ_α is of R type [e.g., in perturbation theory, cf. (4.2)]. We prove the following theorem.

Theorem 8: Let Δ_{I_α}' be an indicatrix of ρ_α of mr and let the order N_α of ρ_α be finite for all α. (For the definition of the order of a spectral function, see Ref. 10.) Suppose

$$N_\alpha \to N, \quad \alpha \to \alpha_0, \tag{4.14}$$

where N is the order of ρ (i.e., $N = \infty$, if ρ is of NR type). Then there exists a sequence of indicatrices Δ'_{I_α} of mr of ρ_α such that

$$\Delta'_{I_\alpha} \to \Delta'_I, \quad \alpha \to \alpha_0 \tag{4.15}$$

uniformly in every compact domain D of the p^2 plane minus T_ρ.

Proof: Let Δ'_I be given in the form

$$\Delta'_I(p) = W(p^2)\int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2 + x^2)} + u(p^2),$$
$$u(p^2) = \sum_0^{N-1} C_\mu (p^2)^\mu. \tag{4.16}$$

Without restriction we may assume that W possesses an order of growth < 1 and that $W(0) = 1$. Then from the theory of entire functions it follows that W is given by

$$W(p^2) = \prod_1^N \left(1 - \frac{p^2}{x_i^2}\right), \tag{4.17}$$

where x_i^2, $|x_1^2| \le |x_2^2| \le |x_3^2| \le \cdots$, are the zeros of W. We define

$$\Delta'_{I_\alpha}(p) = W_\alpha(p^2)\int dx^2 \frac{\rho_\alpha(x^2)}{W_\alpha(x^2)(-p^2 + x^2)} + u_\alpha(p^2), \tag{4.18}$$

where

$$W_\alpha(p^2) = \prod_1^{N_\alpha} \left(1 - \frac{p}{x_i^2}\right), \quad u_\alpha(p^2) = \sum_0^{N_\alpha - 1} C_\mu (p^2)^\mu. \tag{4.19}$$

Then Δ'_{I_α} is an indicatrix of mr of ρ_α. Furthermore we have

$$\left|\int dx^2 \frac{\rho_\alpha(x^2)}{W_\alpha(x^2)(-p^2+x^2)} - \int dx^2 \frac{\rho(x^2)}{W(x^2)(-p^2+x^2)}\right|$$
$$\le \left|\int dx^2 \frac{\rho_\alpha}{W_\alpha(-p^2+x^2)} - \int dx^2 \frac{\rho_\alpha}{W\cdot(-p^2+x^2)}\right|$$
$$+ \left|\int dx^2 \frac{\rho_\alpha}{W\cdot(-p^2+x^2)} - \int dx^2 \frac{\rho}{W\cdot(-p^2+x^2)}\right| \tag{4.20}$$

arbitrary small for α sufficiently close to α_0. Therefore

$$|\Delta'_{I_\alpha} - \Delta'_I| \tag{4.21}$$

is arbitrary small and (4.15) follows. Similarly as in Theorem 6 one sees that the limit is uniform with respect to p^2, $p^2 \in D$. QED

Note that Theorems 5–7, but not Theorem 8, can be applied to a cutoff formulation, for in such a theory one always has $N_\alpha < 0$ and therefore (4.14) cannot hold if the spectral function is of R ($0 \le N < \infty$) or NR ($N = \infty$) type. We remark that Theorems 5–8 permit us to apply all the calculation methods for the indicatrices of spectral functions of R type, developed in Ref. 4, also to NR theories.

5. A SIMPLE EXAMPLE

Suppose[15]

$$\rho(x^2) = \chi(x^2)\theta(x^2),$$
$$\chi(x^2) = \sum_{v\ge1} \frac{C_v}{v!\,(v-1)!}(x^2)^{v-1}. \tag{5.1}$$

The requirement of causality (1.5) is here equivalent to[2]

$$\limsup_{v\to\infty} (C_v)^{1/v} = 0. \tag{5.2}$$

Let us test the various methods to obtain the corresponding propagator. First we look for an indicatrix I of ρ. In (2.14) we choose[16]

$$W(p^2) = W_0(p^2) = (1 + a^2p^2)\chi(p^2), \quad u = 0, \tag{5.3}$$

and obtain

$$I(p^2) = (1 + a^2p^2)\chi(p^2)\int_0^\infty dx^2 \frac{1}{(1 + a^2x^2)(-p^2 + x^2)}$$
$$= -\chi(p^2)\log(-a^2p^2). \tag{5.4}$$

It is easily seen that (5.4) is already of mr: If $W \in \mathcal{M}_\rho$, then (2.15) holds and therefore

$$-\chi(p^2)\log(-a^2p^2) = O(W(p^2)\,|p^2|^{-\epsilon'}), \quad 0 < \epsilon' < \epsilon. \tag{5.5}$$

In the simple case (5.1) the calculation methods of Sec. 4 may also be used to obtain explicit results for the propagator Δ'_I. We write

$$\rho = \lim_{\alpha\to\infty} \rho_\alpha, \tag{5.6}$$

$$\rho_\alpha = \sum_1^\alpha \frac{C_v}{v!\,(v-1)!}(x^2)^{v-1}, \tag{5.7}$$

$$N_\alpha = \alpha, \tag{5.8}$$

the convergence being uniform in every finite interval of the x^2 axis because of (5.2). Using now any method of Ref. 4 for calculating the indicatrix Δ'_{I_α} of mr of ρ_α, we always obtain a result of the form

$$\Delta'_{I_\alpha}(p)$$
$$= -\sum_1^\alpha \frac{C_v}{v!\,(v-1)!}(p^2)^{v-1}\log(-a^2p^2) + \tilde{u}_\alpha(p^2), \tag{5.9}$$

$\tilde{u}_\alpha$ being a polynomial of degree $\leq \alpha - 1$. For example,

$$\tilde{u}_\alpha(p^2) = -\sum_1^\alpha \frac{C_v}{v!}(p^2)^{v-1}\frac{d}{dz}(f(v,z)/(v+z-1)!)_{z=0} \quad (5.10)$$

if to each term in the sum (5.7) the residue prescription developed in Ref. 4 is applied. Of course, Δ'_{I_α} need not converge for $\alpha \to \infty$ {if, e.g.,

$$(d/dz)[f(v,z)/(v+z-1)!]_{z=0} \quad (5.11)$$

grows sufficiently rapidly for $v \to \infty$}. However, Theorem 8 guarantees the existence of a polynomial u_α of degree $\leq \alpha - 1$ such that

$$\Delta'_{I_\alpha} + u_\alpha \to \Delta'_I, \quad (5.12)$$

where $\Delta'_I = I$ is given by (5.4). This is, of course, easily accomplished by choosing

$$u_\alpha = -\tilde{u}_\alpha. \quad (5.13)$$

We obtain

$$\Delta'_{I_\alpha} + u_\alpha = -\sum_1^\alpha \frac{C_v}{v!\,(v-1)!}(p^2)^{v-1}\log(-a^2p^2)$$
$$\to -\chi(p^2)\log(-a^2p^2). \quad (5.14)$$

Furthermore, we see that the above considerations yield an explicit illustration of Theorems 5, 6, and 8 since the lhs of (5.14) is an indicatrix of mr of ρ_α.

It seems worth mentioning that these techniques allow us immediately to calculate the momentum space representation of the Feynman propagator Δ'_F for a large class of entire functions of free fields. The basic idea[3] is to obtain first the corresponding Wightman function and from there the spectral function ρ, and then apply the indicatrix method. To sketch this method for the case of exponentials of free fields, let

$$\Delta'_F(y-y') = (i/g^2)\langle 0|\, T(:e^{g\Phi(y)} - 1::e^{g\Phi(y')} - 1:|0\rangle, \quad (5.15)$$

with g a constant and Φ a free scalar field of mass m. (The factor $1/g^2$ has been introduced in order that Δ'_F approaches the free propagator for $g \to 0$.) Then the positive frequency part of the corresponding commutator Δ' is the Wightman function

$$i\Delta'_+(y-y') = (1/g^2)\langle 0|\, :e^{g\Phi(y)} - 1::e^{g\Phi(y')} - 1:|0\rangle, \quad (5.16)$$

which is readily evaluated to yield

$$i\Delta'_+(x) = (1/g^2)\{\exp[ig^2\Delta_+(x)] - 1\}$$
$$= (1/g^2)\sum_{v\geq 1}(1/v!)g^{2v}[i\Delta_+(x)]^v, \quad (5.17)$$

where $i\Delta_+(y-y') = \langle 0|\,\Phi(y)\Phi(y')\,|0\rangle$. In momentum space (5.17) reads

$$i\Delta_+(p) = (1/g^2)(2\pi)^4\sum_{v\geq 1}(1/v!)(g/4\pi^2)^{2v}[{}^*i\Delta_+(p)]^v, \quad (5.18)$$

where $[{}^*i\Delta_+(p)]^v$ is the v-fold convolution product of $i\Delta_+(p) = 2\pi\theta(p^0)\delta(p^2 - m^2)$ with itself. These convolution products can in principle be calculated[17] and the series in (5.18) can be summed up. Since

$$i\Delta'_+(p) = 2\pi\theta(p^0)\rho(p^2), \quad (5.19)$$

the spectral function ρ can then be obtained. Despite the fact that no closed form solution results, the asymptotic high energy behavior of ρ can be estimated using the results of Ref. 2. We have

$$\rho(x^2) \sim \chi(x^2)\theta(x^2), \quad (5.20)$$

where $\chi(x^2)$ is given by (5.1) with $c_v = (g/4\pi)^{2v}/(v+1)!$. It follows that the causality condition (5.2) is satisfied and that we can again use the weight function W as given in (5.3) to calculate the indicatrix of mr of ρ and the momentum space Feynman propagator $\Delta'_F(p)$.

For the zero mass limit the calculation can be carried out explicitly. We have from (5.17) that

$$i\Delta'_+(x) = (1/g^2)\lim_{\epsilon\to 0}\sum_{v\geq 1}(1/v!)(g/2\pi)^{2v}[-(x - i\epsilon\eta)^2]^{-v}, \quad (5.21)$$

where η is a unit vector of the forward light cone, whence[2]

$$i\Delta'_+(p) = 2\pi\theta(p^0)$$
$$\times\left(\delta(p^2) + \sum_{v\geq 1}\frac{(g/4\pi)^{2v}}{(v+1)!\,v!\,(v-1)!}(p^2)^{v-1}\theta(p^2)\right). \quad (5.22)$$

Therefore,

$$\rho(x^2) = \delta(x^2) + \chi(x^2)\theta(x^2) \quad (5.23)$$

according to (5.19), where χ is the same function as in (5.20). With $W(p^2)$ given by (5.3) and the convenient choice of the arbitrary entire function u according to

$$u(p^2) = [W(p^2) - W(0)]/p^2W(0), \quad (5.24)$$

we obtain the indicatrix of ρ, which, for the same reason as (5.4), is of mr. The Feynman propagator is finally calculated by letting p^2 approach the real axis from above. The result is

$$\Delta'_F(p) = 1/(-p^2 - i0) - \chi(p^2)\log[a^2(-p^2 - i0)]$$
$$= \frac{1}{-p^2 - i0} - \sum_{v\geq 1}\frac{(g/4\pi)^{2v}}{(v+1)!\,v!\,(v-1)!}$$
$$\times (p^2)^{v-1}\log[a^2(-p^2 - i0)]. \quad (5.25)$$

We see that $\Delta_F'(p)$ has a pole of first order with residue -1 at the square of the free field mass $m^2 = 0$, a result which is of a general nature.[2,10]

6. CONCLUSIONS

We conclude that, from the point of view of divergences, unrenormalizable field theories are in no way worse than renormalizable ones and in fact can be dealt with in terms of the same indicatrix techniques as the latter ones. We shall show in a forthcoming paper that the mathematical problems posed by equal time commutators also are entirely within the possibilities provided by the formalism of Refs. 4 and 10.

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* Work supported in part by the Deutsche Forschungsgemeinschaft.

[1] G. Feinberg and A. Pais, Phys. Rev. **131**, 2724 (1963); **133**, B477 (1964); T. D. Lee, *ibid.* **128**, 899 (1962); B. Schroer, J. Math. Phys. **5**, 1361 (1964); K. Bardakci and B. Schroer, *ibid.* **7**, 10, 16 (1966); M. B. Halpern, Phys. Rev. **140**, B1570 (1965); G. V. Efimov, Commun. Math. Phys. **5**, 42 (1967); A. M. Jaffe, Phys. Rev. **158**, 1454 (1967); Phys. Rev. Letters **17**, 661 (1966); Ann. Phys. **32**, 127 (1965); B. Klaiber, Nuovo Cimento **36**, 165 (1965).
[2] E. Pfaffelhuber, thesis, University of Munich (1966); W. Güttinger and E. Pfaffelhuber, Nuovo Cimento **52A**, 389 (1967).
[3] E. Pfaffelhuber, Z. Physik **229**, 264 (1969).
[4] E. Pfaffelhuber, "Propagators in Terms of Generalized Functions," University of Wyoming Preprint (1970).
[5] A. Rieckers and W. Güttinger, Commun. Math. Phys. **7**, 190 (1968).
[6] E. Pfaffelhuber and R. Blomer, Ann. Phys. **45**, 404 (1967); R. Blomer, thesis, University of Munich (1969).
[7] P. Breitenlohner and H. Mitter, Nucl. Phys. **B7**, 443 (1968); E. R. Speer, J. Math. Phys. **9**, 1404 (1968).
[8] F. J. Dyson, Phys. Rev. **75**, 486, 1736 (1949); A. Salam, Phys. Rev. **82**, 217 (1951); **84**, 426 (1951).
[9] A. Rieckers, thesis, University of Munich (1969).
[10] E. Pfaffelhuber, J. Math. Phys. **12**, 311 (1970).
[11] K. Bardakci and B. Schroer, Ref. 1.
[12] G. V. Efimov, Ref. 1.
[13] R. P. Boas, *Entire Functions* (Academic, New York, 1954).
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[17] W. E. Thirring, *Principles of Quantum Electrodynamics* (Academic, New York, 1958), Appendix II.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Remarks on a Paper of Srivastava

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(Received 14 September 1970)

It is pointed out in this note that two series studied by Rosenbaum [J. Math. Phys. **8**, 1977 (1967)] and later given rapid, elementary proofs by the present writer [J. Math. Phys. **10**, 49 (1969)] are virtually the same series because of properties of the factorial ratio involved. This shows that the very complicated generalized series introduced by Srivastava [J. Math. Phys. **11**, 2225 (1970)] is not needed, besides which his general series seems not possible to sum in general and serves no purpose other than to subsume the two original series in a single series. Since the series are, in fact, almost identical, this is simpler than Srivastava's formula makes out. Finally, the proofs in the writer's previous note are again discussed for their value as elementary techniques avoiding complicated infinite series and unnecessary generalizations.

By means of rather involved considerations of commutation relations Rosenbaum[1] was able to sum the two series

$$A = \sum_{n=0}^{\alpha} (-1)^n \binom{n+\epsilon-1}{n} \binom{\epsilon}{\alpha-n} \tag{1}$$

and

$$B = \sum_{n=0}^{\alpha} (-1)^n \binom{n+\epsilon-1}{\alpha-1} \binom{\alpha}{n}, \tag{2}$$

involving binomial coefficients, showing that $A = 0 = B$ for some special cases of the parameters. Then the present writer[2] gave a very simple approach to both series, using the finite Vandermonde series to sum (1) and noting that (2) has the value 0 because it is nothing but a difference of order α of a polynomial of degree less than α.

Srivastava[3] has now published a note proving the results again and claiming to unify the work. He introduces the series

$$S_{p,q,r}^{\nu,\lambda,m} = \sum_{n=0}^{m} (-1)^n \binom{\nu+n}{mp+nq-r} \binom{\lambda}{m-n}, \tag{3}$$

and is then able to sum the series in the very special cases $p = 0$, $q = 1$ and $p = 1$, $q = 0$, thereby obtaining Rosenbaum's results. He uses Gauss' theorem for summation of a certain ${}_2F_1$ hypergeometric series. Along the way, Srivastava finally

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$$\alpha A = \epsilon B \quad \text{for all integers} \quad \alpha \geq 1. \tag{4}$$

We shall remark first of all that introduction of series (3) is a needless complication. The only way in which this unifies things is that it does contain both A and B as special cases. But the general series of Srivastava does not seem possible to get in closed form. I assert this on the basis of many years work with hundreds of different binomial sums. It turns out that Srivastava's general sum is not necessary because in fact the two sums A and B are virtually the same series anyway. This is so because the product of binomial coefficients in series A is really just

$$\epsilon(n + \epsilon - 1)!/n!\,(\alpha - n)!\,(n + \epsilon - \alpha)!, \tag{5}$$

while the product in series B is merely

$$\alpha(n + \epsilon - 1)!/n!\,(\alpha - n)!\,(n + \epsilon - \alpha)!, \tag{6}$$

from which it is evident that relation (4) follows at once. We can then omit the lengthy derivation of (4) given by Srivastava and go at once to the heart of the matter, which is that in both cases the series are zero because they are precisely differences of order α of polynomials of degree less than α as explained in my paper.[2]

Since, moreover, the ratio of factorials in (5) and (6) can be separated a third way and is in fact equal to

$$\binom{n + \epsilon}{\alpha - n}\binom{2n + \epsilon - \alpha}{n}\frac{1}{n + \epsilon}, \tag{7}$$

we hereby obtain a third form of the basic summation which is not covered by the parameters introduced by Srivastava in series (3). It would seem more fruitful to begin a useful generalization by examining the factorial ratio. However, as already pointed out, a "generalization" here seems needless.

This brings us to the question of the purpose of Ref. 2. The purpose I had in mind was to avoid use of infinite series and complicated generalizations. Proof was given to show how some very elementary considerations would suffice. I could have noted (5) and (6) as above but felt that two different finite methods of approach would make a very useful pedagogical note.

Let there be no misunderstanding; I have pointed out to Professor Srivastava (a former colleague here) in private remarks in 1969 that his series (3) would be of interest if it were indeed possible to sum it in general, or if there were really some unifying principle behind it. But as we have seen above, the two series originally studied are virtually one and the same so that the general series (3) is totally uncalled for. If we merely wish to exhibit a general formula that shall contain both A and B on demand for special choices of parameters, we can consider the expression $qA + pB$ which yields A and B for the same values of p and q as in (3). A "generalization" to be useful and interesting must contain some really unifying principle other than a multiplicity of parameters.

[1] D. M. Rosenbaum, J. Math. Phys. **8**, 1977 (1967).
[2] H. W. Gould, J. Math. Phys. **10**, 49 (1969).
[3] H. M. Srivastava, J. Math. Phys. **11**, 2225 (1970).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Off-Shell T Matrix Corresponding to a Sum of Coulomb and Separable Potentials by Expansion in $O(4)$ Harmonics

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(Received 14 January 1971)

Using a group-theoretic approach similar to methods previously used in the pure Coulomb problem, we derive representations for the off-shell "nuclear" T matrix—the difference between the complete T matrix and the Coulomb T matrix—corresponding to the sum of Coulomb and separable potentials, in particular, for the sum of Coulomb and Yamaguchi potentials. These representations have some analogous properties to those representations already known for the pure Coulomb T matrix, especially in the on-shell limit.

I. INTRODUCTION

In the investigation of the three-body problem by means of the Faddeev or Schrödinger equations, one simplifying consideration has been the use of nonlocal separable potentials in place of local potentials.[1] In view of the importance of charged particles in these systems, it is natural to investigate potentials consisting of a sum of a short-range separable potential and the Coulomb potential. Indeed, this problem was previously investigated by Harrington[2] for the sum of a cut-off Coulomb potential and a Yamaguchi potential and subsequently applied to the nuclear obtains the fact that

$$\alpha A = \epsilon B \quad \text{for all integers} \quad \alpha \geq 1. \tag{4}$$

We shall remark first of all that introduction of series (3) is a needless complication. The only way in which this unifies things is that it does contain both A and B as special cases. But the general series of Srivastava does not seem possible to get in closed form. I assert this on the basis of many years work with hundreds of different binomial sums. It turns out that Srivastava's general sum is not necessary because in fact the two sums A and B are virtually the same series anyway. This is so because the product of binomial coefficients in series A is really just

$$\epsilon(n + \epsilon - 1)!/n!\,(\alpha - n)!\,(n + \epsilon - \alpha)!, \tag{5}$$

while the product in series B is merely

$$\alpha(n + \epsilon - 1)!/n!\,(\alpha - n)!\,(n + \epsilon - \alpha)!, \tag{6}$$

from which it is evident that relation (4) follows at once. We can then omit the lengthy derivation of (4) given by Srivastava and go at once to the heart of the matter, which is that in both cases the series are zero because they are precisely differences of order α of polynomials of degree less than α as explained in my paper.[2]

Since, moreover, the ratio of factorials in (5) and (6) can be separated a third way and is in fact equal to

$$\binom{n + \epsilon}{\alpha - n}\binom{2n + \epsilon - \alpha}{n}\frac{1}{n + \epsilon}, \tag{7}$$

we hereby obtain a third form of the basic summation which is not covered by the parameters introduced by Srivastava in series (3). It would seem more fruitful to begin a useful generalization by examining the factorial ratio. However, as already pointed out, a "generalization" here seems needless.

This brings us to the question of the purpose of Ref. 2. The purpose I had in mind was to avoid use of infinite series and complicated generalizations. Proof was given to show how some very elementary considerations would suffice. I could have noted (5) and (6) as above but felt that two different finite methods of approach would make a very useful pedagogical note.

Let there be no misunderstanding; I have pointed out to Professor Srivastava (a former colleague here) in private remarks in 1969 that his series (3) would be of interest if it were indeed possible to sum it in general, or if there were really some unifying principle behind it. But as we have seen above, the two series originally studied are virtually one and the same so that the general series (3) is totally uncalled for. If we merely wish to exhibit a general formula that shall contain both A and B on demand for special choices of parameters, we can consider the expression $qA + pB$ which yields A and B for the same values of p and q as in (3). A "generalization" to be useful and interesting must contain some really unifying principle other than a multiplicity of parameters.

[1] D. M. Rosenbaum, J. Math. Phys. **8**, 1977 (1967).
[2] H. W. Gould, J. Math. Phys. **10**, 49 (1969).
[3] H. M. Srivastava, J. Math. Phys. **11**, 2225 (1970).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Off-Shell T Matrix Corresponding to a Sum of Coulomb and Separable Potentials by Expansion in $O(4)$ Harmonics

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(Received 14 January 1971)

Using a group-theoretic approach similar to methods previously used in the pure Coulomb problem, we derive representations for the off-shell "nuclear" T matrix—the difference between the complete T matrix and the Coulomb T matrix—corresponding to the sum of Coulomb and separable potentials, in particular, for the sum of Coulomb and Yamaguchi potentials. These representations have some analogous properties to those representations already known for the pure Coulomb T matrix, especially in the on-shell limit.

I. INTRODUCTION

In the investigation of the three-body problem by means of the Faddeev or Schrödinger equations, one simplifying consideration has been the use of nonlocal separable potentials in place of local potentials.[1] In view of the importance of charged particles in these systems, it is natural to investigate potentials consisting of a sum of a short-range separable potential and the Coulomb potential. Indeed, this problem was previously investigated by Harrington[2] for the sum of a cut-off Coulomb potential and a Yamaguchi potential and subsequently applied to the nuclear three-body problem.[3] For the pure Coulomb problem, on the other hand, there are momentum space representations of both the Green's function[4,5] and the off-shell T matrix[6–10] which do not involve the use of such a cutoff. These representations for the off-shell Coulomb T matrix have been recently applied to atomic scattering problems from the point of view of the Faddeev equations,[7,8] and a recent paper[11] relates this approach to the eigenfunction expansion approach.[12]

In the present paper we discuss somewhat similar representations for the off-shell T matrix corresponding to the sum of Coulomb and separable potentials. These will be derived by the generalization of a group theoretic method previously used mainly for the pure Coulomb problem.

The group theoretic approach is a natural framework for the treatment of scattering problems involving the Coulomb potential because such problems admit $O(4)$ as a dynamical symmetry group for negative energies and $O(3, 1)$ for positive energies.[13]

This situation was first exploited in nonrelativistic scattering theory by Schwinger[5] by using an $O(4)$ approach based upon the stereographic projection method of Fock.[13] The idea was carried further by Finkelstein and Levy[9] by employing the connection between momentum space and the group space of $O(3)$. These authors also point out that the group theoretic approach can also be used to advantage in problems involving other potentials, even though such potentials do not admit $O(4)$ as a symmetry group. Our work is an illustration of this remark.

Nutt[6] derived the off-shell Coulomb T matrix from one of Schwinger's results[5] for the Coulomb Green's function. The identical result is given by the method of Finkelstein and Levy[9] and also by our approach which is closely related to that of Schwinger.

In using the methods of Finkelstein–Levy and of Schwinger, one first obtains the T matrix corresponding to a given potential from the Lippmann–Schwinger equation for negative energies and then proceeds to positive energies via analytic continuation. Perelomov and Popov[14] have discussed a more direct approach for scattering problems by giving an expansion of the Coulomb Green's function in terms of irreducible representations of $O(3, 1)$.[15] They explicitly demonstrate that this procedure gives the same result as that obtained by analytic continuation of Schwinger's $O(4)$ expansion. These authors also point out that the proper symmetry group for the special case of zero energy is the three-dimensional Euclidean group $E(3)$. The representations of this group can be obtained by contraction from those of either $O(3, 1)$ [14] or $O(4)$.[16]

In Sec. II we give a general discussion of the group theoretic procedure for obtaining the off-shell T matrix corresponding to the sum of Coulomb and separable potentials. Section III is concerned with the pure Coulomb off-shell T matrix. This allows us to derive some of the known representations for this quantity in a systematic way, and also to discuss the analytic continuation procedure in a familiar setting. As a byproduct, we obtain a new representation for the off-shell Coulomb T matrix which is slightly different from those already known. Then, in Sec. IV these methods are applied to the derivation of representations for the off-shell nuclear T matrix corresponding to a sum of Coulomb and Yamaguchi[17] potentials. Section V then consists of some concluding remarks where we indicate how the results of the preceding section would be changed if the Yamaguchi potential were replaced by a separable potential of a different type.

II. GENERAL DISCUSSION

Our starting point is the Lippmann–Schwinger equation in momentum space,

$$T(\mathbf{p}, \mathbf{p}'; E) = V(\mathbf{p}, \mathbf{p}') - \int \frac{V(\mathbf{p}, \mathbf{p}'')T(\mathbf{p}'', \mathbf{p}'; E)d^3p''}{p''^2 - E}, \tag{1}$$

and for convenience we choose units such that $\hbar = 1 = 2m$, where m denotes the reduced mass.

The idea is to first solve (1) for negative energies and then analytically continue to positive energies, as was already mentioned in the Introduction. The connection between momentum space and the group space of $O(4)$ is provided by Fock's stereographic projection[13]

$$\begin{aligned}\zeta_i &= 2p_0p_i/(p_0^2 + p^2)\\ &= (\sin\alpha\sin\theta\cos\varphi, \sin\alpha\sin\theta\sin\varphi, \sin\alpha\cos\theta),\\ \zeta_0 &= (p_0^2 - p^2)/(p_0^2 + p^2) = \cos\alpha,\end{aligned}$$

where α, θ, and φ denote the polar angles on the unit 4-sphere and we have set $E = -p_0^2$. In terms of these angles, the $O(4)$ harmonics are given by

$$Y_{nlm}(\Omega) = N_{nl}^{\frac{1}{2}}\sin^l\alpha\, C_{n-l}^{l+1}(\cos\alpha)Y_l^m(\theta, \varphi), \tag{2}$$

where C_{n-l}^{l+1} and Y_l^m denote, respectively, a Gegenbauer polynomial and the usual spherical harmonic on the unit 3-sphere.

We take the spherical harmonics as normalized to unity,

$$\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi\, Y_l^m(\theta, \varphi)Y_{l'}^{m'*}(\theta, \varphi) = \delta_{l,l'}\delta_{m,m'},$$

so that the normalization constant in (2) is

$$N_{nl} = \frac{2^{2l+1}(n-l)!\,(n+1)(l!)^2}{\pi(n+l+1)!}.$$

It is convenient to define the auxiliary functions,

$$T_a(\Omega, \Omega') = \left(\frac{p_0^2 + p^2}{2p_0}\right) T(\mathbf{p}, \mathbf{p}')\left(\frac{p_0^2 + p'^2}{2p_0}\right),$$
$$V_a(\Omega, \Omega') = \left(\frac{p_0^2 + p^2}{2p_0}\right) V(\mathbf{p}, \mathbf{p}')\left(\frac{p_0^2 + p'^2}{2p_0}\right), \quad (3)$$

and to expand these in terms of $O(4)$ harmonics,[5]

$$T_a(\Omega, \Omega') = \sum_{\mu\nu} Y_\mu(\Omega) T_{\mu\nu} Y_\nu^*(\Omega'),$$
$$V_a(\Omega, \Omega') = \sum_{\mu\nu} Y_\mu(\Omega) V_{\mu\nu} Y_\nu^*(\Omega'), \quad (4)$$

where μ and ν denote the three quantum numbers n, l, and m.

The Lippmann–Schwinger equation (1) now takes the form

$$T_{\mu\nu} = V_{\mu\nu} - \frac{1}{2p_0} \sum_{\mu'} V_{\mu\mu'} T_{\mu'\nu}, \quad (5)$$

when we make use of the orthonormality of the $O(4)$ harmonics and the identity

$$d^3p = [(p_0^2 + p^2)/2p_0]^3\, d\Omega,$$

where $d\Omega$ denotes the element of surface area on the unit 4-sphere,

$$d\Omega = \sin^2 \alpha \sin \theta \, d\alpha \, d\theta \, d\varphi.$$

Corresponding to the usual partial wave expansion for spinless particles

$$V(\mathbf{p}, \mathbf{p}') = \sum_{lm} V_l(p, p') Y_l^m(\hat{p}) Y_l^{m*}(\hat{p}'),$$

one finds from (3) and (4) an expression of the form

$$V_{nlm;n'l'm'} = V_l(n, n')\delta_{l,l'}\delta_{m,m'}. \quad (6)$$

Equation (5) can be easily solved for two classes of potentials, to which we shall restrict ourselves in the present paper. The first class consists of potentials which, in addition to having the property (6), are also diagonal in the third quantum number

$$V_{nlm;n'l'm'} = V_l(n)\delta_{n,n'}\delta_{l,l'}\delta_{m,m'}.$$

Potentials which have the further property that $V_l(n)$ is independent of l have been called "Casimir potentials" by Finkelstein and Levy.[9] The Coulomb potential is an example of such a potential. The second class of potentials for which (5) is easily soluble consists of potentials which are finite sums of terms which are separable in the parameter space of $O(4)$, i.e., potentials of finite rank. For given l and m these potentials have the form (6) with $V_l(n, n')$ a finite sum of the form

$$V_l(n, n') = \sum_j \lambda_j u_{j,l}(n) u_{j,l}(n'). \quad (7)$$

We will be interested in the solution of the Lippmann–Schwinger equation (5) when the potential can be written as the sum of a Coulomb and a separable potential,

$$V = V^c + V^s. \quad (8)$$

Then the off-shell T matrix can be written in the form

$$T = T^c + T^{cs}. \quad (9)$$

Here T^c denotes the Coulomb T matrix and T^{cs} is frequently called the "nuclear" T matrix. This latter quantity satisfies the following equation, which easily follows from the substitution of (9) into (5):

$$T_{\mu\nu}^{cs} = V_{\mu\nu}^s - \frac{1}{2p_0}\sum_{\mu'} V_{\mu\mu'}^s T_{\mu'\nu}^{cs} - \frac{1}{2p_0}\sum_{\mu'} (V_{\mu\mu'}^c + V_{\mu\mu'}^s) T_{\mu'\nu}^{cs}, \quad (10)$$

in which V^s is taken to be of the general form (7). The solution to (10) has the form

$$T_l^{cs}(n, n') = T_l^{cs}(n, n')\delta_{l,l'}\delta_{m,m'}, \quad (11)$$

where the l value corresponds to that of (7) and $T_l^{cs}(n, n')$ has singularities corresponding to bound states of the total potential (8).

Instead of decomposing the T matrix in the form (9), one can, of course, also write

$$T = T^s + T^{sc}, \quad (12)$$

in which T^s denotes the off-shell T matrix corresponding to the separable potential (7). One can then further decompose T^{sc} in (12) as follows:

$$T^{sc} = T^c + T'^{sc}, \quad (13)$$

where T^c again denotes the pure Coulomb T matrix. In general, the quantity T'^{sc} in (13) is much more complicated than the object T^{cs} which appears in (9). Nonetheless, it is somewhat interesting that, when one separates the T matrix corresponding to the separable potential from the total T matrix as in (12), then the Coulomb T matrix *automatically* becomes separated as in (13). When one passes to the on-shell limit $p^2 = k^2 = E = p'^2$, then it is found that T'^{sc} contains a term which exactly cancels the separable on-shell T matrix T^s. The decomposition

$$T = T^s + T^c + T'^{sc}$$

has previously been given in a momentum space representation by Alessandrini *et al.*[3]

III. OFF-SHELL COULOMB T MATRIX

Before proceeding to the discussion of the off-shell T matrix corresponding to the sum of Coulomb and separable potentials in the next section, we want to make a few remarks concerning the pure Coulomb problem. It will be seen that the group theoretic approach affords a unified approach to the derivation of the various representations of the off-shell Coulomb T matrix, including one slightly different from those previously given. Also, the methods of analytic continuation to be used are the same for this problem as for the more general problem to be considered in Sec. IV, so that we have preferred to discuss them in a familiar setting.

Nutt[6] has given an integral representation for the off-shell Coulomb T matrix which was derived from one of Schwinger's representations for the Coulomb Green's function.[5] As we discuss below, this representation can be shown to be equivalent to a representation derived from Hostler's representation of the Green's function.[4] There are corresponding representations to these in terms of hypergeometric functions.[7,10] We will give yet another representation of the latter type. A similar representation is given in the next section for the off-shell nuclear T matrix corresponding to the sum of Coulomb and Yamaguchi potentials.

For the Coulomb potential

$$V^c(\mathbf{p}-\mathbf{p}') = (\lambda_c/2\pi^2)\,|\mathbf{p}-\mathbf{p}'|^{-2};\quad \lambda_c = \pm e^2,$$

we find from (3) and (4)

$$V^c_{nlm;n'l'm'} = [\lambda_c/(n+1)]\delta_{n,n'}\delta_{l,l'}\delta_{m,m'}.$$

In these equations $\lambda_c > 0$ corresponds to a repulsive and $\lambda_c < 0$ to an attractive potential. The T matrix is found from (5) to be

$$T^c_{nlm;n'l'm'} = [\lambda_c/(n+1+\gamma)]\delta_{n,n'}\delta_{l,l'}\delta_{m,m'}, \quad (14)$$

with $\gamma = \lambda_c/2p_0$.

The Coulomb bound states are determined by the vanishing of the denominator in (14),

$$p_0 = |\lambda_c|/2(n+1);\quad \lambda_c < 0,\quad n = 0, 1, 2, \cdots. \quad (15)$$

The representation of (14) in momentum space is obtained by the use of (3) and (4). We find

$$T^c_a(\Omega, \Omega') = \frac{\lambda_c}{2\pi^2}\sum_{n=0}^{\infty}\frac{n+1}{n+1+\gamma}\,\frac{\sin(n+1)\omega}{\sin\omega}, \quad (16)$$

where the angle ω is related to the distance between two points on the surface of the unit 4-sphere by[13]

$$|\zeta - \zeta'| = 2\sin\frac{\omega}{2}$$

and to the polar angles on the sphere by[13]

$$\cos\omega = \cos\alpha\cos\alpha' + \sin\alpha\sin\alpha' \times [\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi-\varphi')].$$

The summation in (16) can be converted into an integral representation by, for example, using a method discussed by Finkelstein and Levy,[9]

$$T^c_a(\Omega, \Omega') = \frac{\lambda_c}{2\pi^2}\left[\frac{1}{(\zeta-\zeta')^2} - \gamma\int_0^1 \frac{y^\gamma\,dy}{(1-y)^2 + y(\zeta-\zeta')^2}\right],\quad \operatorname{Re}\gamma > -1. \quad (17)$$

This representation is of the same type as given by Schwinger[5] for the Coulomb Green's function and, in fact, could have been obtained directly from his work. Equation (17) differs from the expression given by Finkelstein and Levy[9] by a simple integration by parts.

The summation in (16) can also be expressed directly in terms of hypergeometric functions as follows:

$$T^c_a(\Omega, \Omega') = \frac{\lambda_c}{2\pi^2}\,\frac{[e^{i\omega}{}_2F_1(1+\gamma, 2; 2+\gamma; e^{i\omega}) - e^{-i\omega}{}_2F_1(1+\gamma, 2; 2+\gamma; e^{-i\omega})]}{2i(1+\gamma)\sin\omega}$$
$$= \frac{\lambda_c}{2\pi^2}\,\frac{[e^{i\omega}(1-e^{i\omega})^{-1}{}_2F_1(1, \gamma; 2+\gamma; e^{i\omega}) - e^{-i\omega}(1-e^{-i\omega})^{-1}{}_2F_1(1, \gamma; 2+\gamma; e^{-i\omega})]}{2i(1+\gamma)\sin\omega}. \quad (18)$$

The second expression in (18) is obtained from the first by the use of Euler's identity[18]

$${}_2F_1(a, b; c; z) = (1-z)^{c-a-b}{}_2F_1(c-a, c-b; c; z).$$

We now want to analytically continue (17) and (18) to the positive energy region. In the case of (17), the restriction $\operatorname{Re}\gamma > -1$ is removed by use of a transformation given by Schwinger[5] and we find

$$T^c(\mathbf{p}, \mathbf{p}'; k^2) = \frac{\lambda_c}{2\pi^2\,|\mathbf{p}-\mathbf{p}'|^2} \times \left[1 + \frac{4i\mu}{e^{-2\pi\mu}-1}\int_C \frac{y^{i\mu}\,dy}{\epsilon(1-y)^2 - 4y}\right], \quad (19)$$

where $\mu = \lambda_c/2k$, $\epsilon = (p^2-k^2)(p'^2-k^2)/k^2\,|\mathbf{p}-\mathbf{p}'|^2$, and the integration contour, which is the same as that described by Schwinger,[5] starts at $y = 1 + i0$, moves to and encircles the origin and then terminates at $y = 1 - i0$. This representation agrees with that of Nutt[6,19] and can be shown to be equivalent to the representation derived from Hostler's Green's function[8,10] by means of a simple change of variable. Shastry and Rajagopal[11] have given a representation of the off-shell Coulomb T matrix which is the analytic continuation of the expression for $T^c(\mathbf{p}, \mathbf{p}')$ found from (16) by making use of (3). It is amusing to note that they derived this representation by using (19) as a starting point, which just reverses the steps of the present approach.

The analytic continuation of (18) is

$$T^c(\mathbf{p},\mathbf{p}';k^2) = \frac{\lambda_c}{4\pi^2|\mathbf{p}-\mathbf{p}'|^2(1+i\mu)(1+\epsilon)^{\frac{1}{2}}} \frac{\epsilon}{} \times \left[\frac{y_+}{(1+\epsilon)^{\frac{1}{2}}+1}\,{}_2F_1(1,i\mu;2+i\mu;y_+) + \frac{y_-}{(1+\epsilon)^{\frac{1}{2}}-1}\,{}_2F_1(1,i\mu;2+i\mu;y_-)\right], \tag{20}$$

with $y_\pm \equiv 1 + (2/\epsilon)(1 \pm (1+\epsilon)^{\frac{1}{2}})$. We note that the hypergeometric functions in this representation have different parameters and arguments from those in the representations previously given,[7,10] even though the representations are all equivalent.

We will now use the representation (20) to discuss the on-shell limit $p^2 = k^2 = p'^2$ of the Coulomb T matrix. A similar approach has been used previously by Ford[10] in connection with a hypergeometric function form of Hostler's representation. We want to give these details because we use essentially the same method in the next section in connection with the nuclear T matrix corresponding to the sum of Coulomb and Yamaguchi potentials.

In order to pass to the on-shell limit in (20), we note that if k^2 has a nonvanishing imaginary part, then $|y_-| < 1$ and consequently $|y_+| > 1$, since $y_+y_- = 1$. Therefore, we express the first hypergeometric function in (20) in terms of functions with argument y_- by means of the Barnes representation[18] and obtain, after some manipulation,

$$\begin{aligned} T^c(\mathbf{p},\mathbf{p}';k^2) &= \frac{\lambda_c}{4\pi^2|\mathbf{p}-\mathbf{p}'|^2}(1+\epsilon)^{-\frac{1}{2}} \\ &\times \{2|\Gamma(1+i\mu)|^2 e^{\pi\mu} y_-^{i\mu} + \epsilon[(1+\epsilon)^{\frac{1}{2}}+1]^{-1} \\ &\times [(1-i\mu)^{-1}{}_2F_1(1,-i\mu;2-i\mu;y_-) + (1+i\mu)^{-1} \\ &\times {}_2F_1(1,i\mu;2+i\mu;y_-)]\}. \end{aligned} \tag{21}$$

The on-shell limit is now obtained by using the small argument expansion of the hypergeometric functions in (21) and we find

$$T^c(k,k;k^2) = \lim_{\epsilon\to 0}\left[\frac{\lambda_c}{2\pi^2|\mathbf{p}-\mathbf{p}'|^2}|\Gamma(1+i\mu)|^2 e^{\pi\mu}\left(\frac{\epsilon}{4}\right)^{i\mu} + O(\epsilon)\right], \tag{22}$$

a result also given by Ford[10] and Nutt.[6]

We note from (22) the well-known result that the on-shell limit of the off-shell Coulomb T matrix does not yield the correct scattering amplitude. The reason for this has been well understood for some time and is due to the fact that the above calculations were done with momentum eigenstates, which are not the proper asymptotic states for the Coulomb problem. This can be remedied by computing the T matrix with the proper asymptotic states, as Nutt has shown.

IV. OFF-SHELL T MATRIX CORRESPONDING TO A SUM OF COULOMB AND YAMAGUCHI POTENTIALS

We now want to consider the solution of (10). Unfortunately, it is difficult to make detailed statements without specifying the exact form of the separable potential. We have carried out the procedure discussed below for most of the separable potentials normally used in practical calculations and have found that most of the characteristics of these solutions seem to occur in the simplest example. This is also the case treated by Harrington,[2] namely, a rank-one potential of the Yamaguchi type[17]

$$V^Y(p,p') = \lambda(p^2+\beta^2)^{-1}(p'^2+\beta^2)^{-1}, \tag{23}$$

where $\lambda > 0$ corresponds to a repulsive and $\lambda < 0$ to an attractive potential. For the reasons given above we will not give the details of the calculations for other separable potentials but will confine ourselves to a few remarks concerning them in Sec. V.

For the present example (7) reduces to a single term with

$$u_{1,0}(n) = \frac{2\sqrt{2}\,\pi p_0}{p_0^2-\beta^2}\left(\frac{p_0-\beta}{p_0+\beta}\right)^{n+1}. \tag{24}$$

The solution to (10) has the form (11) with

$$T_0^{cs}(n,n') = \frac{\lambda(n+1)(n'+1)u_{1,0}(n)u_{1,0}(n')}{(n+1+\gamma)(n'+1+\gamma)D_{cs}(p_0)}, \tag{25}$$

where

$$D_{cs}(p_0) \equiv 1 + \frac{\lambda}{2p_0}\sum_{n=0}^{\infty}\frac{(n+1)[u_{1,0}(n)]^2}{n+1+\gamma}. \tag{26}$$

The zeros of the function defined in (26) determine the bound states of the total potential (8), $V = V^c + V^Y$, and we recognize the factors of the form $(n + 1 + \gamma)$ in (25) which determine the Coulomb bound states.

The representation of (25) in momentum space is obtained by exactly the same procedure as in the case of the pure Coulomb T matrix in the preceding section. The following results are found:

$$T^{cs}(\mathbf{p}, \mathbf{p}'; k^2) = \frac{\lambda h(p)h(p')}{D_{cs}(p_0)(\beta^2 + p^2)(\beta^2 + p'^2)}, \quad (27)$$

where

$$h(p) = 1 - 4\gamma p_0^2(\beta^2 + p^2)\int_0^1 \frac{y^\gamma\, dy}{a - 2by + cy^2},$$

valid for $\text{Re}\, \gamma > -1$ with

$$a = (p_0 + \beta)^2(p_0^2 + p^2),$$
$$b = (p_0^2 - \beta^2)(p_0^2 - p^2),$$
$$c = (p_0 - \beta)^2(p_0^2 + p^2),$$

and

$$T^{cs}(\mathbf{p}, \mathbf{p}'; k^2) = \frac{-\lambda g(p)g(p')}{4pp'(p_0 + \beta)^2 D_{cs}(p_0)(1 + \gamma)^2}, \quad (28)$$

with

$$g(p) = \frac{p_0 + ip}{\beta - ip}\, {}_2F_1\left(1, \gamma; 2 + \gamma; \left(\frac{p_0 - \beta}{p_0 + \beta}\right)\left(\frac{p_0 + ip}{p_0 - ip}\right)\right) - \frac{p_0 - ip}{\beta + ip}\, {}_2F_1\left(1, \gamma; 2 + \gamma; \left(\frac{p_0 - \beta}{p_0 + \beta}\right)\left(\frac{p_0 - ip}{p_0 + ip}\right)\right).$$

The evaluation of the summation in (26) gives

$$D_{cs}(p_0) = 1 + \frac{\lambda \pi^2}{\beta(p_0 + \beta)^2(1 + \gamma)} \times {}_2F_1\left(1, \gamma; 2 + \gamma; \left(\frac{p_0 - \beta}{p_0 + \beta}\right)^2\right). \quad (29)$$

We note the similarity of (27) and (28) with (17) and (18), respectively, and also that (27) and (28) both reduce to the correct expression for the pure Yamaguchi T matrix when $\lambda_c = 0$, as they should.

Before discussing the analytic continuation of these representations to the positive energy region, we want to make a few remarks concerning the bound states of the Coulomb plus Yamaguchi potential $V = V^c + V^Y$. This topic was not discussed by Harrington.[2] The bound states are determined by solving the equation

$$D_{cs}(p_0) = 0, \quad (30)$$

where D_{cs} is given by (29). It is convenient to rewrite (30) in the following form:

$${}_2F_1\left(1, \frac{\kappa}{y}; 2 + \frac{\kappa}{y}; \left(\frac{y - 1}{y + 1}\right)^2\right) = \pm K f(y, \kappa), \quad (31)$$

where

$$f(y, \kappa) \equiv (y + 1)^2\left(1 + \frac{\kappa}{y}\right), \quad K \equiv \frac{\beta^3}{|\lambda|\, \pi^2}, \quad (32)$$

and we have defined the new variables

$$y \equiv \frac{p_0}{\beta}, \quad \kappa \equiv \frac{\lambda_c}{2\beta}.$$

The positive and negative signs on the right side of (31) correspond, respectively, to attractive and repulsive Yamaguchi potentials, and κ is positive or negative as the Coulomb potential is, respectively, repulsive or attractive.

The solutions of (31) are, of course, obtained by numerical methods. We can, however, make some qualitative remarks indicating the types of solutions which one obtains. By elementary calculus one finds that for fixed κ the critical points of the function $f(y, \kappa)$ occur at $y = -1$ and

$$y_\pm = \frac{-\kappa \pm [\kappa(\kappa + 8)]^{\frac{1}{2}}}{4}. \quad (33)$$

Thus, for positive real y there are no critical points if $-8 < \kappa < 0$. For $\kappa > 0$ or $\kappa < -8$ the critical points (33) may be either maxima, minima, or inflection points depending upon the particular value of κ. For the special case $\kappa = -8$, the two points coalesce to $y_\pm = 2$, which is an inflection point. For all fixed values of κ, $f(y, \kappa)$ is a rapidly varying function of y in comparison with the hypergeometric function.

Now, for $\kappa < 0$, corresponding to an attractive Coulomb potential, we note that $f(|\kappa|, \kappa) = 0$. Then, because of the properties of the functions f and ${}_2F_1$ noted above, it turns out that, for a fixed negative value of κ, there is either no solution or one and only one solution of (31), the choice depending upon the value of K and the sign on the right side of the equation. Thus, there can be solutions for both attractive and repulsive Yamaguchi potentials when the Coulomb potential is attractive. For example, the solution can always be translated to the point $y = 1$ by choosing K to be the reciprocal of $f(1, -|\kappa|)$. We list solutions for a fixed value of K in Table I. For convenience in these calculations we have chosen $K = 1$, thereby locating the bound state of the pure Yamaguchi potential at the origin.

The situation is completely different in the case $\kappa > 0$, corresponding to a repulsive Coulomb

TABLE I. Solutions of Eq. (31) for attractive Coulomb potentials.

κ	y	Type of Yamaguchi potential
$-\frac{1}{4}$	0.44	attractive
$-\frac{1}{2}$	0.74	attractive
$-\frac{3}{4}$	1	attractive
-1	1.24	attractive
$-\frac{5}{4}$	1	repulsive
$-\frac{7}{4}$	1.52	repulsive
$-\frac{9}{4}$	2.06	repulsive
$-\frac{11}{4}$	2.60	repulsive

potential. In this case $f(y, \kappa)$ is strictly positive and its minimum is generally much greater than the maximum value of the hypergeometric function, which is also strictly positive. Nonetheless, solutions of (31) are possible for the positive sign on the right side if the constant K has a sufficiently small value, corresponding to a sufficiently attractive Yamaguchi potential. In fact, it is clear that if, for a given $\kappa > 0$ and a given $y > 0$, the minimum of $Kf(y, \kappa)$ lies below the corresponding value of the hypergeometric function, then *two* solutions may be possible. These remarks are illustrated in Table II. It will be noted that in some of the results of Table II the constant K has been chosen so as to locate one of the bound states at the point $y = 1$.

We now return to the consideration of the analytic continuation of (27) and (28) to the positive energy region. This is accomplished by the same two procedures, respectively, that were used in the preceding section in the case of the pure Coulomb T matrix with the following results. Equation (27) keeps the same general form except that now $D_{cs}(p_0) \to D_{cs}(-ik)$ and $h(p)$ is now given by

$$h(p) = \frac{4i\mu k^2(\beta^2 + p^2)}{e^{-2\pi\mu} - 1} \int_C \frac{y^{i\mu}\, dy}{a - 2by + cy^2}, \tag{34}$$

and now

$$a = (\beta - ik)^2(p^2 - k^2),$$
$$b = (\beta^2 + k^2)(p^2 + k^2),$$
$$c = (\beta + ik)^2(p^2 - k^2).$$

TABLE II. Solutions of Eq. (31) for combinations of repulsive Coulomb and attractive Yamaguchi potentials.

κ	K	y
1	$\frac{1}{8}$	0.094, 1
1	$\frac{1}{9}$	0.075, 1.23
2	$\frac{1}{12}$	0.16, 1
2	$\frac{1}{11}$	0.21, 0.74
3	$\frac{1}{16}$	0.19, 1
3	$\frac{1}{15}$	0.24, 0.71
4	$\frac{1}{20}$	0.22, 1
4	$\frac{1}{19}$	0.26, 0.75

The integration contour in (34) is the same as that of (19). In place of (28) we find

$$T^{cs}(\mathbf{p}, \mathbf{p}'; k^2) = \lambda\bar{g}(p)\bar{g}(p')/4pp'(\beta - ik)^2 D_{cs}(-ik), \tag{35}$$

where now

$$\begin{aligned}\bar{g}(p) &\equiv \frac{-i}{1 + i\mu}\, g(p) \\ &= \frac{1}{1 + i\mu}\Bigg[\frac{p - k}{\beta - ip} \times {}_2F_1\left(1, i\mu; 2 + i\mu; \left(\frac{\beta + ik}{\beta - ik}\right)\left(\frac{p - k}{p + k}\right)\right) \\ &\quad + \frac{p + k}{\beta + ip}\, {}_2F_1 \times \left(1, i\mu; 2 + i\mu; \left(\frac{\beta + ik}{\beta - ik}\right)\left(\frac{p + k}{p - k}\right)\right)\Bigg] \qquad (36a) \\ &= \frac{p - k}{(\beta - ip)(1 + i\mu)}\, {}_2F_1 \times \left(1, i\mu; 2 + i\mu; \left(\frac{\beta + ik}{\beta - ik}\right)\left(\frac{p - k}{p + k}\right)\right) \\ &\quad + \frac{p - k}{(\beta + ip)(1 - i\mu)}\left(\frac{\beta - ik}{\beta + ik}\right) \times {}_2F_1\left(1, i\mu; 2 - i\mu; \left(\frac{\beta - ik}{\beta + ik}\right)\left(\frac{p - k}{p + k}\right)\right) \\ &\quad + \frac{2k}{\beta - ik}\, |\Gamma(1 + i\mu)|^2\, e^{\pi\mu} \times \left(\left(\frac{\beta - ik}{\beta + ik}\right)\left(\frac{p - k}{p + k}\right)\right)^{i\mu}. \qquad (36b)\end{aligned}$$

We can now easily obtain the on-shell limit of (35) by using the small argument expansion of the hypergeometric functions in (36b). For Re k, Im $k > 0$, one easily shows that $\left|\frac{\beta + ik}{\beta - ik}\frac{p - k}{p + k}\right| < 1$ so that

$$\bar{g}(k) = \frac{2k}{\beta + ik}\, |\Gamma(1 + i\mu)|^2\, e^{\pi\mu} \times \left(\frac{\beta - ik}{\beta + ik}\frac{p - k}{p + k}\right)^{i\mu} + O(p - k),$$

and therefore, from (35),

$$T^{cs}(k, k; k^2) = \lim_{\substack{p-k\to 0\\ p'-k\to 0}} \frac{\lambda}{(\beta^2 + k^2)^2 D_{cs}(-ik)}\, |\Gamma(1 + i\mu)|^4 \times \left[\frac{\beta - ik}{\beta + ik}\frac{1}{2k}\right]^{2i\mu} e^{2\pi\mu}(p - k)^{i\mu}(p' - k)^{i\mu}. \tag{37}$$

For the case of real k, the on-shell limits corresponding to (37) are discontinuous:

$$T^{cs}(k, k; k^2) = \frac{\lambda}{(\beta^2 + k^2)^2 D_{cs}(-ik)} |\Gamma(1 + i\mu)|^4 \left[\frac{\beta - ik}{\beta + ik}\frac{1}{2k}\right]^{2i\mu} \times \begin{Bmatrix} e^{2\pi\mu}(p - k)^{i\mu}(p' - k)^{i\mu} \\ (k - p)^{i\mu}(k - p')^{i\mu} \\ e^{\pi\mu}(k - p)^{i\mu}(p' - k)^{i\mu} \end{Bmatrix} \quad (38)$$

or

$$\begin{Bmatrix} p - k \to 0^+, & p' - k \to 0^+ \\ p - k \to 0^-, & p' - k \to 0^- \\ p - k \to 0^-, & p' - k \to 0^+ \end{Bmatrix}.$$

Analogous results to (38) were given by Ford[10,20] for the pure Coulomb T matrix.

The limits (37) and (38) have some similarities with the corresponding results for the pure Coulomb T matrix and the ambiguities of these limits[21] occur for the same reason. Namely, the sum of a short-range potential and the long-range Coulomb potential is again a long-range potential. Thus, the long-range part of the total potential, $V = V^c + V^Y$, dominates the on-shell behavior of the nuclear T matrix and the ambiguities of the limit[21] are due to the fact that momentum eigenstates have been used instead of the proper asymptotic states for the problem, exactly analogous to the situation in the pure Coulomb case. A meaningful limit can be obtained by "folding in" the Coulomb asymptotic states, as is done in the pure Coulomb problem.

V. CONCLUDING REMARKS

In the preceding section we have derived representations for the off-shell nuclear T matrix corresponding to the sum of Coulomb and Yamaguchi potentials. We indicated at the beginning of that section that the consideration of this example is sufficient for the elucidation of the most important ideas connected with the representation of the off-shell T matrix corresponding to the sum of Coulomb and separable potentials. We now give an indication of how the preceding results change when the Yamaguchi potential is replaced by another separable potential.

In general, the dependence of the various formulas on the quantities $\beta \pm ip$, $\beta \pm ip'$, and $\beta \pm ik$ will change, but the long-range behavior of the representations will still remain. For example, the ambiguities noted above for the Yamaguchi potential in the on-shell limit will remain even though the functional form may be changed from that of (37) and (38).

In the bound state problem treated in Sec. IV, we noted that, for an attractive Coulomb potential, at most one bound state can occur for either a repulsive or attractive Yamaguchi potential. The number "one" in this result corresponds to the fact that a pure Yamaguchi potential can support at most one bound state. If one uses instead a separable potential of higher rank, then this number can change. In a similar manner, the number of bound states for the combination of a repulsive Coulomb potential and a sufficiently attractive separable potential may be changed from the number "two" found above for a separable potential of the Yamaguchi type. Similarly, if one considers a separable potential of the type suggested by Tabakin,[22] then the attractiveness or repulsiveness of the potential is energy dependent, but essentially the same conclusions remain.

ACKNOWLEDGMENTS

I wish to thank A. W. Sáenz and R. H. Bassel for discussions concerning this work.

[1] Several reviews of this work are available: I. Duck, in *Advances in Nuclear Physics*, M. Baranger and E. Vogt, Eds. (Plenum, New York, 1968), Vol. I; R. D. Amado, Ann. Rev. Nucl. Sci. **19**, 61 (1969); A. N. Mitra, in *Advances in Nuclear Physics*, M. Baranger and E. Vogt, Eds. (Plenum, New York, 1970), Vol. III.
[2] D. R. Harrington, Phys. Rev. **139**, B691 (1965).
[3] V. A. Alessandrini, C. A. Garcia, and H. Fanchiotti, Phys. Rev. **170**, 935 (1968).
[4] L. Hostler, J. Math. Phys. **5**, 1235 (1964).
[5] J. Schwinger, J. Math. Phys. **5**, 1606 (1964).
[6] G. L. Nutt, J. Math. Phys. **9**, 796 (1968).
[7] C. S. Shastry, L. Kumar, and J. Callaway, Phys. Rev. A **1**, 1137 (1970); *ibid.* (to be published).
[8] C. P. Carpenter and T. F. Tuan, Phys. Rev. A **2**, 1811 (1970).
[9] R. Finkelstein and D. Levy, J. Math. Phys. **8**, 2147 (1967).
[10] W. F. Ford, J. Math. Phys. **7**, 626 (1966).
[11] C. S. Shastry and A. K. Rajagopal, Phys. Rev. A **2**, 781 (1970).
[12] J. S. Ball, J. C. Y. Chen, and D. Y. Wong, Phys. Rev. **173**, 202 (1968); J. C. Y. Chen, K. T. Chung, and P. J. Kramer, *ibid.* **184**, 64 (1969); J. C. Y. Chen and K. T. Chung, Phys. Rev. A **2**, 1449 (1970); P. J. Kramer and J. C. Y. Chen, Phys. Rev. A **3**, 568 (1971).
[13] V. Fock, Z. Physik **98**, 145 (1935).
[14] A. M. Perelomov and V. S. Popov, Zh. Eksp. Teor. Fiz. **50**, 179 (1966) [Sov. Phys. JETP **23**, 118 (1966)].
[15] A similar approach was discussed by D. Zwanziger, J. Math. Phys. **8**, 1858 (1967), who derived the Coulomb scattering amplitude by this method.
[16] J. D. Talman, *Special Functions, A Group Theoretic Approach* (Benjamin, New York, 1968), Chap. 12.
[17] Y. Yamaguchi, Phys. Rev. **95**, 1628 (1954).
[18] L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge U.P., London, 1966).
[19] Our parameter μ is the negative of Nutt's parameter ν.
[20] W. F. Ford, Phys. Rev. **133**, B1616 (1964).
[21] We refer here to the fact that these on-shell limits do not yield the correct scattering amplitude.
[22] F. Tabakin, Phys. Rev. **174**, 1208 (1968).

On the Construction of Orthogonal Matrix Basis Elements of Finite Group Algebras Symmetry Adapted to a Subgroup

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(Received 14 December 1970)

The matrix basis elements of a finite group $g(\Gamma, mn)$ are put in a form $|\Gamma\mathbf{m}\rangle\langle\Gamma\mathbf{n}|$ suggestive of a dyadic in operator space. It is shown that if a subgroup H exists for which $\Gamma\downarrow H = \Sigma\gamma_i$, then these operators may be symmetry adapted to the subgroup via $|\Gamma\gamma_j\mathbf{m}\rangle\,\mathbf{Q}_j^\dagger\mathbf{ba}$. Necessary and sufficient conditions for constructing the elements $\mathbf{Q}_j^\dagger$, $\mathbf{b}$ and $\mathbf{a}$ are given. Particular application of the procedure to the bipartition representations of the symmetric group is made.

I. SYMMETRY ADAPTATION

Application of the representation theory of finite groups is facilitated by use of orthogonal matrix elements, as a basis of the group algebra, because of their simple multiplication rule

$$\mathbf{g}(\Gamma, ij)\mathbf{g}(\Delta, kl) = \delta(\Gamma\Delta)\delta(jk)\mathbf{g}(\Gamma, il).$$

For physical theories which deal with scalar products, it is convenient to use a unitary representation for which

$$\mathbf{g}(\Gamma, ij)^\dagger = \mathbf{g}(\Gamma, ji).$$

For mathematical or physical reasons, one is often interested in using a representation symmetry adapted to a subgroup or a sequence of subgroups.[1] The reciprocal relations between representations of a group and its subgroups implicit in the subduction and induction processes are of interest in themselves for analyzing the structure of the group algebra. Often the most efficient, if not the only, way of constructing an explicit representation of a group is by induction from a known representation of a subgroup. In physical problems a sequence of subgroups often has a perturbative significance and, correspondingly, gives approximately good quantum-number classifications. Melvin[2] discussed the possibility of expressing the matrix basis elements (or any algebraic element) as a product of matrix basis elements of a subgroup and a coset factor, making particular application to the crystallographic point groups. The well-known Young operators of the symmetric group exemplify the construction of persistent algebraic elements by factors induced from subgroups.[3] Klein[4] emphasized the importance of symmetry adaption of the permutation group of a molecular system to permutation subgroups appropriate to the individual constituents (if one wishes to treat consistently the problem with varying internuclear distances).

To the author's knowledge, the only detailed prescription for constructing a group representation by induction from a subgroup is that due to Yamanouchi[5] for the permutation group S_n which results in symmetry adaption to the sequence $S_n \supset S_{n-1} \supset \cdots S_2$. It is the purpose of this paper to give a prescription for constructing the matrix basis elements of an irreducible representation Γ of a group G from those of a subgroup H for which $\Gamma\downarrow H = \Sigma\gamma_j$, i.e., no irreducible representation of H occurs more than once in the reduction of Γ on H. This allows a one-to-one relation to be established between the basis members of Γ and $\Sigma\gamma_j$.

It is convenient to identify vectors within the operator space

$$|\Gamma\mathbf{m}\rangle = \sum_{i,\rho}\alpha U_{\rho i}\mathbf{g}(\Gamma, mi),$$

where U is a unitary matrix so that

$$|\Gamma\mathbf{m}\rangle\langle\Gamma\mathbf{n}| = |\alpha|^2\sum U_{\rho i}U^{-1}_{i'\rho'}\mathbf{g}(\Gamma, mi)\mathbf{g}(\Gamma, i'n) = \mathbf{g}(\Gamma, mn).$$

The number of indices ρ to be included in the summand and the subsequent fixing of $|\alpha|$ is a matter of convenience. Any element $\mathbf{X}$ of the algebra that can be put in dyadic form

$$\mathbf{X} = \sum_{m,n} X_m\,|\Gamma\mathbf{m}\rangle\langle\Gamma\mathbf{n}|\,X_n^*$$

will be a persistent factor of the group algebra, i.e.,

$$\mathbf{XYX} = \sum_{m,n}(X_n^* Y^\Gamma_{nm} X_m)\mathbf{X}.$$

In Sec. II we will prove a theorem giving the necessary and sufficient conditions for constructing such a persistent factor. This allows the construction of symmetry adapted operators

$$|\Gamma\gamma_j\mathbf{m}\rangle = |\gamma_j\mathbf{m}\rangle\,\mathbf{Q}_j^\dagger\sum_i X_i\,|\Gamma\mathbf{i}\rangle.$$

The process can be carried on symmetry adapting to chains of subgroups.

II. CONSTRUCTION OF PERSISTENT FACTORS

Consider the group sublattice chain

$$\begin{array}{ccccc} & \nearrow & B & \searrow & \\ G & & & & L, \\ & \searrow & A & \nearrow & \end{array}$$

where $L \equiv A \cap B$, and let the irreducible representations be denoted by Γ, α, β, and λ, respectively. Let A^Γ and B^Γ be unitary transformations taking the representation G^Γ to forms symmetry adapted to the chains $G \rightarrow A \rightarrow L$ and $G \rightarrow B \rightarrow L$, respectively.

Theorem: $\alpha \uparrow G \cap \beta \uparrow G = \Gamma$ and $\alpha \downarrow L \cap \beta \downarrow L = \lambda$, where Γ and λ occur once and only once in the induction or subduction, are necessary and sufficient conditions such that

$$\begin{aligned} \mathbf{b}(\beta, b_m\lambda_m u, b_i\lambda_i q)\mathbf{a}(\alpha, a_j\lambda_j r, a_k\lambda_k s)\mathbf{b}(\beta, b_l\lambda_l t, b_n\lambda_n v) &= \delta(\lambda_i\lambda_j)\delta(\lambda_i\lambda)\delta(\lambda_k\lambda_l)\delta(\lambda_l\lambda)\delta(qr)\delta(st) \\ &\times \sum_{m,n} B^{\Gamma-1}_{m,b_m\lambda_m u} B^{\Gamma}_{b_n\lambda_n v,n}\mathbf{g}(\Gamma, mn), \quad (1) \end{aligned}$$

where b_m and a_j denote the multiplicities with which λ_m and λ_j occur in the reduction of β and α on L, respectively.

Proof: By use of the orthogonality relations, a matrix basis element of a subgroup when extended to the full group can be shown to have the form

$$\mathbf{a}(\alpha_i, a_j\lambda_j r, a_k\lambda_k s) = \sum_{\Gamma_k \in \alpha_i \uparrow G; f_i; m,n} A^{\Gamma_k -1}_{m,f_i\alpha_i a_j\lambda_j r} A^{\Gamma_k}_{f_i\alpha_i a_k\lambda_k s,n}\mathbf{g}(\Gamma_k, mn).$$

Such an element is not in general a persistent factor of the algebra because more than one irreducible representation occurs in the induction (sum over Γ_k) and with multiple frequency (sum over f_i). Convolution such as in Eq. (1) of matrix basis elements satisfying the conditions of the theorem does produce a persistent element of the algebra. The first condition is seen as necessary and sufficient to obviate the sums over the irreducible representations and their multiplicities. The second condition is necessary for the result to be nonzero as we now show. By Schur's lemma the matrix AB^{-1} is in block diagonal form with respect to the irreducible representations of L. An intertwining number theorem[6] requires

$$i(\alpha \uparrow G, \beta \uparrow G) = \sum_d i(\alpha^d \downarrow L_d, \beta \downarrow L_d),$$

where the sum on d is over the double-coset representatives $G = \bigcup_d A\,dB$, with $L_d = d^{-1}Ld$ and $\alpha^d(\mathbf{d}^{-1}\mathbf{a}\mathbf{d}) = \alpha(\mathbf{a})$. The left-hand side intertwining number is, by hypothesis, 1. If $i(\alpha \downarrow L, \beta \downarrow L) = 0$, all elements of AB^{-1} for that particular (α, β) pair vanish. We therefore require the second condition: Normalize to the nonzero constant multiplier, and the theorem follows. We note the combined conditions $i(\alpha^d \downarrow L_d, \beta \downarrow L_d) = \delta\, dE$ are equivalent to those given by Burrow.[7]

For factors satisfying the conditions of the theorem, a persistent element of the group algebra can be constructed as (equivalent up to a nonzero numerical factor)[8]

$$\begin{aligned} \mathbf{X}(\alpha\beta, pp') &= \mathbf{b}(\beta, p\cdot)\mathbf{a}(\alpha, \cdot\!\!-\!\!\!-\!\!\cdot)\mathbf{b}(\beta, \cdot p') \\ &\sim \sum_{i,j} B^{\Gamma-1}_{i,\beta p} B^{\Gamma}_{\beta p',j}\mathbf{g}(\Gamma, ij). \end{aligned}$$

It can be made Hermitian simply by setting $p' = p$ or by separately summing over these indices.

Our task is completed if we show that the inner indices and the elements $\mathbf{Q}_j$ can be chosen so that

$$\begin{aligned} |\boldsymbol{\Gamma\gamma}_j\mathbf{n}\rangle &= |\boldsymbol{\gamma}_j\mathbf{n}\rangle\, \mathbf{Q}_j^{\dagger}\mathbf{b}(\beta, p\cdot)\mathbf{a}(\alpha, \cdot\!\!-\!\!\!-\!\!\cdot) \\ &\sim \sum_m A^{\Gamma}_{\alpha\lambda\cdot,m}\mathbf{g}(\Gamma, \gamma_j n, m). \end{aligned}$$

This is equivalent to requiring that $(BQ_j)_{\beta p,\gamma_j n'}$ can be chosen to be nonzero and thus normalizable. That such a choice is possible follows from the intertwining number theorem used above. Let $G = \bigcup_q BqH$ and $L_q = q^{-1}Bq \cap H$. Because $i(\beta \uparrow G, \gamma_j \uparrow G) \neq 0$, there is certainly some $\mathbf{q}$ for which $i(\beta^q \downarrow L_q, \gamma_j \downarrow L_q) \neq 0$. Taking this element to be $\mathbf{Q}_j$ guarantees the existence of choices for p and n' such that $(Bq_j)_{\beta p,\gamma_j n'} \neq 0$. By individually summing over the inner indices one obviously obtains a nonzero, and therefore normalizable, result. However, it is well to note the above procedure is not necessary to obtain a nonzero result and there may be more convenient choices for $\mathbf{Q}_j$, p, and n'.

III. DISCUSSION AND EXAMPLES

We have established the following procedure for constructing unitary matrix basis elements for an irreducible representation Γ of a group G from the elements of a subgroup H for which $\Gamma \downarrow H = \Sigma\gamma_j$:

(i) Establish a core by identifying irreducible representations α and β of subgroups A and B for which $\alpha \uparrow G \cap \beta \uparrow G = \Gamma$ and $\alpha \downarrow (A \cap B) \cap \beta \downarrow (A \cap B) = \lambda$. Construct the convolution $\mathbf{b}(\beta, p\cdot)\mathbf{a}(\alpha, \cdot\!\!-\!\!\!-\!\!\cdot)\mathbf{b}(\beta, \cdot p')$.

(ii) For each index $\gamma_j n$, select p' and $\mathbf{Q}_j$ such that $\langle\boldsymbol{\Gamma\gamma}_j\mathbf{n}| \equiv \mathbf{a}(\alpha, \cdot\!\!-\!\!\!-\!\!\cdot)\mathbf{b}(\beta, \cdot p')\mathbf{Q}_j\,\langle\boldsymbol{\gamma}_j\mathbf{n}|$ is nonzero. One way of doing this is by summing over p' and letting $\mathbf{Q}_j$ be any double-coset representative for which $\beta^q \downarrow L_q \cap \gamma_j \downarrow L_q \neq 0$.

(iii) $\mathbf{a}$ and $\mathbf{Q}_j$ can be properly renormalized so that

$$\begin{aligned}\mathbf{g}(\Gamma, \gamma_i m, \gamma_j n) &= |\mathbf{\Gamma\gamma_i m}\rangle\langle\mathbf{\Gamma\gamma_j n}| \\ &= |\mathbf{\gamma_i m}\rangle\, \mathbf{Q}_i^\dagger \mathbf{b}(\beta, p\cdot)\mathbf{a}(\alpha, \cdot\!\!-\!\!\!-\!\!\cdot)\mathbf{b}(\beta, \cdot p')\mathbf{Q}_j \langle\mathbf{\gamma_j n}|.\end{aligned}$$

As an example of the procedure, consider the bipartition representation $[n_1, n_2]$ of the permutation group $S_{(n_1+n_2)}$ and its reduction in the subgroup $S_{n_1} \otimes S_{n_2}$:

$$\begin{aligned}[][n_1, n_2] \downarrow S_{n_1} \otimes S_{n_2} &= \sum [n_1 - j_1, j_1] \otimes [n_2 - j_2, j_2], \\ 0 \le j_1 + j_2 &\le n_2, \quad 0 \le j_1 - j_2 \le n_1 - n_2.\end{aligned}$$

A persistent factored element of the group algebra is given by Young's operator $\mathbf{X} = \mathbf{PNP}$, where $\mathbf{P}$ is the (row) symmetrizer for the group $S_{n_1} \otimes S_{n_2}$ (i.e., in this case the subgroups B and H are identical), and N is the (column) antisymmetrizer of a group $(S_2)^{n_2}$. The double-coset representatives can be chosen as jth-order products of mutually commuting transposes which combine elements from the set (n_1) and those from (n_2), e.g.,[9]

$$q_j = \prod_{i=1}^{j} (i, n_1 + i) \quad \text{for} \quad 0 \le j \le n_2.$$

The irreducible representations $[n_1] \otimes [n_2]$ and $[n_1 - j_1, j_1] \otimes [n_2 - j_2, j_2]$ will intertwine on any subgroup $S_{n_1-j} \otimes S_j \otimes S_{n_2-j} \otimes S_j$, with $j_1 \le j \le n_2$.

Taking $\mathbf{Q}_j \equiv \mathbf{q}_{j_1}$ will give the operators $|\mathbf{\Gamma\gamma_j n}\rangle \sim |\mathbf{\gamma_j n}\rangle\, \mathbf{q}_j\mathbf{PN}$, which obviously yield the desired orthogonality. The required normalization can be found by considering

$$\begin{aligned}&|\mathbf{\Gamma\gamma_j m}\rangle \langle\mathbf{\Gamma\gamma_k p} \mid \mathbf{\Gamma\gamma_k p}\rangle \langle\mathbf{\Gamma\gamma_i n}| \\ &\quad = |\mathbf{\gamma_j m}\rangle\, \mathbf{q}_j\{\mathbf{PNPq}_k \langle\mathbf{\gamma_k p} \mid \mathbf{\gamma_k p}\rangle\mathbf{q}_k\mathbf{PNP}\}\mathbf{q}_i \langle\mathbf{\gamma_i n}|.\end{aligned}$$

Since PNP is a persistent factor of the algebra and in this case is some multiple α of $\mathbf{g}(\Gamma, 11)$, the quantity in curly brackets is

$$\alpha U_{11}^{[n_1,n_2]}(\mathbf{q}_k\langle\mathbf{\gamma_k p} \mid \mathbf{\gamma_k p}\rangle\mathbf{q}_k)\mathbf{PNP}.$$

The coefficient $U_{11}^{[n_1,n_2]}(\mathbf{hq}_j\mathbf{h}') = (-1)^j\binom{n_1}{j}^{-1}$. The element $\langle\mathbf{\gamma_k p} \mid \mathbf{\gamma_k p}\rangle$ belongs to the subgroup algebra and therefore to the $j = 0$ double coset. Let $n(j, k)$ be the number of elements from the jth double coset appearing in the expression $\mathbf{q}_k\langle\mathbf{\gamma_k p} \mid \mathbf{p\gamma_k}\rangle\mathbf{q}_k$. Then the normalizing coefficient is easily evaluated as

$$U_{11}^{[n_1,n_2]}(\mathbf{q}_k\langle\mathbf{\gamma_k p} \mid \mathbf{\gamma_k p}\rangle\mathbf{q}_k) = \sum_{j=0}^{n_2}(-1)^j n(j, k)\binom{n_1}{j}^{-1}.$$

The following table represents a possible reduction scheme for the five-dimensional representation [3, 2] of S_5:

$$[3,2] \begin{cases} \nearrow [3] \otimes [2] \\ \searrow [2, 1] \otimes ([2] + [1^2]) \rightarrow ([2] + [1^2]) \otimes [1] \otimes ([2] + [1^2]) \end{cases}$$

$$\begin{aligned}|\mathbf{3, 2}\rangle &\sim \mathbf{P}_{(123)(45)}\mathbf{N}_{(14)(25)} \equiv \mathbf{PN}, & U &= 1, \\ |\mathbf{2, 1, 2}\rangle &\sim \mathbf{P}_{(12)(45)}\mathbf{N}_{(13)}(\mathbf{14})\mathbf{PN}, & &= 2, \\ |\mathbf{2, 1, 1^2}\rangle &\sim \mathbf{P}_{(12)}\mathbf{N}_{(13)(45)}(\mathbf{14})\mathbf{PN}, & &= 6, \\ |\mathbf{1^2, 1, 2}\rangle &\sim \mathbf{N}_{(12)}(\mathbf{13})\mathbf{P}_{(12)(45)}\mathbf{N}_{(13)}(\mathbf{14})\mathbf{PN}, & &= 6, \\ |\mathbf{1^2, 1, 1^2}\rangle &\sim \mathbf{N}_{(12)}(\mathbf{13})\mathbf{P}_{(12)}\mathbf{N}_{(13)(45)}(\mathbf{14})\mathbf{PN}, & &= 18, \\ & & \alpha &= \tfrac{1}{24}.\end{aligned}$$

[1] F. A. Matsen and O. R. Plummer, in *Group Theory and Its Applications*, edited by E. M. Loebl (Academic, New York, 1968).
[2] M. A. Melvin, Rev. Mod. Phys. **28**, 18 (1956).
[3] H. V. McIntosh, J. Math. Phys. **1**, 453 (1960).
[4] D. J. Klein, J. Chem. Phys. **50**, 5140 (1969).
[5] T. Yamanouchi, Proc. Phys. Math. Soc. Japan **19**, 436 (1937); D. F. Rutherford, *Substitutional Analysis* (Hafner, New York, 1968).
[6] A. J. Coleman, Queens Papers in Pure and Applied Math. No. 4, Queens Univ., Kingston, Ontario, Canada, 1966.
[7] M. D. Burrow, *Representation Theory of Finite Groups* (Academic, New York, 1965); Can. J. Math. **6**, 498 (1954).
[8] We use a convention where a dot $\cdot$ means the index is summed over its range and $\cdot\!\!-\!\!\!-\!\!\cdot$ means the indices are set equal and summed.
[9] J. J. Sullivan, J. Math. Phys. **9**, 1369 (1968). This paper develops the formula used for $U_{11}^{[n_1,n_2]}(j)$.

Exact Results for a Body-Centered Cubic Lattice Green's Function with Applications in Lattice Statistics. I*

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(Received 8 September 1970)

In this paper the body-centered cubic lattice Green's function

$$P(\mathbf{l}, z) = \frac{1}{\pi^3}\iiint_0^\pi (1 - z\cos x_1 \cos x_2 \cos x_3)^{-1}\cos l_1x_1 \cos l_2x_2 \cos l_3x_3\, dx_1\, dx_2\, dx_3,$$

where l_1, l_2, and l_3 are all even, or all odd, is studied. A complete analytic continuation for $P(z) \equiv P(\mathbf{0}, z)$ is derived of the form

$$P(z) = \sum_{n=0}^{\infty} B_n(1 - z^2)^n - (1 - z^2)^{\frac{1}{2}} \sum_{n=0}^{\infty} C_n(1 - z^2)^n,$$

where $|1 - z^2| < 1$. Explicit formulas, recurrence relations, and asymptotic expansions are established for the coefficients B_n and C_n. A similar analytic continuation in powers of $1 - z$ is also investigated. The generalized Watson integral

$$I(m, n) = \frac{1}{\pi^3}\iiint_0^\pi (1 - \cos x_1 \cos x_2 \cos x_3)^{-1}\cos^{2m} x_1 \cos^{2n} x_2\, dx_1\, dx_2\, dx_3,$$

where $m \geq 0$ and $n \geq 0$, is evaluated in closed form. Using this result, we show that $P(\mathbf{l}, 1)$ can, in principle, be evaluated for arbitrary $\mathbf{l}$. Exact expressions and numerical values for $P(\mathbf{l}, 1)$ are given for $0 \leq l_1 \leq l_2 \leq l_3 \leq 8$. Detailed applications of the above results are made in the theory of random walks on a body-centered cubic lattice. In particular, a new asymptotic expansion for the expected number of distinct lattice sites visited during an n-step random walk is obtained. The closely related Green's function

$$\lim_{\epsilon\to 0+}\frac{1}{\pi^3}\iiint_0^\pi (\xi_0 - i\epsilon - \cos x_1 \cos x_2 \cos x_3)^{-1}\, dx_1\, dx_2\, dx_3,$$

where ξ_0 is real, is expressed in terms of complete elliptic integrals for *all* $\xi_0 > 0$, and evaluated numerically in the range $0 < \xi_0 \leq 1$. The behavior of this Green's function in the neighborhood of the singularities at $\xi_0 = 0$ and 1 is also discussed. *No attempt* is made, in the present paper, to discuss $P(\mathbf{l}, z)$ for the general case $\mathbf{l} \neq \mathbf{0}$ *and* $z \neq 1$.

1. INTRODUCTION

In the study of nearest neighbor lattice statistics on the body-centered cubic lattice the Green's function

$$P(\mathbf{l}, z) \equiv P(l_1, l_2, l_3; z) = \frac{1}{\pi^3}\iiint_0^\pi \frac{\cos l_1x_1 \cos l_2x_2 \cos l_3x_3}{1 - z\cos x_1 \cos x_2 \cos x_3}\, dx_1\, dx_2\, dx_3, \tag{1.1}$$

where $|z| \leq 1$ and l_1, l_2, l_3 are all even, or all odd integers, is of frequent occurrence. For example, $P(\mathbf{l}, z)$ appears in the theories of ferromagnetism such as the Ising model,[1–3] Heisenberg model,[4–6] and spherical model.[7–9] The integral $P(\mathbf{l}, z)$ also plays an important role in the theory of random walks on a body-centered cubic lattice, as a probability generating function.[10–12] In view of the physical importance of $P(\mathbf{l}, z)$ it was felt that a detailed investigation of its properties would be a worthwhile project.

We shall restrict our attention in this paper to the particular Green's functions

$$P(z) \equiv P(\mathbf{0}, z) = \frac{1}{\pi^3}\iiint_0^\pi \frac{dx_1\, dx_2\, dx_3}{1 - z\cos x_1 \cos x_2 \cos x_3}, \tag{1.2}$$

and $P(\mathbf{l}, 1)$. *No attempt* will be made to study the Green's function (1.1) for $\mathbf{l} \neq \mathbf{0}$ *and* $z \neq 1$, since it is hoped to discuss this most general case in Paper II of this series. In order to provide a background for the following sections, we now briefly review the results for $P(z)$ that are already available in the literature.

By inspecting the integrand in Eq. (1.2) we see that the integral (1.2), in fact, represents a single-valued analytic function throughout any closed domain of the z^2 plane, cut along the real axis from $+1$ to $+\infty$. Thus for the sake of generality we shall take this analytic function in the cut plane as our *basic definition* of $P(z)$. [It is convenient to consider the z^2 plane since $P(z) = P(-z)$.]

A power series for $P(z)$, valid when $|z| < 1$, may be readily established by expanding the integrand in Eq. (1.2) in powers of z and integrating term by term.[13] We find

$$P(z) = \sum_{n=0}^{\infty} a_n^3 z^{2n}, \quad |z| < 1, \tag{1.3}$$

where

$$a_n = \Gamma(n + \tfrac{1}{2})/\pi^{\frac{1}{2}}\Gamma(n + 1) = (\tfrac{1}{2})_n/(1)_n, \quad n \geq 0, \tag{1.4}$$

and $(\alpha)_n = \Gamma(n + \alpha)/\Gamma(\alpha)$. The coefficients a_n^3 can be interpreted as the probability that a random walker will return to his origin point (not necessarily for the first time) after a walk of $2n$ steps on a body-centered cubic lattice. Since

$$a_n^3 \sim (\pi n)^{-\frac{3}{2}}, \quad \text{as} \quad n \to \infty, \tag{1.5}$$

it follows (Abel's limit theorem) that the range of validity of Eq. (1.3) can be extended to include all points on the circle $|z| = 1$. In particular,

$$P(1) = \sum_{n=0}^{\infty} a_n^3. \tag{1.6}$$

The evaluation of $P(z)$, for $z = 1$, was first carried out by Van Peijpe[14] and later by Watson.[15] Their results are

$$P(1) = (1/4\pi^3)[\Gamma(\tfrac{1}{4})]^4 = (4/\pi^2)K_0^2, \tag{1.7}$$

where K_0 denotes the complete elliptic integral $K(2^{-\frac{1}{2}})$ and $\Gamma(x)$ is the gamma function. The method developed by Watson for the case $z = 1$ may be simply generalized by comparing the series (1.3) with the expansion[15,16]

$$K^2(k) = \tfrac{1}{4}\pi^2 \sum_{n=0}^{\infty} a_n^3 [4\omega(1 - \omega)]^n, \tag{1.8}$$

where $\omega = k^2$ is in the left-hand half of the lemniscate $|\omega(1 - \omega)| = \frac{1}{4}$. It is found[17]

$$P(z) = (4/\pi^2)K^2(k), \quad |z| \leq 1, \tag{1.9}$$

where

$$k^2 = \tfrac{1}{2} - \tfrac{1}{2}(1 - z^2)^{\frac{1}{2}}. \tag{1.10}$$

[The square root in Eq. (1.10) is defined so that its value is real and positive when $0 \leq z^2 < 1$.] This result is particularly convenient for the numerical calculation of $P(z)$, because $K(k)$ can be readily evaluated using the arithmetic–geometric mean procedure.[18]

Since the coefficients a_n^3 in the series (1.3) are positive real numbers, it is clear that $P(z)$ must have singular points at $z = \pm 1$. In the neighborhood of the singular point $z = 1$, it has been shown that[9,19,20]

$$P(z) = P(1) - \frac{2^{\frac{3}{2}}}{\pi}(1 - z)^{\frac{1}{2}} + O(1 - z), \quad z \lessdot 1. \tag{1.11}$$

However, the nature and range of validity of this expansion has not been established and there appear to be no results available for the higher-order coefficients in the expansion. These higher-order coefficients are of considerable importance since they enable one to investigate in detail the critical properties of the spherical model,[21] while in the theory of random walks they are required in certain asymptotic formulas.[12]

The main aims of the present paper are as follows: to establish, in detail, *complete* expansions for $P(z)$ which are valid in the neighborhood of $z = \pm 1$; to develop a procedure for evaluating the Green's function $P(1, 1)$ exactly; and, finally, to apply the results obtained to the theory of random walks.

2. ANALYTIC CONTINUATION OF $P(z)$

We begin by considering the generalized hypergeometric function[22,23]

$$_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; z^2). \tag{2.1}$$

This function, which is analytic throughout the z^2 plane cut along the real axis from $+1$ to $+\infty$, is defined for $|z| \leq 1$ by the series

$$_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; z^2) = \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n(\frac{1}{2})_n(\frac{1}{2})_n}{(1)_n(1)_n} \frac{z^{2n}}{n!}. \tag{2.2}$$

It follows therefore from the *basic definition* of $P(z)$ given above and Eq. (1.3) that

$$P(z) = {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; z^2). \tag{2.3}$$

Thus the inegral (1.2) must be just an integral representation of the $_3F_2$ function. In fact (1.2) can be reduced to a standard representation by performing the integration over x_3. We find

$$P(z) = \frac{4}{\pi^2} \iint_0^{\pi/2} (1 - z^2 \cos^2 x_1 \cos^2 x_2)^{-\frac{1}{2}} dx_1 dx_2, \tag{2.4}$$

where z^2 is in the cut plane. The substitutions $t_1 = \cos^2 x_1$ and $t = \cos^2 x_2$ in Eq. (2.4) yield

$$P(z) = \frac{1}{\pi^2} \iint_0^1 t_1^{-\frac{1}{2}} t_2^{-\frac{1}{2}} (1 - t_1)^{-\frac{1}{2}} (1 - t_2)^{-\frac{1}{2}} \times (1 - z^2 t_1 t_2)^{-\frac{1}{2}} dt_1 dt_2, \tag{2.5}$$

which is the multiple Euler integral[24] for (2.1). It is interesting to note that because the series (2.2) is "well-poised," the evaluation of $P(1)$ can be carried out *directly* using Dixon's theorem (Watson's theorem and Whipple's theorem can also be used).[25]

To establish the analytic continuation of $P(z)$ to the neighborhood of $z^2 = 1$, we first apply Clausen's identity[26]

$$ {}_2F_1(a, b; a + b + \tfrac{1}{2}; z)^2 = {}_3F_2(2a, 2b, a + b; 2a + 2b, a + b + \tfrac{1}{2}; z) \quad (2.6)$$

to Eq. (2.3), with $a = b = \frac{1}{4}$. Hence

$$P(z) = {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; 1; z^2)^2. \quad (2.7)$$

The standard analytic continuation formula[27]

$$\begin{aligned} {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; 1; z^2) &= \frac{[\Gamma(\frac{1}{4})]^2}{2\pi^{\frac{3}{2}}} {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{1}{2}; 1 - z^2) \\ &\quad - 2\pi^{\frac{1}{2}}[\Gamma(\tfrac{1}{4})]^{-2}(1 - z^2)^{\frac{1}{2}} {}_2F_1(\tfrac{3}{4}, \tfrac{3}{4}; \tfrac{3}{2}; 1 - z^2), \quad (2.8)\end{aligned}$$

may now be used in Eq. (2.7) to obtain the following analytic continuation formula for $P(z)$:

$$P(z) = \phi_1(z) - (1 - z^2)^{\frac{1}{2}}\phi_2(z), \quad |\arg (1 - z^2)| < \pi, \quad (2.9)$$

where

$$\begin{aligned}\phi_1(z) = [&(4K_0^2/\pi^2) {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{1}{2}; 1 - z^2)^2 \\ &+ (1/4K_0^2)(1 - z^2) {}_2F_1(\tfrac{3}{4}, \tfrac{3}{4}; \tfrac{3}{2}; 1 - z^2)^2] \end{aligned} \quad (2.10)$$

and

$$\phi_2(z) = \left(\frac{2}{\pi}\right) {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{1}{2}; 1 - z^2) {}_2F_1(\tfrac{3}{4}, \tfrac{3}{4}; \tfrac{3}{2}; 1 - z^2). \quad (2.11)$$

This basic result is valid throughout the cut z^2 plane, provided that z^2 is not on the real negative axis and $z^2 \neq 0$.

Finally, we replace the ${}_2F_1$ functions in Eq. (2.10) by their hypergeometric series and expand $\phi_1(z)$ in the form

$$\phi_1(z) = \sum_{n=0}^{\infty} B_n(1 - z^2)^n, \quad |1 - z^2| < 1, \quad (2.12)$$

where

$$\begin{aligned} B_0 &= \frac{4K_0^2}{\pi^2}, \qquad B_1 = \frac{1}{4}\left(\frac{4K_0^2}{\pi^2} + \frac{1}{K_0^2}\right), \\ B_2 &= \frac{1}{48}\left(\frac{28K_0^2}{\pi^2} + \frac{9}{K_0^2}\right), \quad B_3 = \frac{1}{60}\left(\frac{25K_0^2}{\pi^2} + \frac{9}{K_0^2}\right), \\ B_4 &= \frac{1}{80\,640}\left(\frac{26\,300K_0^2}{\pi^2} + \frac{10\,143}{K_0^2}\right). \end{aligned} \quad (2.13)$$

In a similar manner, we find from Eq. (2.11) that

$$\phi_2(z) = \sum_{n=0}^{\infty} C_n(1 - z^2)^n, \quad |1 - z^2| < 1, \quad (2.14)$$

where

$$\begin{aligned} C_0 &= \frac{2}{\pi}, \quad C_1 = \frac{1}{\pi}, \quad C_2 = \frac{41}{60\pi}, \\ C_3 &= \frac{21}{40\pi}, \quad C_4 = \frac{961}{2240\pi}. \end{aligned} \quad (2.15)$$

Equations (2.9), (2.12), and (2.14), which give the complete analytic continuation of $P(z)$ into the region $|1 - z^2| < 1$, enable one to investigate in detail the behavior of $P(z)$ in the neighborhood of $z^2 = 1$.

Explicit formulas for B_n and C_n can be derived from Eqs. (2.10) and (2.11), respectively, in terms of terminating generalized hypergeometric series. We give the final results below:

$$B_n = B_n^{(0)} + B_n^{(1)}, \quad n \geq 1,$$

where

$$\begin{aligned} B_n^{(0)} &= \left(\frac{4K_0^2}{\pi^2}\right)\frac{(\frac{1}{4})_n^2}{(\frac{1}{2})_n(1)_n} {}_4F_3\left[\begin{matrix}-n, \frac{1}{2} - n, \frac{1}{4}, \frac{1}{4}; \\ \frac{1}{2}, \frac{3}{4} - n, \frac{3}{4} - n;\end{matrix} \; 1\right], \\ B_n^{(1)} &= \left(\frac{1}{4K_0^2}\right)\frac{(\frac{3}{4})_{n-1}^2}{(\frac{3}{2})_{n-1}(1)_{n-1}} \\ &\quad \times {}_4F_3\left[\begin{matrix}-n + 1, \frac{1}{2} - n, \frac{3}{4}, \frac{3}{4}; \\ \frac{3}{2}, \frac{5}{4} - n, \frac{5}{4} - n;\end{matrix} \; 1\right], \end{aligned} \quad (2.16)$$

and

$$\begin{aligned} C_n &= \left(\frac{2}{\pi}\right)\frac{(1)_n}{(\frac{3}{2})_n} \sum_{m=0}^{n} a_m^2 a_{n-m} \\ &= \frac{2}{(2n + 1)\pi} {}_3F_2\left[\begin{matrix}-n, \frac{1}{2}, \frac{1}{2}; \\ \frac{1}{2} - n, 1;\end{matrix} \; 1\right]. \end{aligned} \quad (2.17)$$

The formula for B_n follows directly from a general product theorem,[28] while that for C_n is obtained by applying one of Orr's theorems.[29] It is interesting to note that both the terminating ${}_4F_3$ series in Eq. (2.16) are *"well-poised" and "Saalschützian."*

An analytic continuation formula for a *general* ${}_3F_2$ function has been derived by Olsson.[30] The direct application of this result to the particular case (2.1) enables us to give the following alternative expressions[31] for the coefficients B_n and C_n:

$$B_n = \frac{(\frac{1}{2})_n^2}{n!} \sum_{m=0}^{\infty} \frac{a_m^3}{(\frac{1}{2} - m)_n}, \quad n \geq 0, \quad (2.18)$$

and

$$C_n = \left(\frac{2}{\pi}\right)\frac{(1)_n}{(\frac{3}{2})_n} {}_3F_2\left[\begin{matrix}-n, \frac{1}{2}, \frac{1}{2}; \\ 1, 1;\end{matrix} \; 1\right]. \quad (2.19)$$

We see that this direct procedure does *not* yield the exact closed form result (2.16) for the coefficient B_n. In fact, (2.16) provides us with an exact summation formula (which may be new) for the infinite series in Eq. (2.18)!

This observation has useful consequences. For example, Byrnes *et al.*[32] have recently investigated the integral

$$I_2 = \frac{1}{\pi^3} \iiint_0^\pi \frac{\cos^2 x_1 \cos^2 x_2 \, dx_1 \, dx_2 \, dx_3}{1 - \cos x_1 \cos x_2 \cos x_3} \quad (2.20)$$

$$= \sum_{n=0}^{\infty} a_n a_{n+1}^2, \quad (2.21)$$

and have obtained, using the series (2.21), the numerical estimate $I_2 = 0.55147 \pm 0.00045$. However, if we write the summation (2.21) as

$$I_2 = \sum_{n=0}^{\infty} a_n^3 - \frac{1}{2} \sum_{n=0}^{\infty} \frac{a_n^3}{(\frac{1}{2} - n)}, \quad (2.22)$$

we see immediately from Eq. (2.18) that

$$I_2 = B_0 - 2B_1. \quad (2.23)$$

Hence, we have the exact result

$$I_2 = \left(\frac{2K_0^2}{\pi^2} - \frac{1}{2K_0^2}\right) \simeq 0.551\,151\,350\,638\,50. \quad (2.24)$$

The application of the method of Darboux[33] to Eq. (2.9) provides us with an interesting check on the coefficients $C_0, C_1, \cdots, C_N$. In this method we form [from the singular part of (2.9)] the function

$$f_N(z) = -\sum_{l=0}^{N} C_l (1 - z^2)^{l+\frac{1}{2}}, \quad (2.25)$$

and expand it into the series

$$f_N(z) = \sum_{n=0}^{\infty} D_n(N) z^{2n}, \quad (2.26)$$

where

$$D_n(N) = (-1)^{n+1} \sum_{m=0}^{N} C_m \binom{m + \frac{1}{2}}{n}. \quad (2.27)$$

It may be shown that $D_n(N)$ gives the asymptotic representation

$$a_n^3 \sim D_n(N), \quad \text{as} \quad n \to \infty, \quad (2.28)$$

for the coefficients in the power series (1.2). The substitution of the asymptotic expansion

$$\binom{\alpha}{n} \sim \frac{(-1)^n}{\Gamma(-\alpha) n^{1+\alpha}} \left[1 + \frac{(\alpha)_2}{2n} + \frac{(\alpha)_3(3\alpha + 1)}{24n^2} + \frac{(\alpha)_2(\alpha)_4}{48n^3} + \frac{(\alpha)_5}{5760n^4}(15\alpha^3 + 30\alpha^2 + 5\alpha - 2) + \cdots\right], \quad (2.29)$$

in Eq. (2.27), with $N = 4$, leads to

$$a_n^3 \sim \frac{1}{(\pi n)^{\frac{3}{2}}} \left[1 - \frac{3}{8n} + \frac{9}{128n^2} + \frac{7}{1024n^3} - \frac{165}{32\,768n^4} + \cdots\right]. \quad (2.30)$$

This result is in agreement with that obtained by applying Stirling's series to Eq. (1.4). For the *simple cubic* lattice (with nearest neighbor interactions) this procedure is of considerable importance, since it enables one to derive an asymptotic formula for the probability of return to the origin after a $2n$-step random walk, *without* using the method of steepest descent.[34]

An asymptotic expansion for C_n may also be derived using the method of Darboux providing the behavior of the function $\phi_2(z)$ is known in the neighborhood of the singularity at $z^2 = 0$. This behavior is readily established by substituting the analytic continuation formula

$$_2F_1(a, a; 2a; 1 - z^2) = \frac{\Gamma(2a)}{\Gamma(a)^2} \sum_{n=0}^{\infty} \frac{(a)_n^2}{(n!)^2} [2\psi(n + 1) - 2\psi(n + a) - \ln z^2] z^{2n}, \quad (2.31)$$

in Eq. (2.11). [In this formula $\psi(x)$ denotes the logarithmic derivative of the gamma function.] If the singular part of the resulting expression is formally developed as a power series in $1 - z^2$, then the coefficient of $(1 - z^2)^n$ yields, for large n, the following asymptotic expansion for C_n:

$$C_n \sim \frac{1}{\pi^2 n} g(n) - \frac{1}{8\pi^2 n^2}[5g(n) - 4] + \frac{1}{768\pi^2 n^3}[273g(n) - 277] + \cdots, \quad (2.32)$$

where

$$g(n) = \gamma + 6 \ln 2 + \ln n, \quad (2.33)$$

and γ is Euler's constant. In a similar manner one finds, using Eq. (2.10), that

$$\left.\begin{matrix} B_n^{(0)} \\ B_n^{(1)} \end{matrix}\right\} \sim \frac{1}{2\pi^2 n}[g(n) \pm \pi] - \frac{1}{16\pi^2 n^2}[g(n) \pm \pi] - \frac{1}{1536\pi^2 n^3}[15g(n) \pm 15\pi - 59] + \cdots. \quad (2.34)$$

Hence

$$B_n \sim \frac{g(n)}{\pi^2 n} - \frac{g(n)}{8\pi^2 n^2} - \frac{1}{768\pi^2 n^3}[15g(n) - 59] + \cdots. \quad (2.35)$$

From these results asymptotic expansions for the terminating hypergeometric series in Eqs. (2.16), (2.17), and (2.19) can be readily derived. In Table I the approximate values of $B_n^{(0)}$ and $B_n^{(1)}$ which were obtained using the asymptotic representation (2.34)

TABLE I. Comparison between the exact and asymptotic values of the coefficients $B_n^{(0)}$ and $B_n^{(1)}$.

n	Exact $B_n^{(0)}$	Asymptotic $B_n^{(0)}$	Exact $B_n^{(1)}$	Asymptotic $B_n^{(1)}$
0	1.393 203 929 685 676 9			
1	0.348 300 982 421 419 2	0.345 299 6	0.072 725 307 102 167 7	0.072 995 5
2	0.203 175 573 079 161 2	0.202 959 4	0.054 543 980 326 625 8	0.054 528 8
3	0.145 125 409 342 258 0	0.145 080 9	0.043 635 184 261 300 6	0.043 628 8
4	0.113 595 186 479 207 9	0.113 580 8	0.036 589 920 135 778 1	0.036 587 2
5	0.093 683 634 780 761 2	0.093 677 6	0.031 658 235 247 912 4	0.031 656 9
6	0.079 919 102 246 960 2	0.079 916 2	0.027 999 243 234 334 6	0.027 998 5
7	0.069 810 681 638 857 5	0.069 809 1	0.025 166 787 738 874 1	0.025 166 4
8	0.062 058 363 910 840 0	0.062 057 4	0.022 902 776 414 717 8	0.022 902 5
9	0.055 915 849 764 916 4	0.055 915 3	0.021 047 402 000 266 4	0.021 047 2
10	0.050 923 423 254 356 2	0.050 923 0	0.019 496 258 719 532 6	0.019 496 1

are compared with the exact values. Similar results for the coefficients C_n are given in Table II.

We now attempt to obtain recurrence relations for the coefficients $B_n^{(0)}$, $B_n^{(1)}$, and C_n *directly* from the explicit formulas (2.16) and (2.19). For the coefficients C_n we apply Sister Celine's technique[35] to the polynomials

$$\gamma_n(x) = \frac{1}{n!}\,{}_3F_2\left[\begin{matrix}-n, \frac{1}{2}, \frac{1}{2}; \\ 1, 1;\end{matrix}\; x\right]. \qquad (2.36)$$

This procedure leads to the relation

$$4n^3\gamma_n(x) + [4n(n-1)(x-3) + (x-4)]\gamma_{n-1}(x) + 4(n-1)(3-2x)\gamma_{n-2}(x) + 4(x-1)\gamma_{n-3}(x) = 0. \qquad (2.37)$$

From this result and Eq. (2.19) we see that C_n satisfies the recurrence relation

$$2n(4n^2-1)C_n - (2n-1)(8n^2-8n+3)C_{n-1} + 8(n-1)^3C_{n-2} = 0. \qquad (2.38)$$

In order to investigate the existence of recurrence relations for the coefficients $B_n^{(0)}$ and $B_n^{(1)}$, we first apply the transformation[36]

$$ {}_4F_3\left[\begin{matrix}-n, u-x, u-y, z; \\ \omega, 1-v+z-n, 1-\omega+z-n;\end{matrix}\; 1\right] = \frac{(v)_n(\omega)_n}{(v-z)_n(\omega-z)_n}\,{}_4F_3\left[\begin{matrix}-n, x, y, z; \\ u, v, \omega;\end{matrix}\; 1\right], \qquad (2.39)$$

where

$$u+v+\omega = 1+x+y+z-n, \qquad (2.40)$$

to the Saalschützian ${}_4F_3(1)$ hypergeometric series in Eq. (2.16). The resulting simplified expressions for $B_n^{(0)}$ and $B_{n+1}^{(1)}$ are given below

$$B_n^{(0)} = \left(\frac{4K_0^2}{\pi^2}\right)\frac{(\frac{1}{2})_n}{n!}\,{}_4F_3\left[\begin{matrix}-n, n, \frac{1}{4}, \frac{1}{4}; \\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2};\end{matrix}\; 1\right], \quad n \geq 0, \qquad (2.41)$$

$$B_{n+1}^{(1)} = \left(\frac{1}{K_0^2}\right)\frac{(\frac{3}{2})_n}{n!}\,{}_4F_3\left[\begin{matrix}-n, n+2, \frac{3}{4}, \frac{3}{4}; \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2};\end{matrix}\; 1\right]. \qquad (2.42)$$

We see that $B_n^{(0)}$ and $B_{n+1}^{(1)}$ are basically just generalized Jacobi polynomials

$$f_n(x) \equiv {}_4F_3\left[\begin{matrix}-n, n+\lambda, \sigma, \sigma; \\ 2\sigma, 2\sigma, 2\sigma;\end{matrix}\; x\right] \qquad (2.43)$$

with unit argument.

By applying Sister Celine's technique to the polynomial $f_n(x)$, it is found that there exists a recurrence relation of the form

$$f_n(x) + \sum_{r=0}^{2}(A_{2r+1} + A_{2r+2}x)f_{n-r-1}(x) + A_7 f_{n-4}(x) = 0, \qquad (2.44)$$

where $A_1 \cdots A_7$ depend on n, λ, σ, but not on x. Unfortunately, because of the large amount of algebraic manipulation that is involved, it has not been possible to derive explicit formulas for $A_1 \cdots A_7$.

TABLE II. Comparison between the exact and asymptotic values of the coefficients C_n.

n	Exact C_n	Asymptotic C_n
0	0.636 619 772 367 581 3	
1	0.318 309 886 183 790 7	0.364 644
2	0.217 511 755 558 923 6	0.221 636
3	0.167 112 690 246 490 1	0.168 064
4	0.136 560 625 277 956 6	0.136 891
5	0.115 932 060 481 373 2	0.116 076
6	0.101 005 694 865 241 2	0.101 079
7	0.089 670 877 933 811 4	0.089 712
8	0.080 750 946 694 120 6	0.080 776
9	0.073 536 231 904 598 9	0.073 552
10	0.067 572 393 051 799 9	0.067 583

However, the following *indirect* procedure may be used to establish the required recurrence relations. We first note that the series ${}_3F_2(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1; x)$ is a solution (about $x = 0$) of the differential equation

$$8x^2(1-x)y''' + 12x(2-3x)y'' + 2(4-13x)y' - y = 0. \quad (2.45)$$

Next we apply the method of Frobenius to this equation about the regular singular point $x = 1$, and hence obtain a *general* series solution in powers of $1 - x$. The comparison of this general series solution (for $x = z^2$) with the analytic continuation (2.9) yields the recurrence relation

$$4n(n-1)(2n-1)B_n^{(i)} - 2(n-1)(8n^2-16n+9)B_{n-1}^{(i)} + (2n-3)^3 B_{n-2}^{(i)} = 0, \quad (2.46)$$

where $i = 0, 1$. The initial conditions are

$$\begin{aligned} B_0^{(0)} &= (4K_0^2/\pi^2), & B_1^{(0)} &= (K_0^2/\pi^2), & i &= 0, \\ B_0^{(1)} &= 0, & B_1^{(1)} &= (1/4K_0^2), & i &= 1. \end{aligned} \quad (2.47)$$

For the coefficients C_n one obtains the relation (2.38). We see from Eq. (2.46) that the five-term recurrence relation (2.44) must be an iteration of a three-term relation when $x = 1$.

The basic results given above, which establish the behavior of $P(z)$ in the neighborhood of $z^2 = 1$, will be frequently used in the following sections. We finally note the summation formula

$$P(\pm i) = \sum_{n=0}^{\infty} (-1)^n a_n^3 = \left[\frac{\Gamma(\frac{9}{8})}{\Gamma(\frac{7}{8})\Gamma(\frac{5}{4})}\right]^2 \simeq 0.909\,172\,794\,546\,93, \quad (2.48)$$

which follows directly from Eq. (2.7) by applying Kummer's theorem.[37]

3. RELATED INTEGRALS

In this section we shall study the integrals

$$R(\xi) = \frac{1}{\pi^3} \iiint_0^{\pi} \frac{dx_1\, dx_2\, dx_3}{\xi - \cos x_1 \cos x_2 \cos x_3} \quad (3.1)$$

and

$$E(t) = \frac{1}{\pi^3} \iiint_0^{\pi} \exp(t \cos x_1 \cos x_2 \cos x_3)\, dx_1\, dx_2\, dx_3. \quad (3.2)$$

It is seen by inspection that the first integral defines an analytic function $R(\xi)$ throughout the ξ plane cut along the real axis from -1 to $+1$, while the second integral defines an entire function $E(t)$.

Although $R(\xi)$ is clearly related to $P(z)$ by the equation

$$\xi R(\xi) = P\left(\frac{1}{\xi}\right) = {}_2F_1\left(\tfrac{1}{4}, \tfrac{1}{4}; 1; \frac{1}{\xi^2}\right)^2, \quad (3.3)$$

it is worthwhile considering the analytic continuation of $R(\xi)$ separately since $R(\xi)$ occurs naturally in the theory of the spherical model with ξ as the saddle-point parameter.[8,9] The analytic continuation formula

$$\xi R(\xi) = \sum_{n=0}^{\infty} B_n \left(\frac{\xi^2-1}{\xi^2}\right)^n - \left(\frac{\xi^2-1}{\xi^2}\right)^{\frac{1}{2}} \sum_{n=0}^{\infty} C_n \left(\frac{\xi^2-1}{\xi^2}\right)^n, \quad (3.4)$$

which is valid for $|(\xi^2-1)/\xi^2| < 1$, $\operatorname{Re} \xi^2 > \frac{1}{2}$, follows directly from Eqs. (2.9) and (3.3). An alternative procedure is to substitute the standard result[27]

$$\begin{aligned} {}_2F_1\left(\tfrac{1}{4}, \tfrac{1}{4}; 1; \frac{1}{\xi^2}\right) &= (\xi^2)^{\frac{1}{4}} \left(\frac{\Gamma(\frac{1}{4})^2}{2\pi^{\frac{3}{2}}}\, {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{1}{2}; 1-\xi^2) \right. \\ &\quad \left. - \frac{2\pi^{\frac{1}{2}}}{\Gamma(\frac{1}{4})^2} (\xi^2-1)^{\frac{1}{2}}\, {}_2F_1(\tfrac{3}{4}, \tfrac{3}{4}; \tfrac{3}{2}; 1-\xi^2) \right), \\ &\quad |\arg \xi^2| < \pi, \end{aligned} \quad (3.5)$$

in Eq. (3.3). [The condition $|\arg \xi^2| < \pi$ is not unduly restrictive since $R(-\xi) = -R(\xi)$.] This yields the analytic continuation

$$R(\xi) = \sum_{n=0}^{\infty} (-1)^n [B_n^{(0)} - B_n^{(1)}](\xi^2-1)^n - (\xi^2-1)^{\frac{1}{2}} \times \sum_{n=0}^{\infty} (-1)^n C_n (\xi^2-1)^n, \quad B_0^{(1)} \equiv 0, \quad (3.6)$$

which is valid in the ξ^2 plane cut along the real axis from 0 to $+1$, providing $|\arg \xi^2| < \pi$ and $|\xi^2 - 1| < 1$. General expressions and numerical values for the coefficients in (3.6) have already been given in Sec. 2.

It is now shown that the analytic continuation (3.6) can also be constructed from the integral transform[38]

$$\begin{aligned} R(\xi) &= \frac{1}{\xi}\, {}_3F_2\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; \frac{1}{\xi^2}\right) \\ &= \frac{1}{\pi^{\frac{1}{2}}} \int_0^{\infty} e^{-\xi^2 t} t^{-\frac{1}{2}}\, {}_2F_2\left[\begin{matrix} \frac{1}{2}, \frac{1}{2}; \\ 1, 1; \end{matrix}\ t\right] dt, \end{aligned} \quad (3.7)$$

where $|\arg \xi^2| < \frac{1}{2}\pi$, and $\operatorname{Re} \xi^2 \geq 1$. We first note that the hypergeometric function ${}_2F_2(t)$ in the integrand of (3.7) is an entire function which has a *dominant* asymptotic representation

$${}_2F_2\left[\begin{matrix} \frac{1}{2}, \frac{1}{2}; \\ 1, 1; \end{matrix}\ t\right] \sim \frac{e^t}{\pi t} \sum_{k=0}^{M} \frac{k!}{t^k} d_k, \quad \text{as } |t| \to \infty, \quad (3.8)$$

where $M \geq 0$, $|\arg t| < \frac{1}{2}\pi$, and the coefficients d_k satisfy the recurrence relation

$$4k^2 d_k - (8k^2 - 8k + 3)d_{k-1} + 4(k-1)^2 d_{k-2} = 0, \quad (3.9)$$

with $d_0 = 1$. This asymptotic representation was established using the powerful general theorems derived by Hughes[39] and Riney.[40]

We next follow a method developed by Maradudin *et al.* for the simple cubic lattice Green's function[41] and divide the range of integration in (3.7) into two parts $(0, T)$ and (T, ∞). In the range (T, ∞) the ${}_2F_2(t)$ hypergeometric function may be replaced, to a good approximation, by its asymptotic representation (3.8), provided that T is sufficiently large. Hence, we obtain

$$R(\xi) = I_1 + I_2, \quad (3.10)$$

where

$$I_1 = \frac{1}{\pi^{\frac{1}{2}}} \int_0^T e^{-\xi^2 t} t^{-\frac{1}{2}}\, {}_2F_2\left[\begin{matrix}\frac{1}{2}, \frac{1}{2}; \\ 1, 1;\end{matrix}\; t\right] dt \quad (3.11)$$

and

$$I_2 \simeq \frac{1}{\pi^{\frac{3}{2}} T^{\frac{1}{2}}} \sum_{k=0}^{M} \frac{k!\, d_k}{T^k} \Phi_{-k-\frac{3}{2}}[(\xi^2 - 1)T], \quad (3.12)$$

with

$$\Phi_m(x) = \int_1^\infty t^m e^{-xt}\, dt, \quad \operatorname{Re} x \geq 0, \quad m < -1. \quad (3.13)$$

To derive an analytic continuation formula for $R(\xi)$, which is valid in the neighborhood of $\xi^2 = 1$, we develop the expressions (3.11) and (3.12) as a power series in $\xi^2 - 1$, using the expansion

$$\Phi_m(x) = x^{-m-1}\Gamma(m+1) - \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!\,(n+m+1)}, \quad (3.14)$$

(m not equal to a negative integer). We finally find that

$$R(\xi) = \sum_{n=0}^{\infty} (-1)^n \Theta_n (\xi^2 - 1)^n - (\xi^2 - 1)^{\frac{1}{2}} \times \sum_{n=0}^{\infty} (-1)^n \Omega_n (\xi^2 - 1)^n, \quad (3.15)$$

where

$$\Theta_n \simeq \frac{1}{\pi^{\frac{1}{2}} n!} \left(V_n(T) - \frac{1}{\pi T^{\frac{1}{2}}} \sum_{k=0}^{M} \frac{k!\, d_k T^{n-k}}{(n - k - \frac{1}{2})} \right), \quad M \geq n, \quad (3.16)$$

with

$$V_n(T) = \int_0^T e^{-t} \cdot t^{n-\frac{1}{2}}\, {}_2F_2\left[\begin{matrix}\frac{1}{2}, \frac{1}{2}; \\ 1, 1;\end{matrix}\; t\right] dt \quad (3.17)$$

and

$$\Omega_n = (2/\pi)[n!\, d_n / (\tfrac{3}{2})_n]. \quad (3.18)$$

It follows from Eqs. (3.9) and (3.18) that the coefficients Ω_n satisfy the recurrence relation

$$2n(4n^2 - 1)\Omega_n - (2n - 1)(8n^2 - 8n + 3)\Omega_{n-1} + 8(n-1)^3 \Omega_{n-2} = 0, \quad (3.19)$$

with $\Omega_0 = (2/\pi)$. Hence, we see that the integral transform method enables one to analyze the *singular* part of the analytic continuation (3.15) exactly. However, the coefficients Θ_n have to be calculated numerically by evaluating the expression (3.16) for increasing values of T, with a fixed value of $M \geq n$.[42]

By comparing the two equivalent analytic continuations (3.6) and (3.15) it is clear that we must have

$$\Omega_n \equiv C_n. \quad (3.20)$$

[This result may be proved directly since the recurrence relations (3.19) and (2.38) are identical with the same initial conditions.] It is interesting to note that the relation (3.20), when combined with Eqs. (2.19) and (3.18), gives the solution of the three-term recurrence relation (3.9) as

$$d_n = {}_3F_2\left[\begin{matrix}-n, \frac{1}{2}, \frac{1}{2}; \\ 1, 1;\end{matrix}\; 1\right]. \quad (3.21)$$

Thus we have the *explicit* asymptotic expansion

$${}_2F_2\left[\begin{matrix}\frac{1}{2}, \frac{1}{2}; \\ 1, 1;\end{matrix}\; t\right] \sim \frac{e^t}{\pi t} \sum_{n=0}^{\infty} \frac{n!}{t^n}\, {}_3F_2\left[\begin{matrix}-n, \frac{1}{2}, \frac{1}{2}; \\ 1, 1;\end{matrix}\; 1\right], \quad (3.22)$$

(provided that $|\arg t| < \frac{1}{2}\pi$) which may be a new result.

The integral transform technique (which is closely related to Borel's method of analytic continuation) provides an alternative procedure to that developed by Olsson[30] for deriving the analytic continuation of a ${}_{q+1}F_q$ generalized hypergeometric function. From the particular example given above we see that, although the integral transform method makes use of divergent asymptotic series, the final continuation formula involves Taylor series with a finite radius of convergence.

We now investigate the second integral (3.2) which is related to $R(\xi)$ by the Laplace transform

$$R(\xi) = \int_0^\infty e^{-\xi t} E(t)\, dt, \quad (3.23)$$

provided that $\operatorname{Re} \xi \geq 1$. If the integrand of (3.2) is expanded in powers of t, we find

$$E(t) = \sum_{n=0}^{\infty} \frac{a_n^3}{(2n)!} t^{2n}, \quad |t^2| < \infty, \quad (3.24)$$

where a_n is defined in Eq. (1.4). Thus, $E(t)$ is just the exponential probability generating function for all random walks on a body-centered cubic lattice which start and finish at the same lattice point. From Eq. (3.24) and the duplication formula

$$(2n)! = 2^{2n}(\tfrac{1}{2})_n(1)_n, \tag{3.25}$$

it follows that

$$E(t) = {}_2F_3\left[\begin{matrix}\tfrac{1}{2}, \tfrac{1}{2}; \\ 1, 1, 1;\end{matrix}\ \tfrac{1}{4}t^2\right]. \tag{3.26}$$

It may be shown by applying the general results of Hughes[39] and Riney[40] to the ${}_2F_3$ function in Eq. (3.26) that $E(t)$ has a *dominant* asymptotic representation

$$E(t) \sim \frac{2^{\frac{1}{2}}e^t}{(\pi t)^{\frac{3}{2}}} \sum_{k=0}^{M} \frac{\theta_k}{t^k}, \quad \text{as} \quad |t| \to \infty, \tag{3.27}$$

where $M \geq 0$, $|\arg t| < \frac{1}{2}\pi$, and the coefficients θ_k satisfy the recurrence relation

$$32(k+1)\theta_{k+1} - 4(20k^2 + 20k + 9)\theta_k + 16k(4k^2+1)\theta_{k-1} - (2k-1)^4\theta_{k-2} = 0, \tag{3.28}$$

with $\theta_0 = 1$. The values of the first few coefficients θ_k which were obtained from (3.28) are listed below:

$$\theta_1 = \frac{9}{8}, \quad \theta_2 = \frac{281}{128}, \quad \theta_3 = \frac{6419}{1024}, \quad \theta_4 = \frac{780\,219}{32\,768},$$
$$\theta_5 = \frac{29\,732\,967}{262\,144}, \qquad \theta_6 = \frac{2\,731\,467\,213}{4\,194\,304}. \tag{3.29}$$

The asymptotic expansion (3.27) is of considerable importance and will be used in Sec. 7 to derive an analytic continuation formula for $R(\xi)$ in powers of $\xi - 1$.

We conclude this section by demonstrating that the function $E(t)$ can be evaluated in terms of Mathieu functions. We shall assume that t is real and positive. The integral (3.2) is written in the alternative iterated form

$$E(t) = \frac{1}{\pi^3} \iiint_0^\pi K(x_1, x_2)K(x_2, x_3)\, dx_1\, dx_2\, dx_3, \tag{3.30}$$

where

$$K(x_i, x_j) = \exp(\tfrac{1}{2}t \cos x_i \cos x_j), \tag{3.31}$$

and the homogeneous integral equation

$$\frac{1}{\pi}\int_0^\pi K(x_i, x_j)\psi(x_j)\, dx_j = \lambda\psi(x_i) \tag{3.32}$$

is introduced.

This integral equation possesses a complete set of nontrivial solutions[43,44]

$$\psi_{2n}(x) = ce_{2n}(x, -h^2), \quad n = 0, 1, 2, \cdots,$$
$$\psi_{2n+1}(x) = ce_{2n+1}(x, -h^2), \tag{3.33}$$

where $h = \frac{1}{4}t$, and $ce_n(x, -h^2)$ are periodic even Mathieu functions defined by the Fourier series

$$ce_{2n}(x, q) = \sum_{r=0}^{\infty} A_{2r}^{(2n)}(q) \cos 2rx,$$
$$ce_{2n+1}(x, q) = \sum_{r=0}^{\infty} A_{2r+1}^{(2n+1)}(q) \cos(2r+1)x. \tag{3.34}$$

It is also known that the eigenfunctions (3.33) satisfy the orthogonality relation

$$\frac{2}{\pi}\int_0^\pi \psi_n(x)\psi_m(x)\, dx = \delta_{m,n}. \tag{3.35}$$

The eigenvalues corresponding to the eigenfunctions (3.33) are[43]

$$\lambda_{2n} = A_0^{(2n)}(h^2)/ce_{2n}(0, h^2),$$
$$\lambda_{2n+1} = hB_1^{(2n+1)}(h^2)/se'_{2n+1}(0, h^2), \tag{3.36}$$

where the periodic Mathieu function $se_{2n+1}(x, h^2)$ is given by the Fourier series

$$se_{2n+1}(x, q) = \sum_{r=0}^{\infty} B_{2r+1}^{(2n+1)}(q) \sin(2r+1)x. \tag{3.37}$$

For finite values of $h > 0$ the eigenvalues are positive and nondegenerate with

$$\lambda_0 > \lambda_1 > \lambda_2 > \cdots. \tag{3.38}$$

However, for large h Sips[45] has shown that the eigenvalues become asymptotically degenerate in pairs as follows:

$$\lambda_{2n} \sim \lambda_{2n+1}, \quad \text{as} \quad h \to \infty. \tag{3.39}$$

Since $K(x_i, x_j)$ is a continuous, symmetric, and positive-definite kernel, we can use Mercer's expansion theorem to write

$$K(x_i, x_j) = 2\sum_{n=0}^{\infty} \lambda_n \psi(x_i)\psi(x_j). \tag{3.40}$$

This expansion is absolutely and uniformly convergent with respect to the variables x_i and x_j. If Eq. (3.40) is substituted in Eq. (3.30), the integrations may be readily performed using the orthogonality relation (3.35) and Eq. (3.34). The final result is

$$E(t) = 2\sum_{n=0}^{\infty} [A_0^{(2n)}(h^2)/ce_{2n}(0, h^2)]^2 [A_0^{(2n)}(h^2)]^2, \tag{3.41}$$

with $h = \frac{1}{4}t$.

For small t the nth term in the series (3.41) is $O(t^{4n})$. Thus we should expect the Mathieu function expansion to converge more rapidly than the hypergeometric series (3.26) when t is small. In order to investigate the behavior of the Mathieu function expansion for large t, we now obtain an asymptotic representation for the first term in (3.41). From the work of Sips[45] we find

$$\lambda_0 = \frac{A_0^{(0)}(h^2)}{ce_0(0, h^2)} \sim \frac{e^{\frac{1}{2}t}}{(2\pi t)^{\frac{1}{2}}}\left(1 + \frac{1}{4t} + \frac{1}{4t^2} + \cdots\right). \quad (3.42)$$

It may also be shown[46] that

$$\frac{ce_0(0, h^2)}{ce_0\left(\frac{\pi}{2}, h^2\right)} \sim 2^{\frac{3}{2}} e^{-\frac{1}{2}t}\left(1 + \frac{1}{4t} + \frac{9}{16t^2} + \cdots\right) \quad (3.43)$$

and

$$ce_0\left(\frac{\pi}{2}, h^2\right) \sim (\tfrac{1}{8}\pi t)^{\frac{1}{4}}\left(1 - \frac{3}{16t} - \frac{95}{512t^2} + \cdots\right). \quad (3.44)$$

From these results the asymptotic formula

$$A_0^{(0)}(h^2) \sim \left(\frac{2}{\pi t}\right)^{\frac{1}{4}}\left(1 + \frac{5}{16t} + \frac{305}{512t^2} + \cdots\right) \quad (3.45)$$

is readily derived by multiplying (3.42)–(3.44) together. The combination of Eqs. (3.42) and (3.45) gives the required asymptotic representation

$$2\left(\frac{A_0^{(0)}(h^2)}{ce_0(0, h^2)}\right)^2 [A_0^{(0)}(h^2)]^2 \sim \frac{\sqrt{2}\, e^t}{(\pi t)^{\frac{3}{2}}}\left(1 + \frac{9}{8t} + \frac{277}{128t^2} + \cdots\right). \quad (3.46)$$

By comparing this expression with Eq. (3.27) we see that the behavior of $E(t)$ for large t is described, to a good approximation, by the first term in the Mathieu function expansion (3.41). [For large t, the nth term in (3.41) behaves asymptotically as $e^t/t^{\frac{3}{2}+2n}$.] We conclude from the above arguments that the expansion (3.41) should converge fairly rapidly for *all* $t > 0$. Thus Eq. (3.41) provides us (at least in principle) with a powerful method for the numerical evaluation of $E(t)$.

For numerical purposes it is particularly convenient to convert Eq. (3.41) to the Mathieu function notation adopted by the National Bureau of Standards.[47] In this notation we find

$$E(t) = 2\sum_{n=0}^{\infty} [De_0^{(2n)}(s)]^4 [A_{2n}(s)]^2, \quad (3.47)$$

where $s = \frac{1}{4}t^2$, and $A_{2n}(s)$ is a conversion factor defined by the relation[48]

$$ce_{2n}(x, q) = A_{2n}(s) Se_{2n}(s, x). \quad (3.48)$$

TABLE III. Terms in the Mathieu function expansion (3.47) for $s = 100$.

n	$[De_0^{(2n)}(100)]^4[A_{2n}(100)]^2$
0	7.319 321 55 (+05)
1	9.041 499 72 (+01)
2	2.846 392 94 (−01)
3	6.574 466 78 (−03)
4	1.376 540 08 (−05)
5	4.774 399 83 (−10)
6	2.818 293 93 (−15)
7	4.298 501 79 (−21)

[The conversion factor should not be confused with the Fourier coefficient $A_0^{(2n)}(h^2)$.] Since the Fourier coefficients $De_0^{(2n)}(s)$ *and* $A_{2n}(s)$ have been tabulated[47] for $0 \le s \le 100$, the converted expansion (3.47) can be used to calculate $E(t)$ in the range $0 \le t \le 20$.

As an illustration we evaluate $E(t)$ when $t = 20$. The numerical values of the terms in the expansion (3.47) are listed, for $s = 100$, in Table III. Hence we obtain

$$E(20) \simeq 1\,464\,045.72. \quad (3.49)$$

The expected rapid convergence of the Mathieu function expansion is clearly shown by the results in Table III. The most accurate estimate for $E(20)$ that can be obtained, *in principle*, from the asymptotic expansion (3.27) is

$$E(20) \simeq 1\,464\,045.717. \quad (3.50)$$

This value is achieved by taking the asymptotic representation $M = 20$.

4. ${}_3F_2(1)$ SUMMATION FORMULAS

It has been shown in Sec. 2 that the comparison of the analytic continuation (2.9) with Olsson's general results[30] yields the exact summation formula

$$B_n^{(0)} + B_n^{(1)} = \frac{(\frac{1}{2})_n^2}{n!} \sum_{m=0}^{\infty} \frac{a_m^3}{(\frac{1}{2} - m)_n}. \quad (4.1)$$

In the present section this comparison procedure is developed in a more systematic manner. Further summation formulas, similar to (4.1), are derived and some applications of the results are discussed.

We first rewrite Eq. (4.1) in the standard hypergeometric form

$$B_n^{(0)} + B_n^{(1)} = \frac{(\frac{1}{2})_n}{n!} {}_3F_2\left[\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - n; \\ 1, 1; \end{matrix} \; 1\right], \quad (4.2)$$

using the relation

$$(\tfrac{1}{2} - m)_n = (\tfrac{1}{2})_m (\tfrac{1}{2})_n / (\tfrac{1}{2} - n)_m. \quad (4.3)$$

For $n > 0$, Eq. (4.2) gives a summation formula for a nearly poised ${}_3F_2(1)$ series, which appears to be new. [If $n = 0$, Eq. (4.2) reduces to a special case of Dixon's theorem for a well-poised ${}_3F_2(1)$ series.] The application of the basic transformation[49]

$$ {}_3F_2\left[\begin{matrix} a, b, c; \\ d, e; \end{matrix} \; 1\right] = \frac{\Gamma(d)\Gamma(e)\Gamma(s)}{\Gamma(a)\Gamma(s+b)\Gamma(s+c)} \times {}_3F_2\left[\begin{matrix} d-a, e-a, s; \\ s+b, s+c; \end{matrix} \; 1\right], \tag{4.4} $$

where $s \equiv d + e - a - b - c$, $\mathrm{Re}\,(s) > 0$, and $\mathrm{Re}\,(a) > 0$, to the ${}_3F_2(1)$ series in Eq. (4.2) leads to another nearly poised summation formula

$$ B_n^{(0)} + B_n^{(1)} = \frac{(\frac{1}{2})_n^2}{(n!)^2}\, {}_3F_2\left[\begin{matrix} \frac{1}{2}, \frac{1}{2}, n+\frac{1}{2}; \\ 1, n+1; \end{matrix} \; 1\right]. \tag{4.5} $$

If a direct comparison is made between the analytic continuation formula (3.6) and Olsson's equation (8),[30] it is found that

$$ B_n^{(0)} - B_n^{(1)} = \frac{(\frac{1}{2})_n}{n!}\, {}_3F_2\left[\begin{matrix} \frac{1}{2}, \frac{1}{2}, n+\frac{1}{2}; \\ 1, 1; \end{matrix} \; 1\right]. \tag{4.6} $$

This relation does *not* give a summation formula since the hypergeometric series for the ${}_3F_2(1)$ function is divergent for $n > 0$. However, it does provide the analytic continuation (with respect to a parameter) of the ${}_3F_2(1)$ function in Eq. (4.2) when $n < 0$.

A direct transformation of Eq. (4.6) using the relation (4.4) is not possible because of the occurrence of an indeterminate expression. However, we can avoid this difficulty by applying the transformation to the function[50]

$$ {}_3F_2\left[\begin{matrix} \frac{1}{2}+\epsilon, \frac{1}{2}, n+\frac{1}{2}; \\ 1, 1; \end{matrix} \; 1\right]. \tag{4.7} $$

After some simplification the limit $\epsilon \to 0$ may be taken, and we find

$$ B_n^{(0)} - B_n^{(1)} = \frac{1}{n!} \sum_{m=n}^{\infty} \frac{(\frac{1}{2})_m^2 (\frac{1}{2}-n)_m (-m)_n}{(1)_m^3}. \tag{4.8} $$

The conversion of this equation to hypergeometric form yields the nearly poised summation formula

$$ B_n^{(0)} - B_n^{(1)} = \frac{(\frac{1}{2})_n^3}{(n!)^3}\, {}_3F_2\left[\begin{matrix} \frac{1}{2}, n+\frac{1}{2}, n+\frac{1}{2}; \\ n+1, n+1; \end{matrix} \; 1\right]. \tag{4.9} $$

A second application of the relation (4.4) to the ${}_3F_2(1)$ series in Eq. (4.9), (with $a = n + \frac{1}{2}$) leads to a further nearly poised summation formula:

$$ B_n^{(0)} - B_n^{(1)} = \frac{(\frac{1}{2})_n^2}{(n!)^2}\, {}_3F_2\left[\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \\ 1, n+1; \end{matrix} \; 1\right]. \tag{4.10} $$

The numerical values and asymptotic behavior (for large n) of the nearly poised ${}_3F_1(1)$ series given above are readily obtained from Table I and Eq. (2.34), respectively. It is interesting to note that Eq. (4.10) provides *directly* the asymptotic expansion

$$ B_n^{(0)} - B_n^{(1)} \sim \frac{1}{\pi n}\left(1 - \frac{1}{8n} - \frac{5}{256n^2} - \cdots\right), \tag{4.11} $$

as $n \to \infty$. Since this result agrees with the Darboux analysis given in Sec. 2, we have an excellent check on Eqs. (4.10) and (4.9).

We now show that the ${}_3F_2(1)$ summation formulas can be used to evaluate the generalized Watson integral

$$ I(m, n) = \frac{1}{\pi^3} \iiint_0^{\pi} \frac{\cos^{2m} x_1 \cos^{2n} x_2}{1 - \cos x_1 \cos x_2 \cos x_3}\, dx_1\, dx_2\, dx_3, \tag{4.12} $$

where $m \geq 0$ and $n \geq 0$. Since $I(m, n) = I(n, m)$, it is convenient to take $n \geq m$. If we expand the integrand of Eq. (4.12) as a geometric series and integrate term by term, we find

$$ I(m, n) = \sum_{l=0}^{\infty} a_l a_{l+m} a_{l+n}. \tag{4.13} $$

The conversion of this series to hypergeometric form yields

$$ I(m, n) = \frac{(\frac{1}{2})_m (\frac{1}{2})_n}{(1)_m (1)_n}\, {}_3F_2\left[\begin{matrix} \frac{1}{2}, m+\frac{1}{2}, n+\frac{1}{2}; \\ m+1, n+1; \end{matrix} \; 1\right]. \tag{4.14} $$

The comparison of Eq. (4.14) with Eqs. (4.5) and (4.9) immediately gives

$$ \left.\begin{matrix} I(0, n) \\ I(n, n) \end{matrix}\right\} = \frac{n!}{(\frac{1}{2})_n} [B_n^{(0)} \pm B_n^{(1)}]. \tag{4.15} $$

Using this result and the expressions (2.13) the following list of integrals is readily derived:

$$ \left.\begin{matrix} I(0, 1) \\ I(1, 1) \end{matrix}\right\} = \frac{1}{2}\left(\frac{4K_0^2}{\pi^2} \pm \frac{1}{K_0^2}\right), \tag{4.16} $$

$$ \left.\begin{matrix} I(0, 2) \\ I(2, 2) \end{matrix}\right\} = \frac{1}{18}\left(\frac{28K_0^2}{\pi^2} \pm \frac{9}{K_0^2}\right), \tag{4.17} $$

$$ \left.\begin{matrix} I(0, 3) \\ I(3, 3) \end{matrix}\right\} = \frac{4}{75}\left(\frac{25K_0^2}{\pi^2} \pm \frac{9}{K_0^2}\right), \tag{4.18} $$

$$ \left.\begin{matrix} I(0, 4) \\ I(4, 4) \end{matrix}\right\} = \frac{1}{22\,050}\left(\frac{26\,300K_0^2}{\pi^2} \pm \frac{10\,143}{K_0^2}\right). \tag{4.19} $$

The asymptotic formulas

$$I(0,n)\sim\frac{1}{(\pi^3 n)^{\frac{1}{2}}}\left[g(n)-\frac{1}{768n^2}\{21g(n)-59\}+\cdots\right],\tag{4.20}$$

$$I(n,n)\sim\frac{1}{(\pi n)^{\frac{1}{2}}}\left[1-\frac{7}{256n^2}+\cdots\right],\tag{4.21}$$

as $n\to\infty$, are obtained directly from Eqs. (4.15) and (2.34).

In order to investigate the case $n>m>0$, we first apply the transformation (4.4) to the ${}_3F_2(1)$ series in Eq. (4.14). This procedure leads to the simplified expression

$$I(m,n)=\frac{(\frac{1}{2})_n}{n!}\,{}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},n-m+\frac{1}{2};\\ 1,n+1;\end{matrix}\;1\right].\tag{4.22}$$

The alternative form

$$I(m,n)=\frac{(\frac{1}{2})_m}{m!}\,{}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},m-n+\frac{1}{2};\\ 1,m+1;\end{matrix}\;1\right]\tag{4.23}$$

is also of interest. Next we note the following contiguous function relation[51]:

$$\begin{aligned}(2l-1)\,{}_3F_2&\left[\begin{matrix}\frac{1}{2},\frac{1}{2},l+\frac{1}{2};\\ 1,m+l+1;\end{matrix}\;1\right]\\ &=2(m+l)\,{}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},l-\frac{1}{2};\\ 1,m+l;\end{matrix}\;1\right]\\ &\quad-(2m+1)\,{}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},l-\frac{1}{2};\\ 1,m+l+1;\end{matrix}\;1\right],\end{aligned}\tag{4.24}$$

where l is a positive integer. The substitution of Eq. (4.22) in Eq. (4.24) gives the recurrence relation

$$\begin{aligned}(2l-1)I(m,m+l)&\\ =(2m+2l-1)&I(m,m+l-1)\\ &-(2m+1)I(m+1,m+l).\end{aligned}\tag{4.25}$$

Finally we consider the set of equations formed from Eq. (4.25) by taking $l=1,2,3,\cdots$. If all the integrals $I(m,n)$ which have $m\neq n$ are eliminated successively from the right-hand side of these equations, we find

$$I(m,m+l)=\frac{(m+\frac{1}{2})_l}{(\frac{1}{2})_l}\sum_{r=0}^{l}\binom{l}{r}(-1)^r I(m+r,m+r).\tag{4.26}$$

The substitution of Eq. (4.15) in Eq. (4.26) leads to the general explicit formula

$$I(m,n)=\frac{(m+\frac{1}{2})_{n-m}}{(\frac{1}{2})_{n-m}}\sum_{r=0}^{n-m}\binom{n-m}{r}(-1)^r\times\frac{(m+r)!}{(\frac{1}{2})_{m+r}}[B^{(0)}_{m+r}-B^{(1)}_{m+r}],\tag{4.27}$$

which is valid for $n\geq m\geq 0$. General expressions for the coefficients $B^{(0)}_n$ and $B^{(1)}_n$ are given in Eq. (2.16).

Using Eq. (4.27), we may now readily establish the following list of integrals for the case $n>m>0$:

$$I(1,2)=(4K_0^2/3\pi^2),\tag{4.28}$$

$$\left.\begin{matrix}I(1,3)\\ I(2,3)\end{matrix}\right\}=\frac{1}{90}\left(\frac{100K_0^2}{\pi^2}\pm\frac{9}{K_0^2}\right),\tag{4.29}$$

$$I(2,4)=(20K_0^2/21\pi^2),\tag{4.30}$$

$$\left.\begin{matrix}I(1,4)\\ I(3,4)\end{matrix}\right\}=\frac{1}{3150}\left(\frac{3100K_0^2}{\pi^2}\pm\frac{441}{K_0^2}\right).\tag{4.31}$$

TABLE IV. Numerical values of $I(m,n)$ for $4\geq n\geq m\geq 0$.

m, n	$I(m, n)$
0, 0	1.393 203 929 685 676 9
0, 1	0.842 052 579 047 173 9
1, 1	0.551 151 350 638 502 9
0, 2	0.687 252 142 415 432 1
1, 2	0.464 401 309 895 225 6
2, 2	0.396 350 914 006 761 1
0, 3	0.604 033 899 531 387 7
1, 3	0.416 091 214 420 221 8
2, 3	0.357 910 968 738 487 6
3, 3	0.324 768 720 259 063 5
0, 4	0.549 248 389 906 234 7
1, 4	0.383 498 567 376 070 9
2, 4	0.331 715 221 353 732 6
3, 4	0.302 046 223 421 643 1
4, 4	0.281 619 259 770 257 4

The numerical values of the integrals $I(m,n)$ for $4\geq n\geq m\geq 0$ are given in Table IV.

In the remainder of this section we shall derive more recurrence relations for $I(m,n)$, and give an alternative proof of the recurrence relation (2.46). We begin by substituting Eq. (4.23) in the contiguous relation[51]

$$\begin{aligned}(2l-1)\,{}_3F_2&\left[\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{3}{2}-l;\\ 1,m+1;\end{matrix}\;1\right]\\ &=(2l+2m-1)\,{}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}-l;\\ 1,m+1;\end{matrix}\;1\right]\\ &\quad-2m\,{}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}-l;\\ 1,m;\end{matrix}\;1\right].\end{aligned}\tag{4.32}$$

This procedure leads to the relation

$$\begin{aligned}(2l-1)I(m,m+l-1)&\\ =(2m+2l-1)&I(m,m+l)\\ &-(2m-1)I(m-1,m+l-1).\end{aligned}\tag{4.33}$$

For the special case $m = 1$, Eq. (4.33) becomes

$$I(0, l) = (2l + 1)I(1, l + 1) - (2l - 1)I(1, l). \quad (4.34)$$

The elimination of the integrals $I(m, m + l)$ and $I(m - 1, m + l - 1)$ from Eq. (4.33) via Eq. (4.25) gives a further relation

$$(2m + 1)(2m + 2l - 1)I(m + 1, m + l) - [8m^2 + 8m(l - 1) + 1]I(m, m + l - 1) + (2m - 1)(2m + 2l - 3)I(m - 1, m + l - 2) = 0. \quad (4.35)$$

If $l = 1$, this equation reduces to

$$(2m + 1)^2 I(m + 1, m + 1) - (8m^2 + 1)I(m, m) + (2m - 1)^2 I(m - 1, m - 1) = 0, \quad (4.36)$$

which is a recurrence relation for the "diagonal" integrals $I(m, m)$.

We proceed by noting the recurrence relation for $I(0, l)$:

$$(2l + 1)^2 I(0, l + 1) - (8l^2 + 1)I(0, l) + (2l - 1)^2 I(0, l - 1) = 0, \quad (4.37)$$

which is readily obtained from Eq. (4.34), and Eq. (4.25) with $m = 0$. Finally, we substitute Eq. (4.15) in the recurrence relations (4.36) and (4.37). This procedure yields

$$4n(n - 1)(2n - 1)B_n^{(i)} - 2(n - 1)(8n^2 - 16n + 9)B_{n-1}^{(i)} + (2n - 3)^3 B_{n-2}^{(i)} = 0, \quad (4.38)$$

where $i = 0, 1$. This recurrence relation for the coefficients $B_n^{(0)}$ and $B_n^{(1)}$ was derived in Sec. 2 using the method of Frobenius.

5. EVALUATION OF THE GREEN'S FUNCTION $P(l_1, l_2, l_3; 1)$

In this section the results of Sec. 4 will be used to evaluate the Green's function $P(l_1, l_2, l_3; z)$, for $z = 1$, where l_1, l_2, l_3 are all even, or all odd integers. [This Green's function is defined in Eq. (1.1).] Since $P(l_1, l_2, l_3; z)$ is a symmetric, even function with respect to l_1, l_2, l_3, it will be assumed for convenience that $l_3 \geq l_2 \geq l_1 \geq 0$.

We consider initially the particular Green's function

$$P(0, 2m_2, 2m_3; 1) = \frac{1}{\pi^3} \iiint_0^\pi \frac{\cos 2m_2x_2 \cos 2m_3x_3}{1 - \cos x_1 \cos x_2 \cos x_3}\, dx_1\, dx_2\, dx_3, \quad (5.1)$$

where m_2 and m_3 are positive integers, with $m_3 \geq m_2$. If the numerator of the integrand in Eq. (5.1) is expanded as a finite sum of terms of the type $\Delta_{rs} \cos^{2r} x_2 \cos^{2s} x_3$, it is seen that (5.1) can be written as a sum of integrals of the type $I(m, n)$. Thus it is possible, at least in principle, to evaluate $P(0, 2m_2, 2m_3; 1)$ exactly for arbitrary values of m_2 and m_3.

For example, it is readily found that

$$P(0, 0, 2; 1) = 2I(0, 1) - I(0, 0),$$
$$P(0, 2, 2; 1) = 4I(1, 1) - 4I(0, 1) + I(0, 0),$$
$$P(0, 2, 4; 1) = 16I(1, 2) - 16I(1, 1) - 8I(0, 2) + 10I(0, 1) - I(0, 0). \quad (5.2)$$

Using the results given in Eqs. (4.16), (4.17), and (4.28), we obtain

$$P(0, 0, 2; 1) = \frac{1}{K_0^2},$$
$$P(0, 2, 2; 1) = \left(\frac{4K_0^2}{\pi^2} - \frac{4}{K_0^2}\right), \quad (5.3)$$
$$P(0, 2, 4; 1) = \left(\frac{9}{K_0^2} - \frac{64K_0^2}{9\pi^2}\right).$$

In a similar manner the Green's function (5.1) has been evaluated for $4 \geq m_3 \geq m_2 \geq 0$. The final results are given in Appendix A. It is interesting to note that $P(0, 2m_2, 2m_3; 1)$ is expressible, for $m_2 \neq 0$, as a difference of two squares.[52]

Although the procedure described above for evaluating (5.1) is not particularly *elegant*, it has the *practical* advantage that it only involves elementary algebraic manipulations. In Paper II more general methods will be developed which enable one to express $P(0, 2m_2, 2m_3; z)$ in terms of ${}_2F_1$ hypergeometric functions (even when $z \neq 1$). By using these more powerful techniques, it is possible to evaluate $P(0, 0, 2m; 1)$ in terms of gamma functions. We quote the final result below:

$$P(0, 0, 2m; 1) = \frac{1}{2\pi}\left(\frac{\Gamma(\frac{1}{2}m + \frac{1}{4})}{\Gamma(\frac{1}{2}m + \frac{3}{4})}\right)^2, \quad (5.4)$$

where $m = 0, 1, 2, \cdots$. This expression may be simplified as follows:

$$P(0, 0, 4m; 1) = \left(\frac{1 \cdot 5 \cdot 9 \cdots (4m - 3)}{3 \cdot 7 \cdot 11 \cdots (4m - 1)}\right)^2 \left(\frac{4K_0^2}{\pi^2}\right),$$
$$P(0, 0, 4m + 2; 1) = \left(\frac{3 \cdot 7 \cdot 11 \cdots (4m - 1)}{1 \cdot 5 \cdot 9 \cdots (4m + 1)}\right)^2 \left(\frac{1}{K_0^2}\right). \quad (5.5)$$

[When $m = 0$, the products in (5.5) are replaced by 1.]

TABLE V. Numerical values of the Green's function $P(l_1, l_2, l_3; 1)$ for $8 \geq l_3 \geq l_2 \geq l_1 \geq 0$.

l_1, l_2, l_3	$P(\mathbf{l}, 1)$	l_1, l_2, l_3	$P(\mathbf{l}, 1)$
0, 0, 0	1.393 203 929 685 677	4, 6, 6	0.068 101 112 525 776
1, 1, 1	0.393 203 929 685 677	6, 6, 6	0.061 457 480 402 404
0, 0, 2	0.290 901 228 408 671	1, 1, 7	0.088 446 538 322 424
0, 2, 2	0.229 599 016 050 993	1, 3, 7	0.082 654 773 252 212
2, 2, 2	0.190 926 774 420 746	3, 3, 7	0.077 794 423 305 790
1, 1, 3	0.188 598 527 131 665	1, 5, 7	0.073 588 554 203 926
1, 3, 3	0.147 995 080 254 964	3, 5, 7	0.070 037 165 946 620
3, 3, 3	0.124 429 443 520 405	5, 5, 7	0.064 173 530 979 794
0, 0, 4	0.154 800 436 631 742	1, 7, 7	0.064 080 796 649 657
0, 2, 4	0.141 304 069 570 169	3, 7, 7	0.061 675 815 610 001
2, 2, 4	0.130 353 606 349 838	5, 7, 7	0.057 548 589 097 653
0, 4, 4	0.113 174 214 285 823	7, 7, 7	0.052 630 916 253 723
2, 4, 4	0.106 945 285 442 139	0, 0, 8	0.078 979 814 608 032
4, 4, 4	0.092 612 098 366 566	0, 2, 8	0.076 789 534 214 936
1, 1, 5	0.121 002 346 131 819	2, 2, 8	0.074 756 836 608 861
1, 3, 5	0.107 620 324 762 228	0, 4, 8	0.071 076 843 915 612
3, 3, 5	0.097 567 723 980 431	2, 4, 8	0.069 429 548 828 437
1, 5, 5	0.089 461 127 363 873	4, 4, 8	0.065 053 935 937 817
3, 5, 5	0.083 300 534 912 552	0, 6, 8	0.063 713 709 757 158
5, 5, 5	0.073 862 566 733 171	2, 6, 8	0.062 503 085 308 694
0, 0, 6	0.104 724 442 227 122	4, 6, 8	0.059 226 146 311 942
0, 2, 6	0.099 930 995 617 171	6, 6, 8	0.054 713 107 983 003
2, 2, 6	0.095 670 153 471 168	0, 8, 8	0.056 329 520 539 998
0, 4, 6	0.088 331 194 895 560	2, 8, 8	0.055 482 290 065 564
2, 4, 6	0.085 253 078 465 954	4, 8, 8	0.053 143 444 692 747
4, 4, 6	0.077 509 205 839 691	6, 8, 8	0.049 808 166 570 407
0, 6, 6	0.075 179 758 105 345	8, 8, 8	0.046 026 025 967 152
2, 6, 6	0.073 221 214 354 647		

The asymptotic behavior of $P(0, 0, 2m; 1)$, as $m \to \infty$, is readily established using the expansion[53]

$$\frac{\Gamma(z+\frac{1}{4})}{\Gamma(z+\frac{3}{4})} \sim z^{-\frac{1}{2}} \sum_{k=0}^{\infty} \frac{B_{2k}^{(\frac{1}{2})}(\frac{1}{4}) \cdot (\frac{1}{2})_k}{(2k)!\, z^{2k}}, \tag{5.6}$$

where $B_{2k}^{(2p)}(\rho)$ is a generalized Bernoulli polynomial. We find

$$P(0,0,2m;1) \sim \frac{1}{\pi m}\left(1 - \frac{1}{8m^2} + \frac{11}{128m^4} - \frac{173}{1024m^6} + \cdots\right), \tag{5.7}$$

as $m \to \infty$.

We now turn to the evaluation of the Green's function $P(l_1, l_2, l_3; 1)$, when $l_1 \neq 0$. It can be shown[12] that the Green's function $P(\mathbf{l}, z)$ satisfies the partial finite difference equation

$$P(l_1, l_2, l_3; z) - \tfrac{1}{8}z \sum_{\pm} P(l_1 \pm 1, l_2 \pm 1, l_3 \pm 1; z) = \delta_{\mathbf{l},0}, \tag{5.8}$$

where the summation is over all eight possible arrangements of the plus and minus signs. For $z = 1$, this difference equation is of considerable importance in potential theory, since it is a discrete analog of Poisson's equation with a unit-source function $\delta(\mathbf{r})$.[54,55]

Let us suppose that $P(0, 2m_2, 2m_3; 1)$ is known for $N \geq m_3 \geq m_2 \geq 0$ and that we require $P(l_1, l_2, l_3; 1)$ for $2N \geq l_3 \geq l_2 \geq l_1 \geq 1$. If Eq. (5.8), with $z = 1$, is applied to the row of lattice sites $(0, 0, 2m_3)$, we obtain the set of relations

$$\begin{aligned} P(1,1,1;1) &= P(0,0,0;1) - 1, \\ P(1,1,2m_3+1;1) &= 2P(0,0,2m_3;1) \\ &\quad - P(1,1,2m_3-1;1), \\ &\quad m_3 = 1, 2, \cdots. \end{aligned} \tag{5.9}$$

By solving these equations successively it is seen that $P(\mathbf{l}, 1)$ can be found along the row $(1, 1, 2m_3 + 1)$. Application of this procedure to the rows $(0, 2, 2m_3)$, $(0, 4, 2m_3)$, $\cdots$ enables one to evaluate all the Green's functions $P(1, 2m_2 + 1, 2m_3 + 1; 1)$ that are of interest. The Green's functions for the next plane of lattice sites $(2, 2m_2, 2m_3)$ can now be obtained by applying (5.8) to the rows $(1, 1, 2m_3 + 1)$, $(1, 3, 2m_3 + 1)$, $\cdots$. It is evident that repeated applications of these arguments will yield all the required Green's functions.

In this manner $P(l_1, l_2, l_3; 1)$ has been evaluated for $8 \geq l_3 \geq l_2 \geq l_1 \geq 1$. The final explicit formulas are listed in Appendix A, and the numerical values are given in Table V. Numerical estimates for the particular Green's functions $P(0, 0, 2; 1)$ and $P(0, 2, 2; 1)$ have been derived by Yussouff and Mahanty,[56] and more recently by Byrnes *et al.*[32] However, their results are in poor agreement with the exact values given in Table V.

When $|\mathbf{l}| \equiv (l_1^2 + l_2^2 + l_3^2)^{\frac{1}{2}}$ is large, it can be shown[57] that

$$P(l_1, l_2, l_3; 1) \sim (2/\pi)\, |\mathbf{l}|^{-1} [1 - \tfrac{9}{8} |\mathbf{l}|^{-2} + \tfrac{5}{8} |\mathbf{l}|^{-6} (l_1^4 + l_2^4 + l_3^4) + \tfrac{15}{4} |\mathbf{l}|^{-6} (l_1^2 l_2^2 + l_2^2 l_3^2 + l_3^2 l_1^2) + \cdots]. \quad (5.10)$$

This asymptotic formula [which agrees with (5.7) for $l_1 = l_2 = 0$, and $l_3 = 2m$] provides a useful check on the results in Table V. For example, it gives

$$\begin{aligned} P(7, 7, 7; 1) &\simeq 0.052\,626\,6, \\ P(6, 8, 8; 1) &\simeq 0.049\,805\,3, \\ P(8, 8, 8; 1) &\simeq 0.046\,023\,8. \end{aligned} \quad (5.11)$$

Finally, we note that $P(\mathbf{l}, -1)$ is obtained using the general relation

$$P(l_1, l_2, l_3; -z) = (-1)^{l_1+l_2+l_3} P(l_1, l_2, l_3; z). \quad (5.12)$$

6. EVALUATION OF $R(\xi_0 - i\epsilon)$

In Sec. 3 a Green's function $R(\xi)$ was introduced which for small $|\xi|$ describes the behavior of $P(z)$ at infinity. It was noted that $R(\xi)$ is an analytic function in the ξ plane, cut from -1 to $+1$. For most physical applications ξ is real with $|\xi| \geq 1$. However, in the theory of scattering of phonons from an impurity atom in a body-centered cubic lattice, Yussouff and Mahanty[56] have encountered the Green's function

$$\lim_{\epsilon \to 0+} R(\xi_0 - i\epsilon), \quad (6.1)$$

where ξ_0 is real. (For convenience, we shall assume $\xi_0 > 0$.) Although these authors expressed (6.1) in the interesting form

$$\lim_{\epsilon \to 0+} R(\xi_0 - i\epsilon) = R_1(\xi_0) + iR_2(\xi_0),$$

where

$$R_1(\xi_0) = 2\int_0^\infty J_0^2(x) J_0(2\xi_0 x)\, dx, \quad (6.2)$$

$$R_2(\xi_0) = -2\int_0^\infty J_0^2(x) Y_0(2\xi_0 x)\, dx, \quad (6.3)$$

and $J_0(x)$ and $Y_0(x)$ are Bessel functions of the first and second kind, respectively, no further exact results were obtained. The main aim in this section is to analyze the behavior of $R_1(\xi_0)$ and $R_2(\xi_0)$ for $0 < \xi_0 \leq 1$.

When $\xi_0 \geq 1$, the limit $\epsilon \to 0+$ can be taken without difficulty, and we find, using Eqs. (1.9) and (3.3), that

$$R_1(\xi_0) = (4/\pi^2 \xi_0) K^2(k), \quad (6.4)$$

where

$$k^2 = \tfrac{1}{2} - \tfrac{1}{2}(1 - \xi_0^{-2})^{\frac{1}{2}}, \quad \xi_0 \geq 1. \quad (6.5)$$

[It is evident that $R_2(\xi_0) = 0$, for $\xi_0 \geq 1$.] The behavior of $R_1(\xi_0)$ for $\xi_0 \gtrsim 1$,

$$R_1(\xi_0) = \left(\frac{4K_0^2}{\pi^2}\right) - \left(\frac{2^{\frac{3}{2}}}{\pi}\right)(\xi_0 - 1)^{\frac{1}{2}} - \left(\frac{2K_0^2}{\pi^2} - \frac{1}{2K_0^2}\right)(\xi_0 - 1) + O(\xi_0 - 1)^{\frac{3}{2}}, \quad (6.6)$$

follows directly from the analytic continuation (3.6). It is interesting to note that Eq. (6.4) may be derived from the integral representation (6.2), using a general result due to Bailey.[58]

The evaluation of $R_1(\xi_0)$ and $R_2(\xi_0)$ for $0 < \xi_0 \leq 1$ may be readily carried out by substituting $\xi = \xi_0 - i\epsilon$ in the analytic continuation (3.5). We find

$$R_1(\xi_0) = (4K_0^2/\pi^2)\, {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{1}{2}; 1 - \xi_0^2)^2 - (1/4K_0^2)(1 - \xi_0^2)\, {}_2F_1(\tfrac{3}{4}, \tfrac{3}{4}; \tfrac{3}{2}; 1 - \xi_0^2)^2 \quad (6.7)$$

and

$$R_2(\xi_0) = (2/\pi)(1 - \xi_0^2)^{\frac{1}{2}}\, {}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{1}{2}; 1 - \xi_0^2) \times {}_2F_1(\tfrac{3}{4}, \tfrac{3}{4}; \tfrac{3}{2}; 1 - \xi_0^2). \quad (6.8)$$

Apart from a change of sign in (6.7), we see that $R_1(\xi_0)$ and $R_2(\xi_0)$ are identical to the regular and singular parts, respectively, of the basic analytic continuation (2.9) for $P(z)$.

For $\xi_0 \lessdot 1$, the behavior of $R_1(\xi_0)$ and $R_2(\xi_0)$ is described by the expansions

$$R_1(\xi_0) = \frac{4K_0^2}{\pi^2} + \left(\frac{2K_0^2}{\pi^2} - \frac{1}{2K_0^2}\right)(1 - \xi_0) + \left(\frac{4K_0^2}{3\pi^2} - \frac{1}{2K_0^2}\right)(1 - \xi_0)^2 + O(1 - \xi_0)^3, \quad (6.9)$$

$$R_2(\xi_0) = (2^{\frac{3}{2}}/\pi)(1 - \xi_0)^{\frac{1}{2}} \times [1 + \tfrac{3}{4}(1 - \xi_0) + \tfrac{281}{480}(1 - \xi_0)^2 + O(1 - \xi_0)^3]. \quad (6.10)$$

The behavior of $R_1(\xi_0)$ and $R_2(\xi_0)$ when ξ_0 is small and positive can be established by substituting (2.31) in

Eqs. (6.7) and (6.8). We give the final results below:

$$R_1(\xi_0) = -(1/\pi)\ln \xi_0^2 + (6/\pi)\ln 2 + O(\xi_0^2 \ln \xi_0^2), \tag{6.11}$$

$$R_2(\xi_0) = (1/2\pi^2)(\ln \xi_0^2)^2 - (6\ln 2/\pi^2)\ln \xi_0^2 + (1/2\pi^2)(6\ln 2 + \pi)(6\ln 2 - \pi) + O(\xi_0^2(\ln \xi_0^2)^2). \tag{6.12}$$

Next we apply the following quadratic transformations[59] to Eqs. (6.7) and (6.8):

$$(4K_0/\pi)\,{}_2F_1(\tfrac{1}{4}, \tfrac{1}{4}; \tfrac{1}{2}; 1-\xi_0^2) = {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}; 1; k_+^2) + {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}; 1; k_-^2), \tag{6.13}$$

$$(1/K_0)(1-\xi_0^2)^{\frac{1}{2}}\,{}_2F_1(\tfrac{3}{4}, \tfrac{3}{4}; \tfrac{3}{2}; 1-\xi_0^2) = {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}; 1; k_+^2) - {}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}; 1; k_-^2), \tag{6.14}$$

where

$$k_\pm^2 = \tfrac{1}{2} \pm \tfrac{1}{2}(1-\xi_0^2)^{\frac{1}{2}}. \tag{6.15}$$

This procedure yields

$$R_1(\xi_0) = (4/\pi^2)K(k_+)K(k_-), \tag{6.16}$$

$$R_2(\xi_0) = (2/\pi^2)[K(k_+)^2 - K(k_-)^2], \tag{6.17}$$

where $0 < \xi_0 \leq 1$. Thus we have evaluated indirectly the integrals (6.2) and (6.3) in terms of complete elliptic integrals for $0 < \xi_0 < \infty$. The application of the quadratic transformations to the basic analytic continuation (2.9) leads to the interesting results

$$\left.\begin{matrix}\phi_1(z)\\ (1-z^2)^{\frac{1}{2}}\phi_2(z)\end{matrix}\right\} = \frac{2}{\pi^2}[K(z_+)^2 \pm K(z_-)^2], \tag{6.18}$$

where

$$z_\pm^2 = \tfrac{1}{2} \pm \tfrac{1}{2}(1-z^2)^{\frac{1}{2}} \tag{6.19}$$

and $|z| \leq 1$.

Complete expansions for $R_1(\xi_0)$ and $R_2(\xi_0)$ about $\xi_0 = 0$ may now be obtained from Eqs. (6.16) and (6.17) using Watson's expansions[15,16] for the products $K(k_-)^2$, $K(k_-)K(k_+)$, and $K(k_+)^2$. The final results are

$$R_1(\xi_0) = -\frac{1}{\pi}\ln \xi_0^2 \sum_{n=0}^{\infty} a_n^3 \xi_0^{2n} + \frac{3}{\pi}\sum_{n=0}^{\infty} a_n^3[\psi(n+1) - \psi(n+\tfrac{1}{2})]\xi_0^{2n}, \tag{6.20}$$

$$\begin{aligned}R_2(\xi_0) = {}& \frac{1}{2\pi^2}(\ln \xi_0^2)^2 \sum_{n=0}^{\infty} a_n^3 \xi_0^{2n} + \frac{3}{\pi^2}\ln \xi_0^2 \sum_{n=0}^{\infty} a_n^3[\psi(n+\tfrac{1}{2}) - \psi(n+1)]\xi_0^{2n}\\ &+ \frac{1}{2\pi^2}\sum_{n=0}^{\infty} a_n^3\{3\psi'(n+\tfrac{1}{2}) - 3\psi'(n+1) - 2\pi^2 + 9[\psi(n+\tfrac{1}{2}) - \psi(n+1)]^2\}\xi_0^{2n},\end{aligned} \tag{6.21}$$

where $\psi'(z)$ is the derivative of the digamma function. [The leading order terms in these expressions agree with those given in (6.11) and (6.12).] A complete expansion for $\phi_1(z)$ about $z^2 = 0$ is formally derived from (6.21) by replacing ξ_0 by z and adding the series $\sum a_n^3 z^{2n}$.

The application of Darboux's method[33] to the singular parts of (6.20) and (6.21) yields *directly* asymptotic expansions for the coefficients $B_n^{(0)} - B_n^{(1)}$, and $B_n = B_n^{(0)} + B_n^{(1)}$, respectively. [Note the singular parts of the expansions for $R_2(\xi_0)$ and $\phi_1(z)$ about $\xi_0 = 0$ and $z = 0$ are formally identical.] Thus we have an alternative *simpler* procedure for deriving Eqs. (2.34) and (2.35).

Since the complete elliptic integral $K(k)$ is readily calculated,[18] the expressions (6.16) and (6.17) provide the most convenient means of evaluating $R_1(\xi_0)$ and $R_2(\xi_0)$. A short table of values for $R_1(\xi_0)$ and $R_2(\xi_0)$ in the range $0 < \xi_0 \leq 1$, which was obtained using (6.16) and (6.17), is given in Appendix B. [Numerical values of $R_1(\xi_0) = R(\xi_0)$ for $\xi_0 \geq 1$ can be found in Ref. 19.] Yussouff and Mahanty[56] have calculated $R_1(\xi_0)$ and $R_2(\xi_0)$ by integrating (6.2) and (6.3) numerically. However, their results are, in some cases, only correct to two significant figures. In Fig. 1 we give a graph showing the variation of $R_1(\xi_0)$ and $R_2(\xi_0)$ with ξ_0.

For the sake of completeness we next investigate the behavior of $R(\xi)$ in the neighborhood of $\xi = 0$, for the *general case*, in which ξ is not necessarily on a cut edge. This behavior is essentially determined by the analytic continuation of the series

$${}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; x), \tag{6.22}$$

into the region $|x| > 1$. First we note that (6.22) is a

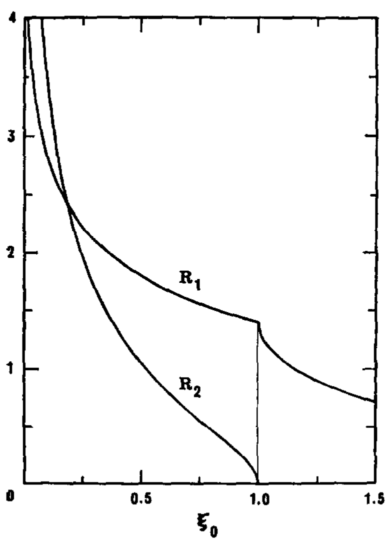

FIG. 1. Real part $R_1(\xi_0)$ and imaginary part $R_2(\xi_0)$ of the Green's function $\lim_{\epsilon\to 0+} R(\xi_0 - i\epsilon)$ for $0 < \xi_0 \leq 1.5$.

solution of the differential equation

$$[\vartheta^3 - x(\vartheta + \tfrac{1}{2})^3]y = 0, \quad \vartheta \equiv x\frac{d}{dx}. \quad (6.23)$$

The application of the transformation $\omega = 1/x$ to this equation gives

$$[\omega\Delta^3 - (\Delta - \tfrac{1}{2})^3]y = 0, \quad \Delta \equiv \omega\frac{d}{d\omega}. \quad (6.24)$$

We now derive the general series solution of (6.24) about the regular singularity at $\omega = 0$, using the method of Frobenius. The particular solution $S(\omega)$, which corresponds to the analytic continuation of the series (6.22) into the region $|x| > 1$, is readily found by "matching" the general solution with the standard expansion[60]

$$\begin{aligned}{}_3F_2\left(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; \frac{1}{\omega}\right) &= {}_2F_1\left(\tfrac{1}{4}, \tfrac{1}{4}; 1; \frac{1}{\omega}\right)^2 \\ &= (1/2\pi^2)(\omega e^{-i\delta\pi})^{\frac{1}{2}} \\ &\quad \times \left(\sum_{n=0}^{\infty}\frac{(\frac{1}{4})_n^2}{(n!)^2}[\ln(\omega e^{-i\delta\pi}) + \psi(\tfrac{3}{4} - n) \right. \\ &\quad \left. + \psi(\tfrac{1}{4} + n) - 2\psi(n+1)]\omega^n\right)^2, \quad (6.25)\end{aligned}$$

where $\delta = \pm 1$, $|\omega| < 1$, and

$$-(1 - \delta)\pi < \arg\omega < (1 + \delta)\pi. \quad (6.26)$$

After replacing ω in $S(\omega)$ by ξ^2 and using Eq. (3.3), we finally obtain the expansion[61]

$$\begin{aligned}R(\xi) = -\frac{i\delta}{2\pi^2}\Bigg([\ln(\xi^2 e^{-i\delta\pi})]^2\sum_{n=0}^{\infty}a_n^3\xi^{2n} + 6\ln(\xi^2 e^{-i\delta\pi}) \\ \times \sum_{n=0}^{\infty}a_n^3[\psi(n + \tfrac{1}{2}) - \psi(n+1)]\xi^{2n} \\ + \sum_{n=0}^{\infty}a_n^3\{3\psi'(n + \tfrac{1}{2}) - 3\psi'(n+1) - \pi^2 \\ + 9[\psi(n + \tfrac{1}{2}) - \psi(n+1)]^2\}\xi^{2n}\Bigg), \quad (6.27)\end{aligned}$$

where $\delta = \pm 1$, $|\xi| < 1$, and

$$-(1 - \delta)\tfrac{1}{2}\pi < \arg\xi < (1 + \delta)\tfrac{1}{2}\pi. \quad (6.28)$$

This result clearly reveals the nature of the discontinuity in the imaginary part of $R(\xi)$ across the cut from -1 to $+1$. If we substitute $\xi = \xi_0 e^{-i\epsilon}$ in (6.27) (where $0 < \xi_0 < 1$ and $\epsilon > 0$) and take the limit $\epsilon \to 0$, we find agreement with the expansions (6.20) and (6.21).

We conclude this section by noting the following formulas for the derivatives of $R_1(\xi_0)$ and $R_2(\xi_0)$:

$$\begin{aligned}\frac{dR_1}{d\xi_0} &= -\frac{4}{\pi^2\xi_0}(\xi_0^2 - 1)^{-\frac{1}{2}}[2K(k)E(k) - K(k)^2], \quad \xi_0 > 1, \\ &= -\frac{4}{\pi^2\xi_0}(1 - \xi_0^2)^{-\frac{1}{2}}[K(k_-)E(k_+) - K(k_+)E(k_-) \\ &\quad + (1 - \xi_0^2)^{\frac{1}{2}}K(k_+)K(k_-)], \quad 0 < \xi_0 < 1, \quad (6.29)\end{aligned}$$

$$\begin{aligned}\frac{dR_2}{d\xi_0} &= -\frac{4}{\pi^2\xi_0}(1 - \xi_0^2)^{-\frac{1}{2}}[K(k_+)E(k_+) + K(k_-)E(k_-) \\ &\quad - k_-^2K(k_+)^2 - k_+^2K(k_-)^2], \quad 0 < \xi_0 < 1, \quad (6.30)\end{aligned}$$

where $E(k)$ is the complete elliptic integral of the second kind, and k and $k_\pm$ are defined in Eqs. (6.5) and (6.15), respectively. The behavior of the derivatives in the neighborhood of $\xi_0 = 0$ and 1 is readily found from the expansions given above.

7. ANALYTIC CONTINUATIONS IN POWERS OF $1 - z$ AND $\xi - 1$

For most applications, one requires analytic continuations for $P(z)$ and $R(\xi)$ in powers of $1 - z$ and $\xi - 1$, respectively. These analytic continuations are readily derived by direct expansion of Eqs. (2.9) and (3.6). We give the final results below:

$$\begin{aligned}P(z) &= \sum_{n=0}^{\infty}[U_n^{(0)} + U_n^{(1)}](1 - z)^n \\ &\quad - (1 - z)^{\frac{1}{2}}\sum_{n=0}^{\infty}V_n(1 - z)^n, \quad |1 - z| < 1 \quad (7.1)\end{aligned}$$

and

$$\begin{aligned}R(\xi) &= \sum_{n=0}^{\infty}(-1)^n[U_n^{(0)} - U_n^{(1)}](\xi - 1)^n \\ &\quad - (\xi - 1)^{\frac{1}{2}}\sum_{n=0}^{\infty}(-1)^nV_n(\xi - 1)^n, \quad |\xi - 1| < 1. \quad (7.2)\end{aligned}$$

The coefficients in these expansions are related to the basic set of coefficients $B_n^{(i)}$ and C_n by the equations

$$U_n^{(i)} = 2^n\sum_{m=0}^{[n/2]}\frac{(-1)^m}{2^{2m}}\binom{n-m}{m}B_{n-m}^{(i)}, \quad i = 0, 1 \quad (7.3)$$

$$V_n = 2^{n+\frac{1}{2}}\sum_{m=0}^{n}\frac{(-1)^m}{2^{2m}}\binom{n - m + \frac{1}{2}}{m}C_{n-m}, \quad (7.4)$$

TABLE VI. Expressions for the coefficients $U_n^{(0)}$, $U_n^{(1)}$, and V_n.

n	$U_n^{(0)}$	$U_n^{(1)}$	V_n
0	$4K_0^2/\pi^2$	0	$2\sqrt{2}/\pi$
1	$2K_0^2/\pi^2$	$1/2K_0^2$	$3\sqrt{2}/2\pi$
2	$4K_0^2/3\pi^2$	$1/2K_0^2$	$281\sqrt{2}/240\pi$
3	K_0^2/π^2	$9/20K_0^2$	$917\sqrt{2}/960\pi$
4	$101K_0^2/126\pi^2$	$2/5K_0^2$	$28\,897\sqrt{2}/35\,840\pi$
5	$169K_0^2/252\pi^2$	$143/400K_0^2$	$100\,111\sqrt{2}/143\,360\pi$
6	$89K_0^2/154\pi^2$	$129/400K_0^2$	$303\,496\,357\sqrt{2}/492\,011\,520\pi$

where $\binom{n}{r}$ denotes the binomial coefficient and $[n/2]$ is equal to $\frac{1}{2}n$ when n is even and $\frac{1}{2}(n-1)$ when n is odd. Explicit expressions for the first few coefficients $U_n^{(0)}$, $U_n^{(1)}$, and V_n are listed in Table VI.

To obtain recurrence relations for $U_n^{(i)}$ and V_n, we first apply the transformation $x = (1-\epsilon)^2$, with $\epsilon = 1 - z$, to the differential equation (2.45). This procedure yields the differential equation

$$\epsilon(2-\epsilon)(1-\epsilon)^2 y''' + 3(1-\epsilon)(2\epsilon^2 - 4\epsilon + 1)y'' - (7\epsilon^2 - 14\epsilon + 6)y' + (1-\epsilon)y = 0. \quad (7.5)$$

We now use the method of Frobenius to derive the general series solution of this equation about the regular singularity at $\epsilon = 0$. The comparison of the general solution with the particular solution (7.1) leads to the recurrence relations:

$$n(n+1)(2n+1)U_{n+1}^{(i)} - n(5n^2+1)U_n^{(i)} + (2n-1)(2n^2-2n+1)U_{n-1}^{(i)} - (n-1)^3 U_{n-2}^{(i)} = 0, \quad n \geq 1, \quad i = 0, 1, \quad (7.6)$$

with the initial conditions

$$U_0^{(0)} = 4K_0^2/\pi^2, \quad U_1^{(0)} = 2K_0^2/\pi^2, \quad U_0^{(1)} = 0, \quad U_1^{(1)} = 1/2K_0^2, \quad (7.7)$$

TABLE VIII. Comparison between the exact and asymptotic values of the coefficients V_n.

n	Exact V_n	Asymptotic V_n
0	0.900 316 316 157 106 1	
1	0.675 237 237 117 829 6	0.789 626
2	0.527 060 176 750 305 8	0.558 076
3	0.429 994 823 914 617 8	0.440 317
4	0.362 952 575 167 297 6	0.366 748
5	0.314 353 957 613 016 3	0.315 836
6	0.277 679 191 435 743 1	0.278 284
7	0.249 071 715 831 021 3	0.249 327
8	0.226 140 724 577 821 7	0.226 252
9	0.207 340 914 829 074 2	0.207 390
10	0.191 636 025 585 644 8	0.191 659

and

$$4(n+1)(2n+1)(2n+3)V_{n+1} - (2n+1)(20n^2+20n+9)V_n + 8n(4n^2+1)V_{n-1} - (2n-1)^3 V_{n-2} = 0, \quad n \geq 0, \quad (7.8)$$

with the initial condition $V_0 = 2^{\frac{3}{2}}/\pi$, and $V_{-1} = V_{-2} \equiv 0$.

The application of the method developed by Maradudin *et al.*[62] to the Laplace transform

$$R(\xi) = \int_0^\infty e^{-\xi t} E(t)\, dt, \quad (7.9)$$

where $E(t)$ is defined in Eq. (3.2), provides an alternative procedure for constructing the analytic continuation (7.2). Although this approach does not lead to exact expressions for the coefficients $U_n^{(i)}$, it does yield the relation

$$V_n = (2^{\frac{3}{2}}/\pi(\tfrac{3}{2})_n)\theta_n, \quad (7.10)$$

where θ_n are the coefficients in the asymptotic expansion for $E(t)$. The substitution of Eq. (7.10) in the recurrence relation (3.28) provides a useful confirmation of the recurrence relation (7.8).

The asymptotic behavior of $U_n^{(0)} - U_n^{(1)}$ and

TABLE VII. Comparison between the exact and asymptotic values of the coefficients $U_n^{(0)}$ and $U_n^{(1)}$.

n	Exact $U_n^{(0)}$	Asymptotic $U_n^{(0)}$	Exact $U_n^{(1)}$	Asymptotic $U_n^{(1)}$
0	1.393 203 929 685 676 9			
1	0.696 601 964 842 838 4	0.800 64	0.145 450 614 204 335 5	
2	0.464 401 309 895 225 6	0.483 28	0.145 450 614 204 335 5	0.145 08
3	0.348 300 982 421 419 2	0.352 24	0.130 905 552 783 901 9	0.134 14
4	0.279 193 644 639 391 6	0.279 87	0.116 360 491 363 468 4	0.118 23
5	0.233 582 801 703 253 4	0.233 52	0.103 997 189 156 099 9	0.104 92
6	0.201 290 827 503 287 7	0.201 11	0.093 815 646 161 796 4	0.094 27
7	0.177 228 908 984 636 3	0.177 06	0.085 433 588 330 405 5	0.085 65
8	0.158 590 121 486 087 5	0.158 47	0.078 468 741 611 774 8	0.078 58
9	0.143 708 484 543 253 1	0.143 62	0.072 611 570 974 261 9	0.072 67
10	0.131 536 464 595 307 0	0.131 47	0.067 625 280 404 734 3	0.067 65

$U_n^{(0)} + U_n^{(1)}$ for large n may be obtained by applying the method of Darboux to the singular parts of the expansions (6.20) and (6.21), respectively. From this analysis we find

$$\left.\begin{matrix} U_n^{(0)} \\ U_n^{(1)} \end{matrix}\right\} \sim (1/\pi^2 n)[2g_0(n) \pm \pi] - (1/\pi^2 n^2) + (1/12\pi^2 n^3)[6g_0(n) \pm 3\pi - 20] + \cdots, \tag{7.11}$$

where

$$g_0(n) = \gamma + 3 \ln 2 + \ln n. \tag{7.12}$$

To investigate the asymptotic behavior of the coefficient V_n, we formally replace ξ_0 by z in Eq. (6.21) and apply Darboux's method to the expansion of $(1 - z)^{-\frac{1}{2}} R_2(z)$ about $z = 0$. The final result is

$$V_n \sim (4/\pi^2 n) g_0(n) - (2/\pi^2 n^2) g_0(n) + (1/6\pi^2 n^3)[12 g_0(n) - 17] + \cdots. \tag{7.13}$$

In Table VII the approximate values of $U_n^{(0)}$ and $U_n^{(1)}$ for $n \leq 10$, which were derived using the asymptotic representation (7.11), are compared with the exact values. Similar results for the coefficients V_n are given in Table VIII.

Since we have now complete analytic continuations for $P(z)$ in powers of $1 - z^2$ and $1 - z$, and exact expressions for $P(\mathbf{0}, 1)$, the main mathematical aims have been achieved. In the remainder of the paper we shall discuss some applications of these results in the theory of random walks. Applications in the theory of ferromagnetism (such as the spherical model) which are of more specialized interest will be considered in detail elsewhere.

8. RANDOM WALK GENERATING FUNCTIONS

A general theory of random walks on lattices has been developed in a clear and systematic manner by Montroll and Weiss.[12] In the following sections we shall use their results to investigate the particular case of a body-centered cubic (bcc) lattice with jumps to nearest neighbor lattice sites.

Consider first a random walk on an infinite simple cubic lattice with unit lattice spacing and lattice sites

$$\mathbf{l} = l_1 \mathbf{e}_1 + l_2 \mathbf{e}_2 + l_3 \mathbf{e}_3, \tag{8.1}$$

where l_1, l_2, l_3 are integers $0, \pm 1, \pm 2, \cdots$ and $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$, and suppose that the probability $p(\mathbf{l}' - \mathbf{l})$ that the walker will make a step from $\mathbf{l}$ to $\mathbf{l}'$ (where $\mathbf{l}'$ is not necessarily a nearest neighbor site of $\mathbf{l}$) is

$$p(\mathbf{l}' - \mathbf{l}) = \tfrac{1}{8}, \quad \text{for } \mathbf{l}' - \mathbf{l} = (\pm 1, \pm 1, \pm 1), \qquad = 0, \quad \text{otherwise.} \tag{8.2}$$

A random walker starting from $\mathbf{l} = \mathbf{0}$ with transition probabilities (8.2) can only reach lattice sites for which l_1, l_2, l_3 are all even or all odd, and thus this random walk is *equivalent* to a random walk on a bcc lattice with nearest neighbor jumps. We shall adopt this alternative formulation for random walks on a bcc lattice since it leads to considerable mathematical simplifications.

Many of the properties of random walks can be described in terms of the probability generating function

$$P(\mathbf{l}, z) = \sum_{n=0}^{\infty} P_n(\mathbf{l}) z^n, \tag{8.3}$$

where $P_n(\mathbf{l})$ is the probability that a random walker, starting at the origin $\mathbf{l} = \mathbf{0}$, will reach the site $\mathbf{l}$ (not necessarily for the first time) after a walk of n steps. For random walks on a bcc lattice we can show,[12] using the equivalent simple cubic random walk (8.2), that

$$P_n(\mathbf{l}) = \frac{1}{\pi^3} \iiint_0^{\pi} (\cos x_1 \cos x_2 \cos x_3)^n \times \cos l_1 x_1 \cos l_2 x_2 \cos l_3 x_3 \, dx_1 \, dx_2 \, dx_3. \tag{8.4}$$

If this integral is substituted in (8.3) and the order of summation and integration is interchanged, we see that the fundamental Green's function (1.1) gives an integral representation for the generating function (8.3).

An explicit expression for (8.4) may be readily derived using standard results. We find

$$P_n(\mathbf{l}) = \Lambda_n(l_1) \Lambda_n(l_2) \Lambda_n(l_3), \tag{8.5}$$

where

$$\Lambda_n(l) = \frac{\Gamma(n+1)}{2^n \Gamma(\frac{1}{2}n + \frac{1}{2}l + 1) \Gamma(\frac{1}{2}n - \frac{1}{2}l + 1)}, \quad l + n \text{ even}, \quad n \geq |l|, \qquad = 0, \quad \text{otherwise.} \tag{8.6}$$

Equation (8.6) shows directly that $P_n(\mathbf{l})$ is zero if l_1, l_2, and l_3 are *not* all even or all odd. We also note that the first nonzero term in the series (8.3) occurs when $n = \max\{|l_1|, |l_2|, |l_3|\}$. Asymptotic expansions for $P_n(\mathbf{l})$, valid when $n \gg |\mathbf{l}|^2$, can be obtained from Eqs. (8.5) and (8.6). For the interesting case $\mathbf{l} = \mathbf{0}$ we find

$$P_{2n}(0) = a_n^3 = \left(\frac{(\frac{1}{2})_n}{(1)_n}\right)^3 \sim \frac{1}{(\pi n)^{\frac{3}{2}}} \left(1 - \frac{3}{8n} + \frac{9}{128 n^2} + \frac{7}{1024 n^3} - \frac{165}{32\,768 n^4} + \cdots\right), \tag{8.7}$$

with $P_{2n+1}(\mathbf{0}) = 0$.

TABLE IX. Values of $F_n^{(r)}(0)$ for the bcc lattice, where $F_n^{(r)}(0)$ is the probability that a random walker will return to the origin for the rth time at step n. [Note that $F_{2n+1}^{(r)}(0) = 0$.]

n/r	1	2	3	4	5	6
2	$1/8$	0	0	0	0	0
4	$19/8^3$	$1/8^2$	0	0	0	0
6	$79/8^4$	$38/8^4$	$1/8^3$	0	0	0
8	$25\,715/8^7$	$1625/8^6$	$57/8^5$	$1/8^4$	0	0
10	$145\,393/8^8$	$75\,446/8^8$	$2979/8^7$	$76/8^6$	$1/8^5$	0

We now introduce a further generating function

$$F(\mathbf{l}, z) = \sum_{n=1}^{\infty} F_n(\mathbf{l}) z^n, \tag{8.8}$$

where $F_n(\mathbf{l})$ is the probability that a random walker, starting at the origin, will reach the lattice site $\mathbf{l}$ for the *first* time at step n. It can be shown that[11,12]

$$F(\mathbf{l}, z) = [P(\mathbf{l}, z) - \delta_{\mathbf{l},\mathbf{0}}]/P(\mathbf{0}, z). \tag{8.9}$$

If the random walker continues to walk indefinitely, then the probability that he will eventually reach the lattice site $\mathbf{l}$ is just $F(\mathbf{l}, 1)$. For the bcc lattice it is possible to evaluate $F(\mathbf{l}, 1)$ exactly using the results listed in Appendix A. Some examples are given below:

$$F(0, 0, 2; 1) = \alpha/4\omega, \quad F(0, 2, 2; 1) = (\omega - \alpha)/\omega,$$
$$F(2, 4, 6; 1) = [(2639/25)\alpha - (1103/9)\omega + 12]/\omega, \tag{8.10}$$

where $\alpha = 1/K_0^2$ and $\omega = K_0^2/\pi^2$. The probability of eventual return to the origin $F(\mathbf{0}, 1)$ has been calculated previously for the bcc lattice by Montroll.[10,11] The results in Appendix A can also be used to evaluate the first passage time[11,12] on the bcc lattice.

Next we investigate the asymptotic behavior of $F_{2n}(\mathbf{0})$ for the bcc lattice, by applying the method of Darboux[33,63] to the generating function $F(\mathbf{0}, z)$. [It is clear from (8.9) that $F_{2n+1}(\mathbf{0}) = 0$.] We first note that, in the z^2 plane, $F(\mathbf{0}, z)$ has *one* singularity on the circle of convergence, at $z^2 = 1$. The behavior of $F(\mathbf{0}, z)$ in the neighborhood of this singularity may be obtained by inverting the basic analytic continuation (2.9) for $P(z) \equiv P(\mathbf{0}, z)$. It is found that

$$\begin{aligned} F(\mathbf{0}, z) = 1 &- (\pi^2/4K_0^2)[1 + (\pi/2K_0^2)(1 - z^2)^{\frac{1}{2}} \\ &+ (1/16K_0^4)(3\pi^2 - 4K_0^4)(1 - z^2) \\ &+ (\pi^3/16K_0^6)(1 - z^2)^{\frac{3}{2}} + (1/768K_0^8) \\ &\times (15\pi^4 + 36\pi^2K_0^4 - 64K_0^8)(1 - z^2)^2 \\ &+ (\pi/2560K_0^{10})(15\pi^4 + 80\pi^2K_0^4 - 16K_0^8) \\ &\times (1 - z^2)^{\frac{5}{2}} + \cdots]. \end{aligned} \tag{8.11}$$

The formal expansion of the *singular* part of this expression in powers of z^2 finally yields the asymptotic representation

$$\begin{aligned} F_{2n}(\mathbf{0}) \sim {} & (\pi^{\frac{3}{2}}/16K_0^4)n^{-\frac{3}{2}} \\ & \times [1 + (3/16K_0^4)(2K_0^4 - \pi^2)n^{-1} + (1/1024K_0^8) \\ & \times (45\pi^4 - 120\pi^2K_0^4 + 152K_0^8)n^{-2} + \cdots]. \end{aligned} \tag{8.12}$$

Montroll and Weiss also considered the generating function

$$F^{(r)}(\mathbf{l}, z) = \sum_{n=1}^{\infty} F_n^{(r)}(\mathbf{l}) z^n, \tag{8.13}$$

where $F_n^{(r)}(\mathbf{l})$ is the probability that a random walker, starting at the origin, will reach $\mathbf{l}$ for the rth time at step n. This generating function may be expressed in terms of $F(\mathbf{l}, z)$ as follows:

$$F^{(r)}(\mathbf{l}, z) = [F(\mathbf{0}, z)]^{r-1} F(\mathbf{l}, z). \tag{8.14}$$

An asymptotic analysis of $F_{2n}^{(r)}(\mathbf{0})$ for the bcc lattice (valid when $n \gg r$) could be readily carried out using Eqs. (8.11) and (8.14). In Table IX the exact values of $F(_{2n}^{(r)}\mathbf{0})$ are listed for $n \leq 5$. The relation

$$\sum_{r=1}^{n} F_{2n}^{(r)}(\mathbf{0}) = P_{2n}(\mathbf{0}) \tag{8.15}$$

provides a useful check on the results.

9. EXPECTED NUMBER OF VISITS TO A LATTICE POINT DURING AN N-STEP RANDOM WALK

The expected or mean number of times a lattice site $\mathbf{l}$ is visited during an n-step random walk is

$$M_n(\mathbf{l}) = \sum_{k=0}^{n} P_k(\mathbf{l}). \tag{9.1}$$

It follows directly from (9.1) that

$$\lim_{n\to\infty} M_n(\mathbf{l}) = P(\mathbf{l}, 1). \tag{9.2}$$

This limit can therefore be evaluated for the bcc lattice using the results in Sec. 5 and Appendix A. If we multiply (9.1) by z^n and sum over n, we see that the generating function

$$M(\mathbf{l}, z) \equiv \sum_{n=0}^{\infty} M_n(\mathbf{l}) z^n = (1 - z)^{-1} P(\mathbf{l}, z). \tag{9.3}$$

For the bcc lattice [and other "loose-packed" lattices which have $P_{2k+1}(\mathbf{0}) = 0$]

$$M_{2n+1}(\mathbf{0}) = M_{2n}(\mathbf{0}). \tag{9.4}$$

Thus, when $\mathbf{l} = \mathbf{0}$ and the lattice is loose-packed, it is convenient to introduce an alternative generating function

$$E(z) \equiv \sum_{n=0}^{\infty} M_{2n}(\mathbf{0})z^{2n} = (1 - z^2)^{-1}P(\mathbf{l}, z). \tag{9.5}$$

For the bcc lattice we find

$$E(z) = 1 + (9/8)z^2 + (603/8^3)z^4 + (4949/8^4)z^6 + (2576763/8^7)z^8 + (20864151/8^8)z^{10} + \cdots. \tag{9.6}$$

We now derive an asymptotic expansion for $M_{2n}(\mathbf{0})$ on the bcc lattice. The generating function $E(z)$ has, in the z^2 plane, one singularity on the circle of convergence, at $z^2 = 1$. In the neighborhood of this singularity the behavior of $E(z)$ is described by the analytic continuation

$$E(z) = \sum_{n=0}^{\infty} B_n(1 - z^2)^{n-1} - \sum_{n=0}^{\infty} C_n(1 - z^2)^{n-\frac{1}{2}}, \tag{9.7}$$

where the coefficients B_n and C_n are defined in Sec. 2. The application of Darboux's method to the singular part of (9.7) yields the required asymptotic expansion

$$M_{2n}(\mathbf{0}) \sim (4K_0^2/\pi^2) - (2/\pi)(\pi n)^{-\frac{1}{2}} \times [1 - (3/8)n^{-1} + (109/640)n^{-2} - (57/1024)n^{-3} - (37/32768)n^{-4} + \cdots]. \tag{9.8}$$

It should be noted that it is possible to derive an asymptotic expansion for $M_n(\mathbf{0})$ on the bcc lattice using the generating function $M(\mathbf{0}, z)$. However, the Darboux analysis in this case is more complicated since $M(\mathbf{0}, z)$ has, *in the z plane, two* singularities on the circle of convergence, at $z = \pm 1$. The final result is presented below:

$$M_n \sim M_n^{(+)} + M_n^{(-)}, \tag{9.9}$$

where

$$M_n^{(+)} = (4K_0^2/\pi^2) - (2^{\frac{3}{2}}/\pi)(\pi n)^{-\frac{1}{2}} \times [1 - (1/2)n^{-1} + (49/160)n^{-2} - (9/64)n^{-3} + (19/2048)n^{-4} + \cdots] \tag{9.10}$$

and

$$M_n^{(-)} = (2^{\frac{3}{2}}/\pi)(\pi n)^{-\frac{1}{2}}(-)^n \times [(1/4)n^{-1} - (3/8)n^{-2} + (39/128)n^{-3} + (7/256)n^{-4} + \cdots], \tag{9.11}$$

are the asymptotic contributions from the singularities at $z = +1$ and -1, respectively. When n is even, the expansion (9.9) agrees with (9.8). The asymptotic analysis of $M_n(\mathbf{0})$ given by Montroll and Weiss[12] is incomplete since the contribution $M_n^{(-)}$ was not discussed. Furthermore, their formula for $M_n^{(+)}$ is in disagreement with (9.10).

An alternative direct procedure for deriving (9.8), which is closely related to the techniques developed by Domb[64] and Byrnes *et al.*[32] is now briefly described. First $M_{2n}(\mathbf{0})$ is written in the form

$$M_{2n}(\mathbf{0}) = \frac{4K_0^2}{\pi^2} - \sum_{k=n+1}^{\infty} P_{2k}(\mathbf{0}). \tag{9.12}$$

Since we are concerned with the case of large n, we may replace $P_{2k}(\mathbf{0})$ by its asymptotic representation (8.7). If the resulting summations

$$\sum_{k=n+1}^{\infty} k^{-m-\frac{3}{2}}, \quad m = 0, 1, \cdots, \tag{9.13}$$

are evaluated using the Euler–Maclaurin summation formula, we finally obtain the asymptotic expansion (9.8).

The probability $\Omega_n^{(r)}$ that a random walker will *return* to his starting point at least r times during an n-step walk is

$$\Omega_n^{(r)} = \sum_{k=1}^{n} F_k^{(r)}(\mathbf{0}), \quad r \geq 1. \tag{9.14}$$

[Note that $\Omega_n^{(r)}$ and $M_n(\mathbf{0})$ are formally rather similar.] It is readily seen from (8.14) that for the generating function

$$\Omega^{(r)}(z) \equiv \sum_{n=1}^{\infty} \Omega_n^{(r)} z^n = (1 - z)^{-1}[F(\mathbf{0}, z)]^r. \tag{9.15}$$

For loose-packed lattices we also define the generating function

$$\sum_{n=0}^{\infty} \Omega_{2n}^{(r)} z^{2n} = (1 - z^2)^{-1}[F(\mathbf{0}, z)]^r, \tag{9.16}$$

since, for this type of lattice,

$$\Omega_{2n+1}^{(r)} = \Omega_{2n}^{(r)}. \tag{9.17}$$

The asymptotic behavior of $\Omega_{2n}^{(r)}$ on the bcc lattice may be determined from (9.16) by using the analytic continuation (8.11) and the method of Darboux. For the particular case $r = 1$, it is found that

$$\Omega_{2n}^{(1)} \sim [1 - (\pi^2/4K_0^2)] - (\pi^{\frac{5}{2}}/8K_0^4)n^{-\frac{1}{2}} \times [1 - (1/16K_0^4)(\pi^2 + 2K_0^4)n^{-1} + (1/5120K_0^8) \times (45\pi^4 + 120\pi^2K_0^4 - 8K_0^8)n^{-2} + \cdots]. \tag{9.18}$$

[This expansion could also be derived directly from (8.12) using the Euler–Maclaurin summation formula.]

TABLE X. Values of $\Theta_n^{(r)}$ for the bcc lattice, where $\Theta_n^{(r)}$ is the probability that a random walker will return to his starting point *exactly r* times during an n step walk. (Note that $\Theta_{2n+1}^{(r)} = \Theta_{2n}^{(r)}$.)

n/r	1	2	3	4	5	6
2	1/8	0	0	0	0	0
4	$75/8^3$	$1/8^2$	0	0	0	0
6	$641/8^4$	$94/8^4$	$1/8^3$	0	0	0
8	$340\,907/8^7$	$7185/8^6$	$113/8^5$	$1/8^4$	0	0
10	$2\,797\,203/8^8$	$511\,454/8^8$	$9603/8^7$	$132/8^6$	$1/8^5$	0

In the limit $n \to \infty$, $\Omega_n^{(1)}$ becomes the probability of eventual return to the origin $F(\mathbf{0}, 1)$. The probability of *not* returning to the origin during an n-step walk is $1 - \Omega_n^{(1)}$.

We conclude this section by considering the probability $\Theta_n^{(r)}$ that a random walker will *return* to the origin *exactly r* times during an n-step walk. It is clear that

$$\Theta_n^{(r)} = \Omega_n^{(r)} - \Omega_n^{(r+1)}. \tag{9.19}$$

The generating function for $\Theta_n^{(1)}$ is therefore

$$\Theta^{(r)}(z) \equiv \sum_{n=0}^{\infty} \Theta_n^{(r)} z^n = (1 - z)^{-1}[F(\mathbf{0}, z)]^r[1 - F(\mathbf{0}, z)]. \tag{9.20}$$

[Note that when $r = 0$, Eq. (9.20) gives the correct generating function for the probability of *not* returning to the origin $1 - \Omega_n^{(1)}$.] For loose-packed lattices we also introduce the generating function

$$\sum_{n=0}^{\infty} \Theta_{2n}^{(r)} z^{2n} = (1 - z^2)^{-1}[F(\mathbf{0}, z)]^r[1 - F(\mathbf{0}, z)]. \tag{9.21}$$

Asymptotic formulas for $\Theta_{2n}^{(r)}$ on the bcc lattice are readily obtained using Eqs. (8.11) and (9.21). In Table X the exact values of $\Theta_{2n}^{(r)}$ are listed for $n \le 5$.

10. EXPECTED NUMBER OF DISTINCT LATTICE SITES VISITED DURING AN N-STEP RANDOM WALK

The problem of finding the expected number of *distinct* lattice sites S_n visited during an n-step random walk was first studied by Dvoretsky and Erdös.[65] These authors proved that for a three-dimensional lattice with nearest neighbor jumps, the behavior of S_n, when n is large, is

$$S_n = a_1 n + O(n^{\frac{1}{2}}), \tag{10.1}$$

where a_1 is a constant which depends on the lattice structure. The values of a_1 were later calculated exactly for the three cubic lattices by Vineyard.[66] A more extensive analysis by Montroll and Weiss[12,11] showed that the higher-order terms in (10.1) were of the form

$$S_n \sim a_1 n + a_2 n^{\frac{1}{2}} + a_3 + a_4 n^{-\frac{1}{2}} + \cdots. \tag{10.2}$$

Montroll and Weiss also calculated a_2 for the three cubic lattices, and a_3 and a_4 for the simple cubic lattice. However, it appears that the only correct higher-order coefficient is a_2 on the simple cubic lattice.

In this section our main aim will be to derive the asymptotic expansion (10.2) for the bcc lattice. We begin with the generating function[12]

$$S(z) \equiv \sum_{n=0}^{\infty} S_n z^n = (1 - z)^{-2}[P(\mathbf{0}, z)]^{-1}. \tag{10.3}$$

This function has, in the z plane, *two* singularities on the circle of convergence, at $z = \pm 1$. The behavior of $S(z)$ in the neighborhood of the singularity at $z = +1$ is readily established by inverting the analytic continuation (7.1). We give the final result below:

$$\begin{aligned} S(z) = (\pi^2/4K_0^2)[&(1 - z)^{-2} + (\pi 2^{\frac{1}{2}}/2K_0^2)(1 - z)^{-\frac{3}{2}} \\ &+ (1/8K_0^4)(3\pi^2 - 4K_0^4)(1 - z)^{-1} \\ &+ (\pi 2^{\frac{1}{2}}/8K_0^6)(\pi^2 - K_0^4)(1 - z)^{-\frac{1}{2}} \\ &+ (1/192K_0^8)(15\pi^4 - 16K_0^8) + (\pi 2^{\frac{1}{2}}/640K_0^{10}) \\ &\times (15\pi^4 + 20\pi^2 K_0^4 - 26K_0^8)(1 - z)^{\frac{1}{2}} + \cdots]. \end{aligned} \tag{10.4}$$

In the neighborhood of the singularity at $z = -1$, we find

$$S(z) = (\pi^2/16K_0^2)[1 + (\pi 2^{\frac{1}{2}}/2K_0^2)(1 + z)^{\frac{1}{2}} + \cdots]. \tag{10.5}$$

The application of the method of Darboux to the singular parts of (10.4) *and* (10.5) yields the required asymptotic expansion

$$\begin{aligned} S_n \sim (\pi^2 n/4K_0^2) \times \{&1 + (1/K_0^2)(2\pi/n)^{\frac{1}{2}} + (1/8K_0^4)(3\pi^2 + 4K_0^4)n^{-1} \\ &+ (1/8K_0^6)(\pi^2 + 2K_0^4)(2\pi/n^3)^{\frac{1}{2}} - (1/1280K_0^{10}) \\ &\times [15\pi^4 + 40\pi^2 K_0^4 + 24K_0^8 + (-)^n 80K_0^8] \\ &\times (2\pi/n^5)^{\frac{1}{2}} + \cdots\}. \end{aligned} \tag{10.6}$$

We see that the "weak" cusplike singularity at $z = -1$ gives rise to significant contributions to the expansion (10.6) of the type $(-)^n/n^{m+\frac{3}{2}}$, where $m = 0, 1, 2, \cdots$. The existence of these oscillatory terms was not discussed by Montroll and Weiss.[12]

It is interesting to note that the behavior of $S(z)$ on the bcc lattice is qualitatively similar to that of the

TABLE XI. Values of $S_n^{(r)}$ for the bcc lattice, where $S_n^{(r)}$ is the expected number of lattice sites visited at least r times during an n-step walk.

n/r	1	2	3	4	5	6
0	1	0	0	0	0	0
1	2	0	0	0	0	0
2	23/8	1/8	0	0	0	0
3	30/8	2/8	0	0	0	0
4	$2349/8^3$	$203/8^3$	$1/8^2$	0	0	0
5	$2778/8^3$	$278/8^3$	$2/8^2$	0	0	0
6	$25\,577/8^4$	$2865/8^4$	$222/8^4$	$1/8^3$	0	0
7	$28\,930/8^4$	$3506/8^4$	$316/8^4$	$2/8^3$	0	0
8	$16\,503\,181/8^7$	$2\,135\,979/8^7$	$27\,409/8^6$	$241/8^5$	$1/8^4$	0

high-temperature susceptibility of the Ising model on a loose-packed lattice.[67] The divergent singularity at $z = 1$ corresponds to a ferromagnetic singularity while the "weaker" singularity at $z = -1$ corresponds to an antiferromagnetic singularity. In fact, since Eqs. (10.4) and (10.5) describe the exact "critical behavior" of the series (10.3), we have a useful example with which to test the accuracy of series extrapolation techniques.[68]

Following Montroll and Weiss,[12] we now define $S_n^{(r)}$ to be the expected number of lattice sites visited at least r times during an n-step walk. The generating function for $S_n^{(r)}$ can be written in the form

$$S^{(r)}(z) \equiv \sum_{n=0}^{\infty} S_n^{(r)} z^n = [F(0, z)]^{r-1} S(z). \qquad (10.7)$$

Thus it would be possible to derive an asymptotic expansion for $S_n^{(r)}$ on the bcc lattice using Eqs. (8.11), (10.4), and (10.5). We list in Table XI the exact values of $S_n^{(r)}$ on this lattice for $n \leq 8$.

We finally consider the expected number of lattice sites $W_n^{(r)}$ that are visited *exactly* r times during an n-step walk. It is clear that

$$W_n^{(r)} = S_n^{(r)} - S_n^{(r+1)}. \qquad (10.8)$$

Hence the generating function for $W_n^{(r)}$ is

$$W^{(r)}(z) \equiv \sum_{n=0}^{\infty} W_n^{(r)} z^n = [F(0, z)]^{r-1}[(1 - z)S(z)]^2. \qquad (10.9)$$

The following asymptotic expansion for $W_n^{(1)}$ on the bcc lattice:

$$W_n^{(1)} \sim (\pi^4 n/16K_0^4) \times \{1 + (2/K_0^2)(2\pi/n)^{\frac{1}{2}} + (5\pi^2/4K_0^4)n^{-1} + (5\pi^2/8K_0^6)(2\pi/n^3)^{\frac{1}{2}} - (1/960K_0^{10})(2\pi/n^5)^{\frac{1}{2}} \times [105\pi^4 - 4K_0^8 + (-)^n 120K_0^8] + \cdots\}, \qquad (10.10)$$

may be readily obtained using Eqs. (10.9), (10.4), and (10.5). For loose-packed lattices $W_n^{(r)}$ and $S_n^{(r)}$ satisfy the simple relations

$$W_{2n}^{(r)} = \tfrac{1}{2}[W_{2n+1}^{(r)} + W_{2n-1}^{(r)}],$$
$$S_{2n}^{(r)} = \tfrac{1}{2}[S_{2n+1}^{(r)} + S_{2n-1}^{(r)}]. \qquad (10.11)$$

This last result may be verified in Table XI.

11. CONCLUDING REMARKS

The results derived in this paper find *direct* application in discrete potential theory, random walks with traps, spin wave theory, the spherical model, and scattering theory. For example, the expressions listed in Appendix A essentially give the critical point correlations for the spherical model with nearest neighbor interactions. Some of these applications will be discussed elsewhere. It is also hoped that the exact analytic continuations, which describe the "critical behavior" of the various random walk generating functions in Secs. 8–10, will help *indirectly* to elucidate the nature of critical point singularities.

Note added in proof. Recently Katsura and Horiguchi[69] have derived expansions for the real part $R_1(\xi_0)$ and imaginary part $R_2(\xi_0)$ of the Green's function (6.1) which are valid in the range $0 < \xi_0 \leq 1$. However, these authors did not obtain the formulas (6.16) and (6.17) which express $R_1(\xi_0)$ and $R_2(\xi_0)$ in terms of complete elliptic integrals. Hence, their "combined subroutine" for calculating $R_1(\xi_0)$ and $R_2(\xi_0)$ is not as convenient as that described in Sec. 6 of the present paper.

Further work on lattice Green's functions for cubic lattices has been carried out by Iwata,[70] Horiguchi and Morita,[71] and Joyce.[72]

APPENDIX A

In this Appendix exact expressions for the body-centered cubic lattice Green's function

$$P(l_1, l_2, l_3; 1) = \frac{1}{\pi^3} \iiint_0^\pi \frac{\cos l_1x_1 \cos l_2x_2 \cos l_3x_3}{1 - \cos x_1 \cos x_2 \cos x_3} dx_1\, dx_2\, dx_3,$$

where l_1, l_2, and l_3 are all even or all odd, are given for $0 \leq l_1 \leq l_2 \leq l_3 \leq 8$. For convenience, the following notation will be introduced:

$$\omega \equiv (K_0^2/\pi^2) \quad \text{and} \quad \alpha \equiv (1/K_0^2),$$

where K_0 denotes the complete elliptic integral $K(2^{-\frac{1}{2}})$;

$P(0,0,0;1) = 4\omega, \quad P(1,1,1;1) = 4\omega - 1,$

$P(0,0,2;1) = \alpha, \quad P(0,2,2;1) = 4\omega - 4\alpha,$

$P(2,2,2;1) = 16\omega + 9\alpha - 8,$

$P(1,1,3;1) = 2\alpha - 4\omega + 1,$

$P(1,3,3;1) = 20\omega - 20\alpha - 1,$

$P(3,3,3;1) = 76\omega + 126\alpha - 63,$

$P(0,0,4;1) = (4/9)\omega,$

$P(0,2,4;1) = 9\alpha - (64/9)\omega,$

$P(2,2,4;1) = 16 - 4\alpha - (380/9)\omega,$

$P(0,4,4;1) = (484/9)\omega - 64\alpha,$

$P(2,4,4;1) = (1664/9)\omega - 111\alpha - 32,$

$P(4,4,4;1) = (1476/9)\omega + 1344\alpha - 448,$

$P(1,1,5;1) = (44/9)\omega - 2\alpha - 1,$

$P(1,3,5;1) = 56\alpha - (444/9)\omega + 1,$

$P(3,3,5;1) = 191 - 230\alpha - (3204/9)\omega,$

$P(1,5,5;1) = (2644/9)\omega - 348\alpha - 1,$

$P(3,5,5;1) = (17100/9)\omega - 298\alpha - 575,$

$P(5,5,5;1) = 12210\alpha - (30564/9)\omega - 2369,$

$P(0,0,6;1) = (9/25)\alpha,$

$P(0,2,6;1) = (100/9)\omega - (324/25)\alpha,$

$P(2,2,6;1) = (656/9)\omega - (111/25)\alpha - 24,$

$P(0,4,6;1) = (5329/25)\alpha - (1600/9)\omega,$

$P(2,4,6;1) = (10\,556/25)\alpha - (4412/9)\omega + 48,$

$P(4,4,6;1) = 1952 - (21\,888/9)\omega - (94\,951/25)\alpha,$

$P(0,6,6;1) = 1156\omega - (34\,596/25)\alpha,$

$P(2,6,6;1) = (20\,624/9)\omega - (62\,399/25)\alpha - 72,$

$P(4,6,6;1) = (165\,636/9)\omega + (140\,764/25)\alpha - 8048,$

$P(6,6,6;1) = (2\,270\,961/25)\alpha - (677\,232/9)\omega - 216,$

$P(1,1,7;1) = (68/25)\alpha - (44/9)\omega + 1,$

$P(1,3,7;1) = (844/9)\omega - (2714/25)\alpha - 1,$

$P(3,3,7;1) = (7652/9)\omega + (7472/25)\alpha - 383,$

$P(1,5,7;1) = (31\,330/25)\alpha - (9\,444/9)\omega + 1,$

$P(3,5,7;1) = (68\,860/25)\alpha - (50\,444/9)\omega + 1151,$

$P(5,5,7;1) = 17\,025 - (82\,300/9)\omega - (1\,189\,400/25)\alpha,$

$P(1,7,7;1) = (57\,860/9)\omega - (192\,344/25)\alpha - 1,$

$P(3,7,7;1) = (207\,164/9)\omega - (491\,078/25)\alpha - 2303,$

$P(5,7,7;1) = (1\,396\,876/9)\omega + (3\,560\,470/25)\alpha - 95\,489,$

$P(7,7,7;1) = (10\,749\,228/25)\alpha - (9\,331\,020/9)\omega + 236\,033,$

$P(0,0,8;1) = (100/441)\omega,$

$P(0,2,8;1) = (441/25)\alpha - (6400/441)\omega,$

$P(2,2,8;1) = 32 + (412/25)\alpha - (46\,492/441)\omega,$

$P(0,4,8;1) = (184\,900/441)\omega - (12\,544/25)\alpha,$

$P(2,4,8;1) = (456\,384/441)\omega - (25\,471/25)\alpha - 64,$

$P(4,4,8;1) = (3\,606\,052/441)\omega + (184\,256/25)\alpha - 4992,$

$P(0,6,8;1) = (137\,641/25)\alpha - (2\,027\,776/441)\omega,$

$P(2,6,8;1) = 96 + (232\,124/25)\alpha - (3\,541\,340/441)\omega,$

$P(4,6,8;1) = 20\,288 + (166\,001/25)\alpha - (28\,133\,184/441)\omega,$

$P(6,6,8;1) = (38\,423\,268/441)\omega - (12\,488\,996/25)\alpha + 114\,976,$

$P(0,8,8;1) = (12\,687\,844/441)\omega - (861\,184/25)\alpha,$

$P(2,8,8;1) = (19\,611\,136/441)\omega - (1\,320\,103/25)\alpha - 128,$

$P(4,8,8;1) = (115\,819\,460/441)\omega - (3\,483\,136/25)\alpha - 50\,944,$

$P(6,8,8;1) = (436\,243\,968/441)\omega + (54\,201\,161/25)\alpha - 975\,232,$

$P(8,8,8;1) = 4\,469\,248 - (41\,413\,632/25)\alpha - (5\,048\,577\,180/441)\omega.$

APPENDIX B

We give below a table of values for the real part $R_1(\xi_0)$ and the imaginary part $R_2(\xi_0)$ of the Green's function

$$\lim_{\epsilon\to 0+} \frac{1}{\pi^3} \iiint_0^\pi \frac{dx_1\,dx_2\,dx_3}{\xi_0 - i\epsilon - \cos x_1 \cos x_2 \cos x_3},$$

in the range $0 < \xi_0 \leq 1$.

ξ_0	$R_1(\xi_0)$	$R_2(\xi_0)$	ξ_0	$R_1(\xi_0)$	$R_2(\xi_0)$
0.02	3.814 427 79	6.774 540 88	0.52	1.769 480 01	0.988 444 98
0.04	3.373 497 52	5.189 004 09	0.54	1.747 034 95	0.943 784 51
0.06	3.115 859 84	4.351 879 16	0.56	1.725 476 73	0.900 941 71
0.08	2.933 327 79	3.798 356 54	0.58	1.704 742 99	0.859 738 08
0.10	2.791 987 13	3.392 081 88	0.60	1.684 777 69	0.820 010 95
0.12	2.676 726 12	3.075 049 68	0.62	1.665 530 26	0.781 610 55
0.14	2.579 480 20	2.817 425 08	0.64	1.646 954 94	0.744 397 55
0.16	2.495 433 18	2.601 935 59	0.66	1.629 010 15	0.708 240 68
0.18	2.421 476 80	2.417 731 88	0.68	1.611 658 04	0.673 014 54
0.20	2.355 487 51	2.257 578 49	0.70	1.594 864 02	0.638 597 37
0.22	2.295 949 69	2.116 422 93	0.72	1.578 596 40	0.604 868 68
0.24	2.241 743 51	1.990 606 01	0.74	1.562 826 11	0.571 706 63
0.26	2.192 017 99	1.877 397 74	0.76	1.547 526 38	0.538 984 91
0.28	2.146 111 13	1.774 710 47	0.78	1.532 672 52	0.506 568 80
0.30	2.103 497 80	1.680 914 12	0.80	1.518 241 69	0.474 309 87
0.32	2.063 754 32	1.594 712 91	0.82	1.504 212 77	0.442 038 69
0.34	2.026 533 90	1.515 060 61	0.84	1.490 566 13	0.409 553 82
0.36	1.991 549 04	1.441 100 87	0.86	1.477 283 53	0.376 604 75
0.38	1.958 558 75	1.372 124 14	0.88	1.464 347 99	0.342 863 44
0.40	1.927 358 97	1.307 536 02	0.90	1.451 743 66	0.307 873 15
0.42	1.897 775 42	1.246 833 56	0.92	1.439 455 75	0.270 947 65
0.44	1.869 658 04	1.189 587 26	0.94	1.427 470 41	0.230 944 21
0.46	1.842 876 69	1.135 427 19	0.96	1.415 774 65	0.185 639 52
0.48	1.817 317 78	1.084 032 05	0.98	1.404 356 30	0.129 264 12
0.50	1.792 881 58	1.035 120 66	1.00	1.393 203 93	0

* This research has been supported in part by the United States Army through its European Office.

[1] R. Brout, Phys. Rev. **118**, 1009 (1960).
[2] G. Horwitz and H. B. Callen, Phys. Rev. **124**, 1757 (1961).
[3] B. V. Thompson and D. A. Lavis, Proc. Phys. Soc. (London) **91**, 645 (1967).
[4] R. Tahir-Kheli and D. ter Haar, Phys. Rev. **127**, 88 (1962).
[5] H. B. Callen, Phys. Rev. **130**, 890 (1963).
[6] N. W. Dalton and D. W. Wood, Proc. Phys. Soc. (London) **90**, 459 (1967).
[7] E. W. Montroll, Nuovo Cimento Suppl. **6**, 265 (1949).
[8] T. H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).
[9] M. Lax, Phys. Rev. **97**, 629 (1955).
[10] E. W. Montroll, J. Soc. Ind. Appl. Math. **4**, 241 (1956).
[11] E. W. Montroll, Proc. Symp. Appl. Math. **16**, 193 (1964).
[12] E. W. Montroll and G. H. Weiss, J. Math. Phys. **6**, 167 (1965).
[13] This procedure is justified since the series is uniformly convergent with respect to the variables x_1, x_2, x_3, for $|z| < 1$.
[14] W. F. Van Peijpe, Physica **5**, 465 (1938).
[15] G. N. Watson, Quart. J. Math. (Oxford) **10**, 266 (1939).
[16] G. N. Watson, Quart. J. Math. **39**, 27 (1908).
[17] The relation (1.8) which was first obtained for z real by A. A. Maradudin (unpublished work) is quoted in Ref. 41.
[18] See M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Natl. Bur. Stds., Washington, D.C., 1964), p. 598.
[19] I. Mannari and C. Kawabata (Physics Research Note No. 15, Okayama University, Okayama, Japan, 1964) have compiled an extensive set of tables for $P(z)$, $0 \leq z \leq 1$, using Eq. (1.8). A Chebyshev interpolation approximation for $P(z)$ has also been obtained by I. Mannari and H. Kageyama, Progr. Theoret. Phys. (Japan) Suppl. Extra No., 269 (1968).
[20] The value given by Montroll and Weiss (in Ref. 12) for the coefficient of $(1 - z)^{\frac{1}{2}}$ in the expansion (1.10) is incorrect.
[21] C. Domb and G. S. Joyce (unpublished).
[22] L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge U.P., Cambridge, 1966).
[23] A. Erdélyi *et al.*, *Higher Transcendental Functions I* (McGraw-Hill, New York, 1953), Chap. IV, p. 182.
[24] See Ref. 22, p. 108.
[25] For details of these special summation theorems see Ref. 22, p. 51.
[26] T. Clausen, J. Reine Angew. Math. **3**, 89 (1828); see also Ref. 22, p. 75.
[27] See Ref. 23, p. 108.
[28] See Ref. 23, p. 187.
[29] The required theorem is given in Ref. 22, p. 75, Theorem II.
[30] P. O. M. Olsson, J. Math. Phys. **7**, 702 (1966).
[31] The relation for C_n is obtained from a formula quoted in Ref. 30, p. 704, which was first derived by N. E. Nørlund in Act. Math. **94**, 289 (1955).
[32] J. S. Byrnes S. Podger, and W. W. Zachary, Proc. Cambridge Phil. Soc. **66**, 377 (1969).
[33] J. G. Darboux, J. Math. (France) **23**, 5, 577 (1878).
[34] G. S. Joyce (unpublished).
[35] This technique is described with examples in E. D. Rainville, *Special Functions* (Macmillan, New York, 1960), Chap. 14.
[36] This transformation is given in Ref. 22, p. 121.
[37] See Ref. 22, p. 51.
[38] Y. L. Luke, *The Special Functions and Their Approximations* (Academic, New York, 1969), p. 59.
[39] H. K. Hughes, Bull. Am. Math. Soc. **50**, 425 (1944).
[40] T. D. Riney, Trans. Am. Math. Soc. **88**, 214 (1958).
[41] A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman, and H. W. Milnes, *Green's Functions for Monoatomic Simple Cubic Lattices* (Académie Royale de Belgique, Bruxelles, 1960).
[42] To obtain accurate results and to avoid large rounding errors, it would be necessary in practice to have M considerably larger than n.
[43] N. W. McLachlan, *Theory and Application of Mathieu Functions* (Dover, New York, 1964), p. 202.
[44] G. S. Joyce, Phys. Rev. Letters **19**, 581 (1967).
[45] R. Sips, Trans. Am. Math. Soc. **90**, 340 (1959).

[46] See Ref. 19, p. 742.
[47] National Bureau of Standards, *Tables Relating to Mathieu Functions* (Columbia U.P., New York, 1951).
[48] The conversion procedure is described in Ref. 47.
[49] This result is proved in Ref. 22, p. 52.
[50] Since we are defining the ${}_3F_2(1)$ function (4.7) by analytic continuation, the condition $\mathrm{Re}\,(s) > 0$ in Eq. (4.4) may be relaxed.
[51] The contiguous function relations for generalized hypergeometric functions have been discussed in detail by E. D. Rainville in Ref. 35, p. 80. The required result Eq. (4.24) is a particular case of Rainville's relation (15), p. 82.
[52] This observation will be discussed in more detail in Paper II.
[53] See Ref. 38, p. 34.
[54] R. J. Duffin, Duke Math. J. **20**, 233 (1953).
[55] H. Davies, Quart. J. Math. (Oxford) **6**, 232 (1955).
[56] M. Yussouff and J. Mahanty, Proc. Phys. Soc. **87**, 689 (1966).
[57] The asymptotic expansion (5.10) was derived using a general technique developed by Montroll and Weiss (see Ref. 12, Appendix A). However, their final expression for $P(l, 1)$ is incorrect due to the omission of a "weighting factor" which counts the "effective" number of singularities in the region of integration. (For the simple cubic, body-centered cubic, and face-centered cubic lattices this weighting factor is 1, 4, and 2, respectively.)
[58] W. N. Bailey, Proc. Math. Soc. (London) **40**, 37 (1935).
[59] See Ref. 23, p. 111.
[60] For details see Ref. 38, p. 86.
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[62] A detailed discussion of this technique is given in Sec. 3.
[63] The first application of the method of Darboux in lattice statistics appears to have been made by B. W. Ninham, J. Math. Phys. **4**, 679 (1963).
[64] C. Domb, Proc. Cambridge Phil. Soc. **50**, 586 (1954).
[65] A. Dvoretzky and E. Erdös, in *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability* (University of California Press, Berkeley, Calif., 1951), p. 353.
[66] G. H. Vineyard, J. Math. Phys. **4**, 1191 (1963).
[67] C. Domb, J. Phys. C **3**, L85 (1970).
[68] M. E. Fisher, Rept. Progr. Phys. **30**, 615 (1967).
[69] S. Katsura and T. Horiguchi, J. Math. Phys. **12**, 230 (1971).
[70] G. Iwata, Natl. Sci. Rept., Ocanomizu Univ., Tokyo, **20**, 13 (1969).
[71] T. Horiguchi and T. Morita, Phys. Letters **32A**, 191 (1970).
[72] G. S. Joyce, J. Phys. C **4**, L53 (1971).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Quadratic Fermion Interaction Hamiltonian

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(Received 23 September 1970)

The interaction Hamiltonian $\lambda \int :\bar{\psi}^{(0)}(\mathbf{x})\psi^{(0)}(\mathbf{x}): g(\mathbf{x})d^s\mathbf{x}, g(\mathbf{x}) \in \mathcal{S}(\mathcal{R}^s)$ is studied. An ultraviolet cutoff is introduced. We remove this cutoff, and take the limit $g \to 1$ in $\mathcal{S}(\mathcal{R}^s)$, by working with the Heisenberg fields. The limiting fields are well defined on the Fock space associated with the bare mass m_0. In the limit we get a new representation of the canonical anticommutation relations which is given by a (generalized) Bogoliubov transformation. The new representation is not always unitarily equivalent to the bare mass Fock representations.

I. INTRODUCTION

The existence of many inequivalent representations of the canonical anticommutation relations (CAR) was pointed out by Friedrichs[1] and van Hove[2]; it was treated rigorously by Gårding and Wightman,[3] Wightman and Schweber,[4] and Golodes.[5] It is well known by now that there is an uncountable number of inequivalent representations of the CAR which are both the hope and the harm of the Hamiltonian approach to quantum field theory. The problem is to find the right representation which makes bona fide a given Hamiltonian. The point is that when one works in the Fock space, translations are not unitarily implementable because of Haag's theorem[6] and/or ultraviolet divergences.[7] The usual approach to find the "correct" representations is to butcher the Hamiltonian by introducing enough cutoffs to develop a well-defined theory in the Fock space, and then try to recover the correct theory by some limiting procedure. This approach has been suggested by Wightman[7] and forms the nucleus of the work of Glimm and Jaffe.[8]

In this note we exemplify Wightman's suggestion in the quadratic fermion interaction Hamiltonian. The method is the same one used by Guenin and Velo.[9]

For space–time dimensions $s + 1$, this model leads to a new representation of the CAR which is given by a (generalized for $s + 1 \geq 4$) Bogoliubov transformation. For $s + 1 \geq 4$ in finite or infinite volume, and for $s = 2$ in infinite volume, the new representation of the CAR is equivalent to the bare mass Fock representation. In all other cases the two representations are equivalent.

In Ref. 10 the same model has been studied by Glimm's method[11] in the form used by Hepp[12] and Fabrey.[13]

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[55] H. Davies, Quart. J. Math. (Oxford) **6**, 232 (1955).
[56] M. Yussouff and J. Mahanty, Proc. Phys. Soc. **87**, 689 (1966).
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[64] C. Domb, Proc. Cambridge Phil. Soc. **50**, 586 (1954).
[65] A. Dvoretzky and E. Erdös, in *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability* (University of California Press, Berkeley, Calif., 1951), p. 353.
[66] G. H. Vineyard, J. Math. Phys. **4**, 1191 (1963).
[67] C. Domb, J. Phys. C **3**, L85 (1970).
[68] M. E. Fisher, Rept. Progr. Phys. **30**, 615 (1967).
[69] S. Katsura and T. Horiguchi, J. Math. Phys. **12**, 230 (1971).
[70] G. Iwata, Natl. Sci. Rept., Ocanomizu Univ., Tokyo, **20**, 13 (1969).
[71] T. Horiguchi and T. Morita, Phys. Letters **32A**, 191 (1970).
[72] G. S. Joyce, J. Phys. C **4**, L53 (1971).

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For space–time dimensions $s + 1$, this model leads to a new representation of the CAR which is given by a (generalized for $s + 1 \geq 4$) Bogoliubov transformation. For $s + 1 \geq 4$ in finite or infinite volume, and for $s = 2$ in infinite volume, the new representation of the CAR is equivalent to the bare mass Fock representation. In all other cases the two representations are equivalent.

In Ref. 10 the same model has been studied by Glimm's method[11] in the form used by Hepp[12] and Fabrey.[13]

The model leads to linear field equations whose solution is trivial. However, working with the Hamiltonian, the model is far from trivial.

II. FORMAL AND CUTOFF HAMILTONIAN

We consider a Dirac field of bare mass m_0 in $(s+1)$-dimensional space–time whose free Hamiltonian H_0 is

$$H_0 = \int d^s s \, :\bar{\psi}^{(0)}(\mathbf{x})(-i\boldsymbol{\gamma}\cdot + m_0)\psi^{(0)}(\mathbf{x}):$$
$$= \sum_r \int d\mathbf{p}\omega(\mathbf{p})[a^*(\mathbf{p}, r)a(\mathbf{p}, r) + b^*(\mathbf{p}, r)b(\mathbf{p}, r)],$$

where

$$\psi^{(0)}(\mathbf{x}) = \frac{1}{(2\pi)^{s/2}} \int \frac{d\mathbf{p}}{\sqrt{\omega_{\mathbf{p}}}} \Big(\sum_r a(\mathbf{p}, r)u(\mathbf{p}, r; m_0)e^{i\mathbf{p}\cdot\mathbf{x}} + \sum_r b^*(\mathbf{p}, r)u(\mathbf{p}, r; m_0)e^{-i\mathbf{p}\cdot\mathbf{x}}\Big),$$

$$\bar{\psi}^{(0)}(\mathbf{x}) = \frac{1}{(2\pi)^{s/2}} \int \frac{d\mathbf{p}}{\sqrt{\omega_{\mathbf{p}}}} \Big(\sum_r b(\mathbf{p}, r)\bar{u}(\mathbf{p}, r; m_0)e^{i\mathbf{p}\cdot\mathbf{x}} + \sum_r a^*(\mathbf{p}, r)\bar{u}(\mathbf{p}, r, m_0)e^{-i\mathbf{p}\cdot\mathbf{x}}\Big),$$

$$\omega_{\mathbf{p}} = \omega(\mathbf{p}) = (p^2 + m_0^2)^{\frac{1}{2}},$$
$$[a(\mathbf{p}, r), a^*(\mathbf{p}', r')]_+ = \delta(\mathbf{p} - \mathbf{p}')\delta_{rr'},$$
$$[b(\mathbf{p}, r), b^*(\mathbf{p}', r')]_+ = \delta(\mathbf{p} - \mathbf{p})\delta_{rr'}.$$

All other anticommutators are equal to zero. We summarize the properties of the Dirac spinors in an appendix. H_0 is a self-adjoint operator on the usual Fock space $\mathcal{H}_{m_0}$, associated with a fermion of mass m_0. $\psi^{(0)}(\mathbf{x})$ and $\bar{\psi}^{(0)}(\mathbf{x})$ are densely defined bilinear forms in $\mathcal{H}_{m_0} \times \mathcal{H}_{m_0}$, and bounded operators when smeared out with test functions in L^2.

We add now to H_0 a new term:

$$H_I = \lambda \int :\bar{\psi}^{(0)}(\mathbf{x})\psi^{(0)}(\mathbf{x}): d\mathbf{x}$$
$$= \int d\mathbf{x} H_I(\mathbf{x})$$
$$= \lambda \sum_{r_1, r_2} \int dp \Big[\frac{\bar{u}(\mathbf{p}, r_1; m_0)u(-\mathbf{p}, r_2; m_0)}{(\omega_p\omega_p)^{\frac{1}{2}}} \times a^*(\mathbf{p}, r_1)b^*(-\mathbf{p}, r_2)$$
$$+ \frac{\bar{u}(\mathbf{p}, r_1; m_0)u(+\mathbf{p}, r_2; m_0)}{\omega_{\mathbf{p}}} a^*(\mathbf{p}, r_1)a(+\mathbf{p}, r_2)$$
$$- \frac{\bar{u}(\mathbf{p}, r, m_0)u(\mathbf{p}, r_2; m_0)}{\omega_{\mathbf{p}}} b^*(\mathbf{p}, r_2)b(+\mathbf{p}, r_2)$$
$$+ \frac{\bar{u}(-\mathbf{p}, r_1)u(+\mathbf{p}, r_2)}{\sqrt{\omega_{\mathbf{p}}}} b(-\mathbf{p}, r_1)a(\mathbf{p}, r_2)\Big]$$
$$= H_{I2} + H_{I1} + H_{I0},$$

which, formally, is the fermion mass renormalization. However, H_I, and therefore $H_0 + H_I$, are not well defined on $\mathcal{H}_{m_0}$ for two reasons: first, because of a simple manifestation of Haag's theorem, namely, if we let Ω_0 be the Fock vacuum, then

$$\|(H_0 + H_I)\Omega_0\|^2 = \int_{x_0=y_0=0} d\mathbf{x}\, d\mathbf{y}[\Omega_0, H_I(\mathbf{x})H_I(\mathbf{y})\Omega_0]$$
$$= \int d\mathbf{x}\, d\mathbf{y} F(\mathbf{x} - \mathbf{y}) = \infty.$$

In the second equality we have used translation invariance. Second, because of ultraviolet divergences, namely, if $g(x) \in \mathfrak{D}$ is a form factor which takes care of the infinite volume divergence, then

$$\|H_I(g)\Omega_0\|^2 \sim \|H_{I2}(g)\Omega_0\|^2$$
$$= \lambda^2 \sum_{r_1, r_2} \int dp_1\, dp_2 \left|\frac{\bar{u}(\mathbf{p}_1, r_1; m_0)u(+\mathbf{p}_2, r_2; m_0)}{(\omega_{\mathbf{p}_1}\omega_{\mathbf{p}_2})^{\frac{1}{2}}}\right|^2 \times |g(\mathbf{p}_1 + \mathbf{p}_2)|^2$$

diverges for $s \geq 1$ since $\left|\frac{u(\mathbf{p}_1, r_1; m_0)u(\mathbf{p}_2, r_2; m_0)}{(\omega_{p_1}\omega_{p_2})^{\frac{1}{2}}}\right|$ is bounded. Thus we must introduce an ultraviolet cutoff κ. We do this by restricting the momentum integrations in $(-\kappa, \kappa)$. Then our cutoff Hamiltonian reads

$$H_\kappa(g) = H_0 + H_{I\kappa}(g)$$
$$= H_0 + \lambda \int d\mathbf{x} :\bar{\psi}_\kappa^{(0)}(\mathbf{x})\psi_\kappa^{(0)}(\mathbf{x}): g(\mathbf{x})$$
$$= H_0 + \lambda \int d\mathbf{p}_1\, d\mathbf{p}_2 \hat{g}(\mathbf{p}_1 + \mathbf{p}_2)\hat{\chi}_\kappa(\mathbf{p}_1, \mathbf{p}_2) \times \Big(\frac{\bar{u}(\mathbf{p}_1, r_1)v(\mathbf{p}_2, r_2)}{(\omega_{\mathbf{p}_1}\omega_{\mathbf{p}_2})^{\frac{1}{2}}} a^*(\mathbf{p}_1, r_1)b^*(\mathbf{p}_2, r_2)$$
$$+ \frac{\bar{u}(-\mathbf{p}_2, r_1)u(\mathbf{p}_1, r_2)}{(\omega_{\mathbf{p}_1}\omega_{\mathbf{p}_2})^{\frac{1}{2}}} a^*(\mathbf{p}_1, r_2)a(-\mathbf{p}_2, r_2)$$
$$- \frac{\bar{v}(-\mathbf{p}_2, r_1)v(\mathbf{p}_1, r_2)}{(\omega_{\mathbf{p}_1}\omega_{\mathbf{p}_2})^{\frac{1}{2}}} b^*(\mathbf{p}_1, r_2)b(-\mathbf{p}_2, r_1)$$
$$+ \frac{\bar{v}(-\mathbf{p}_1 r_1)u(-\mathbf{p}_2, r_2)}{(\omega_{\mathbf{p}_1}\omega_{\mathbf{p}_2})^{\frac{1}{2}}} \times b(-\mathbf{p}_1, r_1)a(-\mathbf{p}_2, r_2)\Big),$$

where $\hat{g}$ is the Fourier transform

$$\hat{g}(\mathbf{p}) = \frac{1}{(2\pi)^s} \int d\mathbf{x} e^{i\mathbf{p}\cdot\mathbf{x}} g(\mathbf{x}),$$

and

$$\hat{\chi}_\kappa(\mathbf{p}_1, \mathbf{p}_2) = 1 \quad \text{for} \quad |\mathbf{p}_1|, |\mathbf{p}_2| \leq \kappa,$$
$$= 0 \quad \text{otherwise}.$$

Simple estimations show that $H_{I\kappa}(g)$, $\kappa < +\infty$, is a self-adjoint bounded operator for real $g(\mathbf{x})$. Thus, $H_\kappa(g) = H_0 + H_{I\kappa}(g)$, $\kappa < +\infty$, is a self-adjoint operator with domain $D[H_\kappa(g)] = D(H_0)$.

III. HEISENBERG FIELDS

Since $H_\kappa(g)$ is a self-adjoint operator, $e^{itH_\kappa(g)}$ is a well-defined unitary operator. Thus we can define

$$\psi_{\kappa g}(\mathbf{x}, i) = e^{itH_\kappa(g)}\psi^{(0)}(\mathbf{x})e^{-itH_\kappa(g)}.$$

Let us write

$$\psi_{\kappa g}(\mathbf{x}, t) = \frac{1}{(2\pi)^{s/2}}\int \frac{dp}{\sqrt{\omega_p}}\Big(\sum_r \tilde{a}_{g\kappa}(\mathbf{p}, r, t)u(\mathbf{p}, r, m_0)e^{i\mathbf{p}\cdot\mathbf{x}} + \sum \tilde{b}^*_{g\kappa}(\mathbf{p}, r, t)v(\mathbf{p}, r, m_0)e^{-i\mathbf{p}\cdot\mathbf{x}}\Big);$$

then

$$\tilde{a}_{g\kappa}(\mathbf{p}, r, t) = e^{itH_\kappa(g)}a(\mathbf{p}, r)e^{-itH_\kappa(g)}$$

satisfies the Heisenberg equations of motion, namely,

$$i\frac{\partial \tilde{a}_{g\kappa}(\mathbf{p}, r, t)}{\partial t} = [\tilde{a}_{g\kappa}(p, r, t), H_\kappa(g)], \tag{1}$$

with the initial conditions

$$\tilde{a}_{g\kappa}(\mathbf{p}, r, 0) = a(\mathbf{p}, r), \quad \tilde{b}^*_{g\kappa}(\mathbf{p}, r, 0) = b(\mathbf{p}, r).$$

To solve these linear equations, we make the following ansatz:

$$\tilde{a}_{\kappa g}(\mathbf{p}, r, t) = \sum_{r'}\int K_1^{(\kappa g)}(t, \mathbf{p}, r, \mathbf{p}', r')a(\mathbf{p}', r')\,d\mathbf{p}' + \sum_{r'}\int K_2^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}', r')b^*(-\mathbf{p}', r')\,d\mathbf{p}'. \tag{2}$$

Substituting (2) into (1), we find that $K_1^{(\kappa,g)}$ and $K_2^{(\kappa,g)}$ satisfy a system of integro-differential equations

$$\begin{aligned}
i\frac{\partial K_1^{(\kappa,g)}(t, \mathbf{p}, r, p', r')}{\partial t} &= \omega(\mathbf{p}')K_1^{(\kappa,g)}(t, \mathbf{p}, r, p', r') + \lambda\int d\mathbf{p}''\hat{g}(\mathbf{p}'' - \mathbf{p}')\chi_\kappa(\mathbf{p}'', -\mathbf{p}') \\
&\times \Big(\sum_{r''}\frac{\bar{u}(\mathbf{p}'', r''; m_0)u(\mathbf{p}', r'; m_0)}{(\omega'\omega'')^{\frac{1}{2}}} \times K_1^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}'', r'') \\
&+ \sum_{r''}\frac{v(-\mathbf{p}'', r'', m_0)u(\mathbf{p}', r', m_0)}{(\omega'\omega'')^{\frac{1}{2}}} \times K_2^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}'', r'')\Big);\\
i\frac{\partial K^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}', r')}{\partial t} &= -\omega(\mathbf{p}')K_2^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}', r') + \lambda\int d\mathbf{p}''\hat{g}(\mathbf{p}'' - \mathbf{p}')\chi_\kappa(\mathbf{p}'', -\mathbf{p}') \\
&\times \Big(\sum_{r''}\frac{u(\mathbf{p}'', r'', m_0)v(-\mathbf{p}', r', m_0)}{(\omega'\omega'')^{\frac{1}{2}}} \times K_1^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}'', r'') \\
&+ \sum_{r''}\frac{v(-\mathbf{p}'', r'', m_0)v(-\mathbf{p}', r', m_0)}{(\omega'\omega'')^{\frac{1}{2}}} \times K_2^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}'', r'')\Big),
\end{aligned} \tag{3}$$

with initial conditions

$$K_1^{(\kappa,g)}(0, \mathbf{p}, r, \mathbf{p}', r') = \delta(\mathbf{p} - \mathbf{p}')\delta_{rr'}, \quad K_2^{(\kappa,g)}(0, \mathbf{p}, r, \mathbf{p}', r') = 0. \tag{4}$$

Define

$$K^{(\kappa,g)}(t, \mathbf{p}, \mathbf{p}', r') = \begin{pmatrix} e^{i\omega_{p'}t}K_1^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}', r') \\ e^{-i\omega_{p'}t}K_2^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}', r')\end{pmatrix} \tag{5}$$

and

$$L^{(\kappa)}(t, \mathbf{p}', r', \mathbf{p}'', r'') = \frac{1}{\lambda}\chi_\kappa(\mathbf{p}'', -\mathbf{p}')\begin{pmatrix} e^{i(\omega'-\omega'')t}\dfrac{\bar{u}(\mathbf{p}'', r''; m_0)u(\mathbf{p}', r'; m_0)}{\omega'\omega''}, & e^{i(\omega'+\omega'')t}\dfrac{\bar{u}(-\mathbf{p}'', r'', m_0)u(\mathbf{p}', r', m_0)}{\omega'\omega''} \\ e^{-i(\omega'+\omega'')t}\dfrac{\bar{u}(\mathbf{p}'', r'', m_0)v(-\mathbf{p}', r', m_0)}{\omega'\omega''}, & e^{-i(\omega'-\omega'')t}\dfrac{\bar{v}(-\mathbf{p}'', r'', m_0)v(-\mathbf{p}', r')}{\omega'\omega''}\end{pmatrix}. \tag{6}$$

Then (3) can be written in the compact form

$$\frac{\partial}{\partial t}K^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}', r') = \lambda\int d\mathbf{p}''\hat{g}(\mathbf{p}'' - \mathbf{p}')\sum_{r''}L^{(\kappa)}(t, \mathbf{p}', r', \mathbf{p}'', r'') \times K^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}'', r''). \tag{7}$$

Theorem 1: (7) with initial conditions (4) has a unique solution, which, smeared out in $\mathbf{p}$ with test functions in $\mathcal{S}(\mathcal{R}^s)$, belongs to $\mathcal{S}(\mathcal{R}^s)$ in $\mathbf{p}'$. Furthermore, this solution, when smeared out in $\mathbf{p}$ with test functions in $\mathcal{S}(\mathcal{R}^s)$, converges in the $\mathcal{S}$ topology as $\kappa \to +\infty$, and $g \to 1$ and the limit is the solution of (7) with $g = 1$ and $\kappa = +\infty$.

Proof: Let

$$f(p) \in \mathcal{S}(\mathfrak{R}^s).$$

Then

$$K^{(\kappa,g)}(t, r, \mathbf{p}', r') = \int d\mathbf{p} f(\mathbf{p}) K^{(\kappa,g)}(t, \mathbf{p}, r, \mathbf{p}', r')$$

is a solution of

$$K^{(\kappa,g)}(t, r, \mathbf{p}', r') = K^{(\kappa,g)}(0, r, \mathbf{p}', r') + \int_0^t dt \int d\mathbf{p}'' \hat{g}(\mathbf{p}'' - \mathbf{p}') \sum_{r''} L^{(\kappa)}(t, \mathbf{p}', r', \mathbf{p}'') K^{(\kappa,g)}(t, r, \mathbf{p}'', r'), \qquad (8)$$

with initial condition

$$K^{(\kappa,g)}(0, r, \mathbf{p}', r') = \begin{pmatrix} \delta_{rr'} f(\mathbf{p}') \\ 0 \end{pmatrix}$$

Iterating (8) we get the Neumann series

$$\begin{aligned} K^{(\kappa,g)}&(t, r, \mathbf{p}', r') \\ &= K^{(\kappa,g)}(0, r, \mathbf{p}', r') + \sum_{n=1}^{+\infty} \lambda^n \int d\mathbf{p}_1 \cdots d\mathbf{p}_n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \hat{g}(\mathbf{p}_1 - \mathbf{p}') \hat{g}(\mathbf{p}_2 - \mathbf{p}_1) \cdots g_n(\mathbf{p} - \mathbf{p}_{n-1}) \\ &\times \left(\sum_{r_1,\cdots,r_n} L^{(\kappa)}(t_1, \mathbf{p}', r', \mathbf{p}_1, r_1) L^{(\kappa)}(t_2, \mathbf{p}_1, r_1, \mathbf{p}_2, r_2) \cdots L^{(\kappa)}(t_n, \mathbf{p}_{n-1}, r_{n-1}\mathbf{p}_n, r_n) K^{(\kappa,g)}(0, r, \mathbf{p}_n, r_n) \right). \end{aligned}$$

From (6) we have

$$\|L^{(\kappa)}(t, \mathbf{p}, r, \mathbf{p}', r')\| \le C_1, \qquad (9)$$

where C_1 is independent of t, $\mathbf{p}$, r, $\mathbf{p}'$, r', and κ. Thus we get

$$|K^{(\kappa,g)}(t, r, \mathbf{p}', r')| \le \sum_{n=0} \frac{C_2^n t^n}{n!} \|K^{(\kappa,g)}(0, r, \mathbf{p}', r')\|_\infty, \qquad (10)$$

where the constant C_2 is independent of t, $\mathbf{p}$, r, $\mathbf{p}'$, r', κ, and g. Therefore the convergence of the Neumann series is uniform in $\mathbf{p}'$, κ, and g. The same kind of estimates we can make for

$$\left\| \left(\prod_{j=1}^{s} p_j'^{\alpha_j} \right) \left(\prod_{i=1}^{s} \frac{\partial^{p_i}}{\partial p_i' p_j} \right) K^{(\kappa,g)}(t, r, p', r') \right\|,$$

proving the convergence in $\mathcal{S}(\mathfrak{R}^s)$ as $\kappa \to +\infty$, $g \to 1$.

IV. LIMITING SOLUTION AND THE ASSOCIATED BOGOLIUBOV TRANSFORMATION

For $\kappa = +\infty$, and $g = 1$, $g(\mathbf{p}'' - \mathbf{p}') = \delta(\mathbf{p}'' - \mathbf{p}')$, (3) becomes

$$\begin{aligned} i \frac{\partial K_1(t, \mathbf{p}, r, \mathbf{p}', r')}{\partial t} &= -\omega(\mathbf{p}') K_1(t, \mathbf{p}, r, \mathbf{p}', r') \\ &+ \frac{\lambda m_0}{\omega(p')} K_1(t, \mathbf{p}, r, \mathbf{p}', r') \\ &+ \lambda \sum_{r''} \frac{\bar{v}(-\mathbf{p}', r'', m_0) u(\mathbf{p}, r', m_0)}{\omega'} \\ &\times K_2(t, \mathbf{p}, r, \mathbf{p}', r''), \end{aligned}$$

$$\begin{aligned} i \frac{\partial K_2(t, \mathbf{p}, r, \mathbf{p}', r')}{\partial t} &= -\omega(\mathbf{p}') K_2(t, \mathbf{p}, r, \mathbf{p}', r') \\ &+ \frac{\lambda m_0}{\omega'} K_2(t, \mathbf{p}, r, \mathbf{p}', r') \\ &+ \lambda \sum_{r''} \frac{\bar{u}(\mathbf{p}', r'', m_0) v(-\mathbf{p}', r', m_0)}{\omega'} \\ &\times K_1(t, \mathbf{p}, r, \mathbf{p}', r''). \end{aligned} \qquad (11)$$

To solve these equations we make the ansatz

$$\begin{aligned} K_1(t, \mathbf{p}, r, \mathbf{p}', r') &= A_1(\mathbf{p}, r, \mathbf{p}', r') e^{-i\Omega t} + A_1'(\mathbf{p}, r, \mathbf{p}', r') e^{i\Omega t}, \\ K_2(t, \mathbf{p}, r, \mathbf{p}', r') &= A_2(\mathbf{p}, r, \mathbf{p}', r') e^{-i\Omega t} + A_2'(\mathbf{p}, r, \mathbf{p}', r') e^{i\Omega t}, \end{aligned}$$

where $\Omega(\mathbf{p}) = (p^2 + (m_0 + \lambda)^2)^{\frac{1}{2}}$. Then

$$\begin{aligned} K_1(t, \mathbf{p}, r, \mathbf{p}', r') &= \left(\frac{\Omega\omega^2 + \omega^2 + \lambda m_0}{2\Omega\omega} e^{-i\Omega t} + \frac{\Omega\omega^2 - \omega^2 - \lambda m_0}{2\Omega\omega} e^{i\Omega t} \right) \\ &\times \delta(p - p') \delta_{rr'}, \\ K_2(t, \mathbf{p}, r, \mathbf{p}', r') &= \frac{\lambda}{2\Omega} \frac{u(\mathbf{p}, r, m_0) v(-\mathbf{p}, r', m_0)}{\omega} (e^{-i\Omega t} - e^{i\Omega t}) \delta(\mathbf{p} - \mathbf{p}') \end{aligned} \qquad (12)$$

Theorem 2:

$$\begin{aligned} \tilde{a}_{\kappa g}(t, \mathbf{p}, r) &= \sum_{r'} \int K_1^{(\kappa g)}(t, \mathbf{p}, r, \mathbf{p}', r') a(\mathbf{p}', r') \, d\mathbf{p}' \\ &+ \sum_{r'} \int K_2^{(\kappa g)}(t, \mathbf{p}, r, \mathbf{p}', r') b^*(-\mathbf{p}', r') \, d\mathbf{p}', \end{aligned}$$

when smeared out with test functions in $\mathcal{S}(\mathcal{R}^s)$, converges, as $\kappa \to +\infty$, $g \to 1$, to

$$\tilde{a}(t, \mathbf{p}, r) = \sum_{r'} \int K_1(t, \mathbf{p}, r, \mathbf{p}', r')a(\mathbf{p}', r')\, d\mathbf{p}' + \sum_{r'} \int K_2(t, \mathbf{p}, r, \mathbf{p}', r')b^*(-\mathbf{p}', r')\, d\mathbf{p}'$$

in the norm topology of $\mathcal{L}(\mathcal{H}_{m_0})$.

Proof: By Theorem 1, it suffices to prove that if $f_n \xrightarrow{\mathcal{S}(\mathcal{R}^s)} f$, then $a^{\#}(f_n) \to a^{\#}(f)$ uniformly. Indeed

$$\|a^{\#}(f_n) - a^{\#}(f)\| = \|a^{\#}(f_n - f)\| \leq \|f_n - f\| \to 0,$$

where $\|f_n - f\|$ is some $\mathcal{S}(\mathcal{R}^s)$ norm.

This theorem implies that $\psi_{\kappa g}(\mathbf{x}, t)$, when smeared out with functions in $L_2(\mathcal{R}^s)$, converges uniformly to

$$\psi(\mathbf{x}, t) = \frac{1}{(2\pi)^{s/2}} \int \frac{d\mathbf{p}}{\sqrt{\omega_\mathbf{p}}} \times \sum_r (\tilde{a}(\mathbf{p}, r, t)u(\mathbf{p}, r, m_0)e^{i\mathbf{p}\cdot\mathbf{x}} + \tilde{b}^*(\mathbf{p}, r, t)v(\mathbf{p}, r, m_0)e^{-i\mathbf{p}\cdot\mathbf{x}})$$

in $\mathcal{L}(\mathcal{H}_{m_0})$.

After some simple manipulations we obtain

$$\psi(x, t) = \frac{1}{(2\pi)^{s/2}} \int \frac{d\mathbf{p}}{(\Omega(\mathbf{p}))^{\frac{1}{2}}} \times \left(\sum_r \tilde{a}(\mathbf{p}, r)u(\mathbf{p}, r; m)e^{-i\Omega t + i\mathbf{p}\cdot\mathbf{x}} + \sum_r \tilde{b}^*(\mathbf{p}, r)v(\mathbf{p}, r, m)e^{i\Omega t - i\mathbf{p}\cdot\mathbf{x}}\right), \quad (13)$$

where $m = m_0 + \lambda$, and

$$\tilde{a}(\mathbf{p}, r) = \sum_{r'} \left(\frac{\bar{u}(\mathbf{p}, r; m)\gamma^0 u(\mathbf{p}, r'; m_0)}{(\omega\Omega)^{\frac{1}{2}}} a(\mathbf{p}, r') + \frac{\bar{u}(\mathbf{p}, r; m)\gamma^0 v(-\mathbf{p}, r'; m_0)}{(\omega\Omega)^{\frac{1}{2}}} b^*(-\mathbf{p}, r')\right),$$

$$\tilde{b}^*(-\mathbf{p}, r) = \sum_{r'} \left(\frac{\bar{u}(-\mathbf{p}, r; m)\gamma^0 u(\mathbf{p}, r'; m_0)}{(\Omega\omega)^{\frac{1}{2}}} a(p, r') + \frac{\bar{v}(-\mathbf{p}, r; m)\gamma^0 v(-\mathbf{p}, r'; m_0)}{(\Omega\omega)^{\frac{1}{2}}} b^*(-\mathbf{p}, r')\right). \quad (14)$$

In two- and three-dimensional space–time, the sum over r' reduces to a single term and the canonical transformation in (14) is the ordinary Bogoliubov transformation. For this transformation, it is known, Uhlenbrock,[14] Ezawa,[15] Klauder and McKenna,[16] and Berezin,[17] that the new representation is unitary equivalent to the original representation if and only if

$$\int d^s\mathbf{p} \left| \frac{\bar{u}(\mathbf{p}; m)\gamma^0 v(-\mathbf{p}; m_0)}{(\Omega\omega)^{\frac{1}{2}}} \right|^2 < +\infty, \quad s = 1, 2. \quad (15)$$

After simple γ gimmics, the integral can be written as

$$\tfrac{1}{2}\int d^s\mathbf{p}\, \frac{\Omega(\mathbf{p})\omega(\mathbf{p}) - p^2 - mm_0}{\Omega(\mathbf{p})\omega(\mathbf{p})},$$

which is convergent for $s = 1$, but divergent for $s = 2$.

In space of finite volume with periodic boundary conditions, criterion (15) reads

$$\sum_\mathbf{p} \left| \frac{\bar{u}(\mathbf{p}; m)\gamma^0 v(-\mathbf{p}, m_0)}{(\Omega\omega)^{\frac{1}{2}}} \right|^2 < +\infty$$

or

$$\tfrac{1}{2}\sum_\mathbf{p} \left(\frac{\Omega(\mathbf{p})\omega(\mathbf{p}) - \mathbf{p}^2 - mm_0}{\Omega(\mathbf{p})\omega(\mathbf{p})}\right) < +\infty, \quad (16)$$

which is satisfied for $s = 1, 2$.

For $s \geq 3$, we get a generalized Bogoliubov transformation. This transformation has been studied in 10. This study shows that the transformation (14) is unitarily inequivalent to the Fock representation associated with a fermion of bare mass m_0.

APPENDIX: CONVENTIONS AND SPINORS

We use the metric

$$g_{00} = 1, \quad g_{ii} = -1, \quad g_{\mu\nu} = 0 \quad \text{for} \quad \mu \neq \nu.$$

The Dirac matrices satisfy

$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2g_{\mu\nu}.$$

They form an irreducible Clifford algebra whenever s is odd. We assume that the γ's are unitary and $\gamma_0^* = \gamma_0$, $\gamma_j^* = -\gamma_j$. We denote $u^*(\mathbf{p})\gamma^0$ by $\bar{u}(\mathbf{p})$. The spinors satisfy

$$(\gamma \cdot p - m)u(\mathbf{p}) = 0, \quad \bar{u}(\mathbf{p})(\gamma \cdot p - m) = 0.$$
$$(\gamma \cdot p + m)v(\mathbf{p}) = 0, \quad \bar{v}(\mathbf{p})(\gamma \cdot p + m) = 0.$$

They are normalized so that

$$u^*(\mathbf{p}, r)u(\mathbf{p}, s) = \omega_p\delta_{rs}, \quad \bar{u}(\mathbf{p}, r)u(\mathbf{p}, s) = m\delta_{rs},$$
$$v^*(\mathbf{p}, r)v(\mathbf{p}, s) = \omega_p\delta_{rs}, \quad \bar{v}(\mathbf{p}, r)v(\mathbf{p}, s) = m\delta_{rs}.$$

The orthogonality is expressed by

$$\sum_r u_\alpha(\mathbf{p}, r)\bar{u}_\beta(\mathbf{p}, r) = (\gamma \cdot p + m)_{\alpha\beta}/2,$$
$$\sum_r v_\alpha(\mathbf{p}, r)\bar{v}_\beta(\mathbf{p}, r) = (\gamma \cdot p - m)_{\alpha\beta}/2.$$

We need the following properties

$$\sum_{r,r'} |u(\mathbf{p}, r)v(\mathbf{p}', r')|^2 = p \cdot p' - m^2 = \omega(\mathbf{p})\omega(\mathbf{p}') - \mathbf{p} \cdot \mathbf{p}' - m,$$

$$u^*(\mathbf{p}, r)v(-\mathbf{p}, s) = 0 = u^*(-\mathbf{p}, r)u(\mathbf{p}, s).$$

[1] K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields* (Interscience, New York, 1953).
[2] L. van Hove, Phys. **18**, 145 (1952).
[3] L. Gårding and A. S. Wightman, Proc. Natl. Acad. Aci. (U.S.) **40**, 617 (1954).
[4] A. S. Wightman and S. S. Schweber, Phys. Rev. **98**, 812 (1955).

[5] V. Golodes, Usp. Mat. Nauk 2, 122 (1965); 6, 126 (1965) (in Russian).
[6] R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics and All That* (Benjamin, New York, 1964).
[7] A. S. Wightman, Cargese lectures, 1964.
[8] J. Glimm and A. Jaffe, "A $\lambda\varphi^4$ Quantum Field Theory without Cutoffs.I, II, III" (unpublished).
[9] M. Guenin and G. Velo, Helv. Phys. Acta 41, 362 (1968).
[10] B. Gidas, thesis, University of Michigan.
[11] J. Glimm, Commun. Math. Phys. 10, 1 (1968).
[12] K Hepp, *Les Systèmes à un nombre infini de degrés de liberté* (C.N.R.S., Paris, 1969).
[13] J. Fabrey, "Exponential Representations of the CCR," thesis, M.I.T., 1969.
[14] D. Uhlenbrock, Commun. Math. Phys. 4, 64 (1967).
[15] H. Ezawa, J. Math. Phys. 6, 380 (1965).
[16] J. Klauder and J. McKenna, J. Math. Phys. 6, 68 (1965); J. Klauder, J. McKenna, and E. Woods, *ibid.* 7, 822 (1966).
[17] F. Berezin, *Methods of Second Quantization* (Academic, New York, 1966).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Microscopic Theory of a Multicomponent System of Charged and Neutral Particles. I. General Quantum Statistical Formulation

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(Received 28 January 1970)

Recent contributions to the Lee–Yang–Mohling theory of single-component quantum fluids have enabled us to develop a new theory of the quantum statistics for a multicomponent nonrelativistic system of charged and neutral particles in thermal equilibrium. With the emphasis as much as possible on the physical content of the theory, this paper presents the new formulation of quantum statistics with explicit rules for calculating the grand potential and particle and photon momentum distributions. The present formalism not only simplifies and corrects an earlier version, but also it has made possible clear and systematic procedures for resolving some divergence difficulties that occur in the many-body theory of fully ionized gases.

1. INTRODUCTION

Interest in controlled thermonuclear reactions, stellar atmospheres and interiors, and, more generally, plasmas has focused attention on the physics of fully ionized gases. Although a theory of the nonequilibrium partially ionized gas should be avidly pursued, the more modest goal of developing a precursory theory of the nonrelativistic fully ionized gas in thermal equilibrium is justified in view of the horrendous complexity of the problem. Moreover, a study of the equilibrium properties of a system can provide important information about nonequilibrium systems—for example, about linear response and transport phenomena.

A few years ago, Mohling and Grandy[1] developed a formalism for calculating thermodynamic properties, momentum distributions, and pair-correlation functions for a nonrelativistic, multicomponent, fully ionized gas in thermal equilibrium, and that theory has been used in several calculations.[2] It was later realized that two classes of photon self-energy structures [called (0, 2) and (2, 0) structures] were accidentally omitted in the self-energy analysis in MG, and it was therefore of interest to amend MG so as to include the missing self-energy structures. However, Mohling, RamaRao, and Shea[3] have recently developed a simple and appealing new master-graph theory of a real quantum fluid in thermal equilibrium; the formalism in MRS applies to a single-component quantum fluid (degenerate or nondegenerate) with a short-range interaction. Moreover, Tuttle[4] has demonstrated that a powerful counterterm technique can be included easily in a quantum statistical theory, such as that of MRS, based upon the Ursell expansion. Thus, rather than revise and correct MG *per se*, we propose, in this paper, to extend MRS to apply to a multicomponent system of charged and neutral particles and concurrently to incorporate the counterterm technique of Tuttle. The results of our development are expressed in terms of diagrammatic expansions for momentum distributions and the grand potential.

It seems characteristic of any many-body theory to be plagued by divergencies and spurious results. For the systems of interest here, the developments in quantum electrodynamics allow us to take cognizance of some prospective troublesome features of the theory. Thus, from the beginning, we address ourselves to the tasks of renormalizing bare masses of charged particles, of dealing with the infrared problem, and of summing the so-called Coulomb ring diagrams.

[5] V. Golodes, Usp. Mat. Nauk 2, 122 (1965); 6, 126 (1965) (in Russian).
[6] R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics and All That* (Benjamin, New York, 1964).
[7] A. S. Wightman, Cargese lectures, 1964.
[8] J. Glimm and A. Jaffe, "A $\lambda\varphi^4$ Quantum Field Theory without Cutoffs.I, II, III" (unpublished).
[9] M. Guenin and G. Velo, Helv. Phys. Acta 41, 362 (1968).
[10] B. Gidas, thesis, University of Michigan.
[11] J. Glimm, Commun. Math. Phys. 10, 1 (1968).
[12] K Hepp, *Les Systèmes à un nombre infini de degrés de liberté* (C.N.R.S., Paris, 1969).
[13] J. Fabrey, "Exponential Representations of the CCR," thesis, M.I.T., 1969.
[14] D. Uhlenbrock, Commun. Math. Phys. 4, 64 (1967).
[15] H. Ezawa, J. Math. Phys. 6, 380 (1965).
[16] J. Klauder and J. McKenna, J. Math. Phys. 6, 68 (1965); J. Klauder, J. McKenna, and E. Woods, *ibid.* 7, 822 (1966).
[17] F. Berezin, *Methods of Second Quantization* (Academic, New York, 1966).

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(Received 28 January 1970)

Recent contributions to the Lee–Yang–Mohling theory of single-component quantum fluids have enabled us to develop a new theory of the quantum statistics for a multicomponent nonrelativistic system of charged and neutral particles in thermal equilibrium. With the emphasis as much as possible on the physical content of the theory, this paper presents the new formulation of quantum statistics with explicit rules for calculating the grand potential and particle and photon momentum distributions. The present formalism not only simplifies and corrects an earlier version, but also it has made possible clear and systematic procedures for resolving some divergence difficulties that occur in the many-body theory of fully ionized gases.

1. INTRODUCTION

Interest in controlled thermonuclear reactions, stellar atmospheres and interiors, and, more generally, plasmas has focused attention on the physics of fully ionized gases. Although a theory of the nonequilibrium partially ionized gas should be avidly pursued, the more modest goal of developing a precursory theory of the nonrelativistic fully ionized gas in thermal equilibrium is justified in view of the horrendous complexity of the problem. Moreover, a study of the equilibrium properties of a system can provide important information about nonequilibrium systems—for example, about linear response and transport phenomena.

A few years ago, Mohling and Grandy[1] developed a formalism for calculating thermodynamic properties, momentum distributions, and pair-correlation functions for a nonrelativistic, multicomponent, fully ionized gas in thermal equilibrium, and that theory has been used in several calculations.[2] It was later realized that two classes of photon self-energy structures [called (0, 2) and (2, 0) structures] were accidentally omitted in the self-energy analysis in MG, and it was therefore of interest to amend MG so as to include the missing self-energy structures. However, Mohling, RamaRao, and Shea[3] have recently developed a simple and appealing new master-graph theory of a real quantum fluid in thermal equilibrium; the formalism in MRS applies to a single-component quantum fluid (degenerate or nondegenerate) with a short-range interaction. Moreover, Tuttle[4] has demonstrated that a powerful counterterm technique can be included easily in a quantum statistical theory, such as that of MRS, based upon the Ursell expansion. Thus, rather than revise and correct MG *per se*, we propose, in this paper, to extend MRS to apply to a multicomponent system of charged and neutral particles and concurrently to incorporate the counterterm technique of Tuttle. The results of our development are expressed in terms of diagrammatic expansions for momentum distributions and the grand potential.

It seems characteristic of any many-body theory to be plagued by divergencies and spurious results. For the systems of interest here, the developments in quantum electrodynamics allow us to take cognizance of some prospective troublesome features of the theory. Thus, from the beginning, we address ourselves to the tasks of renormalizing bare masses of charged particles, of dealing with the infrared problem, and of summing the so-called Coulomb ring diagrams.

The first of these problems will be resolved by means of the counterterm technique (mentioned above), the infrared problem remains to be analyzed in the present formalism, and the Coulomb problem can be treated by techniques developed in MG.

It is our intention to keep this paper as short as possible, but yet of sufficient detail to provide necessary technical background for the second paper in this series. Thus, it may be necessary for the reader to consult MG for notation and a few definitions, MRS for historical perspective and detail of the new self-energy analysis, Tuttle for the development of the counterterm technique (and its relation to Hartree–Fock theory), and all of these papers for references to recent literature on the subject. Further discussion of this problem and our objectives are given in the following paper.

In Sec. 2 of this paper we present some background material which is important for subsequent developments. In Sec. 3 we summarize the quantum statistical theory and discuss the counterterm technique. The rules for the diagrams and the associated vertex functions are given in appendices. An application of the theory given in the next paper will then make use of most of the features of the present development, particularly as discussed in Sec. 3.

2. PRELIMINARY DISCUSSION

The investigations described herein apply to a volume Ω of charged and neutral nonrelativistic particles (with no internal states) in thermal equilibrium; periodic boundary conditions will be used, and the thermodynamic limit will be imposed eventually. The system is considered to be multicomponent, and the constituent particle species are designated by Greek letters $\alpha, \beta, \eta, \cdots$ (the symbol γ is reserved exclusively for photons). All particles are treated as point particles with mass, charge (including zero) and spin (where applicable), but spin-dependent interactions are not considered. For the subsequent analysis it is not necessary to specify the constituents of the system; however, we assume that photons, electrons, and heavy ions are present in the representative system. We complete the definition of the system by the specification of the nonrelativistic Hamiltonian H. In standard notation, the N-particle Hamiltonian has the form[5]

$$H = H_{\text{rad}} + \sum_{i=1}^{N} \frac{1}{2M_i^{(0)}}\left(\mathbf{p}_i - \frac{eZ_i}{c}\mathbf{A}_i\right)^2 + V_2 \quad (2.1)$$

$$= H_0 + V_\gamma + V_2 = H_0 + V. \quad (2.2)$$

In Eq. (2.1) the label i runs over all particles of all species (except photons). Since photons (and, later, quasipârticles) are created and annihilated continually, it is desirable to remove the dependence of the Hamiltonian on particle number by the use of Fock-space methods (in accord with this formulation, statistical averages will be formed over the grand canonical ensemble). The Hamiltonian in Eq. (2.1) is given in occupation number formalism in MG; here, it suffices to state explicitly only the free-particle Hamiltonian H_0:

$$H_0 = \sum_\alpha \sum_{\mathbf{k}^\alpha} a^\dagger(\mathbf{k}^\alpha) a(\mathbf{k}^\alpha) w^{(0)}(\mathbf{k}^\alpha), \quad (2.3)$$

where the single-particle momentum representation is being used and the notation $\mathbf{k}^\alpha$ includes the spin degrees of freedom with each momentum state. In Eq. (2.3) the sum is over all particles and photons, and the (unrenormalized or undressed) free-particle energy–momentum relations are

$$w^{(0)}(\mathbf{k}^\alpha) = (\hbar\mathbf{k})^2/2M_\alpha^{(0)}$$

for α = particles,

$$w^{(0)}(\mathbf{k}^\alpha) = \hbar ck \quad (2.4)$$

for $\alpha = \gamma$(photons). In Eq. (2.1), V_2 includes the Coulomb potential as well as short-range potentials.[6]

Next, we rearrange the Hamiltonian in Eq. (2.2) by the addition and subtraction of a one-particle operator. Thus, we introduce the operator

$$U \equiv \sum_{\mathbf{k}} a^\dagger(\mathbf{k}) a(\mathbf{k}) u(\mathbf{k}) + \sum_{\mathbf{k}} a^\dagger(\mathbf{k}) a(\mathbf{k}) S(\mathbf{k}) \quad (2.5)$$

$$\equiv \sum_\alpha \sum_{\mathbf{k}^\alpha} a^\dagger(\mathbf{k}^\alpha) a(\mathbf{k}^\alpha) C(\mathbf{k}^\alpha) \quad (2.6)$$

and add and subtract it in the Hamiltonian in Eq. (2.2):

$$H = H_0 + U + V - U \equiv H_0' + V - U, \quad (2.7)$$

where

$$H_0' = \sum_\alpha \sum_{\mathbf{k}^\alpha} a^\dagger(\mathbf{k}^\alpha) a(\mathbf{k}^\alpha) w'(\mathbf{k}^\alpha) \quad (2.8)$$

and

$$w'(\mathbf{k}^\alpha) \equiv w_\alpha'(\mathbf{k}) = w_\alpha^{(0)}(\mathbf{k}) + u_\alpha(\mathbf{k}) + S_\alpha(\mathbf{k}). \quad (2.9)$$

It is important to realize that in Eqs. (2.5), (2.6), and (2.8) the sum over particle species includes photons. Thus, $u_\alpha(\mathbf{k})$ and $S_\alpha(\mathbf{k})$ depend upon the particle species, and this dependence is displayed by means of a subscript, as in Eq. (2.9). In Eq. (2.5), U consists of two parts: a part involving $u_\alpha(\mathbf{k})$ (discussed below) and a part involving $S_\alpha(\mathbf{k})$ which is to be chosen specifically to achieve mass renormalization for *charged* particles. Hence, for charged particles we write

$$S_\alpha(\mathbf{k}) = (\hbar^2\mathbf{k}^2/2M_\alpha) D_\alpha, \quad (2.10)$$

where

$$D_\alpha \equiv 1 - M_\alpha/M_\alpha^{(0)} \neq D_\alpha(\mathbf{k}), \qquad (2.11)$$

and M_α is the experimentally observed mass. With Eqs. (2.10) and (2.11) we see that for charged particles

$$w_\alpha^{(0)}(\mathbf{k}) + S_\alpha(\mathbf{k}) = \hbar^2\mathbf{k}^2/2M_\alpha, \qquad (2.12)$$

which is the correct free-particle energy.

The interaction V_γ in the Hamiltonian in Eqs. (2.2) contains the bare masses $M_\alpha^{(0)}$ which also must be mass-renormalized. The mass-renormalization procedure can be completed if we rewrite V_γ as follows:

$$V_\gamma = V_\gamma|_{M_\alpha^{(0)} \to M_\alpha(1-D_\alpha)^{-1}}, \qquad (2.13)$$

with D_α given in Eq. (2.11). Thus, the completion of our mass-renormalization program requires the simple replacement in V_γ of $M_\alpha^{(0)} \to M_\alpha(1 - D_\alpha)^{-1}$. Before discussing the master-graph theory, we wish to make a few qualitative comments about the nature of the counterterms, particularly $u_\alpha(\mathbf{k})$.

It is important to stress that the $u_\alpha(\mathbf{k})$ are completely arbitrary: These functions may be discontinuous, temperature dependent, volume dependent, and so forth. Moreover, the counterterm can be a sum of terms, each of which has a different physical interpretation. The manner in which any arbitrariness of $u_\alpha(\mathbf{k})$ and $S_\alpha(\mathbf{k})$ can be exploited will depend inherently upon the system under consideration. For example, it seems likely that entirely different rearrangements of the Hamiltonian will be useful for the low-temperature electron gas (for which $D_\alpha = 0$) and the high-temperature fully ionized gas. Since this paper concentrates on systems with electromagnetic interactions, it is in order to suggest how counterterms can be used in calculations of the properties of such systems. In Sec. 3 we present the master-graph theory, and there we give a straightforward procedure for identifying and selecting counterterms.

We recall that the masses in H_0 and V_γ in the Hamiltonian in Eq. (2.2) are bare masses, and, as indicated in Eqs. (2.10)–(2.12), the counterterm $S_\alpha(\mathbf{k})$ is introduced to renormalize these masses. Another feature of the theory is that the quantized electromagnetic field leads to the virtual emission and reabsorption of photons by charged particles (in MG, this is called the one-particle problem), and these processes lead to predictions of physical as well as spurious unphysical effects—the unphysical contributions to the theory are to be cancelled by $S_\alpha(\mathbf{k})$. With regard to physical contributions, it should be noted that the electromagnetic potentials V_γ in Eq. (2.2) are divergent for small photon momenta (the infrared problem), and this feature can lead to questions of convergence of the quantum statistical theory; however, the careful summation of infinite series of selected diagrams, along with the density of states factor, usually leads to well-defined physical quantities. Finally, we mention perhaps the most important application of the counterterm technique: If U is selected to contain *all* of the single-particle properties exhibited by V (thus identifying the single-particle self-energies) and thereby $V - U$ is made small, then one can interpret H_0' as describing *quasi-particles* with energies $w_\alpha'(\mathbf{k})$ [see Eq. (2.9)] whose interaction potential is given by $V - U$—this situation is very favorable for the use of perturbation theory. Many of the applications of counterterms alluded to above will be made in the following paper.

3. THE MASTER GRAPH THEORY

In this section we present the extension of the master-graph theory in MRS to a multicomponent system which now contains charged as well as neutral particles. The final form of this theory is a finite temperature nonperturbative theory with interactions which include the electromagnetic interactions, the Coulomb interaction, and short-range interactions (with hard cores, if appropriate). At the same time, we have included in this master-graph theory the counterterm technique developed by Tuttle. In this paper, phase transitions and transport phenomena are not considered; instead, we give diagrammatic expansions for the momentum distribution and the grand potential. In order to avoid excessive use of primes and other affixes, our notation differs slightly from that in MRS.

The master-graph theory is a formulation of quantum statistics in which all self-energy structures have been summed; the self-energy contributions are contained in line factors which are defined by integral equations which are somewhat analogous to Dyson equations. Thus, here, we present the integral equation for the line factors of the master-graph theory; the rules for the master graphs are given in Appendix A, and the associated vertex functions are given in Appendix B. Also, we indicate, in the appropriate places, which quantities were omitted in MG.[7]

The basic line factors for master graphs are defined by[8,9]

$$\mathcal{G}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\alpha) = \delta(t_2^{(-)} - t_1)\delta_{\mu,\nu} + \epsilon_\alpha \mathcal{L}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\alpha), \qquad (3.1)$$

where $(\mu, \nu) = (1, 1), (2, 0), (0, 2)$ (that is, $\mu + \nu = 2$), $\epsilon_\alpha = +1$ if α symbolizes a boson, $\epsilon_\alpha = -1$ if α symbolizes a fermion, and $\mathcal{L}_{\mu,\nu}(t_2, t_1, k^\alpha)$ is defined below. Next, we define the functions

$$\mathcal{M}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\alpha) = \epsilon_\alpha C_\alpha(\mathbf{k})[\theta(t_2 - t_1) + \epsilon_\alpha \nu_\alpha'(\mathbf{k})]\delta_{\mu,\nu} + \mathcal{K}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\alpha), \qquad (3.2)$$

where[10]

$$\mathcal{K}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\alpha) \equiv \sum \begin{pmatrix}\text{all different master} \\ (\mu,\nu)\ L\text{-graphs}\end{pmatrix}_{\mathbf{k}^\alpha}, \quad (3.3)$$

$$\nu'_\alpha(\mathbf{k}) = \{\exp \beta[w'_\alpha(\mathbf{k}) - g_\alpha] - \epsilon_\alpha\}^{-1}, \quad (3.4)$$

$\theta(x > 0) = +1$, $\theta(x \le 0) = 0$, g_α is the partial thermodynamic (or chemical) potential for α-type particles, $g_\gamma = 0$, $\beta \equiv (\kappa T)^{-1}$, κ is the Boltzmann constant, T is the absolute temperature, and $w'_\alpha(\mathbf{k})$ is the quasiparticle energy given in Eq. (2.9). The master (μ, ν) L-graphs, introduced in Eq. (3.3), are defined in Appendix A. The integral equations for the line factors introduced in Eq. (3.1) are now defined by means of the following equations[11]:

$$\mathcal{L}_{1,1}(t_2, t_1, \mathbf{k}^\alpha) = \int_0^\beta ds[\mathcal{G}_{1,1}(t_2, s, \mathbf{k}^\alpha)\mathcal{M}_{1,1}(s, t_1, \mathbf{k}^\alpha) + \delta_{\alpha,\gamma}\mathcal{G}_{2,0}(t_2, s, \mathbf{k}^\alpha)\mathcal{M}_{0,2}(t_1, s, \mathbf{k}^\alpha)], \quad (3.5)$$

$$\mathcal{L}_{0,2}(t_2, t_1, \mathbf{k}^\alpha) = \delta_{\alpha,\gamma}\int_0^\beta ds[\mathcal{G}_{0,2}(t_2, s, \mathbf{k}^\alpha)\overline{\mathcal{M}}_{1,1}(s, t_1, -\mathbf{k}^\alpha) + \mathcal{G}_{1,1}(s, t_2, \mathbf{k}^\alpha)\mathcal{M}_{0,2}(s, t_1, \mathbf{k}^\alpha)], \quad (3.6)$$

$$\mathcal{L}_{2,0}(t_2, t_1, \mathbf{k}^\alpha) = \delta_{\alpha,\gamma}\int_0^\beta ds[\mathcal{G}_{2,0}(t_2, s, \mathbf{k}^\alpha)\overline{\mathcal{M}}_{1,1}(t_1, s, -\mathbf{k}^\alpha) + \mathcal{G}_{1,1}(t_2, s, \mathbf{k}^\alpha)\mathcal{M}_{2,0}(s, t_1, \mathbf{k}^\alpha)]. \quad (3.7)$$

The validity of the preceding equations is established most easily by iteration.

Graphical structures with μ outgoing external lines and ν incoming external lines, where $\mu + \nu = 2$, are called *self-energy graphs*, and the line factors

$$\mathcal{G}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\alpha)$$

in Eq. (3.1) represent sums of all such self-energy structures. We emphasize that, in the present formalism, (0, 2) and (2, 0) structures have only photon external lines.[12] The error in MG stems from the omission of and concomitant failure to sum up structures with only two incoming or two outgoing external photon lines.

For subsequent applications it is useful to decouple the integral equation for the line factor $\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\alpha)$ from the line factors $\mathcal{G}_{0,2}(t_2, t_1, \mathbf{k}^\alpha)$ and $\mathcal{G}_{2,0}(t_2, t_1, \mathbf{k}^\alpha)$. A formal decoupling can be achieved with the aid of the following three functions:

$$\overline{\mathcal{G}}(t_2, t_1, -\mathbf{k}^\gamma) \equiv \delta(t_2^{(-)} - t_1) + \epsilon_\alpha\overline{\mathcal{L}}(t_2, t_1, -\mathbf{k}^\gamma), \quad (3.8)$$

$$\overline{\mathcal{L}}(t_2, t_1, -\mathbf{k}^\gamma) \equiv \int_0^\beta ds\overline{\mathcal{G}}(t_2, s, -\mathbf{k}^\gamma)\overline{\mathcal{M}}_{1,1}(s, t_1, -\mathbf{k}^\gamma), \quad (3.9)$$

$$Q(t_2, t_1, \mathbf{k}^\alpha) \equiv \epsilon_\alpha C_\alpha(\mathbf{k})[\theta(t_2 - t_1) + \epsilon_\alpha\nu'_\alpha(\mathbf{k})] + \mathcal{K}_{1,1}(t_2, t_1, \mathbf{k}^\alpha) + \delta_{\alpha,\gamma}\int_0^\beta ds_1\, ds_2\mathcal{K}_{2,0}(t_2, s_1, \mathbf{k}^\alpha) \times \overline{\mathcal{G}}(s_2, s_1, -\mathbf{k}^\alpha)\mathcal{K}_{0,2}(t_1, s_2, \mathbf{k}^\alpha). \quad (3.10)$$

Now, in terms of these functions, the integral equations for the line factors become

$$\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\alpha) = \delta(t_2^{(-)} - t_1) + \epsilon_\alpha\int_0^\beta ds\mathcal{G}_{1,1}(t_2, s, \mathbf{k}^\alpha)Q(s, t_1, \mathbf{k}^\alpha), \quad (3.11)$$

$$\mathcal{G}_{0,2}(t_2, t_1, \mathbf{k}^\gamma) = \int_0^\beta ds_1\, ds_2\mathcal{K}_{0,2}(s_2, s_1, \mathbf{k}^\gamma) \times \mathcal{G}_{1,1}(s_2, t_2, \mathbf{k}^\gamma)\overline{\mathcal{G}}(s_1, t_1, -\mathbf{k}^\gamma), \quad (3.12)$$

$$\mathcal{G}_{2,0}(t_2, t_1, \mathbf{k}^\gamma) = \int_0^\beta ds_1\, ds_2\mathcal{G}_{1,1}(t_2, s_2, \mathbf{k}^\gamma) \times \overline{\mathcal{G}}(t_1, s_1, -\mathbf{k}^\gamma)\mathcal{K}_{2,0}(s_2, s_1, \mathbf{k}^\gamma). \quad (3.13)$$

Thus, the integral equation in Eq. (3.11) involves, in a sense, only (1, 1) structures owing to the symmetrical manner in which $Q(t_2, t_1, \mathbf{k}^\alpha)$ of Eq. (3.10) combines (0, 2) and (2, 0) structures. The integral equations in Eqs. (3.11)–(3.13) are provided diagrammatically by Figs. 1 and 2.

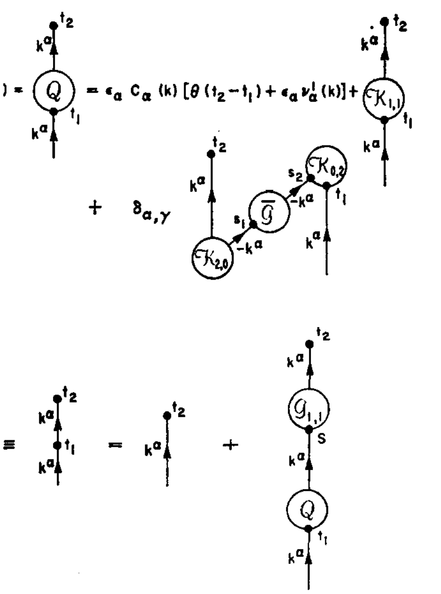

FIG. 1. Diagrammatic representation of Eqs. (3.10) and (3.11). The graphical symbol for $\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\alpha)$ is also defined.

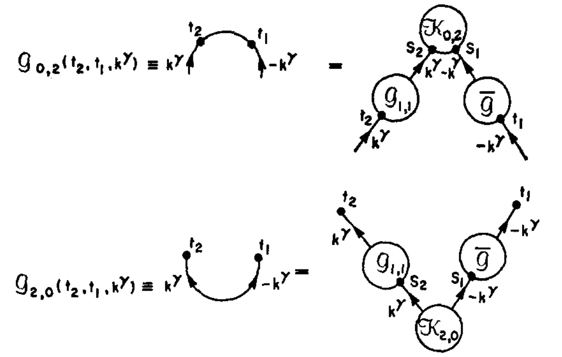

FIG. 2 Diagrammatic representation of Eqs. (3.12) and (3.13). The graphical symbols for $\mathcal{G}_{0,2}(t_2, t_1, \mathbf{k}^\alpha)$ and $\mathcal{G}_{2,0}(t_2, t_1, \mathbf{k}^\alpha)$ are also defined.

In Eqs. (3.6)–(3.13) a bar has been introduced to characterize quantities with $-\mathbf{k}^\gamma$ lines, and this notation will be used henceforth. In the case of photon lines, the difference between the kernels in Eqs. (3.8) [with Eq. (3.9)] and (3.11) results in two different line factors $\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\gamma)$ and $\bar{\mathcal{G}}(t_2, t_1, -\mathbf{k}^\gamma)$. For the same reason the counterterms $\bar{u}_\gamma(-\mathbf{k})$ chosen for the $-\mathbf{k}^\gamma$ lines must differ from the counterterms $u_\gamma(\mathbf{k})$ chosen for the $+\mathbf{k}^\gamma$ lines. Thus, such a notation is necessary. For particle lines, the present comments are not relevant.

The physical quantities which are of interest in this paper are the momentum distribution $\langle n_\alpha(\mathbf{k})\rangle$ (which is the average number of α-type particles with momentum $\mathbf{k}$), defined by

$$\langle n_\alpha(\mathbf{k})\rangle = \mathrm{Tr}\,[a^\dagger(\mathbf{k}^\alpha)a(\mathbf{k}^\alpha)\hat{\rho}], \tag{3.14}$$

and the grand potential f, defined by

$$\Omega f(\beta, g, \Omega) = \ln \mathrm{Tr}\,\hat{\rho}, \tag{3.15}$$

where

$$\hat{\rho} = \exp(-\Omega f)\exp[\beta(G - H)] \tag{3.16}$$

is the density operator for the grand canonical ensemble. In Eq. (3.14) $a^\dagger(\mathbf{k}^\alpha)a(\mathbf{k}^\alpha)$ is the number operator for the number of α-type particles with momentum $\mathbf{k}$, in Eqs. (3.14) and (3.15) Tr indicates the trace in Fock space, and G is the Gibbs potential. Thermodynamic functions can be calculated directly from the grand potential by partial differentiation [see Eqs. (4)–(10) of MG]. In terms of master (1, 1) graphs the momentum distribution is given by

$$\langle n_\alpha(\mathbf{k})\rangle = \nu_\alpha'(\mathbf{k})\int_0^\beta dt\,\mathcal{G}_{1,1}(\beta, t, \mathbf{k}^\alpha). \tag{3.17}$$

The grand potential is given in terms of master (0, 0) and (1, 1) graphs by the following relation:

$$\begin{aligned}\Omega f(\beta, g, \Omega) &= \Omega F(\beta, g, \Omega) + \sum_\alpha \epsilon_\alpha \sum_{\mathbf{k}^\alpha} \ln[1 + \epsilon_\alpha \nu_\alpha'(\mathbf{k})] \\ &+ \sum_\alpha \sum_{\mathbf{k}} \int_0^\beta dt[\mathcal{L}_{1,1}^{(t)}(t, t, \mathbf{k}^\alpha) - \mathcal{L}_{1,1}(t, t, \mathbf{k}^\alpha)] \\ &+ \sum_\alpha \sum_{\mathbf{k}^\alpha} \epsilon_\alpha C_\alpha(\mathbf{k}) \int_0^\beta dt_1\, dt_2[\theta(t_1 - t_2) + \epsilon_\alpha \nu_\alpha'(\mathbf{k})] \\ &\times \mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\alpha),\end{aligned} \tag{3.18}$$

where

$$\Omega F(\beta, g, \Omega) = \sum \begin{pmatrix}\text{all different master} \\ (0, 0)\text{ graphs}\end{pmatrix} \tag{3.19}$$

and the t-dependent functions, such as $\mathcal{L}_{1,1}^{(t)}(t_2, t_1, \mathbf{k}^\alpha)$, needed to calculate the grand potential are defined in analogy with those in Sec. 5 of MRS. Explicit examples of master (μ, ν) graphs, for $\mu + \nu = 2$, are given in the following paper.

The preceding developments mark the end of the presentation of the formal quantum statistical theory, thus achieving the main goal of this paper. The following paper contains further theoretical developments and the explicit calculations of the photon self-energy and momentum distribution. We present now a general procedure for selecting a specific class of counterterms.

We direct attention to Eq. (3.11), the integral equation for the line factor $\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\alpha)$, where the explicit dependence on $Q(t_2, t_1, \mathbf{k}^\alpha)$ is to be noted. Clearly, the convergence or divergence properties of iterative solutions of this integral equation depend quite delicately upon $Q(t_2, t_1, \mathbf{k}^\alpha)$. Moreover, as shown in Eq. (3.10), $Q(t_2, t_1, \mathbf{k}^\alpha)$ depends in a particular additive manner (as well as implicitly) upon the arbitrary functions $C_\alpha(\mathbf{k})$.[13] Thus, the choice of $C_\alpha(\mathbf{k})$ can affect very strongly the iterative solutions of Eq. (3.11). Quantities multiplied by $[\theta(t_2 - t_1) + \epsilon_\alpha \nu_\alpha'(\mathbf{k})]$, but which are otherwise independent of t_2 and t_1, are said to be *temperature independent*. Thus, in Eq. (3.10) for $Q(t_2, t_1, \mathbf{k}^\alpha)$, the $C_\alpha(\mathbf{k})$ can be selected to cancel temperature-independent terms originating from the second and third terms in that equation.[14] The counterterms $\bar{u}_\gamma(-\mathbf{k})$ can be determined by a similar procedure based on Eq. (3.2) for the $-\mathbf{k}^\gamma$ case. Using the above scheme, one can often select counterterms which lead to more convergent iterative solutions for the line factors and which also achieve the correct mass renormalization. After a selection of counterterms one must still examine the properties of the integral equations for the line factors to see how the iterative solutions have been affected[15]—it may occur that additional counterterms, based on further iterations of the line factor equations, must be selected.

The above procedure for cancelling temperature independent contributions to the line factors does not lead to the neglect of any contributions in the theory, since the counterterms reappear elsewhere in the theory. In particular, the counterterms reappear in the Hamiltonian as definite renormalized energies $w_\alpha'(\mathbf{k})$ (including alteration of the masses $M_\alpha^{(0)}$, whose system-independent renormalization is well known in quantum electrodynamics). In the sense that V alone leads to a slowly convergent or divergent theory (thus, V is large) while $V-U$ gives more convergent results (so that $V-U$ is small), one finds already one justification for interpreting the $w_\alpha'(\mathbf{k})$ as quasiparticle energies.

ACKNOWLEDGMENTS

One of us (C. R. S.) would like to thank Professor G. Chew and Professor K. Watson for extending the hospitality of the Lawrence Radiation Laboratory at Berkeley, and Associated Western Universities, Inc., for the faculty fellowship at Lawrence Radiation Laboratory. We are also grateful to Dr. I. RamaRao and Professor W. T. Grandy, Jr., for useful discussions.

APPENDIX A: RULES FOR MASTER (μ, ν) GRAPHS

A Pth-order master (μ, ν) graph is defined to be a graphical structure consisting of P cluster vertices (but no 1-vertices), defined in Fig. 3 and Appendix B, which are entirely interconnected by m internal solid lines and to which are attached μ outgoing external solid lines and ν incoming external solid lines. Each

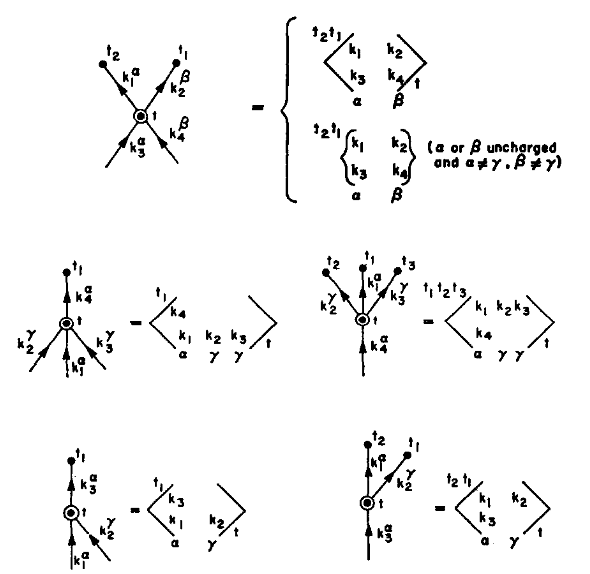

FIG. 3. Symbols for the cluster vertices. The corresponding cluster vertex functions are given explicitly in Appendix B.

external solid line carries a single arrow, and each internal solid line carries two arrows—one at each end. At the head of each arrow there is a dot. If the arrow points toward a vertex, this dot is identical with the vertex. Three different types of internal solid lines are possible, depending upon whether the two arrows point in the same direction, point toward each other, or point away from each other. A master (μ, ν) graph is irreducible and proper in the sense that the cutting of any one or two of its internal lines must not produce two (or three) disconnected graphs, at least one of which is a (1, 1) (0, 2), or (2, 0) graph. Corresponding to each master (μ, ν) graph there is prescribed an analytic term according to the following rules:

Rule 1: To each external solid line assign a pregiven momentum with a particle label; if $(\mu, \nu) \neq (0, 0)$, the incoming particle (not photon) lines refer to the same set of particles as the outgoing lines. External lines with different momentum labels or directions are treated as distinguishable.

Rule 2: Two master (μ, ν) graphs are different if their topological structures (including arrow directions, particle-type labels, and external lines, but not including the momentum labels of internal arrows and the temperature labels which will be assigned below) are different.

Rule 3: To each arrow of the m internal solid lines assign a different integer i, $i = 1, 2, \cdots, 2m$, and a corresponding momentum $\mathbf{k}_i^\alpha$ (the possible choices of α will be fixed by the associated cluster vertices). Assign a different temperature variable t_j to each of the P cluster vertices (encircled dots) and to each of the dots which occur at the head ends of internal arrows that point away from vertices. To each dot of the outgoing external solid lines assign the temperature variable β.

Rule 4: Assign to the entire graph a factor S^{-1}, where S is the symmetry number. The symmetry number is defined to be the total number of permutations of the $2m$ integers (assigned to the arrows of the internal lines) which leave the graph topologically unchanged (including the positions of these integers with respect to the arrows).

Rule 5: Associate with the entire graph the appropriate product of P cluster vertices with the momentum variable assignments of Rules 1 and 3. Assign to the graph an over-all sign factor $\prod_\alpha \epsilon^{P_\alpha}$, where P_α is the parity of the permutation of the bottom row momenta of α-type particles in the vertex functions with respect to the corresponding ones in the top row.

Rule 6: To each *internal* solid line with arrow labels i and j assign a line factor and a momentum conserving Kronecker delta as follows:

$\delta_{\mathbf{k}_i,\mathbf{k}_j}\mathcal{G}_{1,1}(t, s, \mathbf{k}_i^\alpha)$	when the arrows point in the same direction,
$\delta_{\mathbf{k}_i,-\mathbf{k}_j}\mathcal{G}_{0,2}(t, s, \mathbf{k}_i^\gamma)\delta_{\alpha,\gamma}$	when the arrows point toward each other,
$\delta_{\mathbf{k}_i,-\mathbf{k}_j}\mathcal{G}_{2,0}(t, s, \mathbf{k}_i^\gamma)\delta_{\alpha,\gamma}$	when the arrows point away from each other,

where the temperature labels t and s correspond to those assigned by Rule 3. In each case, the arrow labeled i points toward the dot labeled t.

Rule 7: Finally, sum over the $2m$ internal momenta and integrate from 0 to β over the temperature variables t_j assigned in Rule 3.

In one case the Rule 5 above needs to be supplemented:

Rule 5: If two internal lines connect the same two cluster vertices corresponding to pair functions (whose vertices have temperature labels t_3 and t_4) and have for the associated line factor product

$$\mathcal{G}_{1,1}(t_3, t_1, \mathbf{k}_1^\alpha)\mathcal{G}_{1,1}(t_3, t_2, \mathbf{k}_2^\beta),$$

then we must subtract the wiggly-line double bond correction

$$\delta(t_3 - t_1)\delta(t_3 - t_2)\,{}^{t_3t_3}\!\left[\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\\ \alpha & \beta\end{matrix}\right]_{t_4}$$

from the quantity

$$\mathcal{G}_{1,1}(t_3, t_1, \mathbf{k}_1^\alpha)\mathcal{G}_{1,1}(t_3, t_2, \mathbf{k}_2^\beta)\,{}^{t_1t_2}\!\left[\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\\ \alpha & \beta\end{matrix}\right]_{t_4}$$

which would be assigned by the above rules.

A master (μ, ν) L graph, $(\mu, \nu) \neq (0, 0)$, is defined to be a graph with the same structure as a given master (μ, ν) graph except (a) the μ external outgoing lines are assigned temperature variables $t_i \leq \beta$, $i = 0, 1, \cdots, \mu$, and (b) there is no integration over the ν temperature variables t_j, $j = 0, 1, \cdots, \nu$, at the vertices to which the ν incoming external lines attach. If a master (μ, ν) L graph is a subgraph extracted from a larger graphical structure, then there are to be no line factors associated with the $\mu + \nu$ external line factors of this L graph.

APPENDIX B: CLUSTER-VERTEX FUNCTIONS FOR MASTER (μ, ν) GRAPHS

In this appendix we give the explicit expressions for the cluster vertex functions which are involved in the diagrammatic expansions of master (μ, ν) graphs. It should be realized that these vertex functions have evolved directly from the interaction terms in the Hamiltonian.

The generalized cluster-vertex functions are explicitly

$${}^{t_1t_2}\!\left\langle\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\\ \alpha & \beta\end{matrix}\right\rangle_t$$

$$= [\theta(t_1 - t) + \epsilon_\alpha\nu_\alpha'(\mathbf{k}_1)][\theta(t_2 - t) + \epsilon_\beta\nu_\beta'(\mathbf{k}_2)] \times \left(\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\\ \alpha & \beta\end{matrix}\right)_t e^{t[C_\alpha(\mathbf{k}_1)+C_\beta(\mathbf{k}_2)-C_\alpha(\mathbf{k}_3)-C_\beta(\mathbf{k}_4)]}, \quad \text{(B1)}$$

$${}^{t_1t_2}\!\left\langle\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\\ \alpha & \gamma\end{matrix}\right\rangle_t$$

$$= -\frac{2\pi\hbar^2\alpha_0\epsilon_\alpha Z_\alpha^2}{\Omega M_\alpha/(1 - D_\alpha)}\frac{\hat{e}_2\cdot\hat{e}_4}{(k_2k_4)^{\frac{1}{2}}}[\theta(t_1 - t) + \epsilon_\alpha\nu_\alpha'(\mathbf{k}_1)] \times [\theta(t_2 - t) + \nu_\gamma'(\mathbf{k}_2)] \times e^{t[w_\alpha'(\mathbf{k}_1)+w_\gamma'(\mathbf{k}_2)-w_\alpha'(\mathbf{k}_3)-w_\gamma'(\mathbf{k}_4)]}\delta_{(\mathbf{k}_1+\mathbf{k}_2),(\mathbf{k}_3+\mathbf{k}_4)}\delta_{m_1,m_3}, \quad \text{(B2)}$$

$${}^{t_1}\!\left\langle\begin{matrix}\mathbf{k}_4 & & \\ \mathbf{k}_1 & \mathbf{k}_2 & \mathbf{k}_3\\ \alpha & \gamma & \gamma\end{matrix}\right\rangle_t$$

$$= -\frac{2\pi\hbar^2\alpha_0\epsilon_\alpha Z_\alpha^2}{\Omega M_\alpha/(1 - D_\alpha)}\frac{\hat{e}_2\cdot\hat{e}_3}{(k_2k_3)^{\frac{1}{2}}}[\theta(t_1 - t) + \epsilon_\alpha\nu_\alpha'(\mathbf{k}_4)] \times e^{t[w_\alpha'(\mathbf{k}_4)-w_\alpha'(\mathbf{k}_1)-w_\gamma'(\mathbf{k}_2)-w_\gamma'(\mathbf{k}_3)]}\delta_{\mathbf{k}_4,(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)}\delta_{m_1,m_4}, \quad \text{(B3)}$$

$${}^{t_1t_2t_3}\!\left\langle\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2 & \mathbf{k}_3\\ \mathbf{k}_4 & & \\ \alpha & \gamma & \gamma\end{matrix}\right\rangle_t$$

$$= -\frac{2\pi\hbar^2\alpha_0\epsilon_\alpha Z_\alpha^2}{\Omega M_\alpha/(1 - D_\alpha)}\frac{\hat{e}_2\cdot\hat{e}_3}{(k_2k_3)^{\frac{1}{2}}}[\theta(t_1 - t) + \epsilon_\alpha\nu_\alpha'(\mathbf{k}_1)] \times [\theta(t_2 - t) + \nu_\gamma'(\mathbf{k}_2)][\theta(t_3 - t) + \nu_\gamma'(\mathbf{k}_3)] \times e^{t[w_\alpha'(\mathbf{k}_1)+w_\gamma'(\mathbf{k}_2)+w_\gamma'(\mathbf{k}_3)-w_\alpha'(\mathbf{k}_4)]}\delta_{\mathbf{k}_4,(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)}\delta_{m_1,m_4}, \quad \text{(B4)}$$

$${}^{t_1}\!\left\langle\begin{matrix}\mathbf{k}_3 & \\ \mathbf{k}_1 & \mathbf{k}_2\\ \alpha & \gamma\end{matrix}\right\rangle_t$$

$$= \frac{\hbar^2\epsilon_\alpha Z_\alpha}{M_\alpha/(1 - D_\alpha)}\left(\frac{2\pi\alpha_0}{\Omega}\right)^{\frac{1}{2}}\frac{\mathbf{k}_3\cdot\hat{e}_2}{(k_2)^{\frac{1}{2}}}[\theta(t_1 - t) + \epsilon_\alpha\nu_\alpha'(\mathbf{k}_3)] \times e^{t[w_\alpha'(\mathbf{k}_3)-w_\alpha'(\mathbf{k}_1)-w_\gamma'(\mathbf{k}_2)]}\delta_{\mathbf{k}_3,(\mathbf{k}_1+\mathbf{k}_2)}\delta_{m_1,m_3}, \quad \text{(B5)}$$

$$
{}^{t_1t_2}\left\langle\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \end{matrix}\right\rangle_{t}
\begin{matrix}\\ \alpha\quad\gamma\end{matrix}
= \frac{\hbar^2\epsilon_\alpha Z_\alpha}{M_\alpha/(1-D_\alpha)}\left(\frac{2\pi\alpha_0}{\Omega}\right)^{\frac12}\frac{\mathbf{k}_3\cdot\hat{e}_2}{(k_2)^{\frac12}}[\theta(t_1-t)+\epsilon_\alpha\nu'_\alpha(\mathbf{k}_1)]
\times[\theta(t_2-t)+\nu'_\gamma(\mathbf{k}_2)]
\times e^{t[w_\alpha'(\mathbf{k}_1)+w_\gamma'(\mathbf{k}_2)-w_\alpha'(\mathbf{k}_3)]}\delta_{\mathbf{k}_3,(\mathbf{k}_1+\mathbf{k}_2)}\delta_{m_1,m_3},
\tag{B6}
$$

$$
{}^{t_1t_2}\left\{\begin{matrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{matrix}\right\}_{t}
= [\theta(t_1-t_2)+\epsilon_\alpha\nu'_\alpha(\mathbf{k}_1)]
\times {}^{t_2}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}'_t\theta(t_2-t)+[\theta(t_2-t_1)+\epsilon_\beta\nu'_\beta(\mathbf{k}_2)]
\times {}^{t_2}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}'_t\theta(t_1-t)+\epsilon_\alpha\epsilon_\beta\nu'_\alpha(\mathbf{k}_1)\nu'_\beta(\mathbf{k}_2)\,{}^{\beta}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}'_t.
\tag{B7}
$$

(In each bracket symbol the columns are labeled α, β.)

In Eqs. (B2)-(B6), $\alpha_0 = e^2(\hbar c)^{-1}$ is the fine structure constant, and the Kronecker deltas conserve momentum and spin (m_i is the spin projection); the photon polarization vector is represented by $\hat{e}_i$.

The symbol used in Eq. (B1) is defined by

$$
\begin{pmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{pmatrix}_t = -[\langle\mathbf{k}_1,\mathbf{k}_2|\,V_c(t)\,|\mathbf{k}_3,\mathbf{k}_4\rangle + \epsilon_\alpha\langle\mathbf{k}_1,\mathbf{k}_2|\,V_c(t)\,|\mathbf{k}_4,\mathbf{k}_3\rangle]\quad\text{for}\quad\alpha=\beta,
$$
$$
\begin{pmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{pmatrix}_t = -\epsilon_\alpha\epsilon_\beta\langle\mathbf{k}_1^\alpha,\mathbf{k}_2^\beta|\,V_c(t)\,|\mathbf{k}_3^\alpha,\mathbf{k}_4^\beta\rangle\quad\text{for}\quad\alpha\neq\beta.
\tag{B8}
$$

In Eqs. (B1) and (B8), α and β are both charged particles and

$$
\langle\mathbf{k}_1^\alpha,\mathbf{k}_2^\beta|\,V_c(t)\,|\mathbf{k}_3^\alpha,\mathbf{k}_4^\beta\rangle
= (4\pi Z_\alpha Z_\beta e^2/\Omega q^2)
\times\exp t[w_\alpha^{(0)}(\mathbf{k}_1)+w_\beta^{(0)}(\mathbf{k}_2)-w_\alpha^{(0)}(\mathbf{k}_3)-w_\beta^{(0)}(\mathbf{k}_4)]
\times\delta_{(\mathbf{k}_1+\mathbf{k}_2),(\mathbf{k}_3+\mathbf{k}_4)}\delta_{m_1,m_3}\delta_{m_2,m_4},
\tag{B9}
$$

where V_c corresponds to the Coulomb interaction between two particles, one of charge $Z_\alpha e$ and the other of charge $Z_\beta e$; $\mathbf{q}=\mathbf{k}_3-\mathbf{k}_1$ is the momentum transfer.

In Eq. (B7) the primed bracket symbol (excluding hard-core potentials) is

$$
{}^{t_2}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}'_t
= \exp t[-u_\alpha(\mathbf{k}_3)-u_\beta(\mathbf{k}_4)]
\times\Big\{\exp t[u_\alpha(\mathbf{k}_1)+u_\beta(\mathbf{k}_2)]\,{}^{t_2}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}_t
+[-u_\alpha(\mathbf{k}_1)-u_\beta(\mathbf{k}_2)]
\times\int_{t_1}^{t_2}ds\,\exp s[u_\alpha(\mathbf{k}_1)+u_\beta(\mathbf{k}_2)]\,{}^{s}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}_t\Big\},
\tag{B10}
$$

where

$$
{}^{t_1}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}_t = \langle\mathbf{k}_1,\mathbf{k}_2|\,R(t_1,t)\,|\mathbf{k}_3,\mathbf{k}_4\rangle + \epsilon_\alpha\langle\mathbf{k}_1,\mathbf{k}_2|\,R(t_1,t)\,|\mathbf{k}_4,\mathbf{k}_3\rangle\quad\text{for}\quad\alpha=\beta,
$$
$$
{}^{t_1}\begin{bmatrix}\mathbf{k}_1 & \mathbf{k}_2\\ \mathbf{k}_3 & \mathbf{k}_4\end{bmatrix}_t = \epsilon_\alpha\epsilon_\beta\langle\mathbf{k}_1^\alpha,\mathbf{k}_2^\beta|\,R(t_1,t)\,|\mathbf{k}_3^\alpha,\mathbf{k}_4^\beta\rangle\quad\text{for}\quad\alpha\neq\beta.
\tag{B11}
$$

In Eq. (B11), the operator $R(t_1,t)$ is defined by

$$
R(t_1,t) = -\frac{\partial}{\partial t}\exp[t_1H_0^{(2)}]\times\exp[-(t_1-t)H^{(2)}]\exp[-tH_0^{(2)}],
\tag{B12}
$$

where the superscript on $H_0^{(2)}$ and $H^{(2)}$ means "two-particle"—compare Eq. (2.1) with $N=2$. The operator $R(t_1,t)$ is discussed in detail in MI, and its matrix elements (called pair functions) will not be analyzed here. It is worth observing that the pair function represents the effective interaction for short-range forces and, being expressible in terms of wave-functions or reaction matrices, is well behaved even when a hard-core interaction is present. In Eq. (B11) neither α nor β can be a photon, and the operator $R(t_1,t)$ is defined only for nonelectromagnetic interactions.

* This research was begun while at the University of Wyoming; the final stages were completed at Lawrence Radiation Laboratory (Berkeley) while supported by Associated Western Universities, Inc., through contract with the U.S. Atomic Energy Commission.

[1] F. Mohling and W. T. Grandy, Jr., J. Math. Phys. **6**, 348 (1965), hereafter referred to as MG.

[2] See, for example: W. T. Grandy, Jr., and F. Mohling, Ann. Phys. (N.Y.) **34**, 424 (1965); C. R. Smith, Ph.D. thesis, University of Colorado, 1967, unpublished; I. K. Hwang and W. T. Grandy, Jr., Phys. Rev. **177**, 359 (1969); and E. A. Nosal and W. T. Grandy, Jr., Ann. Phys. (N.Y.) **55**, 1 (1969).

[3] F. Mohling, I. RamaRao, and D. W. J. Shea, Phys. Rev. A **1**, 177 (1970), hereafter referred to as MRS.

[4] E. R. Tuttle, Phys. Rev. A **1**, 1243, 1758 (1970), hereafter referred to as Tuttle.

[5] The notation $M_i^{(0)}$ is used for the bare mass of the ith particle. Omission of the superscript zero means that the dressed or renormalized mass is to be used.

[6] In this paper we concentrate on systems containing charged particles; in particular, we do not treat degenerate Bose systems (which are discussed quite adequately in MRS), nor do we discuss the short-range interaction, since this is treated in MRS and F. Monling, Phys. Rev. **122**, 1043 (1961), hereafter referred to as MI. Moreover, it seems unrealistic to include the possibility of Bose–Einstein condensation in a fully ionized gas. For the sake of completeness, the pair function is included in the definitions of the cluster vertex functions in Appendix B; however, explicit rules to prevent the occurrence of forbidden wiggly-line double bonds are given in MRS.

[7] It is important to note that while this paper, in effect, simplifies and corrects the self-energy analysis in MG, the diagrams and the integral equations for the line factors are now entirely different from those in MG.

[8] In Eq. (3.1) the delta function represents a single internal line (and the dummy temperature variable is removed in this case), and the presence of $t_2^{(-)}$ requires $t_2 > t_1$ to prevent the occurrence of certain forbidden loops which otherwise would not be eliminated explicitly by the rules.

[9] In Eq. (3.1) the momentum $\mathbf{k}^\alpha$ is the momentum preassigned to the external lines. Conservation of momentum requires that the

external lines of (1, 1) structures have the same momentum and that the external lines of (0, 2) and (2, 0) structures have momenta equal in magnitude and oppositely directed.

[10] On the right-hand side of Eq. (3.3), a factor of $\delta(t_2 - t_1)$ is to be included with the term corresponding to an (0, 2) L graph which has both external lines attached to the same vertex.

[11] It is seen from Eqs. (3.5)–(3.7), with Eqs. (3.1)–(3.3), that the quasiparticle energy distributions $\nu'_\alpha(\mathbf{k})$ of Eq. (3.4) enter the theory in a very explicit manner.

[12] In MRS the existence of (0, 2) and (2, 0) structures is tantamount to high quantum mechanical degeneracy in Bose fluids (at extremely low temperatures); it is interesting to note that these structures are important (for photons) in ionized gases at all temperatures.

[13] The quantities in Eq. (3.10) are actually functionals of the $C_\alpha(\mathbf{k})$; thus, a selection of $C_\alpha(\mathbf{k})$ on the basis of the above procedure leads in general to integral equations for the counterterms.

[14] It is reasonable to inquire whether there will arise terms in $Q(t_2, t_1, \mathbf{k}^\alpha)$ of a form which can be cancelled by the counterterm in Eq. (3.10). The general answer to this question is not known, but explicit calculations show that such terms usually occur and that their cancellation by counterterms eliminates most divergences in the theory.

[15] In essence, this procedure regroups terms in the integral equations for the line factors in such a way that an analytic continuation of the line factors is achieved. In this process of analytic continuation, single-particle energies $w_\alpha^{(0)}(\mathbf{k})$ are renormalized to quasiparticle energies $w'_\alpha(\mathbf{k})$.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Microscopic Theory of a Multicomponent System of Charged and Neutral Particles. II. Investigation of Properties of Photons*†

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(Received 4 May 1970)

On the basis of the master-graph formulation of quantum statistics in the preceding paper, the properties of photons in a nonrelativistic, multicomponent, fully ionized gas in thermal equilibrium are investigated. The photon self-energy is calculated by summation, to all orders, of selected diagrams, and it is proposed that the solution is formally exact. Next, the photon momentum distribution is calculated, in the high-temperature, low-density limit, to second order in the fine-structure constant. Several nonperturbative results are obtained which are significant even in lowest order. The lowest-order results have an interesting relation to the pair-Hamiltonian approximation and the Bogoliubov transformation, and this relation is discussed. Finally, the counterterm technique of the master-graph theory is employed to accomplish mass renormalization through second order in the fine-structure constant. The investigation is valid for particle densities $\rho \ll 10^{24}$ particles/cm^3 and for absolute temperatures $T \leq 10^8$ °K (but large enough for a high degree of ionization).

1. INTRODUCTION

It is reasonable to expect that quantum mechanics and quantized Maxwell–Lorentz electrodynamics can serve as a basis for a microscopic theory for calculating accurately the properties of a nonrelativistic fully ionized gas in thermal equilibrium. In the preceding paper[1] such a theory was proposed, where the goal has been to develop a theory that is not only rigorous, but also is tractable *in practice*.

Three type of divergences are prominent in a many-body theory of the equilibrium fully ionized gas: the ultraviolet, the Coulomb, and the infrared divergences—all are of electromagnetic origin. Thus, we are concerned with developing techniques for dealing with these divergences. The counterterm technique developed in I can be used to remove the ultraviolet divergence by means of mass renormalization, and the Coulomb divergence has been effectively approached by selective summation of the so-called ring diagrams.[2] In a nonrelativistic theory, the infrared divergence has not yet been eliminated in a fundamental manner. In this paper, we avoid certain perturbation theoretic difficulties arising from the infrared divergence by finding noniterative solutions or by selective summations of diagrams. In some applications the infrared divergence can be isolated by a Bogoliubov transformation of the photon operators, and relevant aspects of this technique will be discussed.

For the system of interest in this paper, there has been considerable activity directed toward the calculation of the photon momentum distribution in the high-temperature, low-density region[3–8]; of course, a comprehensive treatment has not yet been achieved owing to the inherent complexity of the problem. Several of the recent investigations[4–7] have been based on the master-graph formalism of MG, and a renewed interest in the problem was created by the discovery that MG is substantially in error for certain self-energy structures [called (2, 0) and (0, 2) structures]. These self-energy structures are included properly in I, and it is of interest in this paper to use the master-graph theory of I to learn the effects of a external lines of (1, 1) structures have the same momentum and that the external lines of (0, 2) and (2, 0) structures have momenta equal in magnitude and oppositely directed.

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In this paper we present results of calculations of the photon self-energy and momentum distribution. Thus, in Sec. 2 we give necessary preliminary details about the system. In Sec. 3 we outline the calculation of the photon self-energy; the result obtained is based on an extensive partial summation procedure, and it is suggested that our solution may be formally exact. Next, in Sec. 4, we calculate the photon momentum distribution to second order in the fine-structure constant. In both Secs. 3 and 4, the effects of the (2, 0) and (0, 2) structures are investigated. In the final section, Sec. 5, we summarize the general nature of these studies. The counterterm which achieves mass renormalization to second order in the fine-structure constant is presented in the Appendix.

2. THE MODEL SYSTEM

In this section we discuss briefly the properties of the system under study and the ranges of certain physical parameters which characterize the system. The basic model of the system is discussed in detail in I; here, we simplify that model by neglecting short-range forces and by imposing the high-temperature, low-density limit so that the Coulomb interaction can be neglected. Thus, we are interested in a multicomponent, nonrelativistic fully ionized gas in thermal equilibrium, where the dominant interaction is the transverse electromagnetic interaction between particles and photons.

Since the system is nonrelativistic, thermal energies must be much less than particle rest energies, and photon energies must be insufficient for pair production; thus, we have the conditions

$$\eta_\alpha \equiv (\beta M_\alpha c^2)^{-1} \ll 1 \tag{2.1}$$

and

$$w_\alpha(\mathbf{k}) \ll w_\gamma(\mathbf{k}), \tag{2.2}$$

where $\beta \equiv (\kappa T)^{-1}$, κ is the Boltzmann constant, T is the absolute temperature, M_α is the mass of α-type particles and c is the speed of light in vacuo. In Eq. (2.2) we have introduced the particle energy $w_\alpha(\mathbf{k}) = \hbar^2k^2/2M_\alpha$ and the photon energy $w_\gamma(\mathbf{k}) = \hbar ck$ ($\hbar\mathbf{k}$ is momentum). In the high-temperature, low-density limit the fugacity z_α for α-type particles is given approximately by[2]

$$z_\alpha \equiv \exp(\beta g_\alpha) \simeq \rho_\alpha\lambda_\alpha^3(2S_\alpha + 1)^{-1} \ll 1, \tag{2.3}$$

where g_α is the chemical potential (and $g_\gamma = 0$), ρ_α is the number density, λ_α is the thermal wavelength, given by

$$\lambda_\alpha = (2\pi\hbar^2\beta/M_\alpha)^{\frac{1}{2}}, \tag{2.4}$$

and S_α is the spin quantum number. The inequality in Eq. (2.3) implies that the average interparticle spacing $\rho_\alpha^{-\frac{1}{3}}$ is much larger than the thermal wavelength λ_α and reflects that in the high-temperature, low-density limit, particle states are weighted statistically by the Boltzmann factor. On the other hand, photon statistics and dynamics are treated entirely quantum mechanically.

The definition of the high-temperature, low-density limit is completed by requiring the Debye length to be much larger than the interparticle spacing; this restriction, with Eq. (2.3), is equivalent to the condition

$$\beta\hbar\omega_p \ll 1, \tag{2.5}$$

where the composite plasma frequency ω_p is defined by

$$\omega_p^2 = \sum_\alpha \omega_p^2(\alpha) = \sum_\alpha 4\pi\rho_\alpha e^2 Z_\alpha^2/M_\alpha, \tag{2.6}$$

$\omega_p(\alpha)$ is the plasma frequency and Z_α the charge number of α-type particles. The inequalities in Eqs. (2.1), (2.2), and (2.5) are mutually compatible for the following temperature and density regions:

$$0^\circ \ll T < 10^6\,{}^\circ\mathrm{K}, \qquad \rho \ll 10^{24}\ \text{particles/cm}^3. \tag{2.7}$$

3. THE PHOTON SELF ENERGY

The basic quantities in the master-graph theory of I are the line factors $\mathcal{G}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\alpha)$ [throughout this paper $\mu + \nu = 2$]. In this section we concentrate on $\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\gamma)$, defined as the solution of the integral equation, Eq. (I.3.11),[1,9]

$$\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\gamma) = \delta(t_2 - t_1) + \int_0^\beta ds\,\mathcal{G}_{1,1}(t_2, s, \mathbf{k}^\gamma)Q(s, t_1, \mathbf{k}^\gamma), \tag{3.1}$$

where the kernel $Q(t_2, t_1, \mathbf{k}^\gamma)$ [Eq. (I.3.10) with $\alpha = \gamma$] is

$$Q(t_2, t_1, \mathbf{k}^\gamma) = u_\gamma(\mathbf{k})[\theta(t_2 - t_1) + \nu_\gamma'(\mathbf{k})] + \mathcal{K}_{1,1}(t_2, t_1, \mathbf{k}^\gamma) + \int_0^\beta ds_1\,ds_2\mathcal{K}_{2,0}(t_2, s_1, \mathbf{k}^\gamma) \times \bar{\mathcal{G}}(s_2, s_1, -\mathbf{k}^\gamma)\mathcal{K}_{0,2}(t_1, s_2, \mathbf{k}^\gamma). \tag{3.2}$$

In Eq. (3.2) $\mathcal{K}_{\mu,\nu}(t_2, t_1, \mathbf{k}^\gamma)$ is given by the sum of all different master (μ, ν) L graphs and $\bar{\mathcal{G}}(t_2, t_1, -\mathbf{k}^\gamma)$ is given by [see Eqs. (I.3.8) and (I.3.9)][10]

$$\bar{\mathcal{G}}(t_2, t_1, -\mathbf{k}^\gamma) = \delta(t_2 - t_1) + \int_0^\beta ds\bar{\mathcal{G}}(t_2, s, -\mathbf{k}^\gamma)\bar{\mathcal{K}}_{1,1}(s, t_1, -\mathbf{k}^\gamma). \tag{3.3}$$

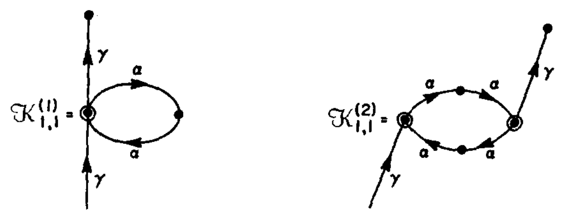

FIG. 1. The two master (1, 1) graphs of order α_0

In Eq. (3.3) we have

$$\mathcal{M}_{1,1}(t_2, t_1, -\mathbf{k}^\gamma) = \bar{u}_\gamma(-\mathbf{k})[\theta(t_2 - t_1) + \bar{\nu}_\gamma(-\mathbf{k})] + \bar{\mathcal{K}}_{1,1}(t_2, t_1, -\mathbf{k}^\gamma), \tag{3.4}$$

where $\bar{\mathcal{K}}_{1,1}(t_2, t_1, -\mathbf{k}^\gamma)$ is defined diagrammatically analogously to $\mathcal{K}_{1,1}(t_2, t_1, \mathbf{k}^\gamma)$. Our objective now is to calculate the photon self energy; to do this we first examine the contributions to the photon counterterm[11] $u_\gamma(\mathbf{k})$ in Eq. (3.2) through second order in the fine-structure constant α_0, where $\alpha_0 = e^2/\hbar c$. Thus, as seen from Eqs. (I.2.4) and (I.2.9), this amounts to a renormalization or dressing of the vacuum photon energy $\hbar ck$ to

$$w'_\gamma(\mathbf{k}) = \hbar ck + u_\gamma(\mathbf{k}). \tag{3.5}$$

There are 18 master (μ, ν) graphs of order α_0 and α_0^2, and these are given in Figs. 1–4. [The rules for writing down the analytical expressions for master

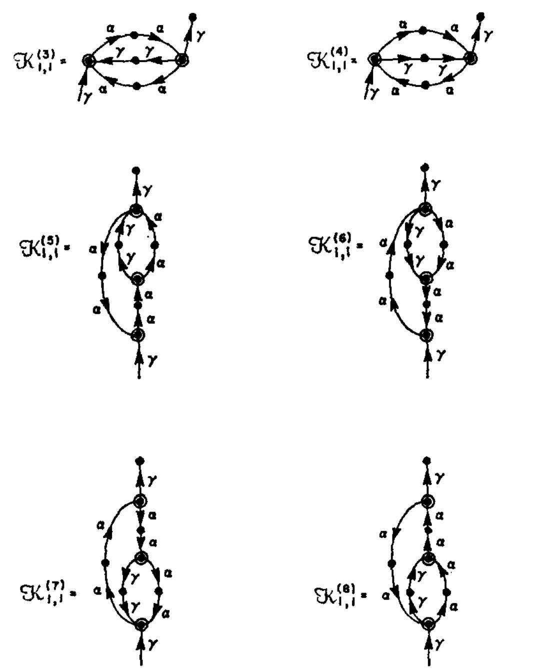

FIG. 2. The six master (1, 1) graphs of order α_0^2 which contain ultraviolet divergences.

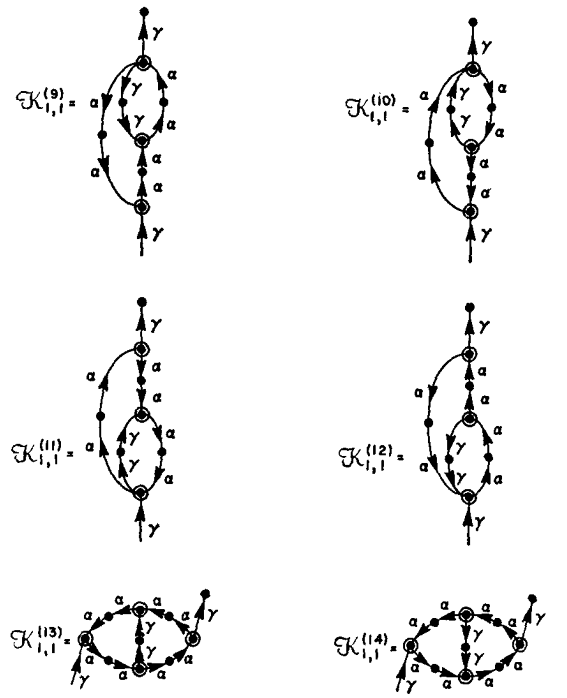

FIG. 3. The remaining six master (1, 1) graphs of order α_0^2—these graphs do not lead to ultraviolet divergences.

(μ, ν) graphs are given in Appendix A of I.] In order to gain insight into the general *structure* of the photon self-energy, we must go beyond the diagrams in Figs. 1–4 and examine contributions to the second and third terms in Eq. (3.2) which arise from higher-order iterations. Thus, we iterate Eq. (3.3) to obtain

$$\bar{\mathcal{G}}(t_2, t_1, -\mathbf{k}^\gamma) = \delta(t_2 - t_1) + \bar{\mathcal{M}}_{1,1}(t_2, t_1, -\mathbf{k}^\gamma) + \int_0^\beta ds \bar{\mathcal{M}}_{1,1}(t_2, s, -\mathbf{k}^\gamma)\bar{\mathcal{M}}_{1,1}(s, t_1, -\mathbf{k}^\gamma) + \cdots, \tag{3.6}$$

where $\bar{\mathcal{M}}_{1,1}(t_2, t_1, -\mathbf{k}^\gamma)$ is defined in Eq. (3.4). We

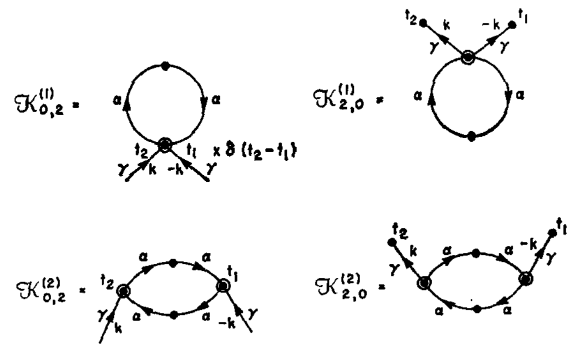

FIG. 4. The four master (2, 0) and (0, 2) graphs of order α_0

use Eq. (3.6) and rewrite Eq. (3.2) in the iterated form

$$Q(t_2, t_1, \mathbf{k}^\gamma) = u_\gamma(\mathbf{k})[\theta(t_2 - t_1) + \nu_\gamma'(\mathbf{k})] + \sum_i \mathcal{K}_{1,1}^{(i)}(t_2, t_1, \mathbf{k}^\gamma) + \int_0^\beta ds_1 ds_2 \Big\{ \Big[\sum_j \mathcal{K}_{2,0}^{(j)}(t_2, s_1, \mathbf{k}^\gamma) \Big] \times \Big[\delta(s_2 - s_1) + \bar{\mathcal{M}}_{1,1}(s_2, s_1, -\mathbf{k}^\gamma) + \int_0^\beta ds \bar{\mathcal{M}}_{1,1}(s_2, s, -\mathbf{k}^\gamma) \bar{\mathcal{M}}_{1,1}(s, s_1, -\mathbf{k}^\gamma) + \cdots \Big] \times \Big[\sum_l \mathcal{K}_{0,2}^{(l)}(t_1, s_2, \mathbf{k}^\gamma) \Big] \Big\}. \quad (3.7)$$

In this paper we discuss explicitly the iterations which arise from the graphs in Figs. 1–4; thus, in Eq. (3.7), i runs over the 14 graphs in Figs. 1–3, j runs over the two (2, 0) graphs in Fig. 4, l runs over the two (0, 2) graphs in Fig. 4, and $\bar{\mathcal{M}}_{1,1}(t_2, t_1, -\mathbf{k}^\gamma)$ will be approximated by $\bar{\mathcal{M}}_{1,1}^{(2)}(t_2, t_1, -\mathbf{k}^\gamma)$ [see Eq. (3.4) and the second graph in Fig. 1], since

$$\bar{\mathcal{M}}_{1,1}^{(1)}(t_2, t_1, -\mathbf{k}^\gamma) \simeq 0$$

[see Eq. (3.18), below]. Next, it is convenient to separate $u_\gamma(\mathbf{k})$ into two parts

$$u_\gamma(\mathbf{k}) = u_\gamma(\mathbf{k})_1 + u_\gamma'(\mathbf{k}), \quad (3.8)$$

where $u_\gamma(\mathbf{k})_1$ is the contribution to $u_\gamma(\mathbf{k})$ from (1, 1) graphs [the first sum in Eq. (3.7)], and $u_\gamma'(\mathbf{k})$ is the remaining contribution which involves the (2, 0) and (0, 2) graphs [arising from the sums over j and l in Eq. (3.7)].

It is straightforward to write down the analytic expression for $\mathcal{K}_{1,1}^{(i)}(t_2, t_1, \mathbf{k}^\gamma)$, $i = 1, 2, \cdots, 14$, in Eq. (3.7) and then to identify the corresponding self energies $u_\gamma^{(i)}(\mathbf{k})$.[8] Here, for the sake of illustration, we give the approximate expressions for the two graphs in Fig. 1. We use

$$\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\alpha) \simeq \delta(t_2 - t_1), \quad (3.9)$$

the lowest order approximation to the particle line factor in Eq. (I-3.11), to obtain, assuming mass renormalization has been performed (see the Appendix),[12,13]

$$\mathcal{K}_{1,1}^{(1)}(t_2, t_1, \mathbf{k}^\gamma) \simeq -\frac{2\pi\hbar^2\alpha_0}{\Omega k} \sum_\alpha Z_\alpha^2(2S_\alpha + 1)M_\alpha^{-1} \times \sum_{\mathbf{k}_1} \nu_\alpha(\mathbf{k}_1)[\theta(t_2 - t_1) + \nu_\gamma'(\mathbf{k})], \quad (3.10)$$

$$\mathcal{K}_{1,1}^{(2)}(t_2, t_1, \mathbf{k}^\gamma) \simeq \frac{2\pi\hbar^4\alpha_0}{\Omega k} \sum_\alpha Z_\alpha^2(2S_\alpha + 1)M_\alpha^{-2} \times \sum_{\mathbf{k}_1,\mathbf{k}_2} (\mathbf{k}_2 \cdot \hat{e}_\mathbf{k})^2 W_1^{-1} \delta_{\mathbf{k}_1,(\mathbf{k}_2+\mathbf{k})} \times [\nu_\alpha(\mathbf{k}_2) - \nu_\alpha(\mathbf{k}_1)][\theta(t_2 - t_1) + \nu_\gamma'(\mathbf{k})] + F(t_2, t_1, \mathbf{k}^\gamma), \quad (3.11)$$

where

$$F(t_2, t_1, \mathbf{k}^\gamma) = -\frac{2\pi\hbar^4\alpha_0}{\Omega k} \sum_\alpha Z_\alpha^2(2S_\alpha + 1)M_\alpha^{-2} \times \sum_{\mathbf{k}_1,\mathbf{k}_2} (\mathbf{k}_2 \cdot \hat{e}_\mathbf{k})^2 W_1^{-1} \delta_{\mathbf{k}_1,(\mathbf{k}_2+\mathbf{k})} \times [\theta(t_2 - t_1)\nu_\alpha(\mathbf{k}_2) + \theta(t_1 - t_2)\nu_\alpha(\mathbf{k}_1) + \epsilon_\alpha \nu_\alpha(\mathbf{k}_1)\nu_\alpha(\mathbf{k}_2)] \exp[(t_1 - t_2)W_1], \quad (3.12)$$

$$W_1 = w_\alpha(\mathbf{k}_1) - w_\alpha(\mathbf{k}_2) - w_\gamma'(\mathbf{k}), \quad (3.13)$$

$$\nu_\gamma'(\mathbf{k}) = [e^{\beta w_\gamma'(\mathbf{k})} - 1]^{-1}, \quad (3.14)$$

$$\nu_\alpha(\mathbf{k}) = \{e^{\beta[w_\alpha(\mathbf{k}) - g_\alpha]} - \epsilon_\alpha\}^{-1}, \quad (3.15)$$

$\epsilon_\alpha = +1$ for α = boson, $\epsilon_\alpha = -1$ for α = fermion, and $\hat{e}_\mathbf{k}$ is the photon unit polarization vector (as in I, we are using the Coulomb gauge). In the high-temperature, low-density limit as expressed by Eq. (2.3) and with the nonrelativistic condition in Eq. (2.2), we have from Eqs. (3.10) and (3.11) the approximate photon self-energy contributions[11]

$$u_\gamma^{(1)}(\mathbf{k})_1 \simeq \hbar^2\omega_p^2/2\hbar ck, \quad (3.16)$$

$$u_\gamma^{(2)}(\mathbf{k})_1 \simeq 16\pi^2\hbar^2\alpha_0 k^{-3} \times \sum_\alpha \rho_\alpha Z_\alpha^2 M_\alpha^{-1} \lambda_\alpha^{-2} \frac{[w_\alpha(\mathbf{k})]^2}{[w_\gamma'(\mathbf{k})]^2 - [w_\alpha(\mathbf{k})]^2}. \quad (3.17)$$

Here, we see that the choice in Eq. (3.16) leads to the result

$$\bar{\mathcal{M}}_{1,1}^{(1)}(t_2, t_1, -\mathbf{k}^\gamma) \simeq \mathcal{M}_{1,1}^{(1)}(t_2, t_1, \mathbf{k}^\gamma) \simeq 0. \quad (3.18)$$

Once the mass-renormalization counterterm has been introduced, a straightforward, but tedious, calculation leads to the conclusions

$$\sum_{i=3}^{14} u_\gamma^{(i)}(\mathbf{k})_1 \ll u_\gamma^{(2)}(\mathbf{k})_1 \ll u_\gamma^{(1)}(\mathbf{k}). \quad (3.19)$$

Thus, the contributions $u_\gamma^{(i)}(\mathbf{k})_1$, $i = 3, \cdots, 14$, can be neglected.

Now, we examine the contributions to $u_\gamma'(\mathbf{k})$ which arise from the temperature independent parts of $\int ds \mathcal{K}_{2,0}^{(j)} \mathcal{G} \mathcal{K}_{0,2}^{(l)}$ in Eq. (3.7). To do this, it is useful to simplify the notation; thus, corresponding to the appropriate terms in Eq. (3.7), we identify symbolically the following *temperature independent* quantities[11]:

$$u_\gamma'(\mathbf{k}) = \sum_{j,l,p,r,\cdots} u_\gamma'(\mathbf{k})_{jlpr\cdots}, \quad (3.20)$$

where, in simplified notation,

$$u_\gamma'(\mathbf{k})_{jlpr\cdots} = -\Big\{ \int_0^\beta ds_1\, ds_2 \mathcal{K}_{2,0}^{(j)}(s_1) \mathcal{K}_{0,2}^{(l)}(s_2) \times \Big[\delta(s_2 - s_1) + \bar{\mathcal{M}}_{1,1}^{(p)}(s_2, s_1) + \int_0^\beta ds \bar{\mathcal{M}}_{1,1}^{(p)}(s_2, s) \bar{\mathcal{M}}_{1,1}^{(r)}(s, s_1) + \cdots \Big] \Big\}_{\mathrm{TIP}}, \quad (3.21)$$

and TIP denotes the temperature-independent part. In what follows, we examine Eq. (3.21) with $p = r = 2$ [recall Eq. (3.18)], and the p and r subscripts used in Eq. (3.20) will be suppressed.

Next, we attempt to discover the general structure of $u_\gamma(\mathbf{k})$; in order to do this, we start with a detailed examination of the three leading order contributions to Eq. (3.20) given in Figs. 5–7. We find, after some tedious manipulations,[14]

$$u_\gamma'(\mathbf{k})_{11} = -[u_\gamma^{(1)}(\mathbf{k})_1]^2 W^{-1}(1 - R)^{-1}, \tag{3.22}$$

$$u_\gamma'(\mathbf{k})_{12} = u_\gamma'(\mathbf{k})_{21} \tag{3.23}$$

$$= -[u_\gamma^{(1)}(\mathbf{k})_1 u_\gamma^{(2)}(\mathbf{k})_1] W^{-1}(1 - R)^{-1}, \tag{3.24}$$

where

$$R = 2\pi\hbar^4\alpha_0\Omega^{-1}k^{-1}\sum_\alpha Z_\alpha^2(2S_\alpha + 1)M_\alpha^{-2} \times \sum_{\mathbf{k}_1,\mathbf{k}_2}(\mathbf{k}_1\cdot\hat{e}_\mathbf{k})^2\delta_{\mathbf{k}_1,(\mathbf{k}_2-\mathbf{k})}[\nu_\alpha(\mathbf{k}_1) - \nu_\alpha(\mathbf{k}_2)]\overline{W}_1^{-1}W_4^{-1}, \tag{3.25}$$

$$W = w_\gamma'(\mathbf{k}) + \bar{w}_\gamma(-\mathbf{k}), \tag{3.26}$$

$$W_4 = w_\alpha(\mathbf{k}_1) - w_\alpha(\mathbf{k}_2) + w_\gamma'(\mathbf{k}),$$
$$\overline{W}_1 = w_\alpha(\mathbf{k}_1) - w_\alpha(\mathbf{k}_2) - \bar{w}_\gamma(-\mathbf{k}), \tag{3.27}$$

and W_1 is given in Eq. (3.13). The important point here is that temperature integrals and momentum sums have decoupled in such a way as to enable factorization of terms in Eq. (3.21) and the summation of the resultant geometric series. With the results in Eqs. (3.22)–(3.24), we obtain for Eq. (3.20)

$$u_\gamma'(\mathbf{k}) \simeq -[u_\gamma^{(1)}(\mathbf{k})_1 + u_\gamma^{(2)}(\mathbf{k})_1]^2 W^{-1}(1 - R)^{-1}. \tag{3.28}$$

We have examined Eq. (3.20) for all combinations of the graphs in Figs. 1 through 4 (as well as for a few more complicated graphical structures) and have

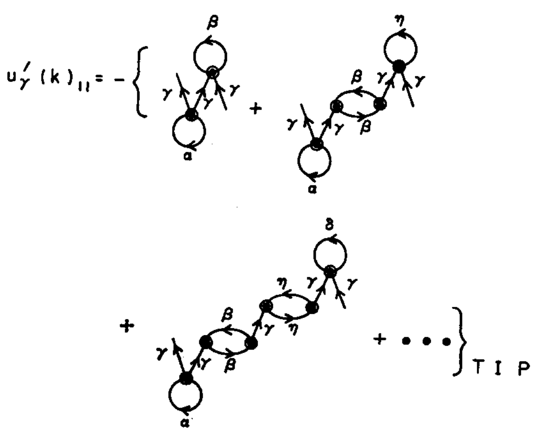

FIG. 5. The diagrammatic form of the series in Eq. (3.21) for $j = 1$, $l = 1$.

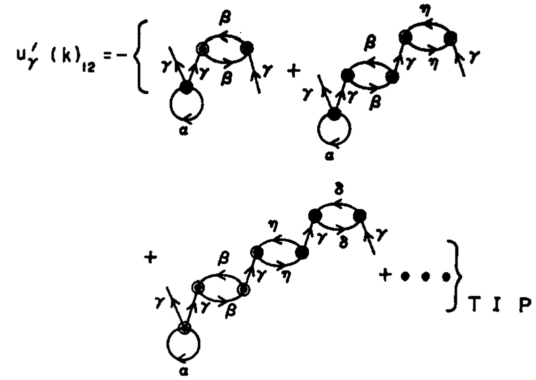

FIG. 6. The diagrammatic form of the series in Eq. (3.21) for $j = 1$, $l = 2$.

obtained the more general result

$$u_\gamma'(\mathbf{k}) = [u_\gamma(\mathbf{k})_1]^2 W^{-1}\{[\bar{u}_\gamma(-\mathbf{k})_1 - \tilde{u}_\gamma(\mathbf{k})_1]W^{-1} - 1\}^{-1}, \tag{3.29}$$

where $\tilde{u}_\gamma(\mathbf{k})_1$ is to be obtained from $u_\gamma(\mathbf{k})_1$ by changing $\mathbf{k}$ to $-\mathbf{k}$ and then replacing $w_\gamma'(-\mathbf{k})$ by $-w_\gamma'(\mathbf{k})$ wherever this quantity occurs inside momentum sums. Now, we introduce[15]

$$w_\gamma'(\mathbf{k}) \equiv \hbar ck + u_\gamma(\mathbf{k})_1 + u_\gamma'(\mathbf{k}) \equiv w_\gamma'(\mathbf{k})_1 + u_\gamma'(\mathbf{k}), \tag{3.30}$$

$$\bar{w}_\gamma(-\mathbf{k}) \equiv \hbar ck + \bar{u}_\gamma(-\mathbf{k})_1, \tag{3.31}$$

$$\tilde{w}_\gamma(\mathbf{k})_1 \equiv \hbar ck + \tilde{u}_\gamma(\mathbf{k})_1, \tag{3.32}$$

and use Eq. (3.29) to rewrite Eq. (3.8) in the form

$$w_\gamma'(\mathbf{k}) = w_\gamma'(\mathbf{k})_1 - [u_\gamma(\mathbf{k})_1]^2[w_\gamma'(\mathbf{k}) + \tilde{w}_\gamma(\mathbf{k})_1]^{-1}, \tag{3.33}$$

which, in turn, can be solved for $w_\gamma'(\mathbf{k})$ to give

$$w_\gamma'(\mathbf{k}) = \tfrac{1}{2}[u_\gamma(\mathbf{k})_1 - \tilde{u}_\gamma(\mathbf{k})_1] + \tfrac{1}{2}\{[w_\gamma'(\mathbf{k})_1 + \tilde{w}_\gamma(\mathbf{k})_1]^2 - 4[u_\gamma(\mathbf{k})_1]^2\}^{\frac{1}{2}}. \tag{3.34}$$

Here, it is to be realized that the simple form of Eq. (3.34) is deceptive, since it is actually a nonlinear integral equation.

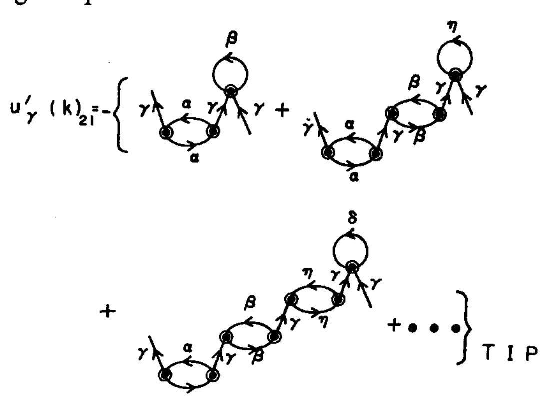

FIG. 7. The diagrammatic form of the series in Eq. (3.21) for $j = 2$, $l = 1$.

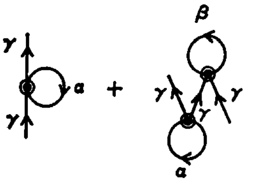

FIG. 8. The diagrams which, in lowest order, are equivalent to the pair-Hamiltonian approximation.

We suggest that Eq. (3.29) and, hence, Eq. (3.34) are formally exact. Of course, this assertion is based only on the experience gained by the detailed examination of the perturbation series in Eqs. (3.7) and (3.21) with the approximation given in Eq. (3.9). Also, we note that the inclusion of the Coulomb interaction would not alter the procedures used above. A general proof of this assertion, if one exists, has not yet been developed. The main question is whether energy denominators occurring in Eq. (3.21) can be factorized (to give decoupling).

For the 14 graphs in Figs. 1–3, relabeling leads to the result

$$u_\gamma(\mathbf{k})_1 - \tilde{u}_\gamma(\mathbf{k})_1 \simeq \sum_{i=1}^{14} [u_\gamma^{(i)}(\mathbf{k})_1 - \tilde{u}_\gamma^{(i)}(\mathbf{k})_1] = 0. \quad (3.35)$$

Moreover, using Eq. (3.19) and the analogous relation for $\tilde{u}_\gamma^{(i)}(\mathbf{k})$ and assuming the high-temperature, low-density limit, we have for Eq. (3.34)

$$w_\gamma'(\mathbf{k}) \simeq [(\hbar ck)^2 + \hbar^2\omega_p^2 + 2\hbar cku_\gamma^{(2)}(\mathbf{k})_1]^{\frac{1}{2}}, \quad (3.36)$$

where $u_\gamma^{(2)}(\mathbf{k})_1$ is given by Eq. (3.17), and Eqs. (3.16) and (3.35) have been used. In fact, Eq. (3.36) is given, to a good approximation, by

$$w_\gamma'(\mathbf{k}) \simeq [(\hbar ck)^2 + \hbar^2\omega_p^2]^{\frac{1}{2}} \equiv w_\Gamma(\mathbf{k}), \quad (3.37)$$

because, for all k, $|2\hbar cku_\gamma^{(2)}(\mathbf{k})_1[w_\Gamma(\mathbf{k})]^{-2}|$ is bounded by $(2\omega_p^2)^{-1}\sum_\alpha \eta_\alpha\omega_p^2(\alpha)$ which is always small, since $\omega_p^2 \geq \omega_p^2(\alpha)$ and $\eta_\alpha \ll 1$ [see Eq. (2.1)]. Thus, in conclusion, Eq. (3.37) represents accurately the photon self energy (in the high-temperature, low-density limit).

It is interesting to note that the photon self-energy in Eq. (3.37) corresponds precisely to that obtained in the pair-Hamiltonian approximation, which is diagrammatically equivalent to considering only the two graphs in Fig. 8. Moreover, as will be indicated in Sec. 4, the pair Hamiltonian can be diagonalized by a Bogoliubov transformation,[16] and the resulting quasiphoton energy is that given by Eq. (3.37). The dominant nature of Eq. (3.37) as an approximation to $w_\gamma'(\mathbf{k})$ in Eq. (3.34) suggests that the pair Hamiltonian is a good starting point for a perturbation theoretic development—this point of view will be adopted henceforth. At the end of the following section, the pair Hamiltonian and the Bogoliubov transformation are discussed in detail.

4. THE PHOTON MOMENTUM DISTRIBUTION

In this section we calculate the photon momentum distribution $\langle n_\gamma(\mathbf{k})\rangle$ [which is the average number of photons with momentum $\mathbf{k}$—see Eq. (4.16), below]. Thus, we are to evaluate [see Eqs. (I.3.14) and (I.3.17)]

$$\langle n_\gamma(\mathbf{k})\rangle = \nu_\gamma'(\mathbf{k})\int_0^\beta ds\mathcal{G}_{1,1}(\beta, s, \mathbf{k}^\gamma), \quad (4.1)$$

where $\nu_\gamma'(\mathbf{k})$ is given in Eq. (3.14), and the line factor $\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\gamma)$ is given by Eq. (3.1). The choice of counterterms made in the preceding section leads to the cancellation of all temperature independent parts of Eq. (3.2), so that the kernel $Q(t_2, t_1, \mathbf{k}^\gamma)$ in Eqs. (3.1) and (3.2) involves now only temperature dependent parts (TDP).[11]

First, we observe that the vertex functions for the electromagnetic interactions [Eqs. (I.B2)–(I.B6)] give rise to factors of $1/k$ in Eq. (3.2) so that the iterative solution of Eq. (3.1) is not valid for $k \to 0$; thus, we should always seek noniterative solutions of Eq. (3.1). It is easy to find the exact, noniterative solution of Eq. (3.1) in the pair-Hamiltonian approximation (which corresponds to the two graphs in Fig. 8). However, since the contributions of the (2, 0) and (0, 2) photon self-energy structures are of particular interest, we go beyond the simple pair-Hamiltonian approximation and include the leading order contributions to $\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\gamma)$ which arise from these structures. Thus, instead of the graphs in Fig. 8, we examine those in Fig. 9. Corresponding to the diagrams in Fig. 9 and for the selection of counterterms made in the preceding section, the kernel in Eq. (3.2) is approximately

$$Q(t_2, t_1, \mathbf{k}^\gamma) \simeq [\theta(t_1 - t_2) + \bar{\nu}_\gamma(-\mathbf{k})]E \exp[(t_2 - t_1)W], \quad (4.2)$$

where

$$E = [\bar{u}_\gamma^{(1)}(-\mathbf{k})_1 + \bar{u}_\gamma^{(2)}(-\mathbf{k})_1]^2 W^{-1} \quad (4.3)$$

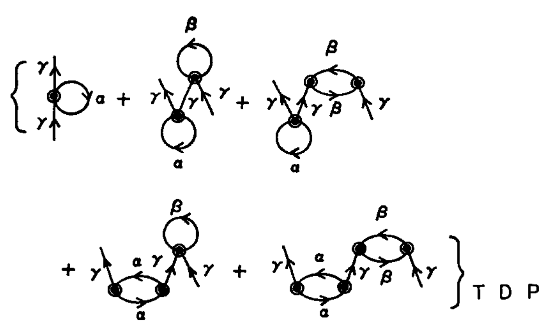

FIG. 9. The diagrams considered in the calculation of the line factor in Eq. (4.5).

and W is given in Eq. (3.26). Now, with Eq. (4.2), the line factor in Eq. (3.1) is obtained by solving the integral equation

$$\mathcal{G}'_{1,1}(t_2, t_1, \mathbf{k}^\gamma) \simeq \delta(t_2 - t_1) + \int_0^\beta ds \mathcal{G}'_{1,1}(t_2, s, \mathbf{k}^\gamma) E \times [\theta(t_1 - s) + \bar{\nu}_\gamma(-\mathbf{k})] \exp[(s - t_1)W]. \quad (4.4)$$

In the high-temperature, low-density limit $\bar{u}_\gamma^{(1)}(-\mathbf{k})_1$ is given approximately by Eq. (3.16) and $\bar{u}_\gamma^{(2)}(-\mathbf{k})_1$ by Eq. (3.17); thus, in this case, the kernel of Eq. (4.4) diverges for $k \to 0$. This causes no problem since the exact, noniterative solution to Eq. (4.4) is found to be

$$\mathcal{G}'_{1,1}(t_2, t_1, \mathbf{k}^\gamma) = \delta(t_2 - t_1) + E[\theta(t_1 - t_2) + M] \times \exp[(t_2 - t_1)(W - E)], \quad (4.5)$$

where

$$M^{-1} = \exp(-\beta E)\{1 + [\bar{\nu}_\gamma(-\mathbf{k})]^{-1}\} - 1. \quad (4.6)$$

Next, we use Eq. (4.5) as an approximate solution to Eq. (3.1) and introduce the lowest order temperature dependent contribution of the diagrams in Figs. 1–3, namely that from the second diagram in Fig. 1. Thus, to this order, we obtain

$$\mathcal{G}_{1,1}(t_2, t_1, \mathbf{k}^\gamma) \simeq \mathcal{G}'_{1,1}(t_2, t_1, \mathbf{k}^\gamma) + F(t_2, t_1, \mathbf{k}^\gamma), \quad (4.7)$$

where $F(t_2, t_1, \mathbf{k}^\gamma)$ is given by Eq. (3.12). Since Eq. (3.12) has a factor of k^{-1}, Eq. (4.7) cannot be used to construct an iterative solution of Eq. (3.1) for small k. Analogous to the procedures used in the preceding section, we have developed a partial summation program to obtain solutions to Eq. (3.1) which cause no problem for small k. However, the resulting analytical expressions are not particularly illuminating and are perhaps not useful, since it is difficult to assess the relative importance of neglected terms in the integral equation. With these points in mind, we use Eq. (4.7) to estimate the photon momentum distribution in Eq. (4.1). In the high-temperature, low-density limit we obtain, for Eq. (4.1) with Eq. (4.7),

$$\langle n_\gamma(\mathbf{k})\rangle \simeq \nu'_\gamma(\mathbf{k}) + \nu'_\gamma(\mathbf{k}) EM(W - E)^{-1} \times \{\exp[\beta(W - E)] - 1\} + (2\beta\hbar ck)^{-1} \times \sum_\alpha \hbar^2\omega_p^2(\alpha)[w'_\gamma(\mathbf{k}) + w_\alpha(\mathbf{k})]^{-2}. \quad (4.8)$$

We wish to explore the meaning of this result, by examining its lowest-order approximation; thus, we use Eq. (3.19), Eq. (3.16) for $\bar{u}_\gamma^{(1)}(-\mathbf{k})_1$ and Eq. (3.37) for $w'_\gamma(\mathbf{k})$ to obtain[17]

$$\langle n_\gamma(\mathbf{k})\rangle \simeq [f_-(\mathbf{k})]^2 + \{[f_+(\mathbf{k})]^2 + [f_-(\mathbf{k})]^2\}\nu_\Gamma(\mathbf{k}) + (2\beta\hbar ck)^{-1} \sum_\alpha \hbar^2\omega_p^2(\alpha)[w_\Gamma(\mathbf{k}) + w_\alpha(\mathbf{k})]^{-2}, \quad (4.9)$$

where

$$[f_+(\mathbf{k})]^2 - [f_-(\mathbf{k})]^2 = 1, \quad (4.10)$$

$$[f_+(\mathbf{k})]^2 = [w_\Gamma(\mathbf{k}) + \bar{w}_\gamma^{(1)}(-\mathbf{k})][2w_\Gamma(\mathbf{k})]^{-1}, \quad (4.11)$$

$$\nu_\Gamma(\mathbf{k}) = \{\exp[\beta w_\Gamma(\mathbf{k})] - 1\}^{-1}, \quad (4.12)$$

with $\bar{w}_\gamma^{(1)}(-\mathbf{k}) = \hbar ck + \bar{u}_\gamma^{(1)}(-\mathbf{k})_1$. We see that Eqs. (4.8) and (4.9) diverge as k^{-1} for small k; this same divergence is also exhibited by the Planck or free-photon distribution function. However, this kind of behavior is of no consequence, since in calculations of all measurable quantities the divergence is removed by the density-of-states factor. Thus, in lowest order, we have obtained a result which does not suffer from the infrared divergence. It is interesting to note that the first term in Eq. (4.9) is independent of the system temperature; the electrodynamic origin of this term is not clear.

In closing this section we wish to indicate the connection between Eqs. (3.37), (4.9), and the pair Hamiltonian H_p. It is straightforward to extract H_p from the system Hamiltonian[16]; the result is

$$H_p = \sum_{\mathbf{k}} \{(\hbar ck + \hbar^2\omega_p^2/2\hbar ck)a^\dagger(\mathbf{k})a(\mathbf{k}) + \hbar^2\omega_p^2(2\hbar ck)^{-1}[a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k}) + a(\mathbf{k})a(-\mathbf{k})]\}, \quad (4.13)$$

where $a^\dagger(\mathbf{k})$ and $a(\mathbf{k})$ are photon creation and annihilation operators. The pair Hamiltonian can be diagonalized by means of a Bogoliubov transformation; thus, one introduces the quasiphoton creation and annihilation operators $b^\dagger(\mathbf{k})$ and $b(\mathbf{k})$ as follows:

$$a^\dagger(\mathbf{k}) \to Ua^\dagger(\mathbf{k})U^\dagger \equiv f_+(\mathbf{k})b^\dagger(\mathbf{k}) - f_-(\mathbf{k})b(-\mathbf{k}),$$
$$a(\mathbf{k}) \to Ua(\mathbf{k})U^\dagger \equiv f_+(\mathbf{k})b(\mathbf{k}) - f_-(\mathbf{k})b^\dagger(-\mathbf{k}), \quad (4.14)$$

where $f_+(\mathbf{k})$ and $f_-(\mathbf{k})$ are given by Eqs. (4.10)–(4.11). One readily verifies that

$$H'_p = UH_pU^\dagger = \sum_{\mathbf{k}} w_\Gamma(\mathbf{k})b^\dagger(\mathbf{k})b(\mathbf{k}), \quad (4.15)$$

where $w_\Gamma(\mathbf{k})$ is given in Eq. (3.37). Now, we can also relate the *true photon* momentum distribution and the *quasiphoton* momentum distribution. If we introduce the transformation in Eq. (4.14) into the definition of the photon momentum distribution, namely

$$\langle n_\gamma(\mathbf{k})\rangle \equiv \mathrm{Tr}[\rho a^\dagger(\mathbf{k}^\gamma)a(\mathbf{k}^\gamma)], \quad (4.16)$$

we obtain

$$\langle n_\gamma(\mathbf{k})\rangle = [f_-(\mathbf{k})]^2 + \{[f_+(\mathbf{k})]^2 + [f_-(\mathbf{k})]^2\} \times \mathrm{Tr}[\rho' b^\dagger(\mathbf{k})b(\mathbf{k})] - f_-(\mathbf{k})f_+(\mathbf{k})\,\mathrm{Tr}\{\rho'[b^\dagger(\mathbf{k})b^\dagger(-\mathbf{k}) + b(\mathbf{k})b(-\mathbf{k})]\}. \quad (4.17)$$

In Eq. (4.16) ρ is the density operator for the grand canonical ensemble, and in Eq. (4.17)

$$\rho' = U\rho U^\dagger. \tag{4.18}$$

One observes that Tr $[\rho' b^\dagger(\mathbf{k})b(\mathbf{k})]$ is the quasiphoton momentum distribution. The quasiphoton momentum distribution has been calculated earlier (for the two diagrams in Fig. 1, as well as for a Coulomb correction),[6] and, on the basis of Eq. (4.17), the result is in accord with our lowest-order results for the true photon momentum distribution.

We see that Eq. (4.17) is, in lowest order, equivalent to Eq. (4.9); this suggests that the pair Hamiltonian is a useful choice of unperturbed Hamiltonian for a perturbation theory of interacting radiation and charges.[18] Moreover, Eq. (4.17) provides the formal relation between the photon and quasiphoton momentum distributions; however, this relation is not as useful as it may appear, since it is now necessary to construct a calculational scheme for evaluating the last two terms in Eq. (4.17) [note that these terms are inherently (2, 0) and (0, 2) structures]. Finally, we observe that the infrared divergence does not occur in the quasiphoton representation[16]; thus, in Eq. (4.17), the infrared divergence has been relegated completely to the factors involving $f_+(\mathbf{k})$ and $f_-(\mathbf{k})$.

5. DISCUSSION

A principal goal of this investigation was to determine the importance of the complete photon self-energy analysis on the calculations of the properties of photons in a fully ionized gas. The most interesting result of this study is the photon energy–momentum relation given in Eq. (3.34), and we note that the *form* of this expression is determined primarily by the analysis of the (2, 0) and (0, 2) photon structures; thus, these structures, which have not been included completely in any of the prior investigations,[3–7] play a very significant role in determining the dressed photon energy.

The expression for the momentum distribution in Eq. (4.8) also has certain features not observed before, since earlier calculations[3–7] did not include the self-energy analysis of (2, 0) and (0, 2) structures, and since some of these calculations[6,7] were for the quasiphoton momentum distribution. It is recalled that the noniterative result in Eq. (4.5) was important in determining the result in Eq. (4.8). At this point, we remark that a complete understanding of the properties of photons in an interacting system (as considered herein) cannot be based solely on the quantities which we have investigated, and additional functions must be determined. In particular, knowledge of the dynamic structure factor is of extreme value, since this can be used to understand the modes of propagation of photons and also the related lifetimes.

In Sec. 4 we have indicated that in the photon momentum distribution the infrared divergence can be extracted by means of a Bogoliubov transformation, but that it will be difficult to calculate the resulting expression. Since the infrared divergence is of electrodynamic origin, it would be more pleasing to analyze this problem on a more fundamental level. Thus, we are currently pursuing the infrared problem, along the lines initiated by Kibble,[19] by using a nonseparable Hilbert space for describing photon states.

As a result of this investigation, we conclude that the new formalism in I, in addition to performing a *complete* self-energy analysis, is much simpler in practice than its predecessor.[2] As a direct outcome of the simplifications introduced by the new formalism, it has been possible to sum certain important infinite series to all orders. Another important feature of the theory in I is the counterterm technique. It is apparent that the technique is particularly well suited for investigating the self-energy properties associated with single particles or photons (as opposed to collective excitations); examples of this type of self-energy problem are provided by mass renormalization, the dressed photon energy and the one-particle problem of MG.[20] The Coulomb and infrared divergences seem to be less susceptible to a direct application of the counterterm technique.

The connections between the line factors in I and single-particle Green functions have been established recently.[21] Thus, starting with the line factors in Sec. 4, we could now calculate the normal and anomalous single-particle Green functions for the equilibrium fully ionized gas—such calculations have been performed.[22] However, in the present paper, we have observed consistently the $(t_2 - t_1)$-temperature dependence established in the Green function theory.[21]

ACKNOWLEDGMENTS

The authors would like to thank Professor G. Chew and Professor K. Watson for extending the hospitality of the Lawrence Radiation Laboratory at Berkeley. One of us (C. R. S.) wishes to thank Associated Western Universities, Inc., for the faculty fellowship at Lawrence Radiation Laboratory. Finally, we express our appreciation to Professor F. Mohling and Professor W. T. Grandy, Jr., and Dr. I. RamaRao and Dr. I. K. Hwang for illuminating discussions.

APPENDIX

In the calculations of this paper no use is made of the *explicit* expressions for the (1, 1) graphs of order α_0^2 in Figs. 2 and 3, since (after mass renormalization) they are much smaller than the other contributions which are taken into account. On the other hand, if the expressions for the graphs in Fig. 2 are examined, it is found that (before mass renormalization) these expressions diverge for large photon momentum—this is a manifestation of the ultraviolet divergence of quantum electrodynamics. The need for mass renormalization occurs because in the Hamiltonian the electromagnetic field associated with each charged particle is separated from the particle so that *bare* particles interact with the total electromagnetic field. Since it is meaningless from an experimental standpoint to separate a charged particle and its associated field, it is clear that the separation mentioned above must be a mathematical convenience and can be of no further consequence. The mass-renormalization technique developed in I is designed to replace bare-particle masses by their experimentally observed masses. Below, we outline how mass renormalization is used to cancel the ultraviolet divergences in the graphs in Fig. 2 to obtain the finite contributions from these graphs.

The mass-renormalization procedure developed in I is quite straightforward; however, since some skill may be involved in applying the technique, we now indicate how one approaches the selection of the mass-renormalization counterterm. Thus, following I, we combine the kinetic energy of the bare particle

$$w_\alpha^{(0)}(k) = \hbar^2k^2/2M_\alpha^{(0)} \tag{A1}$$

and the mass-renormalization counterterm

$$S_\alpha(k) = (\hbar^2k^2/2M_\alpha)D_\alpha \tag{A2}$$

so as to achieve the correct single-particle kinetic energy:

$$w_\alpha(k) = w_\alpha^{(0)}(k) + S_\alpha(k) = \hbar^2k^2/2M_\alpha. \tag{A3}$$

Above, $M_\alpha^{(0)}$ is the bare mass, M_α is the observed mass, and

$$1/M_\alpha^{(0)} \equiv (1 - D_\alpha)/M_\alpha. \tag{A4}$$

As noted earlier,[5] the kinetic energy in Eq. (A3) is to be quadratic in k so that D_α must be independent of k. Then, the identity in Eq. (A4) is used to re-express the bare masses in the interaction vertices in terms of M_α and D_α, which in turn determine $S_\alpha(k)$.

Next, we combine the diagrams in Figs. 1 and 2 as follows:

$$\mathcal{K}_{1,1}^{(1)} + \mathcal{K}_{1,1}^{(3)} + \mathcal{K}_{1,1}^{(4)} \tag{A5}$$

$$\mathcal{K}_{1,1}^{(2)} + \mathcal{K}_{1,1}^{(5)} + \cdots + \mathcal{K}_{1,1}^{(8)}. \tag{A6}$$

By relabeling, one can extract a factor $\mathcal{K}_{1,1}^{(1)}$ in Eq. (A5) and a factor $\mathcal{K}_{1,1}^{(2)}$ in Eq. (A6); in the remaining factors in Eqs. (A5) and (A6) it is possible to select the quantity D_α to cancel the ultraviolet divergences in these terms. We state the result:

$$D_\alpha = (4\pi\alpha_0\hbar^2Z_\alpha^2/M_\alpha\Omega) \times \sum_{\mathbf{k}_4} (\hat{e}_\mathbf{k}\cdot\hat{e}_4)^2 k_4^{-1}[w_\alpha(\mathbf{k}_4) + w_\gamma'(\mathbf{k}_4)]^{-1}. \tag{A7}$$

This defines a counterterm, Eq. (A2), which cancels, through order α_0^2, the ultraviolet divergences everywhere in the theory. In order to obtain Eq. (A7) the following identities (relating to the angular integrations) are useful:

$$\int_{-1}^{1} d\mu_4 \int_0^{2\pi} d\phi_4 \sum_{\lambda_4} (\hat{e}_4\cdot\hat{e}_\mathbf{k})^2 = 8\pi/3,$$

$$\int_{-1}^{1} d\mu_4 \int_0^{2\pi} d\phi_4 \sum_{\lambda_4} (\hat{e}_4\cdot\hat{e}_\mathbf{k})(\mathbf{k}_2\cdot\hat{e}_4)(\mathbf{k}_2\cdot\hat{e}_\mathbf{k})^{-1} = 8\pi/3,$$

where $\sum_{\lambda_4}$ is the sum over polarizations of the photon with momentum $\mathbf{k}_4$.

* Based in part on a thesis (A. B.) submitted to the faculty of the graduate school of the University of Wyoming in partial fulfillment of the requirements for the Ph.D. degree, 1970.

† The final stages of this research were completed at Lawrence Radiation Laboratory (Berkeley), while one of us (C. R. S.) was supported by Associated Western Universities, Inc., through contract with the U.S. Atomic Energy Commission and the other (A. B.) was supported by a research assistantship from the Physics Department of the University of Wyoming.

[1] The preceding paper will be referred to as I. Equation (*n*) of I will be referred to as Eq. (I.*n*).

[2] F. Mohling and W. T. Grandy, Jr., J. Math. Phys. **6**, 348 (1965), hereafter referred to as MG.

[3] S. Nakai, Nucl. Phys. **63**, 131 (1965).

[4] W. T. Grandy, Jr., Nuovo Cimento **40**, 265 (1965).

[5] C. R. Smith, Ph.D. thesis, University of Colorado, 1967, unpublished.

[6] I. K. Hwang and W. T. Grandy, Jr., Phys. Rev. **177**, 359 (1969).

[7] W. T. Grandy, Jr., Phys. Rev. **177**, 371 (1969).

[8] A. Bhowmik, Ph.D. thesis, University of Wyoming, 1970, unpublished.

[9] Throughout this paper the notation $\delta(t_2^{(-)} - t_1)$ is simplified to $\delta(t_2 - t_1)$.

[10] We comment here on the notation. A bar is always placed over quantities associated with $-\mathbf{k}^\gamma$ lines. This is necessary since in general the difference between the kernels in Eqs. (3.1) and (3.3) results in two different line factors $\mathcal{G}_{1,1}$ and $\bar{\mathcal{G}}$; for the same reason $\bar{w}_\gamma(-\mathbf{k}) \neq w_\gamma'(-\mathbf{k})$ [also, see Eqs. (3.30) and (3.31)].

[11] Quantities multiplied by $[\theta(t_2 - t_1) + \nu_\gamma'(\mathbf{k})]$, but which are otherwise independent of t_2 and t_1, are said to be *temperature independent* (and analogously for $-\mathbf{k}^\gamma$ lines). Thus, in Eq. (3.2) for $Q(t_2, t_1, \mathbf{k}^\gamma)$ [or in Eq. (3.4) for $\bar{\mathcal{K}}_{1,1}(t_2, t_1, -\mathbf{k}^\gamma)$], the counterterms are selected to cancel the temperature independent parts. It should be clear that the counterterm extracts contributions to the interaction potential which are of a single-particle nature [see Eq. (I.2.7)].

[12] The mass-renormalization counterterm $S_\alpha(k)$ is suppressed throughout the main text, but is discussed and identified in the Appendix.

[13] The approximation in Eq. (3.9) permits us to neglect the particle self-energies $u_\alpha(\mathbf{k})$ so that $w_\alpha'(\mathbf{k}) \simeq w_\alpha(\mathbf{k})$.

[14] In arriving at Eqs. (3.28) and (3.29), we must rearrange energy denominators by repeated use of the identity $(ab)^{-1} = [a(a+b)]^{-1} + [b(a+b)]^{-1}$, as well as other analogous identities involving momentum sums.

[15] The form in Eq. (3.31) follows from Eq. (3.4); thus, $\bar{w}_\gamma(-\mathbf{k})$ contains no contribution analogous to $u_\gamma'(\mathbf{k})$—this clarifies further why, in general, $w_\gamma'(-\mathbf{k}) \neq \bar{w}_\gamma(-\mathbf{k})$.

[16] W. R. Chappell, W. E. Brittin, and S. J. Glass, Nuovo Cimento 38, 1186 (1965).

[17] Rayleigh–Schrödinger perturbation theory has been applied to a fully ionized gas in a pure state, and the expression for the average number of photons has a form analogous to Eq. (4.9).

[18] There are some disadvantages in partially diagonalizing the Hamiltonian by means of the Bogoliubov (or any other) transformation, since the explicit appearance of some interaction terms is prevented, thereby obscuring the physical consequences of these interactions. For example, Hwang and Grandy (Ref. 6, Sec. 5) were unable to achieve mass renormalization in the transformed theory, and found it necessary to appeal to the untransformed theory.

[19] T. W. B. Kibble, J. Math. Phys. 9, 315 (1968).

[20] If iterations of the line factor of a charged particle are introduced, then processes involving the emission and reabsorption of photons by the charged particle are introduced. Such iterations, called radiative corrections, give rise to physical effects as well as to unobservable (system independent) electromagnetic self energies. The one-particle problem is concerned with the cancellation of these spurious, particle self energies. The Λ_s transformation of Sec. 4 of MG was developed to treat this problem, and we note here that the counterterm technique of I encompasses the Λ_s transformation.

[21] I. RamaRao and C. R. Smith, Phys. Rev. A 2, 843 (1970).

[22] C. R. Smith, unpublished.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Conformal Group in a Poincaré Basis. I. Principal Continuous Series

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(Received 9 October 1970)

In the first of a series of papers on the global representation theory of $SU(2, 2)$, with particular emphasis on the Poincaré subgroup, we study the two principal continuous series of unitary irreducible representations. These are defined by operators on Hilbert spaces of functions over a six-dimensional manifold, and after an automorphism of the group by a real orthogonal transformation [in precise analogy to that used in the mapping $SU(1, 1) \rightarrow SL(2, R)$] we display these in such a form that the Poincaré subgroup $SL(2, C) \times T_4$ appears in a simple fashion. The generators of translations, dilations, Lorentz and special conformal transformations are given as differential operators, and by using these we find explicit expressions for the eigenvalues of the three Casimir operators of the group. Finally, we perform the reduction of the two series when restricted to the Poincaré group. It is found that all those principal series representations of $\mathbb{P}$ enter which allow a certain value of helicity.

I. INTRODUCTION

There has been recently[1] considerable interest in the conformal group[2] $O(4, 2)$ and its spin-covering group $SU(2, 2)$, together with much speculation as to its precise role in physics. There are at least two ways in which this group arises—in internal symmetries as a subgroup of $SU(6, 6)$ and as a dynamical group acting on the space–time coordinates—and its physical significance in the two cases is best expressed by entirely different reductions—to the maximal compact subgroup $SU(2) \times SU(2) \times U(1)$ in the former case and to the Poincaré group $\mathbb{P}$ in the latter. Although almost all the applications so far have used only the degenerate representations of $SU(2, 2)$, it is certainly of considerable importance and interest, both physically and mathematically, to have a detailed knowledge of the entire representation theory; and so in a series of papers we shall present this, with special attention being paid to the Poincaré subgroup.

Much previous work (see, e.g., Refs. 3, 4) on the representation theory of $SU(2, 2)$ has concentrated on the Lie algebra. The most inclusive material on this topic is by Yao[3] (where references to earlier work on these lines may be found), who discusses the reduction to the maximal compact subgroup, evaluates the matrix elements of all the generators in terms of certain constants, and, by imposing on these suitable reality conditions, obtains conditions for the representation to be unitary and irreducible. This method naturally raises questions of completeness, because of the amount of algebra involved, and indeed Yao has omitted one principal series of representations. Globally, the theory is very ill known; there is a solitary paper by Klink[5] (which treats only the series omitted by Yao) and treatments of sundry degenerate representations by various authors,[6,7] but otherwise it is far from the completeness attained algebraically.

There is, however, a little-known paper by Graev[8] on the theory of $U(p, q)$, and in this paper we take that as our basis of studying the global representation theory and the reduction of a given representation with respect to the Poincaré group when the group elements are restricted to the latter. Because the material,

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There is, however, a little-known paper by Graev[8] on the theory of $U(p, q)$, and in this paper we take that as our basis of studying the global representation theory and the reduction of a given representation with respect to the Poincaré group when the group elements are restricted to the latter. Because the material, otherwise rather lengthy, falls into several parts, we shall in the present paper treat only the two principal continuous series; subsequent papers will examine the principal discrete series and, finally, the complementary and degenerate representations. Our treatment has but little in common with the algebraic approach, and so we shall not discuss the latter further.

The principal series of representations of a group is the set of all those that occur in the reduction of the regular representation, whether they are continuous or discrete. All other (unitary-irreducible) representations are termed supplementary, and are recognizable by two features: the existence of a two-point measure in the scalar product defining the Hilbert space (complementary series) or definition over some lower-dimensional transitive manifold (degenerate series); the two classes are not exclusive. The complementary series are familiar from the groups $SL(2, C)$ and $SL(2, R)$, but the degenerate are not so well known because, for these groups, they reduce to trivialities. The mere fact of being degenerate need not exclude a representation from the principal series [contrast the timelike representation of $\mathbb{P}$ induced by the trivial representation of $SO(3)$ with the spacelike one induced by the trivial representation of $SO(2, 1)$]; but, with $SU(2, 2)$, the two classes are indeed disjoint, and we shall consider them separately.

The principal series then are induced by representations of the nonisomorphic Cartan subgroups of $SU(2, 2)$; since there are three of these (with three, two, and one compact generators, respectively), we expect three distinct series of unitary irreducible representations—the principal discrete series d_0 and the first and second principal continuous series d_1 and d_2. Representations of all three can be specified by a single ansatz involving constants whose ranges differ in each case; but these transformations are, of course, upon different Hilbert spaces, and it is found that the ansatz is reducible in the discrete series. We shall treat this in a later paper, and here concentrate upon d_1 and d_2.

It proves convenient to follow Graev[8] and choose a different realization of the group as that set of transformations leaving invariant the form $\bar{z}_1 z_4 + \bar{z}_2 z_3 + \bar{z}_3 z_2 + \bar{z}_4 z_1$; unfamiliar though this may be, it is derived from the usual matrix realization by a real orthogonal transformation, and bears precisely the relation to $SU(2, 2)$ that $SL(2, R)$ bears to $SU(1, 1)$. In this formalism, the Poincaré subgroup [or, rather, its spin-covering group $SL(2, C) \times T_4$] appears in a very simple fashion; not only is the representation made more transparent, but the reduction under $\mathbb{P}$ is displayed clearly in the case of d_2. For d_1 the situation is more complicated because of the definition of the appropriate Hilbert space, but we continue to use the same realization. In Sec. II we discuss this group of matrices and introduce some subgroups, and then in Sec. III define the representations d_1 and d_2.

In Sec. IV we give the generators of the group as differential operators, and calculate the three Casimir operators and their eigenvalues. While these are not so important in this paper, they will be necessary later when we wish to compare our degenerate representations with the formalism of other workers—in particular with the list of Yao.[3] Finally, Sec. V shows how the representations reduce when restricted to the Poincaré group. One subset of d_2 has indeed been treated by Klink,[5] but he notes only the absence of lightlike particles (which can be deduced at once from the fact that these are principal-series representations) and does not discuss any remaining restrictions. We find that, in fact, the only restriction upon the principal-series representations of $\mathbb{P}$ occurring in d_1 and d_2 is given by that label m of the representations of $SU(2, 2)$, which is always integral. This appears through a covariance condition involving a certain $SL(2, C)$ subgroup, and the result is that only those representations of $\mathbb{P}$ enter which allow a helicity of $\frac{1}{2}m$, and these have unit multiplicity.

After completion of this work we have received a preprint by Yao which deals with the same problems.[9] His approach is algebraic, and his results, which are in complete contradiction to ours, are derived by considering the matrix elements of the generators. For the principal series his results are left implicit, and we cannot comment on them except to remind the reader that there are actually six principal discrete series[8] of $SU(2, 2)$. For his 14 degenerate series, however, he finds that *only* spacelike *or* timelike *or* lightlike representations of $\mathbb{P}$ occur, and this is very different from our results, which will be presented in a subsequent paper. We believe that this discrepancy is due to nonintegrability of his representations of the algebra to those of the group. Thus, it is known that in the reduction $SL(2, R) \supset O(1, 1)$ the subgroup is degenerate, and is labeled by a discrete parameter t; but all matrix elements of *generators* between subspaces of different t vanish identically. (See Mukunda, Ref. 10.) We believe that a similar situation holds here when taking matrix elements between states with differing signs of M^2.

II. $SU(2, 2)$ AND MATRIX REALIZATIONS

The pseudo-orthogonal group $SO(4, 2)$ has 15 generators, whose commutation relations in canonical form can be written

$$[J_{\alpha\beta}, J_{\gamma\delta}] = g_{\alpha\gamma}J_{\beta\delta} + g_{\beta\delta}J_{\alpha\gamma} - g_{\beta\gamma}J_{\alpha\delta} - g_{\alpha\delta}J_{\beta\gamma}, \quad (1)$$

where the indices run from 1 to 6 and the metric is $(++++-+-)$. This is not very transparent physically, and so we define the new generators

$$\begin{aligned} J_{\mu 5} + J_{\mu 6} &= -2L_\mu, \\ J_{\mu 5} - J_{\mu 6} &= -P_\mu, \\ J_{56} &= D. \end{aligned} \quad (2)$$

Replacing the label 4 by 0 and the metric by $(+---)$, we then find that $J_{\mu\nu}$ and P_ρ generate the Poincaré group:

$$\begin{aligned} &[J_{\mu\nu}, J_{\rho\sigma}] = -g_{\mu\rho}J_{\nu\sigma} - g_{\nu\sigma}J_{\mu\rho} + g_{\mu\sigma}J_{\nu\rho} + g_{\nu\rho}J_{\mu\sigma}, \\ &[J_{\mu\nu}, P_\rho] = -g_{\mu\rho}P_\nu + g_{\nu\rho}P_\mu, \\ &[P_\mu, P_\nu] = 0; \quad \mu, \nu = 0 \cdots 3, \end{aligned} \quad (3)$$

while the remaining commutation relations are

$$\begin{aligned} &[P_\mu, L_\nu] = J_{\mu\nu} - Dg_{\mu\nu} \; [P_\mu, D] = P_\mu, \\ &[L_\rho, J_{\mu\nu}] = g_{\mu\rho}L_\nu - g_{\nu\rho}L_\mu \; [L_\mu, D] = -L_\mu, \\ &[L_\mu, L_\nu] = 0 = [J_{\mu\nu}, D]. \end{aligned} \quad (4)$$

In the remainder of this work we shall use the relations (3) and (4), often replacing the quantities $J_{\mu\nu}$ by the rotations $J_i = \frac{1}{2}\epsilon_{ijk}J_{jk}$ and the boosts $K_i = J_{0i}$. Notice that our definition of L_μ differs by a factor of 2 from that of some authors.

Under the one-parameter subgroups generated by these elements of the Lie algebra, a position vector x_μ is transformed as follows:

$$\begin{aligned} &\exp(\theta J_3): x_\mu \\ &\quad = (x_0, x_1 \cos\theta + x_2 \sin\theta, x_2\cos\theta - x_1 \sin\theta, x_3), \\ &\exp(\zeta K_3): x_\mu \\ &= (x_0 \cosh\zeta + x_3 \sinh\zeta, x_1, x_2, x_0 \sinh\zeta + x_3\cosh\zeta), \\ &\quad \exp(y_\mu P^\mu): x_\mu = x_\mu + y_\mu, \\ &\quad \exp(dD): x_\mu = dx_\mu, \\ &\quad \exp(s_\nu L^\nu): x_\mu = \frac{x_\mu + s_\mu x^2}{1 + 2s_\mu x^\mu + s^2x^2}. \end{aligned} \quad (5)$$

The four L_μ, which generate an Abelian group, are known as special conformal transformations or vector accelerations; D is a dilatation. The Lie algebra can be integrated to give (among other possibilities) either $O(4, 2)$ or its spin-covering group $SU(2, 2)$—that is, that connected component of each which includes the identity. We shall consider the latter.

This is defined as the set of transformations leaving invariant the Hermitian form $|z_1^2| + |z_2^2| - |z_3^2| - |z_4^2|$. It proves convenient to carry out an automorphism of the group by a real orthogonal matrix and consider instead the isomorphic group $\mathcal{G}$ defined by the metric tensor

$$S = \begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{pmatrix} \equiv \begin{pmatrix} & s \\ s & \end{pmatrix}, \quad (6)$$

which corresponds to the form $\bar{z}_1 z_4 + \bar{z}_2 z_3 + \bar{z}_3 z_2 + \bar{z}_4 z_1$. $\mathcal{G}$ is then the set of all (unimodular) matrices g which satisfy the condition

$$g^\dagger S g = S. \quad (7)$$

We now enumerate some subgroups of $\mathcal{G}$. For compactness, we write the matrices with elements which are themselves matrices of appropriate order:

$$\begin{aligned} &K \ni k = \begin{pmatrix} k_{-1} & k_0 \\ & k_1 \end{pmatrix}, \\ &Z \ni z = \begin{pmatrix} 1 & \\ z & 1 \end{pmatrix}, \\ &\qquad z = \begin{pmatrix} a & b \\ c & -\bar{a} \end{pmatrix}, \quad \operatorname{Re} b = 0 = \operatorname{Re} c, \\ &D \ni d = \begin{pmatrix} k_{-1} & \\ & k_1 \end{pmatrix}, \quad k_1 \in GL(2, c)/U(1), \; k_{-1}^\dagger s k_1 = s. \end{aligned} \quad (8)$$

The unimodularity condition restricts k_1 to have real determinant; if this is relaxed, the group becomes isomorphic to $U(2, 2)$. In all of the above definitions the submatrices were themselves 2×2: We now pass on to some other subgroups,

$$\mathcal{K} \ni \kappa = \left(\begin{array}{c|c|c} \kappa_{-1} & \kappa_{-10} & \kappa_{-11} \\ \hline & \kappa_0 & \kappa_{01} \\ \hline & & \kappa_1 \end{array}\right),$$

$$Z \ni \zeta = \left(\begin{array}{c|c|c} 1 & & \\ \hline -\beta & 1 & \\ -\bar{\alpha} & & \\ \hline c & \alpha \;\; \beta & 1 \end{array}\right),$$

$$c + \bar{c} + \alpha\bar{\beta} + \bar{\alpha}\beta = 0. \quad (9)$$

In $\mathcal{K}$, the submatrix κ_0 is 2×2. We need not give explicitly the remaining restrictions on the elements of these matrices, for they can all be obtained from (7).

Finally, we shall need two further subgroups:

$$\mathit{\Lambda} \ni \Lambda = \left(\begin{array}{cc|cc} \bar{\lambda}^{-1} & -\bar{\mu}/\bar{\Delta} & \lambda_1 & \\ & \bar{\lambda}/\bar{\Delta} & & \\ \hline & & \lambda^{-1}\Delta & \mu \\ & & & \lambda \end{array}\right),$$

$$\mathrm{Y} \ni y = \left(\begin{array}{cc|cc} 1 & & & \\ -\bar{\omega} & 1 & & \\ \hline a & b & 1 & \\ \omega a + c & \omega b - \bar{a} & \omega & 1 \end{array}\right),$$

$$\operatorname{Re} b = 0 = \operatorname{Re} c. \quad (10)$$

It is not difficult to show that, except for a lower-dimensional manifold, any element $g \in \mathcal{G}$ can be written uniquely as a product of these matrices. Some forms that we shall use are

$$g = kz = \not{k}\zeta = \mathit{\Lambda} y$$

and

$$k = z^{\mathrm{T}} d \quad (11)$$

where the superscript T denotes matrix transposition. We shall need various invariant measures: By direct computation[8] we find that on the subgroups z, Z, Y these are

$$\begin{aligned} d\mu(z) &= -Da\, db\, dc, \\ d\mu(\zeta) &= D\alpha\, D\beta d(\operatorname{Im} c), \\ d\mu(y) &= d\mu(z)\, D\omega. \end{aligned} \quad (12)$$

Because of the factorization (11), any element of the group defines a transformation of these manifolds, $z \to z'$, etc.:

$$zg = kz', \quad \zeta g = \not{k}\zeta', \quad yg = \mathit{\Lambda} y', \quad (13)$$

under which the invariant measures (12) behave as

$$\begin{aligned} d\mu(z')/d\mu(z) &= |\Delta|^{-4}, \\ d\mu(\zeta')/d\mu(\zeta) &= |\not{k}_1|^{-6}, \\ d\mu(y')/d\mu(y) &= |\lambda^2\Delta|^{-2}. \end{aligned} \quad (14)$$

Now consider further the subgroup z. This is a four-parameter Abelian group, and it is convenient to map it onto the translation subgroup $T_4 \subset \mathbb{P}$ of the Poincaré group by setting

$$\begin{aligned} a &= ix_1 - x_2, \\ b &= i(x_0 + x_3), \\ c &= i(x_0 - x_3). \end{aligned} \quad (15)$$

Then under the transformation (13), this manifold of 2×2 matrices z is mapped by the block-diagonal group D into

$$z \to z' : (zs)' = k_1^{-1} z s k_1^{-1\dagger}. \quad (16)$$

Restrict k_1 to $SL(2, C)$; then this is precisely the mapping of a position vector dictated by a homogeneous Lorentz transformation. Hence the Poincaré subgroup of $\mathcal{G}$ is realized by the matrices d and z (that is, by k^{T}), and allowing det k_1 to vary in magnitude enlarges this to the similitude group.

III. CONTINUOUS NONDEGENERATE REPRESENTATION OF G

The representations in the principal series of the group $U(p, q)$ are induced by representations of a Cartan subgroup. Since there are $(q + 1)$ of these that are nonisomorphic, there are $(q + 1)$ distinct principal nondegenerate series of unitary irreducible representations (UIR's) of $U(p, q)$; of these, one is discrete while the others are specified by $p + q - r$ integers and r real parameters. These considerations apply also to the unimodular groups (except that here one less integer is needed), and so $\mathcal{G}$ has two nondegenerate principal continuous series that we label (following Graev) d_1 and d_2. Some representations of the latter have been examined by Klink[5]; we are not aware of a global treatment of the former.

It turns out that the description of the representations d_1 reduces entirely to a consideration of the discrete series of $SU(1, 1)$ together with the principal series of $GL(1, C)$; d_2, on the other hand, needs only the representations of $GL(2, C)$. Graev[8] discusses each continuous series separately, finding it convenient to select a matrix realization of the group in which the subgroup of diagonal matrices coincides with the relevant Cartan subgroup; but since we wish to obtain a single realization, wherein the Poincaré group appears explicitly, we shall not do this but keep to the metric of (6). This corresponds to Graev's discussion of d_2 and is, as we have seen, particularly convenient in displaying $\mathbb{P}$.

A. The Series d_2

We therefore start by considering the second continuous series d_2. Let H_z be the space of all C^∞ functions $f(z)$, $z \in \mathrm{Z}$, square-integrable with respect to the invariant measure $d\mu(z)$; and let $\hat{H}$ be the space of functions $f(\omega)$ upon which is realized by $\hat{T}$ a given UIR $(m_1 m_2 \rho_1 \rho_2)$ of $GL(2, C)$.[11] Then the representation $(m_1 m_2 \rho_1 \rho_2)$ of $U(2, 2)$ is defined on the tensor product space

$$\mathcal{H}_2 = \hat{H} \otimes H_z \quad (17)$$

by

$$T_g^2 : f(\omega, z) = \hat{T}_{k_1} : f(\omega, z') \cdot \left(\frac{d\mu(z')}{d\mu(z)}\right)^{\frac{1}{2}},$$

where

$$zg = kz' \quad (18)$$

and $\hat{T}$ acts on f as a function of ω: That is,

$$\hat{T}_{k_1}: f(\omega) = |\Delta|^{m_1+i\rho_1+1}\Delta^{-m_1}|\lambda|^{m_2-m_1+i\rho_2-i\rho_1-2}\lambda^{m_1-m_2}f(\omega'),$$

$$\omega k_1 = k'\omega', \tag{19}$$

$$\omega \equiv \begin{pmatrix} 1 & \\ \omega & 1 \end{pmatrix}, \quad k' = \begin{pmatrix} \lambda^{-1}\Delta & \mu \\ & \lambda \end{pmatrix}. \tag{20}$$

This specifies a representation of $U(2, 2)$; we assert (but do not prove here) that it is irreducible. When restricted to $SU(2, 2) \sim \mathcal{G}$ by the requirement that $\det k_1$ (i.e., Δ) be real, it remains irreducible. Combining the transformations of the manifolds z and ω, we are led at last to the representation of $\mathcal{G}$ by operators on functions defined over the manifold Y:

$$T_g^2: f(y) = |\Delta|^{i\rho_1-1}(\operatorname{sgn}\Delta)^\epsilon |\lambda|^{m-i\rho_1+i\rho_2-2}\lambda^{-m}\cdot f(y'),$$

$$yg = \Lambda y', \tag{21}$$

$$f \in \mathcal{H}_2 \subset L^2(y).$$

This is clearly unitary; for $\rho_1 \neq \rho_2$, it is also irreducible (in the case of equality we may be led to degenerate representations, as will be shown in a subsequent paper). When the sign parameter ϵ is zero, we have the representation treated by Klink.[5] Notice that it is specified by one integer, two real parameters, and a parity.

B. The Series d_1

In the second series d_2, the Cartan subgroup was generated by $\{D, J_3, K_3\}$; here we take instead that given by $\{J_3, D - K_3, P_0 + P_3 - 2L_0 + 2L_3\}$, which has only one noncompact generator. Graev's treatment of this series is not directly applicable with the metric (6), and so we present a modified version.

Consider first the matrix k_0 of (9). This has the form

$$k_0 = e^{i\phi}\begin{pmatrix} a & ib \\ ic & d \end{pmatrix},$$

$$ad + bc = 1, \tag{22}$$

with all parameters real, and so forms a subgroup isomorphic to $SL(2, R) \times U(1) \sim U(1, 1)$. Given the strictly positive integer $2k$ and integer n of the same parity, we can define its representations (n, k) in the discrete series in the usual way[11] upon the space H_k of functions defined modulo polynomials of degree less than $2k - 1$ and square-integrable with the inner product

$$(f, g)_k = i^{2k-1}\int \overline{f(x)}g^{(2k-1)}(x)\,dx, \tag{23}$$

by

$$T_{k_0}^k: f(x) = e^{in\phi}\lambda^{2k-2}f(x'), \tag{24}$$

where

$$\begin{pmatrix} 1 & \\ ix & 1 \end{pmatrix} k_0 = \begin{pmatrix} \lambda^{-1} & i\mu \\ & \lambda \end{pmatrix}\begin{pmatrix} 1 & \\ ix' & 1 \end{pmatrix} e^{i\phi}; \tag{25}$$

x, λ, μ are all real. Define H_ζ to be the space of all C^∞ functions $f(\zeta)$, $\zeta \in Z$, that are square-integrable with respect to the measure $d\mu(\zeta)$; then $\mathcal{H}_1$ is defined as the completion of the tensor product

$$\mathcal{H}_1 = H_k \otimes H_\zeta. \tag{26}$$

The representation (m, n, ρ, k) of $U(2, 2)$ is then defined upon $\mathcal{H}_1$ by

$$T_g^1: f(x, \zeta) = |k_1|^{m+i\rho-3}k_1^{-m}T_{k_0}^k: f(x, \zeta'),$$

$$\zeta g = k\zeta', \tag{27}$$

where k_1, k_0 are defined from k by (9) and T^k acts upon f as a function of x. The factors in front we recognize as a representation of $GL(1, C)$.

Once again, we can combine the transformations of the manifolds ζ and x by multiplying together the appropriate matrices. If we now identify this product manifold with Y and change notation accordingly, the partial derivative in (23) is transformed into a more complicated quantity and the new realization of $\mathcal{H}_1$ is given by the scalar product

$$(f, g)_k = -\int \overline{f(y)}\delta^{2k-1}g(y)d\mu(y), \tag{28}$$

where

$$-i\delta = \omega\frac{\partial}{\partial\bar{a}} - \bar{\omega}\frac{\partial}{\partial a} + \frac{\partial}{\partial b} + \omega\bar{\omega}\frac{\partial}{\partial c}. \tag{29}$$

The functions $f \in \mathcal{H}_1(y)$ are now defined only modulo multinomials in a, $\bar{a}$, b, c of total degree less than $2k - 1$. Upon this space the representation (27), when restricted to $\mathcal{G}$, becomes

$$T_g^1: f(y) = \Delta^{2k-2}|\lambda|^{m+i\rho-2k-1}\lambda^{-m}f(y'). \tag{30}$$

Now this representation is reducible. It is easy to show, by choosing a representative set of elements of $\mathcal{G}$, that, with the variables

$$\rho = a + \bar{\omega}b,$$
$$\sigma = b,$$
$$\tau = \omega a - \overline{\omega a} + c + \omega\bar{\omega}b,$$
$$\omega,$$

the space $\mathcal{H}_1$ has two invariant subspaces: of functions which are analytic in the right or left half-planes of σ, respectively. We shall call these spaces $\mathcal{H}_1^+$ and $\mathcal{H}_1^-$; the corresponding restrictions d_1^+ and d_1^- are then irreducible.

Notice that the differential operator δ of (29) becomes just $\partial/\partial\sigma$. The positivity of the norm in the spaces $\mathcal{H}_1^\pm$ separately now follows by passing to the

Fourier transform and using the Plancherel formula, in exact analogy to the principal discrete series of the groups $SU(1, 1)$.

IV. REPRESENTATIONS OF THE LIE ALGEBRA

We shall need later the eigenvalues of the Casimir operators in order to compare our degenerate representations with those of other authors—in particular, with the algebraic constructions of Yao.[3] To find these, we must first know the generators themselves as differential operators; these can be obtained in a straightforward manner by direct differentiation of the transformations (21) induced by the relevant one-parameter subgroups, and we list them below. In each case the subgroup is defined uniquely by (5):

$$\begin{aligned}
&P_\mu: \frac{\partial}{\partial x_\mu},\\
&D: \sum x_\mu \frac{\partial}{\partial x_\mu} - \tfrac{1}{2}(\sigma + 2i\rho_1 - 2),\\
&J_1: x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3} + \tfrac{1}{2}i(1-\omega^2)\frac{\partial}{\partial\omega} - \tfrac{1}{2}i(1-\bar\omega^2)\frac{\partial}{\partial\bar\omega} + \tfrac{1}{4}i\sigma(\omega-\bar\omega) - \tfrac{1}{4}im(\omega+\bar\omega),\\
&J_2: x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1} + \tfrac{1}{2}(1+\omega^2)\frac{\partial}{\partial\omega} + \tfrac{1}{2}(1+\bar\omega^2)\frac{\partial}{\partial\bar\omega} - \tfrac{1}{4}\sigma(\omega+\bar\omega) + \tfrac{1}{4}m(\omega-\bar\omega),\\
&J_3: x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2} + \tfrac{1}{2}im + i\omega\frac{\partial}{\partial\omega} - i\bar\omega\frac{\partial}{\partial\bar\omega},\\
&K_1: x_0\frac{\partial}{\partial x_1} + x_1\frac{\partial}{\partial x_0} - \tfrac{1}{2}(1-\omega^2)\frac{\partial}{\partial\omega} - \tfrac{1}{2}(1-\bar\omega^2)\frac{\partial}{\partial\bar\omega} - \tfrac{1}{4}\sigma(\omega+\bar\omega) + \tfrac{1}{4}m(\omega-\bar\omega),\\
&K_2: x_0\frac{\partial}{\partial x_2} + x_2\frac{\partial}{\partial x_0} + \tfrac{1}{2}i(1+\omega^2)\frac{\partial}{\partial\omega} - \tfrac{1}{2}i(1+\bar\omega^2)\frac{\partial}{\partial\bar\omega} - \tfrac{1}{4}i\sigma(\omega-\bar\omega) + \tfrac{1}{4}im(\omega+\bar\omega),\\
&K_3: x_0\frac{\partial}{\partial x_3} + x_3\frac{\partial}{\partial x_0} + \tfrac{1}{2}\sigma - \omega\frac{\partial}{\partial\omega} - \bar\omega\frac{\partial}{\partial\bar\omega}.
\end{aligned} \tag{31}$$

The special conformal generators are more complicated:

$$\begin{aligned}
L_1:\ & x_1 D + \tfrac{1}{2}x^2\frac{\partial}{\partial x_1} - \tfrac{1}{2}imx_2 + \tfrac{1}{4}(x_0+x_3)[m(\omega-\bar\omega) - \sigma(\omega+\bar\omega)]\\
&+ \tfrac{1}{2}[x_3(1+\omega^2) - x_0(1-\omega^2) - 2i\omega x_2]\frac{\partial}{\partial\omega} + \tfrac{1}{2}[x_3(1+\bar\omega^2) - x_0(1-\bar\omega^2) + 2i\bar\omega x_2]\frac{\partial}{\partial\bar\omega},\\
L_2:\ & x_2 D + \tfrac{1}{2}x^2\frac{\partial}{\partial x_2} + \tfrac{1}{2}imx_1 + \tfrac{1}{4}i(x_0+x_3)[m(\omega+\bar\omega) - \sigma(\omega-\bar\omega)]\\
&+ \tfrac{1}{2}i[x_0(1+\omega^2) - x_3(1-\omega^2) + 2\omega x_1]\frac{\partial}{\partial\omega} - \tfrac{1}{2}i[x_0(1+\bar\omega^2) - x_3(1-\bar\omega^2) + 2\bar\omega x_1]\frac{\partial}{\partial\bar\omega},\\
L_3:\ & x_3 D + \tfrac{1}{2}x^2\frac{\partial}{\partial x_3} + \tfrac{1}{2}i\sigma x_0 + \tfrac{1}{4}(\omega+\bar\omega)(\sigma x_1 - imx_2) + \tfrac{1}{4}i(\omega-\bar\omega)(\sigma x_2 + imx_1)\\
&- \tfrac{1}{2}[x_1(1+\omega^2) - ix_2(1-\omega^2) + 2\omega x_0]\frac{\partial}{\partial\omega} - \tfrac{1}{2}[x_1(1+\bar\omega^2) + ix_2(1-\bar\omega^2) + 2\bar\omega x_0]\frac{\partial}{\partial\bar\omega},\\
L_0:\ & -x_0 D + \tfrac{1}{2}x^2\frac{\partial}{\partial x_0} - \tfrac{1}{2}\sigma x_3 - \tfrac{1}{4}(\omega+\bar\omega)(\sigma x_1 - imx_2) - \tfrac{1}{4}i(\omega-\bar\omega)(\sigma x_2 + imx_1)\\
&- \tfrac{1}{2}[x_1(1-\omega^2) - ix_2(1+\omega^2) + 2\omega x_3]\frac{\partial}{\partial\omega} - \tfrac{1}{2}[x_1(1-\bar\omega^2) + ix_2(1+\bar\omega^2) + 2\bar\omega x_3]\frac{\partial}{\partial\bar\omega}.
\end{aligned} \tag{32}$$

In these relations we have parametrized the matrices z by (15), in order to cast the results into a more familiar guise. By x^2 we mean $x_\mu x^\mu$ (the metric is still $+---$), and the sum in the first term of D is to be taken *with all signs positive*. The quantity σ is given by $\sigma = i\rho_2 - i\rho_1 - 2$. If $i\rho_1$ is replaced everywhere by $2k - 1$, the generators take the form appropriate to d_1—they are here derived from d_2. Notice finally the interesting feature that $\rho_1 + \rho_2$ appears nowhere except in D.

Casimir Operators

$\mathcal{G}$ has three independent Casimir operators. They are easily defined from the generators of $O(4, 2)$ in canonical form:

$$2C_2 = J_{\mu\nu}J^{\mu\nu},$$

$$48C_3 = \epsilon^{\mu\nu\xi\rho\sigma\tau}J_{\mu\nu}J_{\xi\rho}J_{\sigma\tau}, \qquad (33)$$

$$C_4 = \sum_{i_1<i_2<i_3<i_4} J^2(i_1, i_2, i_3, i_4), \qquad (34)$$

where (e.g.)

$$J(1, 2, 3, 4) = J_{12}J_{34} - J_{13}J_{24} + J_{23}J_{14}.$$

The first two are well known; but there is some ambiguity in the definition of the fourth-order operator, not only because of the possibility of adding a term $(C_2)^2$ but also because definitions with different orderings of the indices may introduce multiples of C_2. Our definition is that given by Castell.[12] Using (2), we can write these as

$$C_2 = \mathbf{J}^2 - \mathbf{K}^2 - P_\mu L^\mu - L_\mu P^\mu - D^2, \qquad (35)$$

$$C_3 = \mathbf{J}\cdot\mathbf{K}D - \mathbf{K}\cdot\mathbf{P}\wedge\mathbf{L} + \mathbf{J}\cdot\mathbf{L}P_0 - \mathbf{J}\cdot\mathbf{P}L_0 - \mathbf{J}\cdot\mathbf{K}, \qquad (36)$$

$$\begin{aligned} C_4 = {} & -(\mathbf{J}\cdot\mathbf{K})^2 + \mathbf{J}\cdot\mathbf{P}\mathbf{J}\cdot\mathbf{L} + \mathbf{J}\cdot\mathbf{L}\mathbf{J}\cdot\mathbf{P} - 2\mathbf{J}^2P_0L_0 \\ & - \mathbf{K}\wedge\mathbf{P}\cdot\mathbf{K}\wedge\mathbf{L} - \mathbf{K}\wedge\mathbf{L}\cdot\mathbf{K}\wedge\mathbf{P} \\ & - \mathbf{K}\wedge\mathbf{L}\cdot\mathbf{J}(P_0 + L_0) - (P_0 + L_0)\mathbf{J}\cdot\mathbf{K}\wedge\mathbf{L} - (\mathbf{L}\wedge\mathbf{P} + \mathbf{J}D)^2 \\ & + L_0\mathbf{P}\cdot\mathbf{K}D + D\mathbf{K}\cdot\mathbf{P}L_0 - P_0\mathbf{L}\cdot\mathbf{K}D - D\mathbf{K}\cdot\mathbf{L}P_0 \\ & - \mathbf{L}\cdot\mathbf{P}P_0L_0 - \mathbf{P}\cdot\mathbf{L}L_0P_0 + \mathbf{P}^2L_0^2 + \mathbf{L}^2P_0^2 + \mathbf{K}^2D^2 \\ & + \mathbf{J}^2D + \mathbf{J}\cdot\mathbf{L}\wedge\mathbf{P} + \mathbf{L}\wedge\mathbf{P}\cdot\mathbf{J} + \mathbf{P}\cdot\mathbf{K}L_0 + \mathbf{L}\cdot\mathbf{K}P_0 - \mathbf{J}^2. \end{aligned} \qquad (37)$$

There are obviously very many ways of writing (38): We have used a 3-vector notation largely out of personal preference. The lower-order terms have arisen because of commutators needed in order to express the operators simply with this notation.

With the representation of the generators by (31) and (32), it is now a simple matter to obtain the eigenvalues of the Casimir operators, since these are pure numbers. A brief calculation gives for the series d_2

$$\begin{aligned} C_2 &= \tfrac{1}{2}(\rho_1^2 + \rho_2^2) - \tfrac{1}{4}m^2 + 5, \\ C_3 &= -\tfrac{1}{8}im(\rho_1^2 - \rho_2^2), \\ C_4 &= -\tfrac{1}{8}m^2(2 + \rho_1^2 + \rho_2^2) + \tfrac{1}{2}(\rho_1^2 + \rho_2^2) \\ &\quad + \tfrac{1}{16}(\rho_1^2 - \rho_2^2)^2 + 1, \end{aligned} \qquad (38)$$

and we remark again that the substitution $i\rho_1 \to 2k - 1$ gives the values of these operators in the series d_1. Our Casimir operators as defined above differ from those of Yao[3] (which we call Y) by

$$\begin{aligned} Y_2 &= -C_2, \\ Y_3 &= \pm iC_3, \\ Y_4 &= -C_4 + \tfrac{1}{4}C_2^2 - C_2. \end{aligned} \qquad (39)$$

Although this makes comparison with Yao's list rather more difficult, we prefer to retain our C_4 since on the most degenerate principal continuous series only C_2 is then nonzero; this agrees with the conventions of Ref. 7.

V. REDUCTION UNDER $\mathbb{P}$

Recall that the Poincaré subgroup is expressed by the four-parameter Abelian group $z \sim T_4$ and the block-diagonal matrices D, where the blocks are restricted to be unimodular. Define the inhomogeneous transform (a, z) by

$$(a, z) = kz, \quad z \in Z, \quad a \in SL(2, C),$$

$$k = \begin{pmatrix} sa^{-1\dagger}s & \\ & a \end{pmatrix} \in D;$$

then we find

$$(a_1, z_1)(a_2, z_2) = (a_1a_2, z_2 + a_2^{-1}z_1sa_2^{-1\dagger}s)$$

or, under the parametrization (15),

$$(a_1, x_1)(a_2, x_2) = (a_1a_2, x_2 + A_2^{-1}x_1), \qquad (40)$$

which is just the product law of the Poincaré group. The apparent inversion of order is because we have chosen to consider the right regular representation rather than the left.

A. Second Series d_2

When g in (21) is restricted to $\mathbb{P}$, we obtain

$$T^2_{g\in\mathbb{P}}: f(y) = \lambda^{-\frac{1}{2}m+\frac{1}{2}i\rho-1}\bar{\lambda}^{\frac{1}{2}m+\frac{1}{2}i\rho-1}f(y'), \qquad (41)$$

where we have set $\rho \equiv \rho_2 - \rho_1$. Clearly this representation of $\mathbb{P}$ is specified by the parameters m, ρ associated with $\mathcal{G}$ itself; and we notice that the way these enter is to make $\hat{T}$ of (18) a unitary irreducible representation[13] of the principal series of $SL(2, C)$.

This is just the expression of a covariance condition. Instead of defining the representation (41) over $Y = WZ$, let us realize it on the manifold $P = kz$:

$$P \ni p = \begin{pmatrix} k_{-1} & \\ k_1 z & k_1 \end{pmatrix} = \begin{pmatrix} sa^{-1\dagger}s & \\ az & a \end{pmatrix}, \quad (42)$$

which is isomorphic to the group $\mathbb{P}$ and can be parametrized by $p = (a, x)$. Then (21) becomes

$$T_g^2: f(p) = |\Delta|^{i\rho_1 - 1} (\operatorname{sgn} \Delta)^\epsilon \, |\lambda|^{m+i\rho-2} \, \lambda^{-m} f(p'),$$
$$pg = \Lambda p', \quad (43)$$

and p' is no longer uniquely defined. Hence this is a representation of $\mathcal{G}$ only with the covariance condition

$$f(\lambda_0 a, x) = |\lambda|^{m+i\rho-2} \, \lambda^{-m} f(a, x),$$
$$\lambda_0 = \begin{pmatrix} \lambda^{-1} & \mu \\ & \lambda \end{pmatrix} \in SL(2, C). \quad (44)$$

This is precisely analogous to the constraint required in the representation of $SL(2, C)$ by means of operators on functions defined over $SU(2)$:

$$\phi(e^{i\alpha J_3} u) = e^{i\alpha j_0} \phi(u).$$

In that well-known case we expand $\phi(u)$ in the matrix elements $\mathfrak{D}^j_{j_0, m}(u)$ of the rotation group; here we require the analog of that result and the expansion of an otherwise arbitrary function on $\mathbb{P}$ that transforms irreducibly under the left-representation of $SL(2, C)$. A further restriction on $f(a, x)$ comes from the observation that T^2 is a principal-series representation of $\mathcal{G}$: in other words, that it is contained in the regular representation by means of operators on functions square-integrable over $\mathcal{G}$ itself. Therefore (41) must be contained in the regular representation of $\mathbb{P}$, and hence is a direct integral of representations in the principal series of that group, so that we need to determine all such which transform under the representation (m, ρ) of $SL(2, C)$ "from the left." The problem is solved in the Appendix, and we find the following result.

Theorem 1: When restricted to $\mathbb{P}$, the representation (m, ρ_1, ρ_2) in the second principal continuous series d_2 of $\mathcal{G}$ contains a direct integral and sum over all the principal-series representations of $\mathbb{P}$ allowing a helicity of $m/2$. Each representation enters with unit multiplicity.

That is, all masses (real and imaginary) appear in the reduction, but the lightlike representations are omitted[14] because they enter with vanishing invariant measure. (They appear explicitly in other series of $\mathcal{G}$.) For timelike representations, all spins $s \geq |\frac{1}{2}m|$ occur; for spacelike representations, all continuous spins, and discrete spins $0 < k \leq |\frac{1}{2}m| - 1$ only. The parity of the representations of the little groups is that of m.

B. First Series d_1

The problem here is more interesting. When restricted to $\mathbb{P}$, (30) becomes

$$T^1_{g \in \mathbb{P}}: f(y) = |\lambda|^{m+i\rho-2k-1} \, \lambda^{-m} f(y'), \quad f \in \mathcal{H}_1, \quad (45)$$

and the scalar product is given by (28). This representation of $\mathbb{P}$ is clearly unitary, but the definition of $\mathcal{H}_1$ makes it difficult to see how it reduces because of the derivatives in the scalar product. We shall, however, show that it is equivalent to a representation (of $\mathbb{P}$) on the space $\mathcal{H}_2$, and the results of the previous section will then solve the problem.

Consider then the operator A defined by

$$A: f(y) = \int d\mu(p) e^{-i \operatorname{Tr}(p^{\mathrm{T}} z)} \{\Omega(p, \omega)\}^{k-\frac{1}{2}} \times \int d\mu(z_0) e^{i \operatorname{Tr}(p^{\mathrm{T}} z_0)} f(z_0, \omega), \quad (46)$$

where

$$-i\Omega(p, \omega) = \omega \bar{p}_a - \bar{\omega} p_a + p_b + \omega \bar{\omega} p_c, \quad (47)$$

p is a matrix of the same form as z with elements p_a, etc., and the superscript T indicates transposition of the matrix. It is trivial to show that

$$A T^1_{z_0}: f(z, \omega) = A f(z + z_0, \omega); \quad (48)$$

let us now investigate the action of T^1_a, $a \in SL(2, C) \subset \mathbb{P}$. Define the matrix $p' = a^{\mathrm{T}} p s \bar{a} s$; then clearly

$$\operatorname{Tr}(p^{\mathrm{T}} z) = \operatorname{Tr}(p'^{\mathrm{T}} z'),$$

where $ya = \Lambda y'$ defines z'. We also find, by direct calculation, the remarkable result

$$\Omega(p', \omega') = |\lambda|^{-2} \, \Omega(p, \omega),$$

so that, using these identities, we obtain

$$A T^1_a: f(z, \omega)$$
$$= \int d\mu(p) e^{-i \operatorname{Tr}(p^{\mathrm{T}} z)} \Omega(p, \omega)^{k-\frac{1}{2}} \times \int d\mu(z_0') e^{i \operatorname{Tr}(p'^{\mathrm{T}} z_0')} \, |\lambda|^{m+i\rho-2k-1} \, \lambda^{-m} f(z_0', \omega')$$
$$= |\lambda|^{m+i\rho-2} \, \lambda^{-m} A f(z', \omega'). \quad (49)$$

In other words, we have shown by (42) and (49) that

$$A T^1_p = T^2_p A, \quad (50)$$

so that A intertwines the representations (45) and (41) of $\mathbb{P}$. Notice that this important result hinges on the fact that when $g \in \mathcal{G}$ is restricted to $\mathbb{P}$, then λ and ω' are independent of z; hence no similar program can be developed for $\mathcal{G}$ itself.

We must now show that the representations are equivalent—that is, that

$$A:\mathcal{H}_1(m, \rho, k) \to \mathcal{H}_2(m, \rho, -k-1)$$

is an isometry as well as one to one and onto. To establish this, we remark that $\mathcal{H}_1$ was defined in Sec. 3B only modulo multinomials of total degree $2k-2$ or less in the elements of z; hence, the Fourier transform with respect to these variables certainly converges in the classical sense. Consider the subspaces $K_1 \subset \mathcal{H}_1$ and $K_2 \subset \mathcal{H}_2$ of C^∞ functions of compact support in all variables; these are dense subspaces,[15] and, by the Riemann—Lebesgue lemma and (46), $A:K_1 \to K_2$. By virtue of the classical theorems on Fourier transforms we know that, on K, A is invertible; that it is isometric (we ignore irrelevant numerical factors) follows from its definition. Therefore, $A:\mathcal{H}_1 \to \mathcal{H}_2$ is indeed an isometric isomorphism, and the representations (41) and (45) of $\mathbb{P}$ are equivalent as we asserted.

It remains only to examine the consequences of the reducibility of d_1. Consider the variables ρ, σ, τ introduced in Sec. 3B, and define $\hat{f}(\rho, \sigma, \tau; \omega) = f(a, b, c; \omega)$. Because the Fourier transform with respect to $(-i\sigma)$ of a function $\hat{f} \in \mathcal{H}_1^+$ is concentrated on the positive axis, the integral over p in (46) is over only that region where $\Omega(p, \omega)$ is positive; for $\mathcal{H}_1^-$ the situation is reversed. This establishes the single-valuedness of (46), and shows that $A:\mathcal{H}_1^+ \to \mathcal{H}_2^+$, where $\mathcal{H}_1^+ \subset \mathcal{H}_2$ contains only those functions which are analytic in $\operatorname{Re} \sigma > 0$. Now suppose $f \in \mathcal{H}_2^+$. Then $T_g:f \in \mathcal{H}_2^+$ for all $g \in \mathcal{G}$, so that we can examine any $T_g f$ to determine whether or not f lies in the space. Consider in particular

$$\begin{aligned}[T_{\omega^{-1}}:f](z, \omega) &= f(a + b\bar{\omega}, b, c + a\omega - \bar{a}\bar{\omega} + b\omega\bar{\omega}; 0)\\ &= f(\rho, \sigma, \tau; 0) = \hat{f}(\rho, \sigma, \tau; 0),\end{aligned}$$

where ω^{-1} is an element of $SL(2, C) \in \mathbb{P}$ specified by $a_{11} = a_{22} = 1$, $a_{21} = -\omega$; then we see that analyticity in $\operatorname{Re} \sigma > 0$ implies that, upon the cross section $\omega = 0$, f is analytic in $\operatorname{Re} b > 0$. In other words, $f(a, b, c; \omega) \in \mathcal{H}_2^+$ is analytic in the b coordinate of that point on the surface $\omega = 0$ which is mapped onto $(a, b, c; \omega)$ by transformation under $\omega \in SL(2, C)$.

Therefore, by choosing correct analyticity for $f(a, b, c; 0)$, we ensure that f belongs to $\mathcal{H}_1^+$; since by (15) b is just $i(x_0 + x_3)$, we see, by passing to the Fourier transform with respect to $z \sim x_\mu$ of $f \in \mathcal{H}_2^+$, that in this subspace we have just the restriction $(p_0 + p_3) > 0$, where p_μ is the μ component of the 4-momentum. We remark that intuitively this procedure corresponds to choosing a standard orientation for the spin of a particle and then in that frame examining its momentum.

We now ask how this restricts the representations of the Poincaré group occurring in d_1^+. Suppose first that $p_\mu p^\mu < 0$ so that we have a spacelike representation of $\mathbb{P}$; then the restriction is not Lorentz invariant and does not eliminate any masses. If, however, $p_\mu p^\mu > 0$, we have a timelike representation, and now the restriction is indeed real and tells us that only positive masses occur. For d_1^- the situation is, of course, reversed and only negative masses arise.

Now the ω dependence of $f(z, \omega)$ is still quite unrestricted. With these results upon the coordinate dependence of the functions in $\mathcal{H}_1^+$, we can therefore make use of the results of the last section to reduce d_1^+ and d_1^- with respect to $\mathbb{P}$. We find the following theorem.

Theorem 2: When restricted to $\mathbb{P}$, the representation (m, ρ, k^+) of the positive first principal continuous series d_1^+ of $\mathcal{G}$ contains a direct sum and integral over all the principal series representations of $\mathbb{P}$ which both allow a helicity of $\frac{1}{2}m$ and have either an imaginary or a real and positive rest mass. The representation (m, ρ, k^-) of the negative series d_1^- contains all such representations which both allow a helicity of $\frac{1}{2}m$ and have either an imaginary or a real and negative rest mass.

APPENDIX

It is clear from (43) that no irreducible representation $[M, S]$ of $\mathbb{P}$ occurs more than once in the reduction. In order to see which of these are allowed by our covariance condition (44), we must express the basis functions $f(a, x)$ in terms of the (generalized) matrix elements of $\mathbb{P}$ in an $SL(2, C)$ basis—or, equivalently, know how $\mathbb{P}$ reduces with respect to $SL(2, C)$. This latter is, of course, well known[16] for timelike representations, but the spacelike case $M^2 < 0$ does not seem to have been studied and so we shall use the former approach.

Suppose then that we know the generalized matrix elements

$$\langle m\rho j\mu |\, T_p^{[M,S]}\, | m'\rho' j'\mu' \rangle$$

of the Poincaré group in such a basis, together with the appropriate Fourier inversion theorem and measure $d\omega$. Then (44) tells us that $f(p)$ must be expanded as

$$f(p) = \int \tilde{f}(m'\rho'j'\mu'; MS)\, \langle m\rho j\mu |\, T_p^{[M,S]}\, | m'\rho'j'\mu' \rangle\, d\omega,$$

where the labels (m, ρ) of the matrix element are those of $\mathcal{G}$, and j, μ [specifying some basis of $SL(2, C)$] are irrelevant. By virtue of the Plancherel theorem[14] for $\mathbb{P}$ (a Type I group), this is an isometry, and hence solves the reduction problem once we know the possible values of $[M, S]$ for fixed (m, ρ).

To find these, we use the following prescription for calculating the matrix elements:

$$\langle\ \rangle = \int \overline{Y^{[M,S]}_{m\rho j\mu}(p')} Y^{[M,S]}_{m'\rho' j'\mu'}(p'p)\, d\mu(p'),$$

where $Y(p)$ is a spherical function of $\mathbb{P}$ in an $SL(2, C)$ basis and $d\mu(p)$ is the invariant measure. The details of this procedure are irrelevant to our present purpose: What we need is only a knowledge of the spherical functions. For timelike representations these have been given by Rühl[17]: In our notation

$$Y^{[M,S]}_{m\rho j\mu}(p) = \mathfrak{D}^{m\rho}_{s\mu' j\mu}(a) \cdot \exp\,[iM(A^{-1}x)^0],$$

where $\mathfrak{D}(a)$ is a representation function of $SL(2, C)$ in the canonical basis and $(A^{-1}x)^0$ is just the 0-component of the vector x^μ after the transformation $A^{-1} \in O(3, 1)$ conjugate to $a^{-1} \in SL(2, C)$. The label μ' is unimportant. A similar procedure can be outlined for $M^2 < 0$ using the "cross-basis" matrix elements of $SL(2, C)$ between an $SU(1, 1)$ and an $SU(2)$ basis,[17] which are the spherical functions for the reduction $SL(2, C) \supset SU(1, 1)$:

$$Y^{[M^2<0,S]}_{m\rho j\mu;\tau}(p) = \mathfrak{D}^{m\rho}_{s\mu'\tau;j\mu}(a) \cdot \exp\,[i\,|M|\,(A^{-1}x)^3];$$

s is now on the principal series of the $SU(1, 1)$ subgroup, while j still refers to $SU(2)$. The label τ is related to parity.

We can now deduce the allowed values of $[M, S]$ by examining the spherical functions. For $M^2 > 0$, it is clear that for fixed (m, ρ) there occur only those spins with $2S \geq |m|$: this, of course, agrees with the results of Joos.[13] For $M^2 < 0$, we find that all continuous S are allowed, but discrete $S \leq |\frac{1}{2}m| - 1$ only.[18] Since there are no restrictions on the x dependence of our functions $f(a, x)$, every (real and imaginary) mass M occurs, entering with invariant measure $M^2\, dM^2$; hence, the lightlike representations $M^2 = 0$ can be neglected[14] as being a lower-dimensional manifold with vanishing invariant measure. The problem is solved.

[1] Proceedings of Boulder symposium on de Sitter and Conformal Groups, University of Colorado, 1970.
[2] L. Castell, Nucl. Phys. **B13**, 231 (1969).
[3] T. Yao, J. Math. Phys. **8**, 1931 (1967); **9**, 1605 (1968).
[4] A. Kihlberg, V. F. Muller, and F. Halbwachs, Commun. Math. Phys. **3**, 194 (1966), Y. Murai, Progr. Theoret. Phys. (Kyoto) **9**, 147 (1953).
[5] W. H. Klink, J. Math. Phys. **10**, 606 (1969).
[6] G. Mack and I. Todorov, J. Math. Phys. **10**, 2078 (1969).
[7] R. Rączka, N. Limić, and J. Niederle, J. Math. Phys. **7**, 1861, 2026 (1966).
[8] M. I. Graev, Am. Math. Soc. Transl. **66**, 1 (1968); Tr. Mosc. Mat. Obshch. **7**, 335 (1958).
[9] *Note added in proof:* In the published version of this paper [J. Math. Phys. **12**, 315 (1971)] Yao has inserted a footnote modifying his results. Our strictures no longer apply.
[10] N. Mukunda, J. Math. Phys. **9**, 50 (1968).
[11] I. M. Gel'fand and M. A. Naimark, Tr. Mat. Inst. Akad. Nauk SSSR, No. 36 (1950) (German transl., Akademie-Verlag Berlin, 1957).
[12] L. Castell, Nuovo Cimento **46A**, 1 (1966).
[13] In the notation of a previous paper [N. W. Macfadyen, J. Math. Phys. **12**, 492 (1971)], $m = 2j_0$, $i\rho = 2\sigma$; our parameter m is always an integer.
[14] G. Rideau, Commun. Math. Phys. **3**, 218 (1966).
[15] This is not strictly true: See I. M. Gel'fand *et al.*, *Generalized Functions* (Academic, New York, 1966), Vol. V, Chap. III, Sec. 5.3. As shown there, the distinction is irrelevant for our purposes.
[16] H. Joos, Fortschr. Physik **10**, 65 (1962); W. Rühl, Nuovo Cimento **63**, 1131 (1969), Sec. 2.1.
[17] R. Delbourgo, K. Koller, and P. Mahanta, Nuovo Cimento **52A**, 1254 (1967).
[18] This is in agreement with the results of A. Chakrabarti, preprint, Ecole Polytechnique, 1970, which has just come to our attention.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Addendum: Simple Procedure for Determining the Number of Components of an Irreducible Tensor

[J. Math. Phys. 12, 1 (1971)]

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The theorem proved in our paper was previously noted by L. C. Biedenharn, A. Giovannini, and J. D. Louck [J. Math. Phys. **8**, 691 (1967)], who attribute the result to G. de B. Robinson [*Representation Theory of the Symmetric Group* (University of Toronto Press, Toronto, 1961)]. We thank Professor C. M. Andersen for calling these references to our attention.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Erratum: $O(5)$ Harmonics and Abnormal Solutions in the Bethe–Salpeter Equation

[J. Math. Phys. 11, 1204 (1970)]

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Due to the invariance of Eq. (10) under reflection $x \to \pi - x$, we have $f(\pi - x) = \pm f(x)$. This ensures that the series

$$\sum_{k\text{ even}} a_k P^{(3)}_{N+k,n} \quad\text{and}\quad \sum_{k\text{ odd}} a_k P^{(3)}_{N+k,n}$$

separately constitute the eigensolutions of our integral equation. The evaluation of the normalization integral now modifies the expression (19) to read

$$|a_\alpha|^2\, S_{N+\alpha}(-)^\kappa,$$

where $\kappa = N + \alpha - n$ and $\alpha = 0$ or 1 according as the series is even or odd.

Since this does not affect the difference equation, our eigenvalue solutions and other conclusions remain unaffected.

The authors are grateful to Professor V. Singh and Professor G. R. Allock for drawing their attention to this point.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 7 JULY 1971

Erratum: Random Operator Equations in Mathematical Physics. I

[J. Math. Phys. 11, 1069 (1970)]

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The following line was inadvertently omitted from the Acknowledgment: The project has received support from the Office of Naval Research (Contract No. N00014-69-A-0423 Themis).